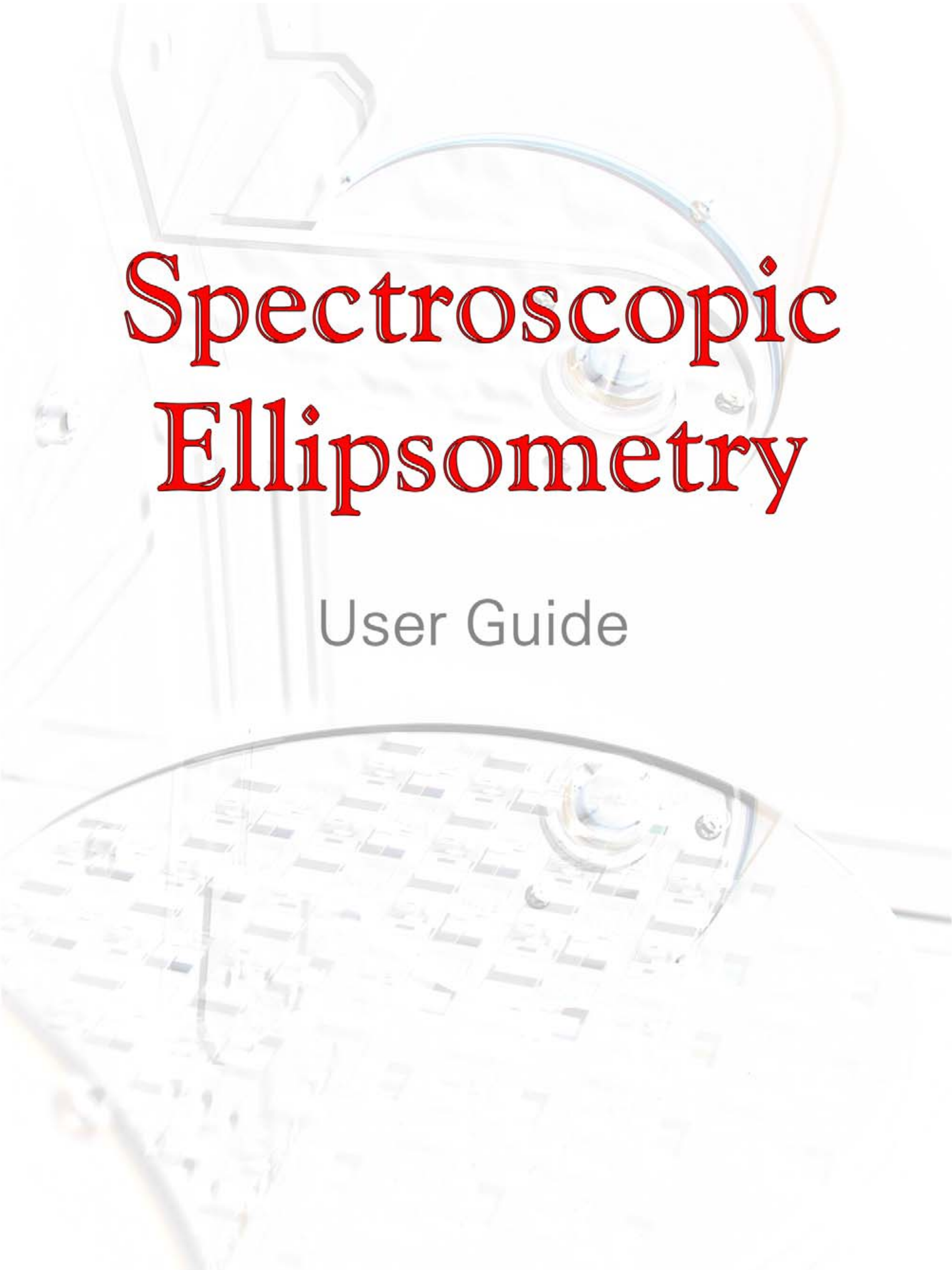
HORIBA JOBIN YVON



Spectroscopic Ellipsometry

User Guide

P/N: 31 087 134

HORIBA JOBIN YVON

Explore the future

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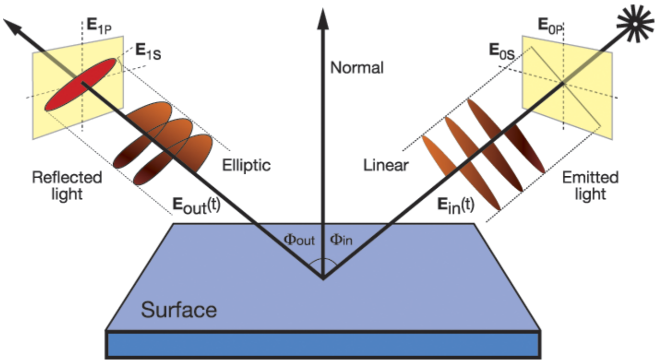
1 Introduction

1.1 General Aspects

1.1.1 What is ellipsometry?

Ellipsometry is an optical technique for surface and thin films analysis. It is based on the measurement of the change in polarization state of a light beam caused by the reflection on the material surface or the transmission through the material. From the change in state of polarization one can deduce film thickness and optical properties of the material. The principle was discovered already more than a century ago. However, over the past few decades the technique has progressed rapidly due to the availability of computers and thus automation of high accuracy ellipsometers. The field of applications is wide: microelectronics, display, opto-electronics, photovoltaics, chemistry, metallurgy etc. Ellipsometry is especially suited to the characterization of semi-conductors where we have massive substrates, thin film layers ranging from few nanometers to tens of micrometers, and also multi-layer structures. Furthermore ellipsometry is a fast and non-destructive technique that allows the monitoring of film growth in real time.



1.1.2 What does it measure?

Ellipsometry measures Ψ and Δ

Ellipsometry measures the change in state of polarization of a light beam caused by the reflection on the sample surface (or the transmission through the sample). The measured parameters are the so-called ellipsometric angles Ψ and Δ. They are related to the ratio of the complex Fresnel reflection coefficients r_s and r_p. Thereby r_s is the reflection coefficient for light polarized perpendicular (German: "senkrecht") to the plane of incidence and r_p is the reflection coefficient for light polarized parallel to the plane of incidence. This is expressed by the fundamental equation of ellipsometry:

fundamental equation of ellipsometry

$$\rho = \frac{r_p}{r_s} = \tan\Psi e^{i\Delta}$$

where

$$\tan\Psi = \frac{|r_p|}{|r_s|} \qquad 0^\circ \le \Psi \le 90^\circ$$

and

$$\Delta = \delta_p - \delta_s \quad 0^\circ \leq \Delta \leq 360^\circ$$

From the measured parameters Ψ and Δ the optical and structural properties of the sample can be determined by appropriate modeling. Sample parameters of interest are for example:

- optical constants in near UV, visible, and near IR wavelength ranges
- mono- or multi-layer thickness
- thickness of layers in superlattice structure
- surface and interface roughness
- anisotropy
- gradient of optical constants in single layers

Ellipsometry is a highly accurate and precise metrology technique because it measures the change in state of polarization (expressed by the ratio of reflection coefficient magnitudes and difference in phase change) rather than simply an intensity.

1.1.3 Limits of applicability

Very rough and inhomogeneous samples are difficult to analyze by ellipsometry

The major limiting factors come from the state of the sample surface. Ellipsometry excludes all scattering effects and only deals with specular reflection. Therefore the roughness of the surface and also of interfaces between two media must not exceed the wavelength of the light. Otherwise non-specular scattering of the incident beam occurs which causes depolarization of the reflected light beam.

The thickness of the film must have low variation over the width of the light spot otherwise the assumption of parallel interfaces is no more valid; it means that the surface must be as plane as possible. That is why the different steps of surface preparation must not be neglected.

Assuming a perfect optical surface the minimum thickness of a film that can be determined is related to the sensitivity of the ellipsometer. This is in the sub-monolayer range.

The maximum thickness of a film that can be determined depends mainly on the wavelength range and the spectral resolution that is used. Typically films up to several tens of μm can be analyzed.

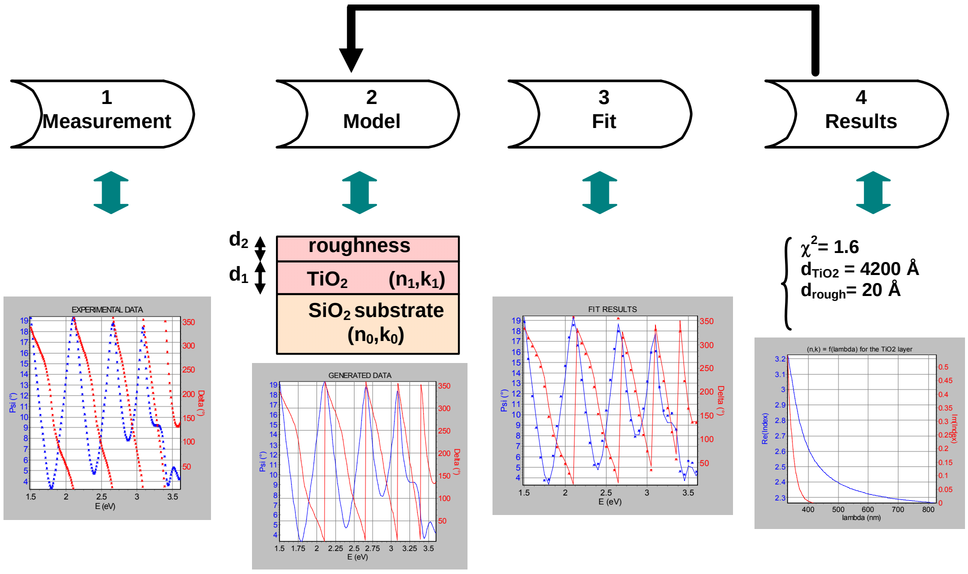
1.1.4 Procedure of ellipsometric experiments

1)Acquire
2)Model
3)Fit
4)Results

An ellipsometric experiment follows always the same procedure:

1. an ellipsometer measurement yields the ellipsometric angles Ψ and Δ not the required sample parameters like thickness and optical constants.
2. It is necessary to create a model of the sample to determine the sample parameters.
3. Once the model is built, calculated data must be fitted to the experimental data and the best match between the two sets has to be found.
4. The user has to evaluate the best-fit model in order to decide whether the predictive model is physically reasonable and whether the different parameters are unique and not correlated.

SE data analysis flowchart:



1.1.5 Accuracy of ellipsometric measurements

Ellipsometry is a very sensitive and highly reproducible technique, but the absolute accuracy is hard to define

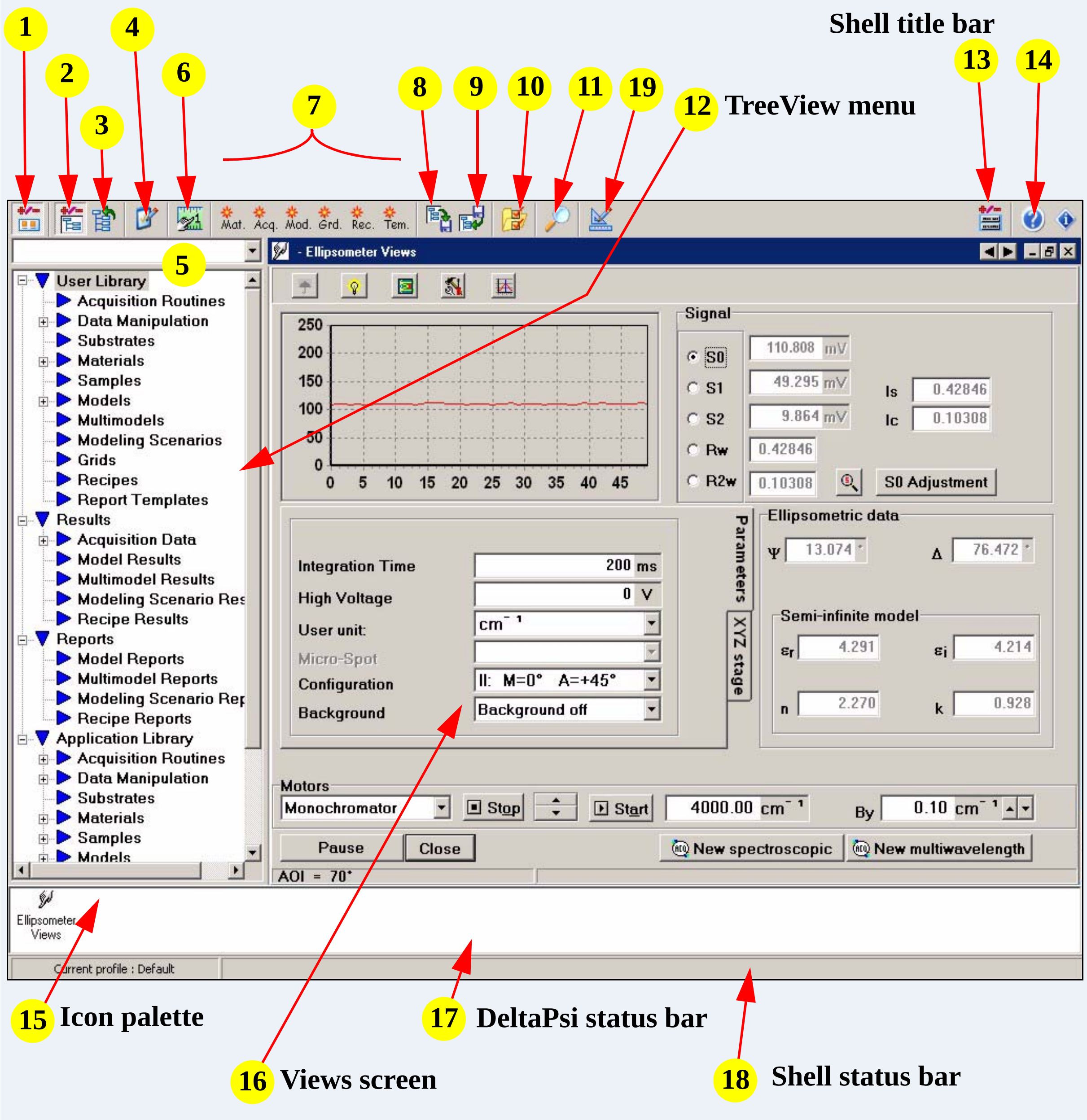
Ellipsometry is a very sensitive and reproducible technique. However, it is very difficult to determine the absolute accuracy of an ellipsometer. One way is to compare results with **certified standard samples**. However, the thickness of these samples is usually certified not better than +/-5Å. This values are well above the sensitivity of an ellipsometer. Another way is to compare results with complementary methods such as AFM or RBS microscopy.

1.1.6 Final words

Ellipsometry is a very powerful but not an all mighty technique: we cannot determine the structure of a complex sample without any input information of the sample. There are some limits of applicability regarding maximum and minimum thickness and absolute accuracy. **Nevertheless ellipsometry is one of the most sensitive and precise tool for thin film thickness measurements. Furthermore, ellipsometry allows the determination of the optical constants (n and k) over a broad spectral range, from near IR to UV. And this can be done all in a non-destructive way which is important for research and much more for industrial applications.**

1.2 General Introduction to DP2 Software

The graph below shows the general user interface of DP2 software:



S0 110.808 mV
S1 49.295 mV
S2 9.864 mV
Rw 0.42846
R2w 0.10308
Is 0.42846
Ic 0.10308

Ψ 13.074 °
Δ 76.472 °

ε_r 4.291
ε_i 4.214
n 2.270
k 0.928

Integration Time 200 ms
High Voltage 0 V
User unit: cm^{-1}
Micro-Spot
Configuration II: M=0° A=+45°
Background Background off

Monochromator 4000.00 cm^{-1} By 0.10 cm^{-1}

AOI = 70°

Current profile : Default

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1
15 The Show/Hide icon palette is a toggle command which hides the area located below the TreeView and the Main Screen. This area displays an icon for every file which has been loaded. Thus, it becomes easy to take a look and switch between the currently loaded files.

2 The Show/Hide ***TreeView*** icon is a toggle command which hides the TreeView menu. This is useful as it magnifies the working View screen.

3 This command is a short-cut which closes the opened ***TreeView Explorer*** folders.

4 Open the ***Options Software*** screen.

5 The ***TreeView Explorer*** simplifies the access to the TreeView. Click on the field to activate the scroll bar, then select the node to open it.

6 The ***Manual Measurement*** icon launches the ***Views*** screen . The Views screen is in fact the Real Time Acquisition panel. Depending on your System(s), an intermediate screen could ask for the acquisition to launch.

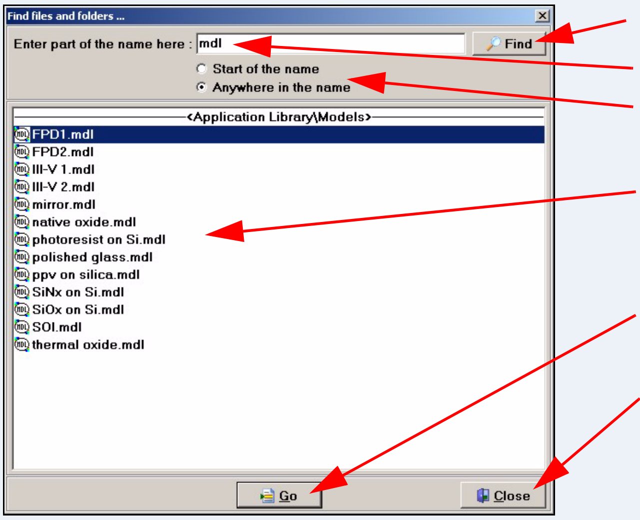
7 Mat. Acq. Mod. Grd. Rec. Tem. ***Creation*** icons: from these «short-cut» icons, the user can create a new material, acquisition routine, model, grid, recipe or report template.

8 Launch the ***Export*** files package feature.

9 Launch the ***Import*** files package feature.

10 The Check Files Integrity is a very powerful feature which is recommended for experimented users only. This feature analyzes the files integrity and verify the links between built models, recipes etc...

11 Click on the ***Search*** feature to find a DeltaPsi2 file. The following screen will be displayed:



Enter part of the name here : mdl

○ Start of the name
● Anywhere in the name

<Application Library\Models>

FPD1.mdl
FPD2.mdl
III-V 1.mdl
III-V 2.mdl
mirror.mdl
native oxide.mdl
photoresist on Si.mdl
polished glass.mdl
ppv on silica.mdl
SiNx on Si.mdl
SiOx on Si.mdl
SOI.mdl
thermal oxide.mdl

Activates the search

Enter the query string to find

Select specific criteria

Select the searched file in the list, then click on the Go icon to select this file in the TreeView. Double-click goes directly to the file.

Close the **Search** screen and select the searched file in the TreeView

Close the **Search** screen

NOTICE: the * sign must not be used in the search query string

12 ***TreeView*** Main Menu allows the user to access files. It contains nodes which are detailed below:

▼ ▶ Functional node which is used to browse through the files of the software. There are three possibilities to open/close the functional node:

- Using the left button of the mouse, double-click the node name,
- Left-click on the +/- indicator in front of the icon. If this indicator does not exist, the node is empty,
- DeltaPsi files: each file node represents a DeltaPsi file located on the hard disk. To open the file, double-click with the left button of the mouse.

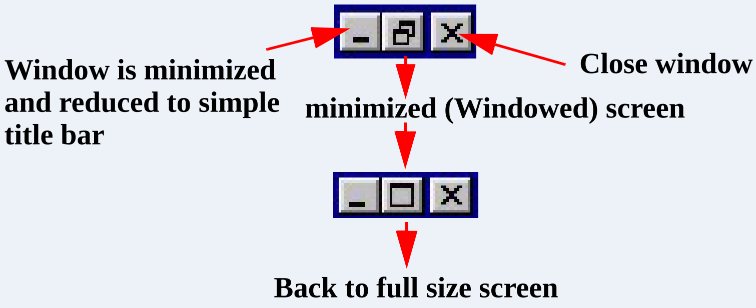
  Each type of file is marked on the icon: i.e. SPE for spectroscopy, REF for reference...
- Unknown file: this icon signifies that an unknown file has been found.

NOTICE: Right-clicking on an element name will display a popup menu. This menu contains specific options related to the node. Do not hesitate to try features included in this menu.

13 ***Shell Title Bar***: includes the ***Print*** command, the ***About*** button (DeltaPsi version information) and the ***Help*** button which is not active.

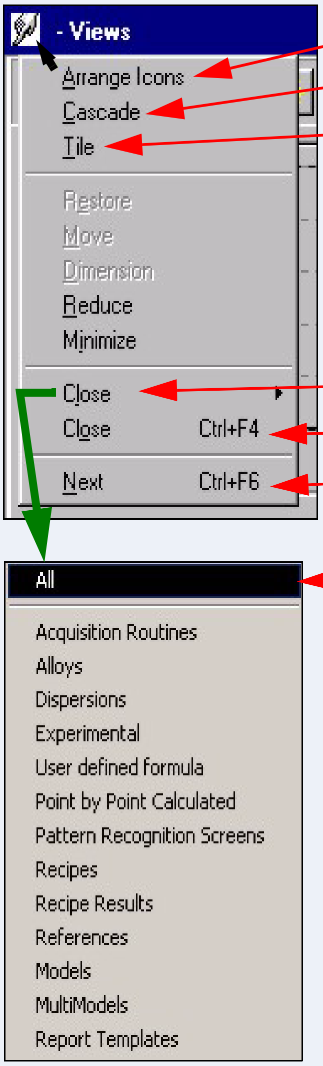
14 Help online is available by clicking the icon located on the ***Button Bar.***

16 Views screen: this is the main working area. This screen is in fact an independent window which can be resized using the following icon located on the upper right hand side of the screen:



◀ ▶ If several windows have been opened, these two buttons switch between the windows.

Additional options can be accessed by clicking on the icon located on the upper left hand side of the window. Depending on your size status, some options cannot be activated (greyed). Here below is an example of such of screen:



Arrange all minimized windows to make them visible

Arrange all windows in ¬¨¬¥windowed¬¨¬™ state wi same size with cascaded display

Arrange all windows in ¬¨¬¥windowed¬¨¬™ state an the size to be all visible at once

Standard Windows management options

Open a sub-menu detailed below

Close the active window

Activate next window

Close all windows

Each listed choice will close the related window, e.g. ¬¨¬¥Dispersions¬¨¬™ will close all dispersion f windows

17 DeltaPsi2 status bar information.

18 Shell status bar information.

19 Data manipulation feature

2 Basic Principles of Optics

2.1 The electromagnetic wave according to Maxwell equations

An electromagnetic wave is a transverse wave consisting of an electric field vector and a magnetic field vector. The magnitude of both vectors is a function of position and time. These two vectors are mutually perpendicular and both are perpendicular to the direction of propagation. The frequencies are ranging from ca. 3 10^{11} to 3 10^{16}Hz. The important quantity describing the light wave is the electric field vector. The magnetic field vector is not important because the induced magnetization in the material can be neglected since the motion of magnetic moments of electrons and nuclei is too slow to follow the rapid optical oscillations.

The electromagnetic field is described by Maxwell's equations:

Maxwell equations

$$\vec{\nabla} \cdot \vec{E} = 0$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0$$

$$\vec{\nabla} \times \vec{B} - \frac{\mu\varepsilon}{c} \frac{\partial \vec{E}}{\partial t} = 0$$

where E and B are the electric and magnetic field, c is the speed of light, μ is the permeability and is the dielectric function.

Combining these equations leads to the electric field wave equation:

$$\vec{\nabla}^2 \vec{E} - \frac{1}{\upsilon^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

with the optical impedance

$$\upsilon = \frac{c}{\sqrt{\mu\varepsilon}}$$

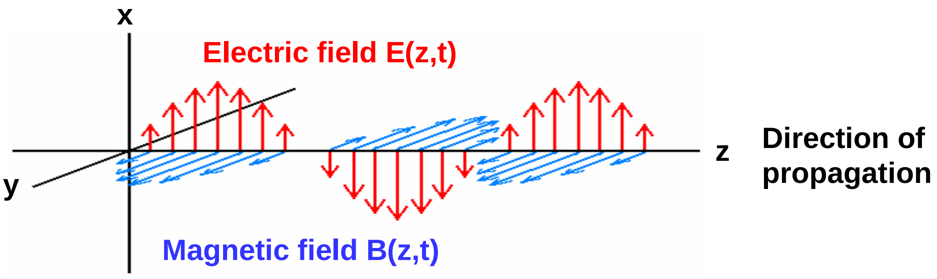
The electromagnetic plane wave is a solution of the electric field wave equation

$$\vec{E}(\vec{r}, t) = \vec{E}_0 \exp\left(\frac{i2\pi \cdot \tilde{n}}{\lambda} \vec{q}.\vec{r} \right) \exp(-i\omega \cdot t)$$

where $\vec{r}$ is the position vector along the direction of propagation, t is the time, the vector q is a unit vector along the propagation of the wave, $\tilde{n} = n + ik$ is the complex index of refraction, is the angular frequency of the wave, is the wavelength and is $\vec{E}_0$ a complex vector constant specifying the amplitude and polarization state of the wave. A plane wave propagating along the z-axis of an orthogonal coordinate system can be described by:

$$\vec{E}(z,t)=\vec{E}_0\exp\left(\frac{i2\pi\cdot\tilde{n}}{\lambda}q_z z\right)\exp(-i\omega\cdot t)$$

Linearly polarized plane wave propagating along the z-axis



2.2 Interaction of light with matter: complex index of refraction

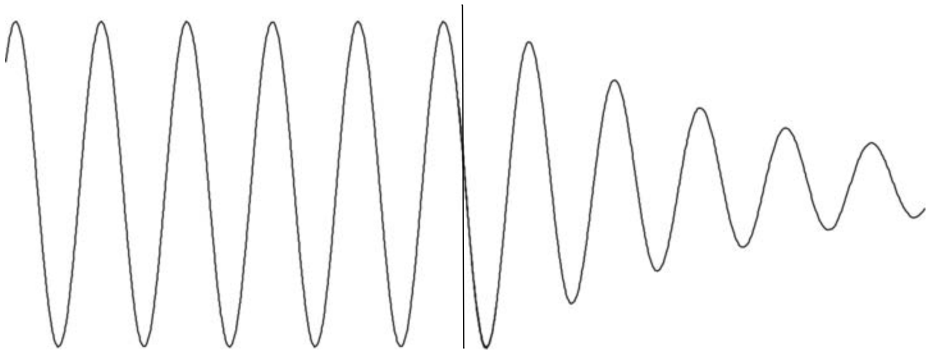
n: index of refraction
k: coefficient of absorption

When a light beam hits an interface between two media several phenomena can be observed. The wave in general slows down, changes direction, can be absorbed and/or reflected by the second medium. Optically the media are described by their complex index of refraction $\tilde{n}$ and their thickness.

The complex index of refraction $\tilde{n}=n+ik$ consists of the index of refraction n and the extinction coefficient k. It describes the interaction of light and matter. Both, n and k, are functions of the wavelength. The index of refraction describes the phase velocity of light in a material. The extinction coefficient describes how the intensity decreases as the light passes through the material.

0: Transparent medium $\tilde{n}_0 = n_0$

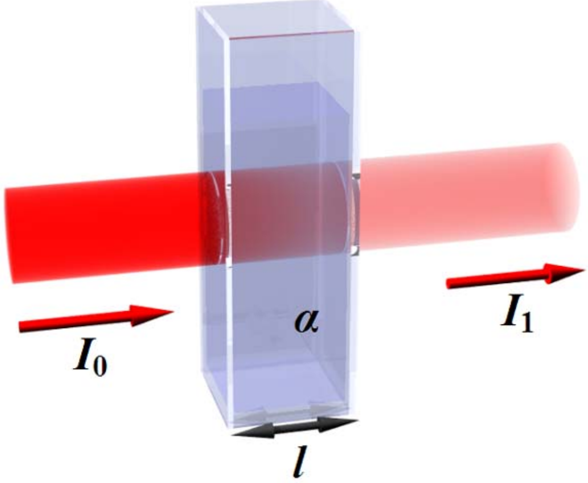
1: Absorbing medium $\tilde{n}_1 = n_1 - ik_1$



depth penetration

The decrease in intensity in an absorbing medium can be described by the following law:

$$I=I_0\exp(-\alpha\cdot z)$$



With the absorption coefficient α:

$$\alpha = \frac{4\pi \cdot k}{\lambda}$$

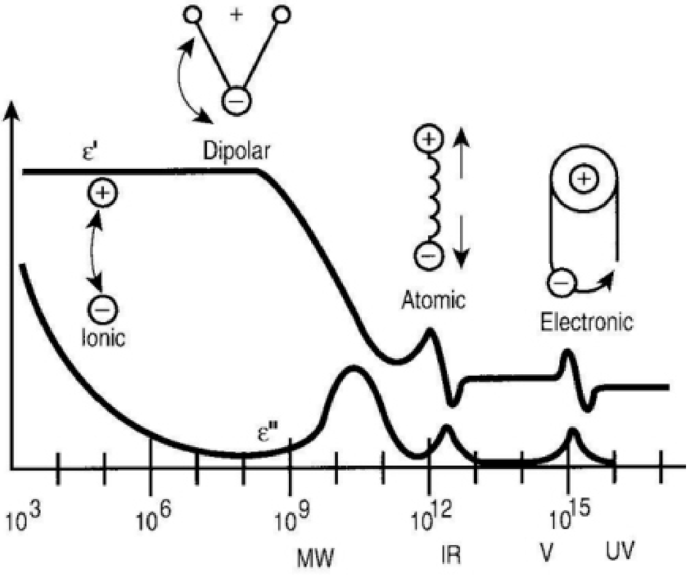
The penetration depth is defined by:

$$D_p = \frac{\lambda}{4\pi \cdot k}$$

When the thickness of the film is greater than ca. 4x the penetration depth the film can be treated as a substrate because too less light reflected from the interface reaches the detector. In this case the thickness cannot be determined, only the optical constants n and k.

There are mainly three processes causing the interaction of light with matter:

1. electronic transitions
2. molecular or lattice vibrations
3. free carrier absorption



2.3 Reflection and Refraction of Light

2.3.1 Law of reflection

The angle of reflection θ_r is equal to the angle of incidence θ_i :

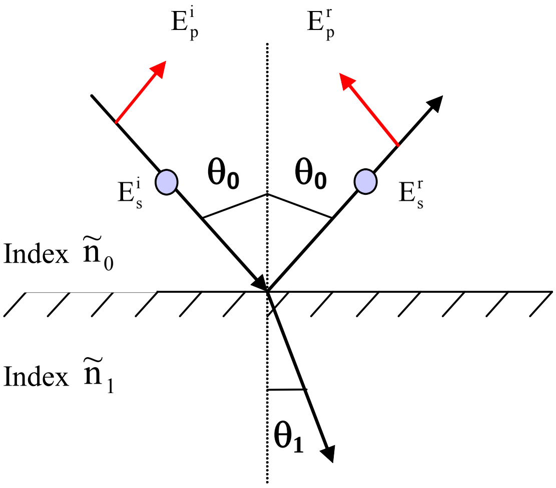
$$\theta_r = \theta_i$$

2.3.2 Law of refraction:

The light that is transmitted through the interface changes its direction according to the Snell-Descartes law:

$$\tilde{n}_0 \sin\theta_0 = \tilde{n}_1 \sin\theta_1$$

The knowledge of this law will allow us to determine the Fresnel coefficients.

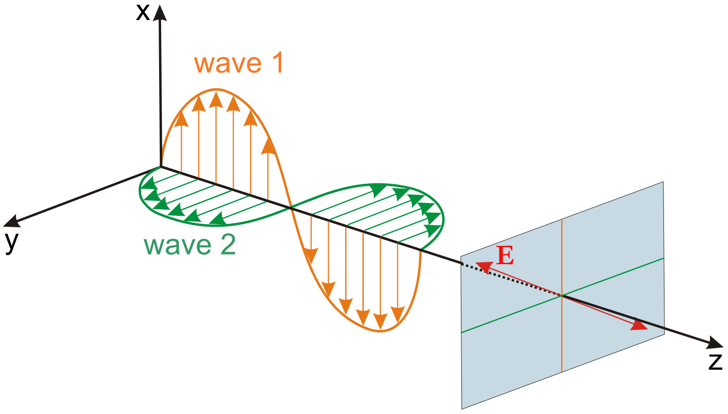


2.4 Polarization

Polarization refers to the behaviour with time of the electric field vector observed at a fixed point in space.

2.4.1 Linearly polarized light

Light with its electric field oriented in a constant transverse direction - although its magnitude and sign vary with time - is called linearly polarized. The transverse direction could be for example the x- or y- direction or any other direction perpendicular to the direction of propagation (z). In general any linearly polarized light can be described by the superposition of components polarized in the x-direction and in the y-direction. The amplitudes can be different however they must be in phase.

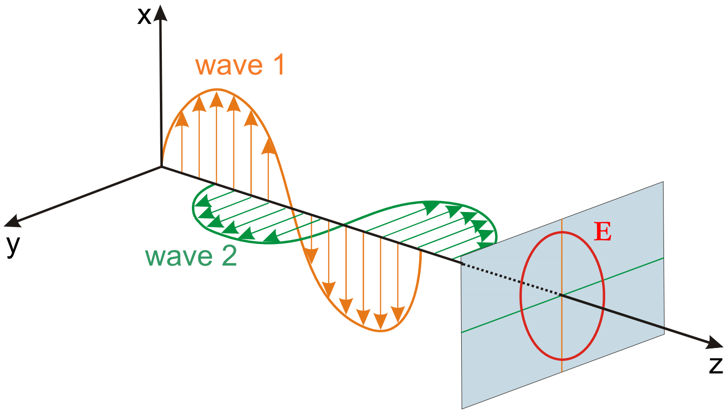


2.4.2 Circularly polarized light

If the amplitudes of the two components are equal and their relative phase difference is for example equal to /2 then the light is circularly polarized.

If the phase difference is equal to $-/2 + 2m$ (m=0, ±1, ±2,…) then the electric field vector is rotating clockwise at the frequency of the light as seen by an observer toward whom the wave is moving. This is called right-circularly polarized light. The electric field vector makes one complete rotation as the wave advances through one wavelength.

If the phase difference is equal to $+/2 + 2m$ (m=0, ±1, ±2,…) then the electric field vector is rotating counterclockwise at the frequency of the light as seen by an observer toward whom the wave is moving. This is called ***left-circularly polarized*** light.

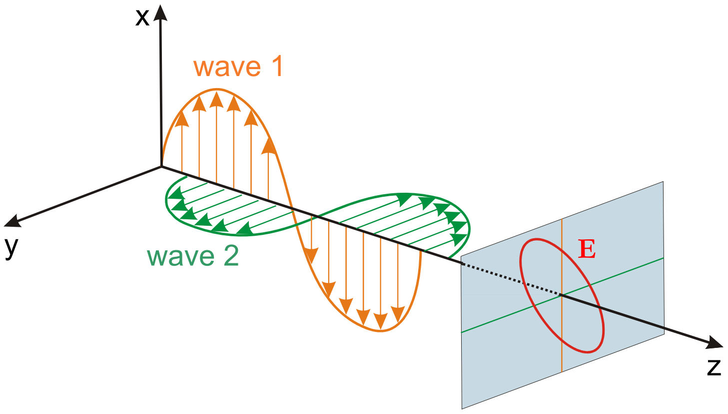


2.4.3 Elliptically polarized light

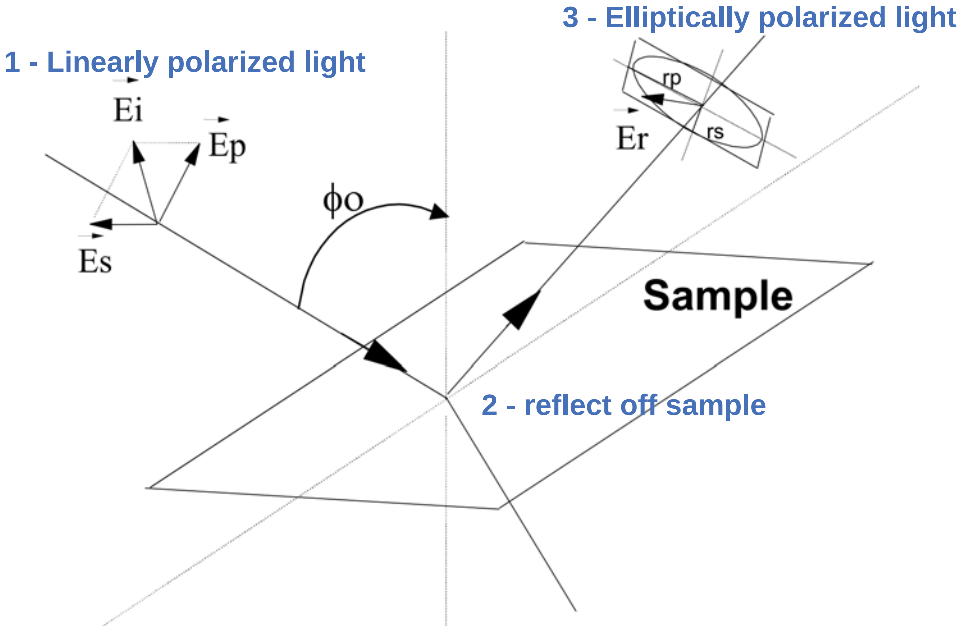
In general the two components of the light wave have different amplitudes and are out of phase. The result is elliptically polarized light. The tip of the electric field vector describes an ellipse in the projection on the x-y plane.

The most common components to describe the state of polarization are the component along the x-direction and the component along the y-direction. However, in general any two orthogonal polarization states can be used to describe the polarization of the light wave. For example also the two oppositely polarized circular waves can be used.

Elliptically polarized light can be formed for example by the reflection of linearly polarized light on a surface.



So usually in ellipsometry we see elliptically polarized light after reflection on the sample at the detector when the incoming light is linearly polarized:



2.4.4 Partially polarized light

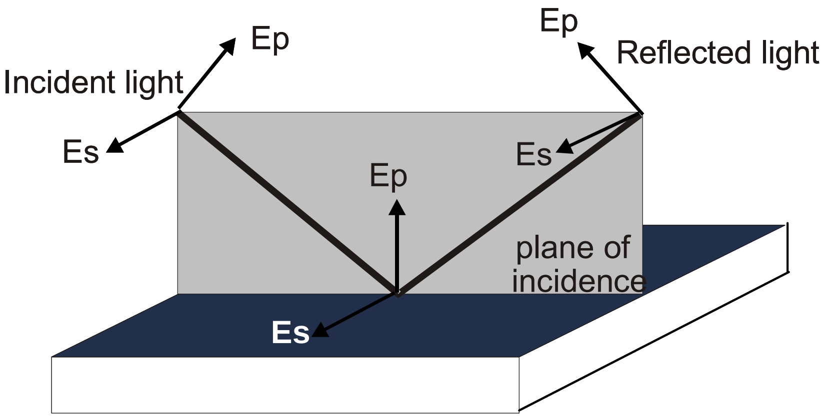
The electric fields of photons emitted from an incandescent light source are oriented in all different directions. This is called ***unpolarized light***. In general the electric field varies in a way that is neither totally regular nor totally irregular, it is ***partially polarized***. This partial polarization can be expressed by the ***degree of polarization***.

2.5 The Fresnel coefficients

Assuming a plane wave arrives at the sample surface, one part of the wave is reflected and the other part is transmitted. The electric field vector can be decomposed in two components as mentioned above, in a component E_s perpendicular to plane of incidence (s – for German “senkrecht”) and in a component E_p parallel to the plane of incidence. Both components show different behaviour during reflection and thus reflection leads to a modification of the light polarization. The reflection of the components is described by the Fresnel coefficients of reflection r_p and r_s :

The complex Fresnel coefficients

$$r_p = \frac{E_p^{\,r}}{E_p^{\,i}} = |r_p| \exp(i\delta_p) \qquad r_s = \frac{E_s^{\,r}}{E_s^{\,i}} = |r_s| \exp(i\delta_s)$$



The modules of the coefficients give the amplitude modifications of the electric field components. Their phases give the phase shift caused by the reflection.

The ratio ρ of these two coefficients is exactly what an ellipsometer measures:

Fundamental equation of ellipsometry

$$\rho = \frac{r_p}{r_s} = \tan\Psi e^{i\Delta}$$

with

$$\tan\Psi = \frac{|r_p|}{|r_s|}$$

$$\Delta = \delta_p - \delta_s$$

and $\in [0;90°]$ & $\in [0;360°]$.

The parameters Ψ and Δ are called the ***ellipsometric angles***. The analysis of Ψ and Δ allows to obtain optical properties of the sample.

2.6 Relation of Fresnel coefficients to material properties

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For a homogeneous sample the Snell-Descartes equation is

$$\tilde{n}_0 \sin\theta_0 = \tilde{n}_1 \sin\theta_1$$

where θ_0 and θ_1 are the angle of incidence and refraction and is $\tilde{n}_1$ the refractive index of the sample and $\tilde{n}_0$ f the surrounding material. By using this equation and the properties of the electromagnetic field at an interface one obtains the Fresnel coefficients for reflection and transmission:

Fresnel coefficients

reflection

$$r_p = \frac{\tilde{n}_1 \cos\theta_0 - \tilde{n}_0 \cos\theta_1}{\tilde{n}_0 \cos\theta_0 + \tilde{n}_1 \cos\theta_1}$$

$$r_s = \frac{\tilde{n}_0 \cos\theta_0 - \tilde{n}_1 \cos\theta_1}{\tilde{n}_0 \cos\theta_0 + \tilde{n}_1 \cos\theta_1}$$

transmission

$$t_p = \frac{2\tilde{n}_0 \cos\theta_0}{\tilde{n}_1 \cos\theta_0 + \tilde{n}_0 \cos\theta_1}$$

$$t_s = \frac{2\tilde{n}_0 \cos\theta_0}{\tilde{n}_0 \cos\theta_0 + \tilde{n}_1 \cos\theta_1}$$

In this simple case of a semi-infinite sample without top layer it is possible to calculate the dielectric function of the material directly from the ratio $\rho = r_p/r_s$:

$$\tilde{\varepsilon} = \tilde{n}_1{}^2 = \tilde{n}_0{}^2 \sin^2\theta_0 \left[1 + \left(\frac{1-\rho}{1+\rho} \right)^2 \tan^2\theta_0 \right]$$

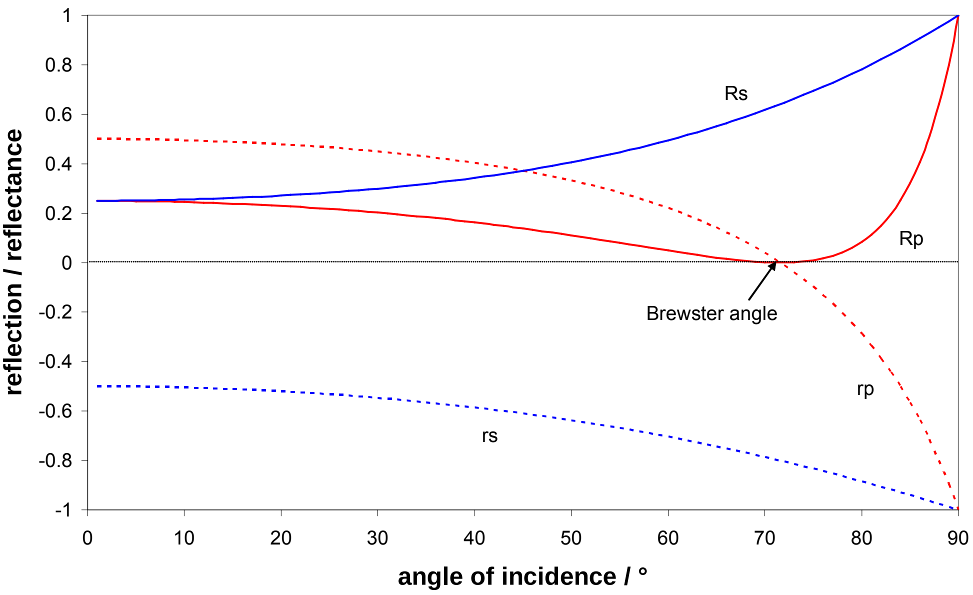
2.7 The Brewster angle

The ***reflectance*** *R* is calculated from the reflection coefficients *r* by:

$R^s = |r^s|$ and $R^p = |r^p|$

If we plot the reflectance *R* versus the angle of incidence (*AOI*) we see that R^p shows a minimum for a certain AOI and gets equal to 0 for a certain AOI in the case of a dielectric (k =0) whereas R^s increases with *AOI*.

The AOI where R^p shows a minimum is called the ***principle angle*** and in the case of dielectric materials ($R^p = 0$) the ***Brewster angle***.

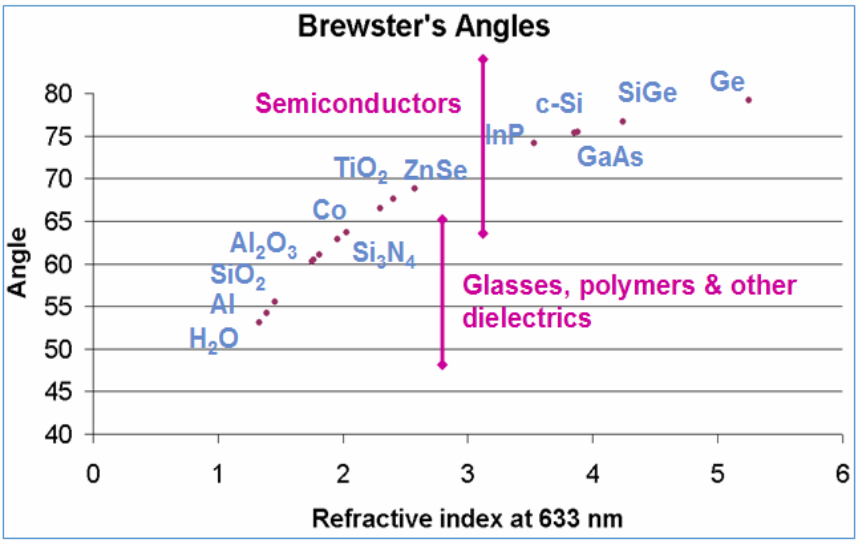


The Brewster angle can be calculated from the indices of the two media by:

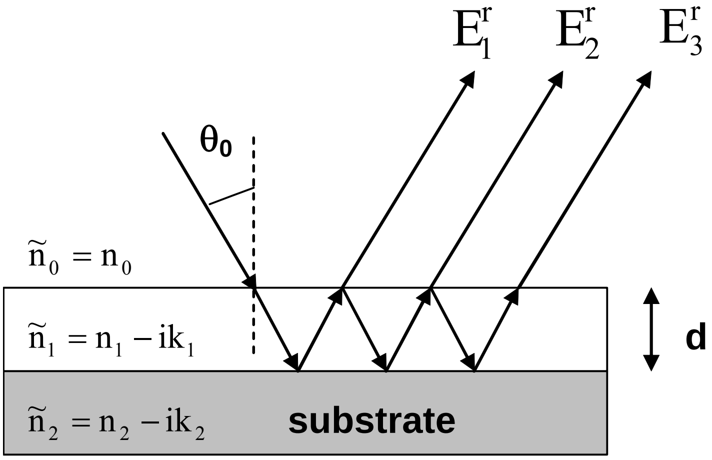
$$\tan\theta_B = \frac{n_1}{n_0}$$

The phase retardation of the p-wave shifts abruptly from zero to 180° at the Brewster angle for dielectrics.

The Brewster angle for some materials is shown in the next graph:



2.8 Reflection with films



In the case of a deposited film on a substrate, the part of light which is transmitted cannot be ignored as it is the case for a bulk material because it is reflected on the film-substrate interface.

The resulting reflected wave returning to the medium 0 is composed of light which is reflected from the first interface as well as light transmitted by the first interface, reflected by the second one and then transmitted by the first one, and so on. Assuming the previous derivation for the Fresnel reflection and transmission coefficients of a bulk material is locally valid for the reflection and transmission of a beam from any interface, we can now calculate the Fresnel coefficients which are functions of the optical properties of the film and the ambient. The calculation of the coefficient for the p-polarization is independent from the one for the s-polarization; any arbitrary incident light beam can be described as a linear combination of the two polarization states. For a single film, the ratio of the amplitude of the outgoing resulting wave to the amplitude of the incoming light beam is defined as total reflection coefficient:

Total reflection coefficients

$$r_{total}^{p} = \frac{E_p{}^{r}{}_{total}}{E_p{}^{i}} = \frac{r_{01}{}^{p} + r_{12}{}^{p}\exp(-i\cdot 2\beta)}{1 + r_{01}{}^{p}r_{12}{}^{p}\exp(-i\cdot 2\beta)}$$

$$r_{total}^{s} = \frac{E_s{}^{r}{}_{total}}{E_s{}^{i}} = \frac{r_{01}{}^{s} + r_{12}{}^{s}\exp(-i\cdot 2\beta)}{1 + r_{01}{}^{s}r_{12}{}^{s}\exp(-i\cdot 2\beta)}$$

where

Fundamental equation of ellipsometry

β is the phase change from the top of the film to the bottom of the film

$$\beta = \left(\frac{2\pi\cdot d}{\lambda}\right)\tilde{n}_1\cos\theta_1$$

2.9 Effect of film thickness

For normal incidence the total reflection coefficient for a single film system is give by:

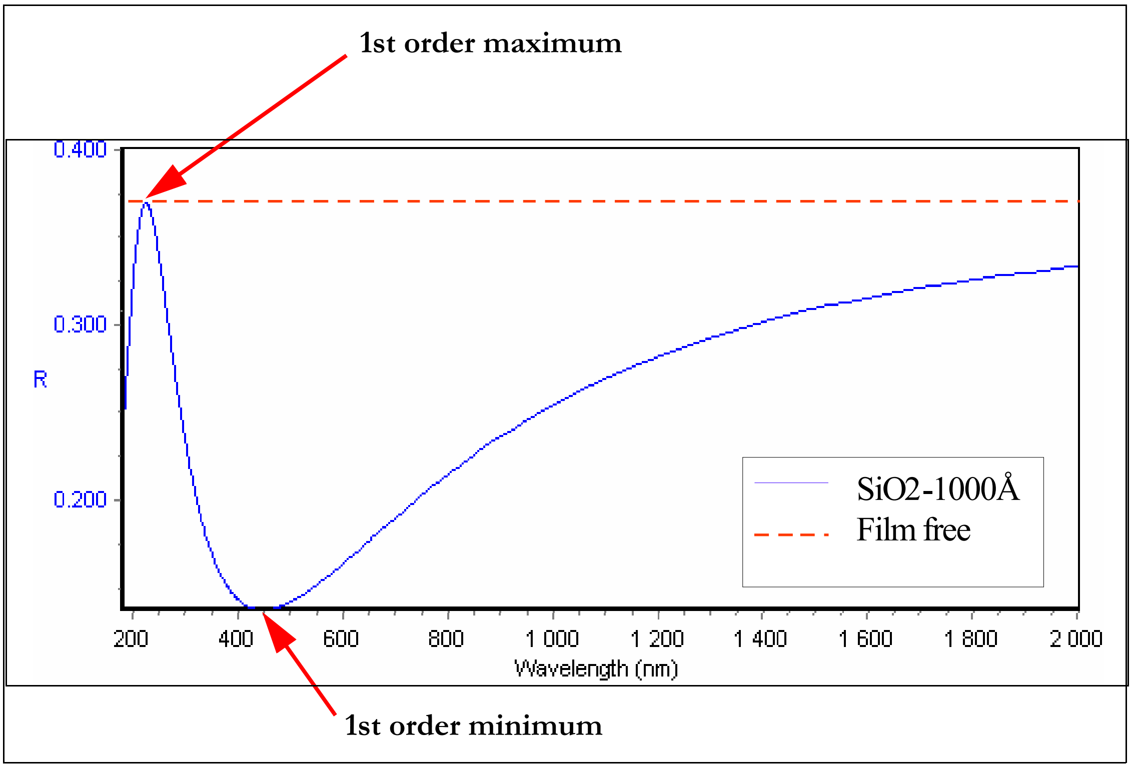
$$r_{total} = \frac{r_{01} + r_{12}\exp(-i \cdot 2\beta)}{1 + r_{01}r_{12}\exp(-i \cdot 2\beta)}$$

When the thickness and wavelength are such that the light reflecting from the top surface and the light reflecting from the interface layer-substrate or layer1-layer2 are 180° out of phase, which is the equivalent to $2\beta = \pi$, the exponential term of the reflectance is -1 and we have the greatest amount of destructive interference. It results in the first order minimum on the reflectance spectrum.

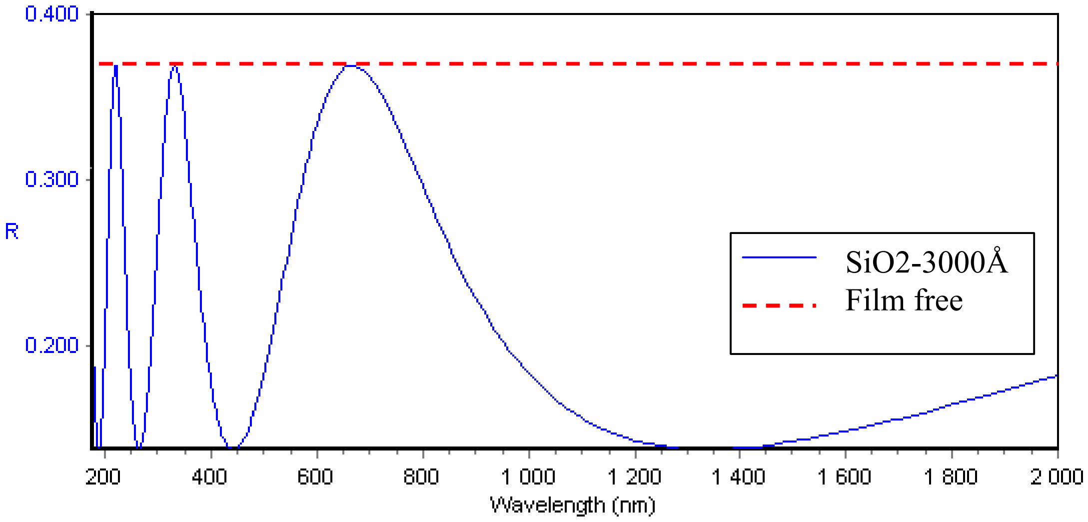
When $2\beta = 2\pi$, the value of the exponential term is +1, the reflectance is the same as the reflectance of a film free substrate and we have a first order maximum.

The minima occur for $2\beta = \pi, 3\pi, 5\pi, 7\pi\ldots$ and the maxima occur for $2\beta = 2\pi, 4\pi, 6\pi, 8\pi\ldots$

For the following illustration we plotted the reflectance of a 1000Å thick SiO_2 layer on a substrate whose index of refraction "n" is 3.87 and whose extinction coefficient "k" is 0.0165.



If we increase the thickness of the SiO_2 layer several higher-order maxima and minima appear successively. The reflectance spectrum of a 3000Å SiO_2 layer on the same substrate as above is shown in the next figure:



We can make the following observations:

- the spacing between maxima and minima increases with wavelength
- increasing the thickness causes all the positions of the maxima and minima to move toward a longer wavelength
- thicker films provide more maxima and minima than thinner films for any wavelength range

3 Ellipsometry Basics

3.1 Definition Ellipsometry

Ellipsometry measures the change in state of polarization in reflection and transmission experiments.

3.2 Fundamental equation of ellipsometry

Fundamental equation of ellipsometry

The relation between ellipsometric angles Ψ and Δ with the reflection coefficients for parallel and perpendicular polarization is given by:

$$\rho = \frac{r^p}{r^s} = \tan\Psi \cdot e^{i\Delta}$$

This equation is called the fundamental equation of ellipsometry.

3.3 Dependence on Sample Properties (single wavelength)

In this chapter Psi-Delta curves are shown as functions of substrates, film thickness and optical constants.

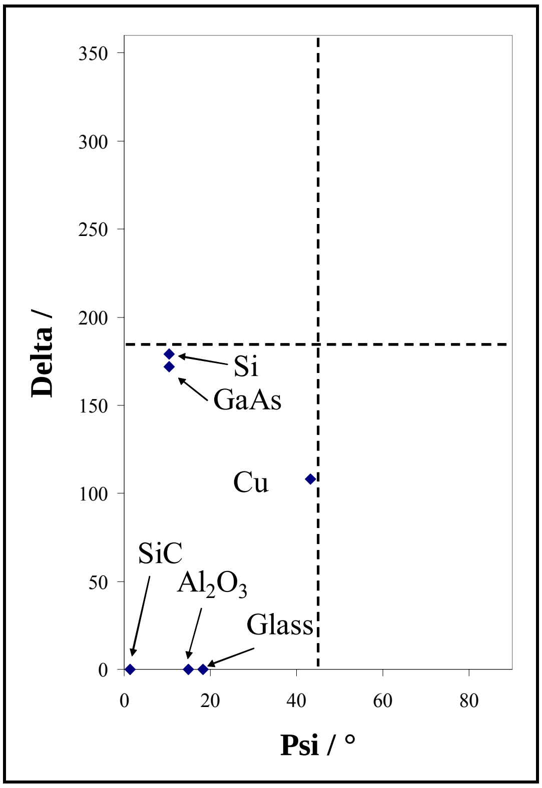
3.3.1 Substrates

For pure substrates the measured Psi-Delta values must be in the following intervals:

$0 \leq \Psi \leq 45°$

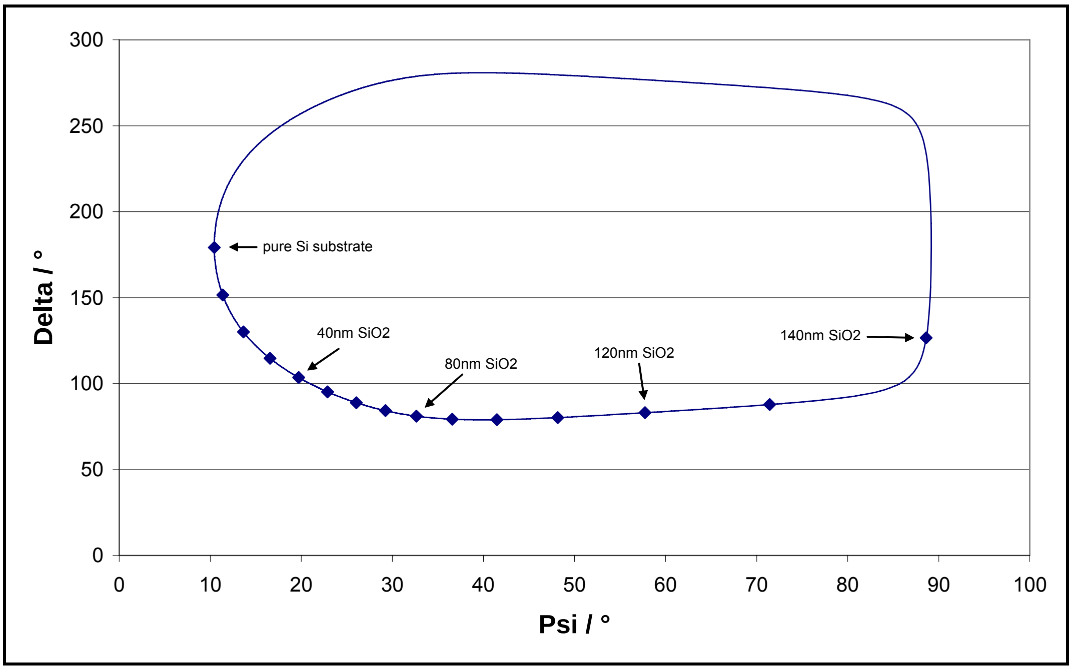
$0 \leq \Delta \leq 180°$

This is shown for some examples in the following graph:



3.3.2 Single films: thickness variation

When growing a thin film on a substrate the Ψ–Δ trajectory describes a closed curve if the film is transparent. This is shown for SiO_2 on Si substrate (AOI: 70°, 633nm):



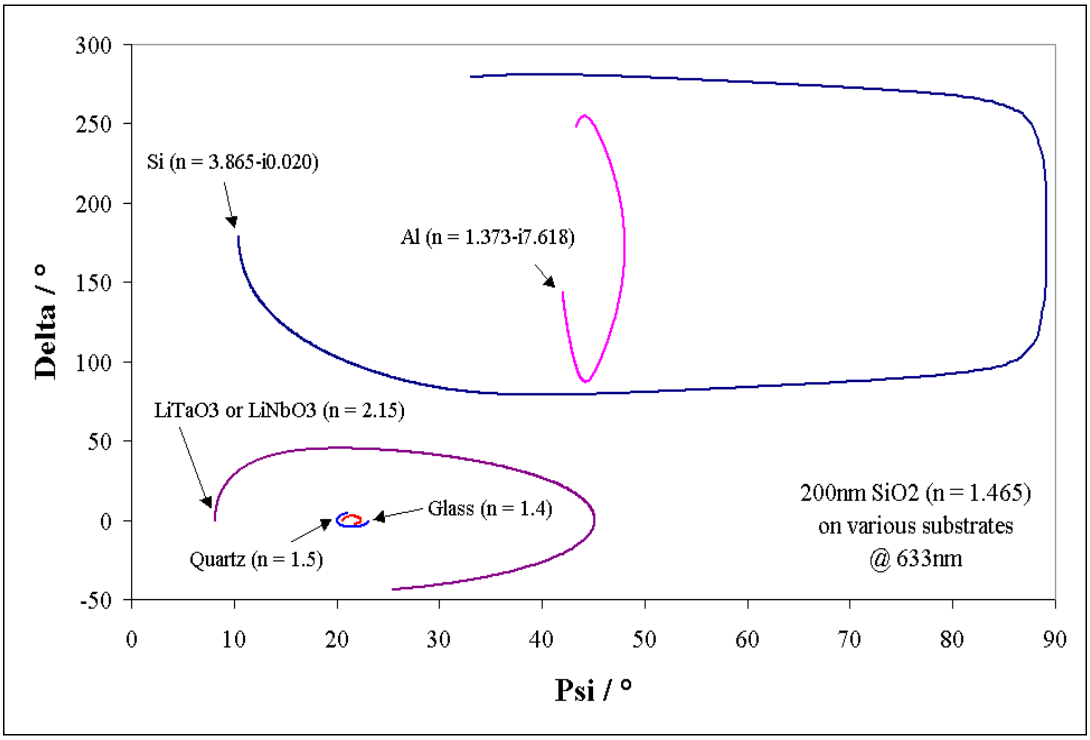
After one «period» (P) the curve reaches the starting point. The period depends on wavelength, AOI and refractive index of the material:

$$P = \frac{\lambda}{2\sqrt{n_1^2 - n_0^2 \sin(AOI)}}$$

For SiO_2 on Si substrate (AOI = 70°, 633nm) the period is ca. 280nm. So it is actually not possible to distinguish a SiO_2 layer of a certain thickness t and a layer of thickness t + nP. For example the following SiO_2 layers would give the same - values: 20nm, 300nm, 580nm, ...

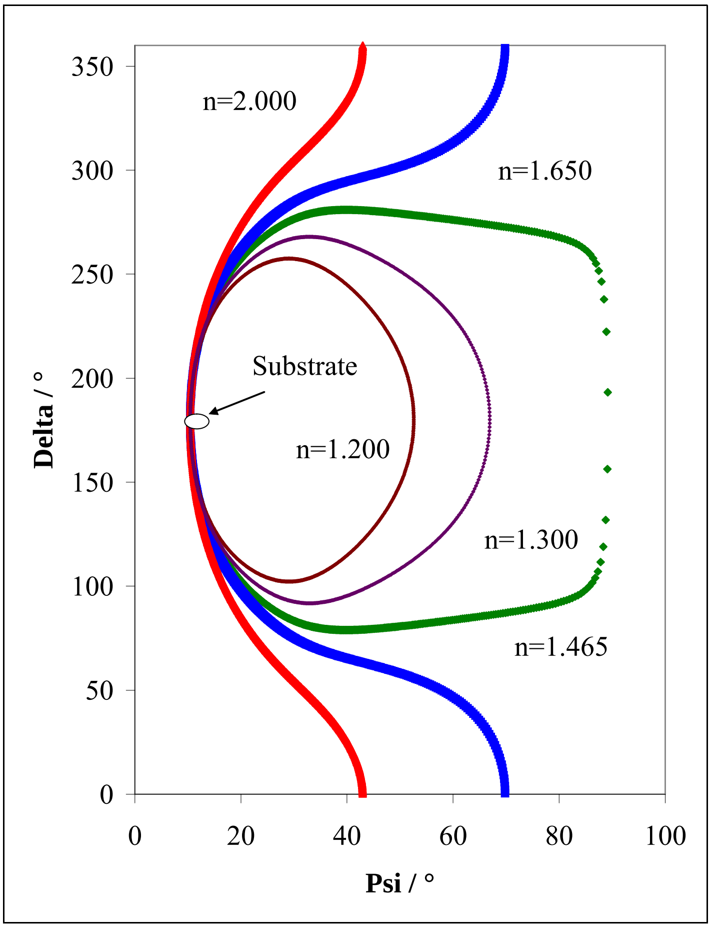
This is called the «period problem» of single wavelength ellipsometry.

The period does not depend on the substrate. For example the next graph shows $\Psi - \Delta$ trajectories of SiO_2 on different substrates. Although the curves look quite different the period length is always the same.



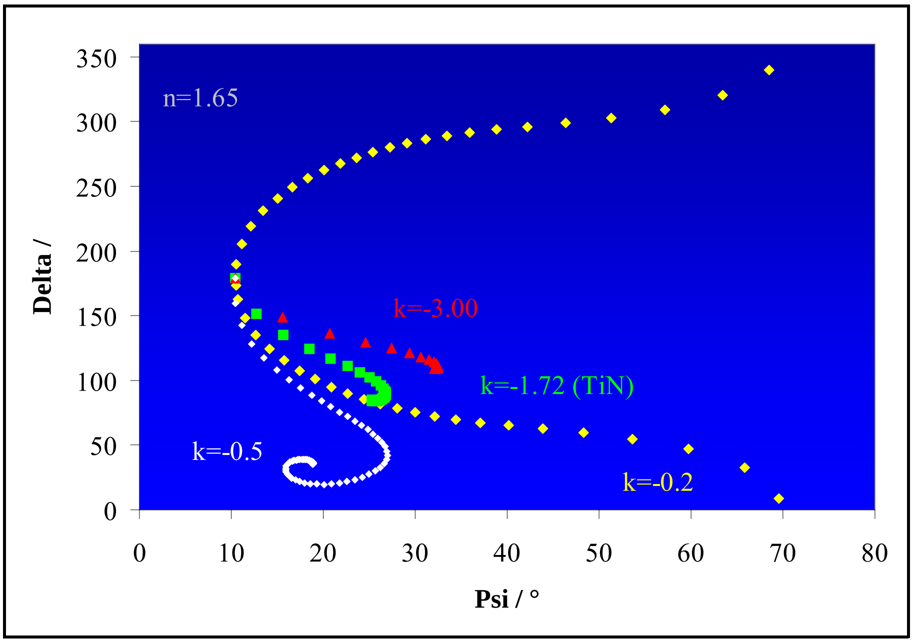
3.3.3 Single films: variation in n

The dependency of the $\Psi - \Delta$ trajectories on the refractive index n is shown in the next graph. As long as k = 0 the curves are closed with a period that depends on n.



3.3.4 Single films: variation in k

If k > 0 the Ψ–Δ trajectories are not closed any more they converge into the Ψ–Δ values that represent the film as pure substrate:



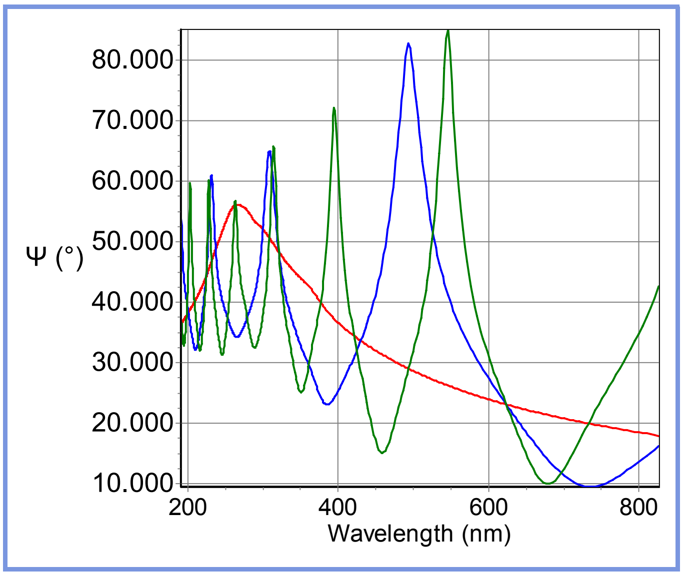
For films thicker than the ca. 4x the penetration depth it is not possible any more to determine the thickness of the film. It can be regarded as a substrate. That means that one can determine n & k of this film directly from $\Psi-\Delta$ values.

Remember the penetration depth is defined by:

$$D_p = \frac{\lambda}{4\pi \cdot k}$$

3.4 Spectroscopic information

The spectroscopic information eliminates the period problem because the period is wavelength dependant. The following graph shows the Ψ-values of SiO_2 films on Si substrate (red: 50nm, blue: 330nm, green: 610nm) at AOI = 70°:



One can see that the curves coincide at 633nm but are different at the other wavelengths. Again, the thicker the layer the more “interference fringes” appear.

3.5 Different ellipsometer types

The different ellipsometers have components in common

There are three major techniques to measure the ellipsometric angles Ψ and Δ:

- null ellipsometry
- rotating element analyzer
- polarization modulation ellipsometer

All types of ellipsometers consist of a light source of some sort, a device that defines the state of polarization before the light strikes the sample and a device that determines the state of polarization after reflection.

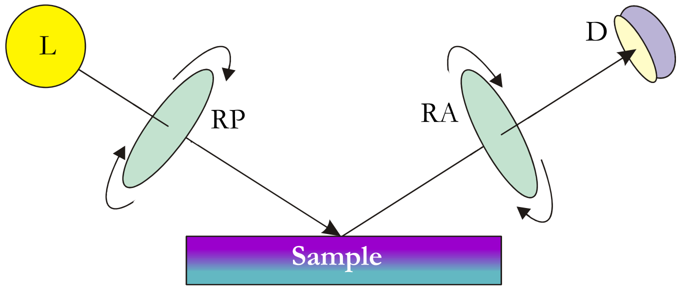
3.5.1 Null ellipsometer

This kind of ellipsometer is based on the principle of signal extinction. The azimuths of a polarizer and an analyzer are manually adjustable to obtain the configuration where the light intensity that is detected is minimized.

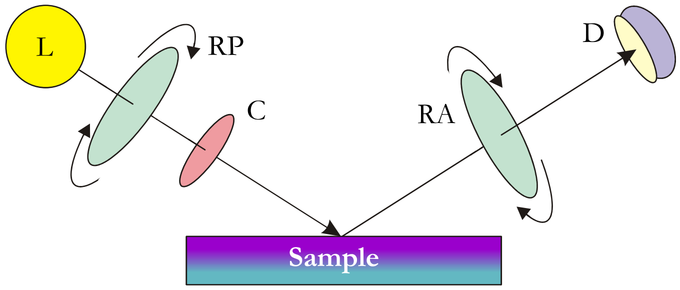
3.5.2 Rotating element ellipsometer

This is a very common type of ellipsometer. One of the polarizing elements (polarizer, analyzer or compensator) rotates at a frequency of ca. 10 to 300Hz. This leads already to an improvement of acquisition time compared to null ellipsometers but acquisition is still rather slow. The range of frequencies is prone to noise caused by mechanical vibrations, requiring an elaborate signal treatment.

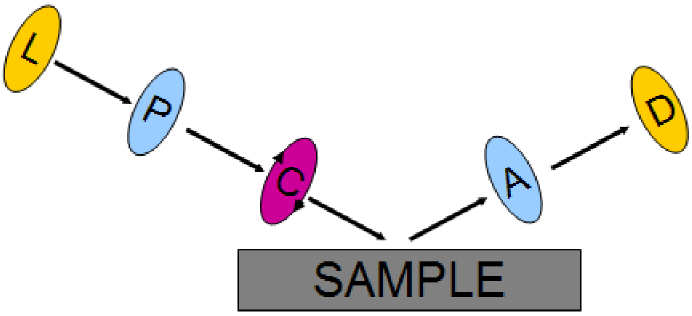
Rotating polarizer (RP) or analyzer (RA)



Rotating polarizer (RP) or analyzer (RA) with compensator (C)



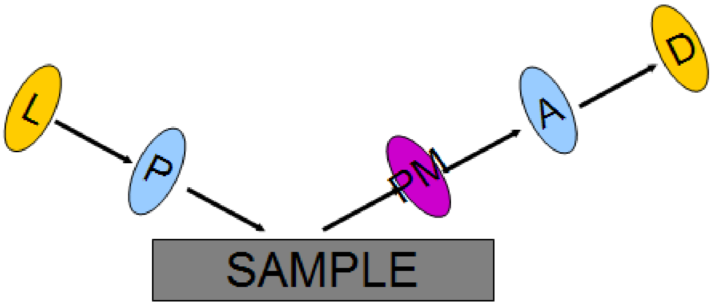
Rotating compensator (RC)



3.5.3 Polarization modulation ellipsometer (PME)

The PEM allows very fast measurements

This ellipsometer shows optimized acquisition speed and a large spectral range from the IR to the UV. The high acquisition speed is due to the presence of a photoelastic modulator (PEM) whose acquisition frequency is around 50kHz. The drawbacks of this ellipsometer are the chromatic behaviour of the modulator and the sophisticated optical calibrations. This type of ellipsometer allows extremely accurate results, thanks to a high performing electronic system.



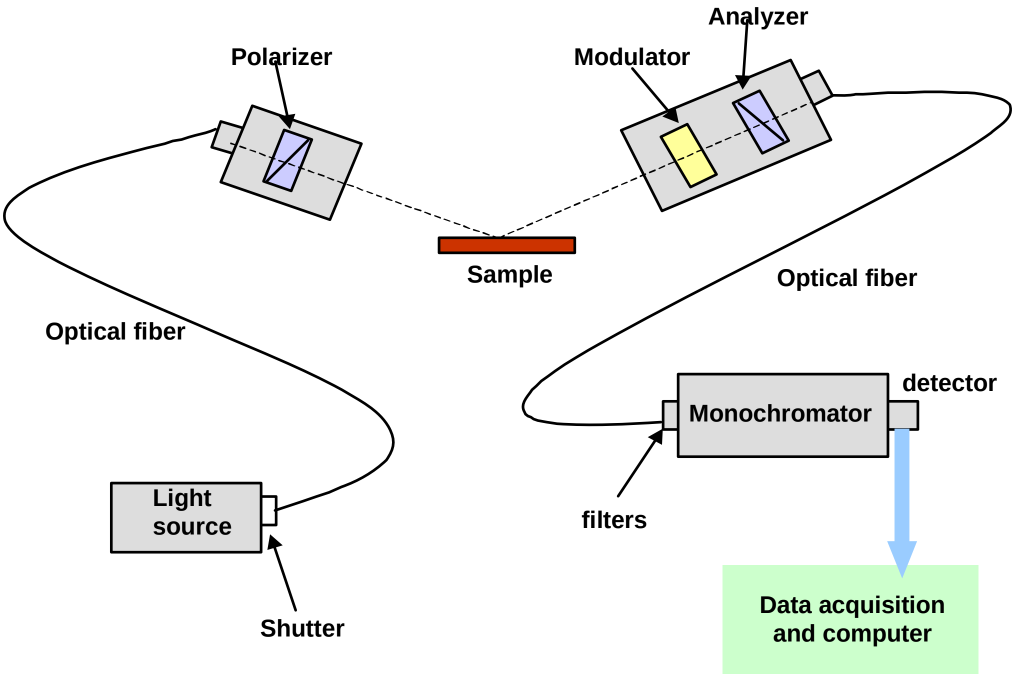
3.5.4 Summary

Technique	**RA / RP**	**RA / RP and compensator**	**RC**	**PME**
Modulation frequency	10 - 300Hz	10 - 300Hz	10 - 300Hz	50kHz
Measured parameters	tanΨ - cosΔ	tanΨ - tanΔ	tanΨ – tanΔ	sin2Ψ - cosΔ sin2Ψ - sinΔ cos2Ψ

Strength	Simple design Easy calibration Large spectral range No wavelength dependent optics CCD detection possible	High accuracy also at $\Delta \approx 0°$ or $180°$ (thin transparent films)	High accuracy CCD detection possible	No rotating elements Wide spectral range High accuracy for all Ψ and Δ Fast acquisition: 1ms
Weakness	Not accurate for $\Delta \approx 0°$ or $180°$ Errors due to residual polarization Moving part	Complicated calibration CCD detection not possible Moving part	Difficult technology Difficult calibration Moving part	Difficult technology Difficult calibration CCD detection not possible

3.5.4.1 Detailed description of the Polarization modulation (PM) ellipsometer

The layout of a classical PM ellipsometer is as follows:



Elliptically modulated polarized light

Source

The typical light source is a Xenon arc lamp of 75 Watt with a spectral range from the near IR to the UV.

Optical fibers

The optical fibers are used to couple the light beam from the output of the light source to the input of the polarizer and from the output of the analyzer to the input of the monochromator. Generally the optical fibers have a 1mm core diameter and are of two types:

- UV fibers which cover the range 190 - 880nm
- NIR fibers which cover the range 260nm – 2100nm

Polarizer

The polarizer defines the state of polarization before the light strikes the sample.

Photoelastic Modulator (PEM)

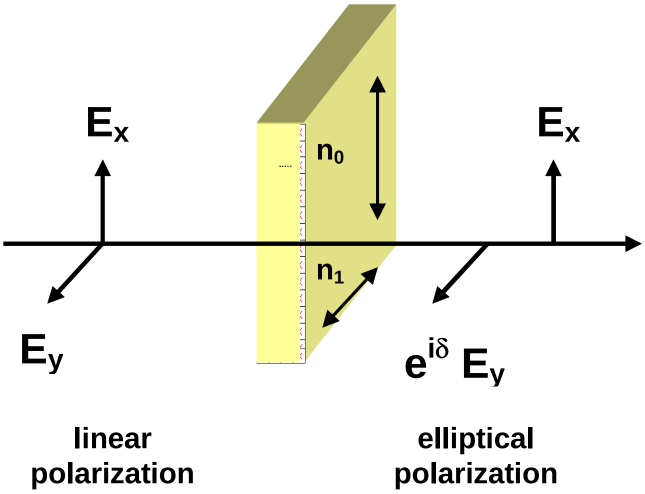
The polarization modulator induces a modulation of the state of polarization that means that the ellipticity of the polarization varies as a function of time.

The modulator used in the spectroscopic ellipsometers of HORIBA JOBIN YVON is based on the photoelastic effect: Stress is applied to a silica bar so that its optical properties are modified. In its equilibrium state, the modulator is optically isotropic with one index of refraction, and becomes birefringent (with two indices) under mono-axial stress. A cosine variation of the stress modulates the birefringent state of the silica bar (resonance frequency $f = \Omega/2\pi \approx 50$ kHz). The phase retardation between the two components of the electric field is:

$$\delta(t) = A \sin \Omega t$$

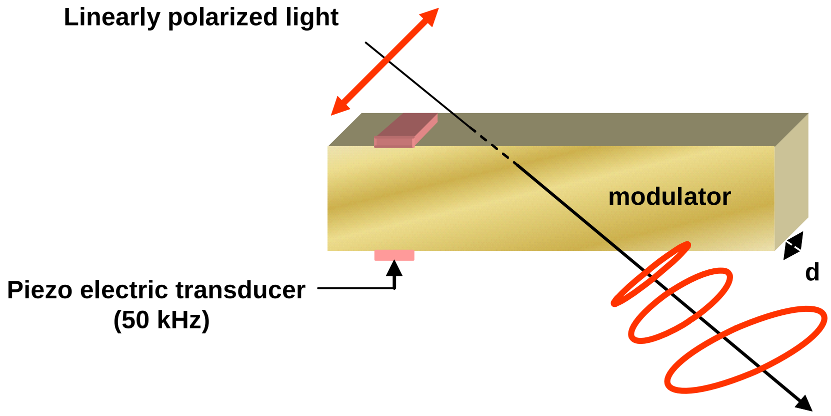
whereby

$$A = \frac{2\pi \cdot d(n_1 - n_0)}{\lambda}$$



The applied stress is wavelength dependent. It is regulated with a modulation voltage, so that the modulation amplitude is kept constant.

The modulator temperature must be controlled and kept constant. The advantages of the photoelastic modulation are: very fast acquisition, high accuracy and working frequency far from ambient noise sources.



Analyzer

The analyzer is similar to the polarizer of the entry and is located just after the sample and photoelastic modulator.

Monochromator

The monochromator separates the light into its various components before it reaches the detector.

Detector

The detection system is composed of various elements:

- photomultipliers for the UV and the visible spectral range
- a InGaAs detector for the IR spectral range

Acquisition interface

Except for the sample placement, the operation of the ellipsometer is entirely automated.

The computer interface owns command modules to control:

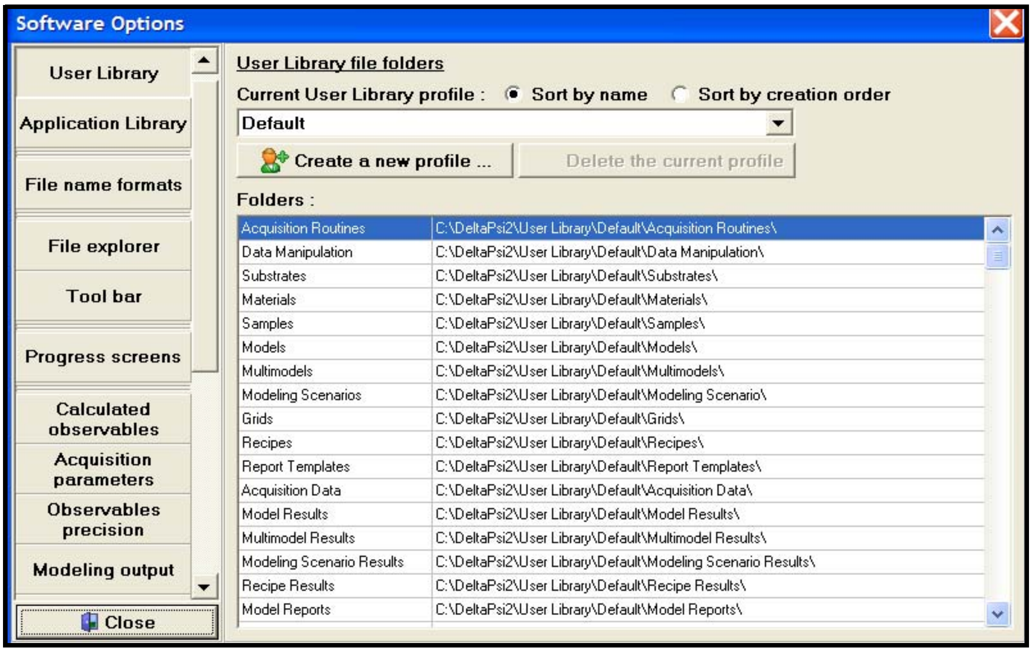
- step motors for azimuths of analyzer, polarizer and modulator
- goniometer for the angle of incidence
- amplitude of the photoelastic modulator
- shutters and filters
- high voltage of the photomultipliers
- slits of the IR monochromators

4 Measurement QuickStart

Preparation of System

- Switch on the controller unit and the computer where the ***DeltaPsi2*** software is installed.
- Turn on the ***light source*** (usually a Xe arc lamp) and wait 15min to let it stabilize.
- Open the ***DeltaPsi2*** software and click on the "software options" tab:

The following window will appear:



User Library file folders

Current User Library profile : ● Sort by name ○ Sort by creation order

Default

Folders :

Acquisition Routines	C:\DeltaPsi2\User Library\Default\Acquisition Routines\
Data Manipulation	C:\DeltaPsi2\User Library\Default\Data Manipulation\
Substrates	C:\DeltaPsi2\User Library\Default\Substrates\
Materials	C:\DeltaPsi2\User Library\Default\Materials\
Samples	C:\DeltaPsi2\User Library\Default\Samples\
Models	C:\DeltaPsi2\User Library\Default\Models\
Multimodels	C:\DeltaPsi2\User Library\Default\Multimodels\
Modeling Scenarios	C:\DeltaPsi2\User Library\Default\Modeling Scenario\
Grids	C:\DeltaPsi2\User Library\Default\Grids\
Recipes	C:\DeltaPsi2\User Library\Default\Recipes\
Report Templates	C:\DeltaPsi2\User Library\Default\Report Templates\
Acquisition Data	C:\DeltaPsi2\User Library\Default\Acquisition Data\
Model Results	C:\DeltaPsi2\User Library\Default\Model Results\
Multimodel Results	C:\DeltaPsi2\User Library\Default\Multimodel Results\
Modeling Scenario Results	C:\DeltaPsi2\User Library\Default\Modeling Scenario Results\
Recipe Results	C:\DeltaPsi2\User Library\Default\Recipe Results\
Model Reports	C:\DeltaPsi2\User Library\Default\Model Reports\

- Choose "user library" and choose an existing user library profile in the drop-down menu or "Create a new profile…".
- Close the "software options" window and click the "manual measurement" tab to open the "Views" screen:

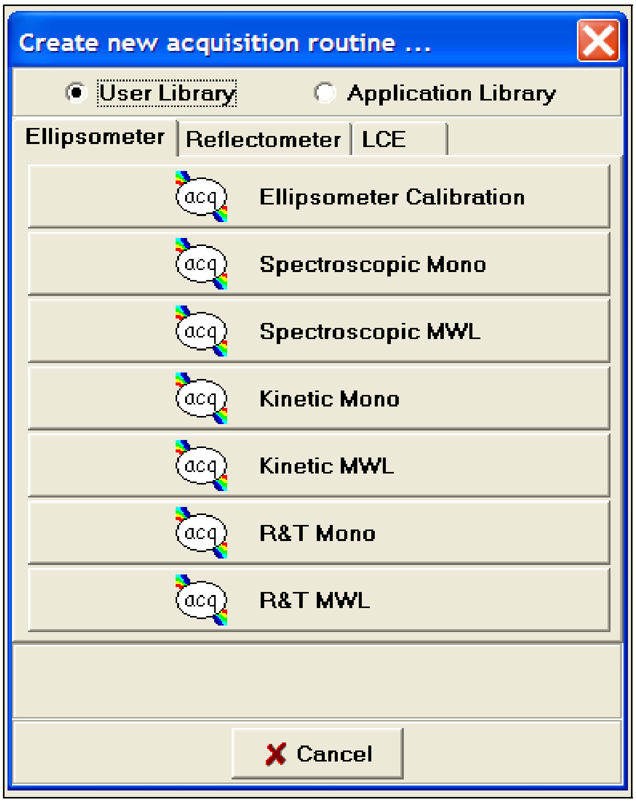
Sample Positioning

- Place your ***sample*** on the ***stage*** and switch on the ***autocollimator illumination***.
- Look through the eyepiece of the autocollimator and align the crosshairs so that the centers overlap by adjusting the two knobs underneath the stage.
- In the views screen set the monochromator to 2.75eV (or 450nm if you prefer to work with wavelength).
- Adjust now the height of the stage by turning the corresponding knob underneath the stage. Try to find the position where S0 is at its maximum
- In the views screen click "S0 adjustment" or manually set the high voltage so that S0 is between 60 and 80mV.

DeltaPsi2 Software: Acquisition Interface

- Click on the «Create a new acquisition routine...» tab:

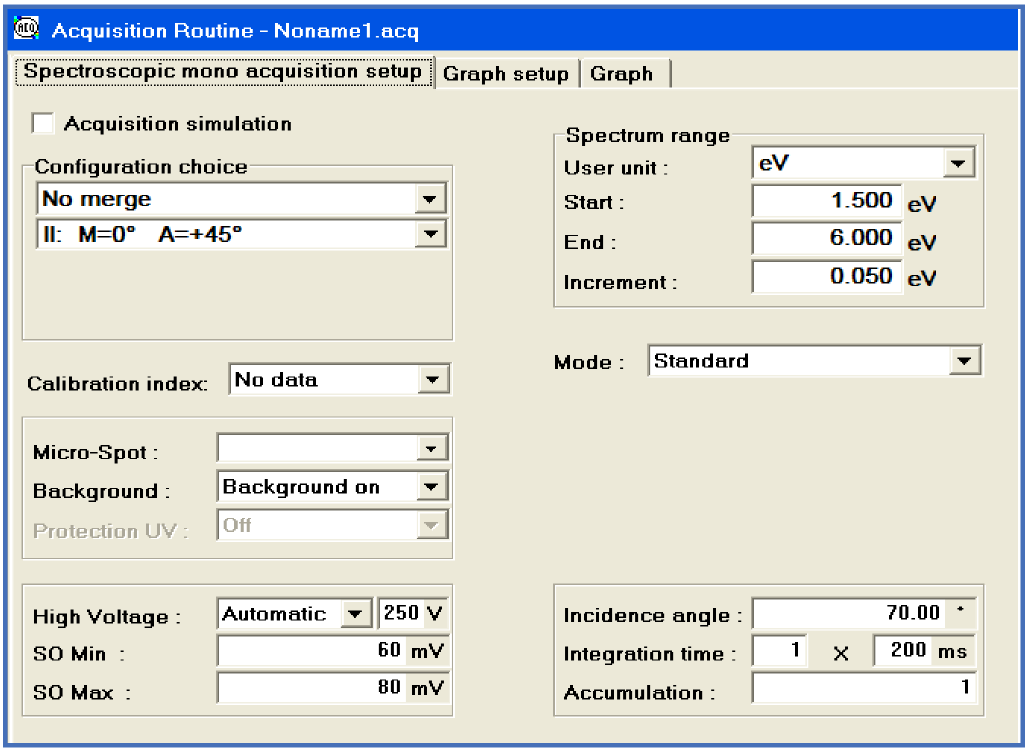
- The following options will appear (they will be explained for scanning systems – for MWL systems the main points are mostly identical):



They allow you to choose the data type you wish to acquire.

> **Ellipsometric Calibration:** For calibration of your system

> **Spectroscopic Mono:** Choose this option if you want to acquire ellipsometric data over a certain wavelength range.



☐ Acquisition simulation

Configuration choice
No merge
II: M=0° A=+45°

Calibration index: No data

Micro-Spot :
Background : Background on
Protection UV : Off

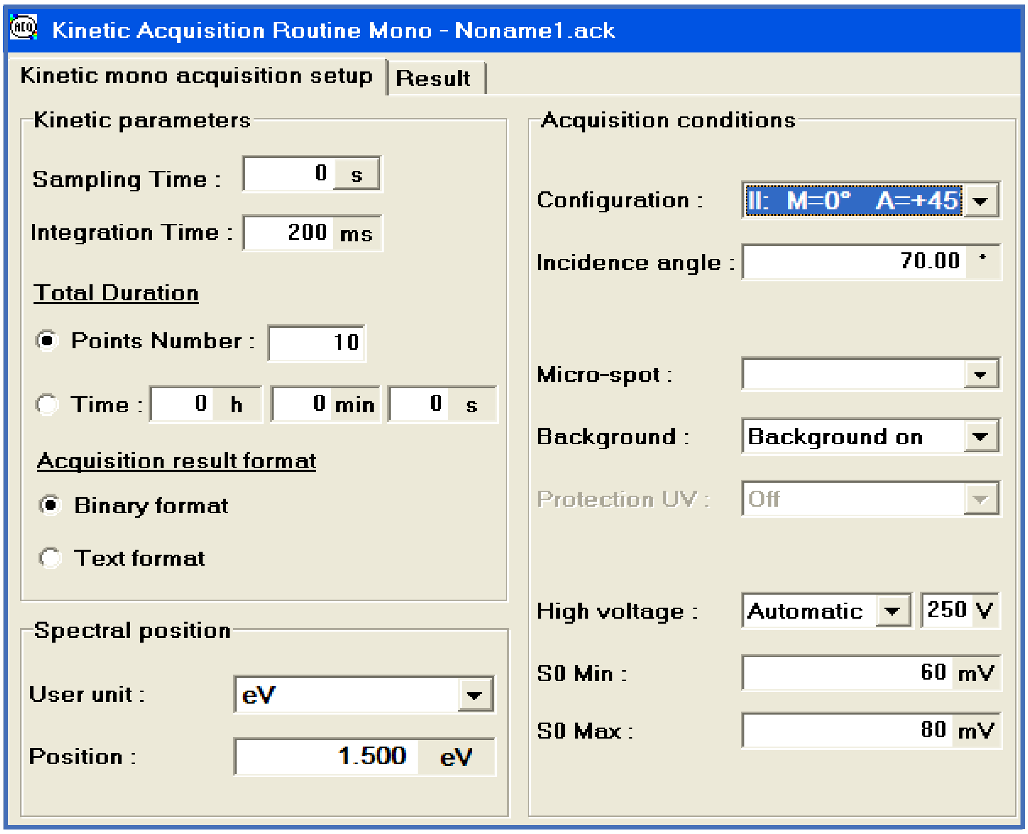
High Voltage : Automatic 250 V
SO Min : 60 mV
SO Max : 80 mV

Spectrum range
User unit : eV
Start : 1.500 eV
End : 6.000 eV
Increment : 0.050 eV

Mode : Standard

Incidence angle : 70.00 °
Integration time : 1 x 200 ms
Accumulation : 1

> **Kinetic Mono:** Choose this option if you want to acquire ellipsometric data as a function of time.



Kinetic Acquisition Routine Mono - Noname1.ack

Kinetic parameters

Sampling Time : 0 s

Integration Time : 200 ms

Total Duration

● Points Number : 10

○ Time : 0 h 0 min 0 s

Acquisition result format

● Binary format

○ Text format

Spectral position

User unit : eV

Position : 1.500 eV

Acquisition conditions

Configuration : II: M=0° A=+45

Incidence angle : 70.00 °

Micro-spot :

Background : Background on

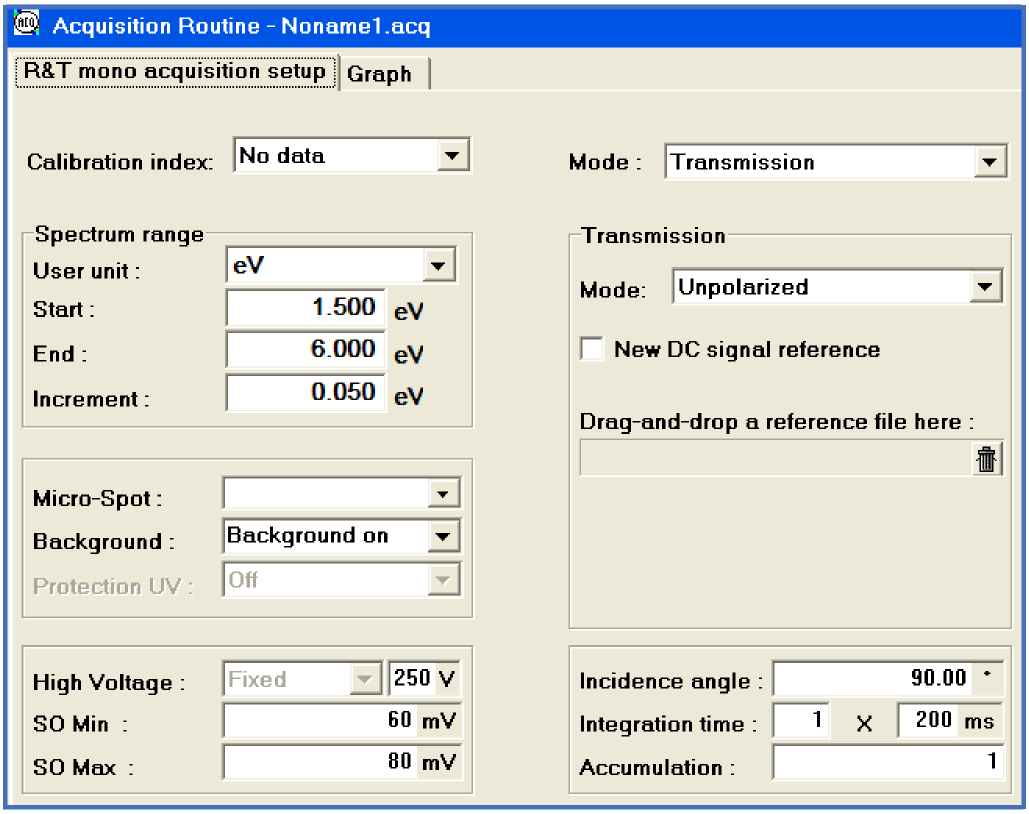
Protection UV : Off

High voltage : Automatic 250 V

S0 Min : 60 mV

S0 Max : 80 mV

> **R & T Mono:** Choose this option if you want to acquire reflection or transmission data over a certain wavelength range.



Acquisition Routine - Noname1.acq

Calibration index: No data

Mode : Transmission

Spectrum range

User unit : eV

Start : 1.500 eV

End : 6.000 eV

Increment : 0.050 eV

Transmission

Mode: Unpolarized

☐ New DC signal reference

Drag-and-drop a reference file here :

Micro-Spot :

Background : Background on

Protection UV : Off

High Voltage : Fixed 250 V

SO Min : 60 mV

SO Max : 80 mV

Incidence angle : 90.00 °

Integration time : 1 X 200 ms

Accumulation : 1

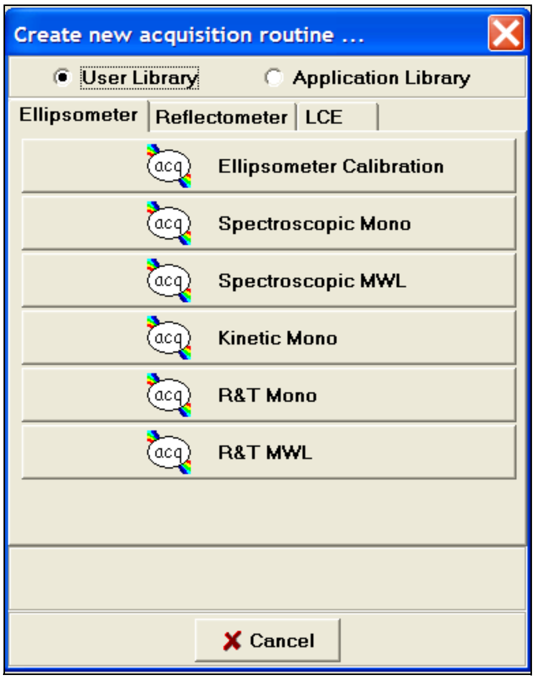
5 Advanced Acquisition

5.1 Introduction

The UVISEL system is able to acquire data basically from any given sample. Moreover besides ellipsometric data we can also acquire reflectance and transmittance data.

If you click on the Acq. Tab on top of the page:

The following window will appear:


● User Library ○ Application Library

The different options for the UVISEL ellipsometer are:

Ellipsometric Calibration: system calibration

Spectroscopic Mono: acquisition of ellipsometric data in reflection and/or transmission with a scanning monochromator

Spectroscopic MWL: acquisition of ellipsometric data in reflection and/or transmission with detection at fixed multiple wavelengths

Kinetic Mono: acquisition of ellipsometric data in reflection and/or transmission at a specified wavelength as a function of time

R&T Mono: acquisition of reflectance and/or transmittance data with a scanning monochromator

R&T MWL: acquisition of reflectance and/or transmittance data with detection at fixed multiple wavelengths

To optimize the data acquisition (in terms of data quality and measurement time) the following parameters have to be set before the measurement:

- ***spectral range***
- ***angles of incidence***
- ***spectral step size***: equal increments in wavelengths or energy?
- ***detector settings***
- ***spot size***
- ***measurement parameters (experimental data types)***

This parameters will be discussed in detail for the most important acquisition mode, the spectroscopic mono, but most of the information is also relevant for the other acquisition modes.

5.2 Sample preparation

Before the data acquisition is started the sample has to be prepared and positioned on the sample support.

5.2.1 Surface cleaning

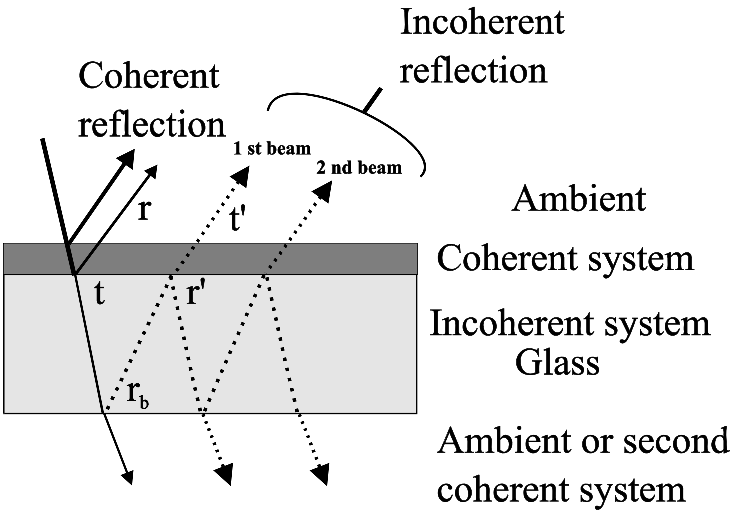
Ellipsometry is very sensitive to the microscopic surface state whereas it is rather insensitive to macroscopic particles: large objects only scatter the light away from the detector. But surface roughness or oxidation layers may have strong effects on the specularly reflected beam.

Overlayers including native oxides or surface roughness can be removed by chemical or mechanical treatment. The user should refer to a library of surface treatments for the considered material.

If the overlayer cannot be removed it can be included in the layer model.

5.2.2 Back surface reflections

In the case of transparent samples that are polished on both sides the light beam reflected from the backside reaches the detector and affects the measurement.



One way to avoid this backside reflection is **roughening** the backside surface. Roughening provides a scattering effect and a non-specular surface which prevents the penetrating beams to be reflected from the back.

Backside roughening can be applied for example to samples based on plastic substrates especially when these are optically anisotropic.

Roughening can be achieved with sandpaper assuming that it does not leave residue such as inclusions in the sample.

Note that backside reflections are not necessarily a problem. In some particular cases (thin transparent substrates with both sides polished) the backside reflections can be included in the layer model.

Assuming the optical properties of the transparent material are isotropic we can distinguish three cases:

- the case of substrates whose thickness is < 1 mm:

The detection head will collect several incoherent reflected beams; the exact amount of them is not critical as far as there are at least two collected beams. The modeling will assume infinite number of backside reflected beams. The problem can therefore be solved by proper modeling.

- the case of substrates whose thickness is between 1 and 2 mm:

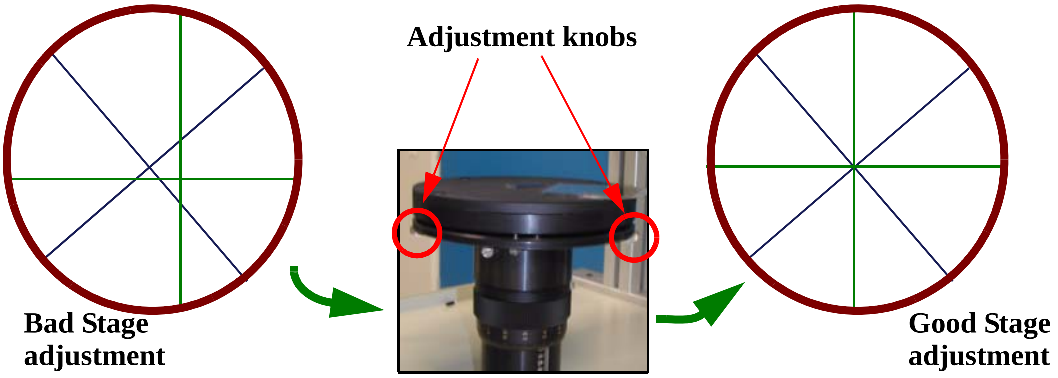
In this case the backside reflected beams tend to be separated. The backside reflected beam can be suppressed mechanically with an appropriate spot size and angle of incidence. If this is not possible the only solution is to roughen the backside.

- the case of substrates whose thickness is > 2 mm:

In this case, the back surface beams are sufficiently separated so that the backside reflected beam can be clearly suppressed mechanically with an appropriate spot size and angle of incidence.

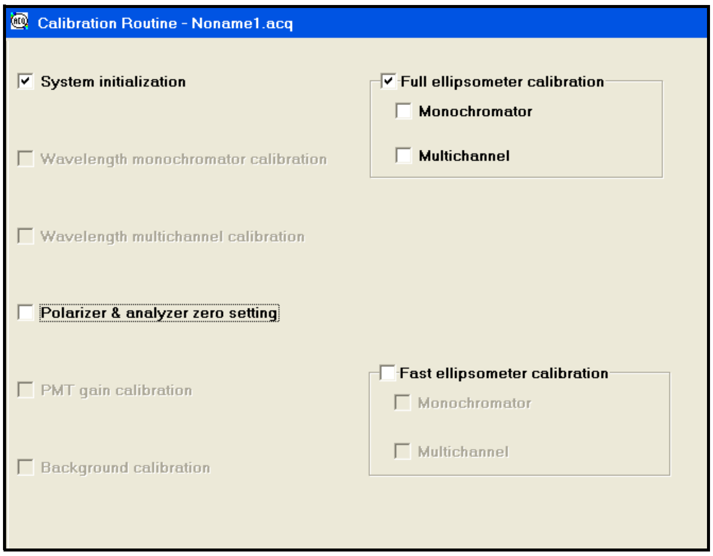
5.2.3 Sample positioning

The levelling of the sample is performed with the **Autocollimator**. Adjust the screws of the stage so that crossing points of both reticules coincide:



5.3 Ellipsometric calibration acquisition mode

This mode is used for calibration of system devices. It is used only in extraordinary situations when the ellipsometer needs to be fully calibrated. For this type of calibration, it is advised to ask for the assistance of HJY Service Engineers. Do not perform this calibration for routine measurements.



Calibration Routine - Noname1.acq

☑ System initialization

☑ Full ellipsometer calibration
- ☐ Monochromator
- ☐ Multichannel

☐ Wavelength monochromator calibration

☐ Wavelength multichannel calibration

☐ Polarizer & analyzer zero setting

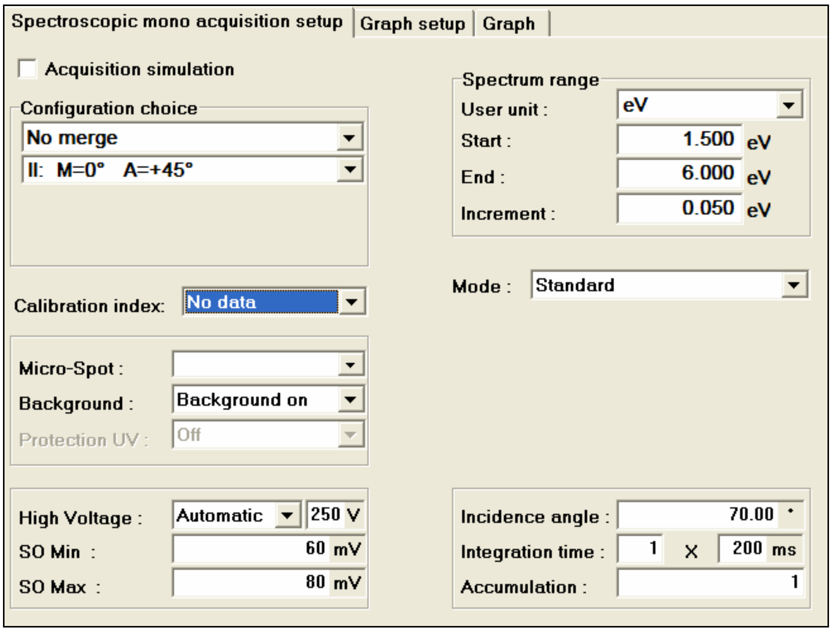
☐ Fast ellipsometer calibration
- ☐ Monochromator
- ☐ Multichannel

☐ PMT gain calibration

☐ Background calibration

5.4 Spectroscopic Mono acquisition mode

The following figure shows the DP2 page for setting the acquisition parameters:



☐ Acquisition simulation

Configuration choice: No merge; II: M=0° A=+45°

Calibration index: No data

Micro-Spot :

Background : Background on

Protection UV : Off

High Voltage : Automatic 250 V

SO Min : 60 mV

SO Max : 80 mV

Spectrum range

User unit : eV

Start : 1.500 eV

End : 6.000 eV

Increment : 0.050 eV

Mode : Standard

Incidence angle : 70.00 °

Integration time : 1 x 200 ms

Accumulation : 1

5.4.1 Spectral range

1 *Set wavelength range*

The spectral range option allows the user to define the range of wavelength or photon energy over which he wants to have measurement points.

The choice of optimal spectral range depends directly on the **material** under study and of course on the information that is needed (thickness and/or optical constant in a certain spectral region).

5.4.1.1 Optimal spectral: thickness and/or optical constants

If the user is attempting to determine the thickness(es) of layer(s) in the sample, few well chosen wavelengths might be enough to obtain the correct information. Of course, the acquisition over multiple wavelengths allows the overdetermination of the thickness and thus lead to a higher accuracy.

If the user is attempting to determine the optical constant at certain wavelengths, data must be acquired in the corresponding spectral range. Assuming DeltaPsi2 linearly interpolates optical constant between two points of measurement, one has to see how sharp absorption peaks are. The wavelength or energy increments have to be set so that these peaks can be sufficiently resolved. Typically, the increment in energy for data acquisition ranges between 0.1 eV to 0.905 eV.

It is always preferable to acquire data in the transparent spectral range of the material, as this allows to reduce the correlation between the different fitting parameters and to eliminate the determination of material absorption from the analysis. It is important to repeat that ellipsometric data must be acquired in the transparent spectral range of the material to determine the thickness of the film. Therefore the appropriate spectral range for various types of materials is discussed in the following section.

5.4.1.2 Optimal spectral range for various material types

Dielectric materials

Dielectric materials are, along with semiconductors, the most commonly encountered class of materials. Examples for dielectric materials are SiO_2, $SrTiO_3$, SiC, Si_3N_4, HfO_2, LaO_3, Ta_2O_5, TiO_2, MgO or Al_2O_3 .... These materials are transparent over a wide spectral range from IR to deep UV. Ellipsometric measurements from IR to UV The measurement of these materials can be done over a very broad part of the spectral range because they are transparent from IR to UV and even deep UV. Ellipsometric maesureemnts from IR to UV provide a wealth of information. Al_2O_3 for example is transparent from IR to deep UV due to its wide energy band-gap. Silicon dioxyde instead is transparent for wavelengths > 250nm.

The transparent region for low-k materials is in general smaller than that for high-k materials ranging from the near IR to the visible/near UV, thus for energies < 3 - 4eV. Transparent organic materials have an absorption tail in the UV region which can be described by dispersion functions.

Semiconductors

Semiconductor materials exhibit a band gap. In general we can basically decompose the spectra of semiconductors into two regions:

- energy > band gap: the material begins to absorb and the absorption increases smoothly
- energy < band gap: the absorption coefficient of the material approaches zero (material becomes transparent) and the index of refraction decreases monotonically with decreasing photon energies.

The absorption processes for semiconductors are mainly due to interband transitions above the energy band gap.

Semiconducting material can have crystalline or amorphous structure. For **crystalline semiconductors** the transition from the transparent region to the absorbing region at the band gap is very **sharp**. **Amorphous semiconductors instead have broad absorption bands**. In fact, amorphous solids exhibit absorption tails below the band gap (Urbach tails), which are far more extensive than the absorption tails of crystalline solids.

Metals

The classical model used to describe metals is the Drude model assuming a gas of free carriers. The absorption of energy of an incident beam by the free carriers can be explained by the fact that the electric field of the light beam induces a conducting current whose dissipation leads to the absorption of incident energy. When resolving the Maxwell equation, we obtain the following dependency:

$$\varepsilon = 1 - \frac{\omega_p^{\ 2}}{\omega^2 + i\gamma\omega}$$

where $\omega = 2\pi \frac{E}{h}$ and ω_p as the plasma frequency:

$$\omega_p^{\ 2} = \frac{Ne^2}{m\varepsilon_0}$$

with:

- N the density per volume unit of free carriers
- ε_0 the dielectric permittivity of the void
- m the mass of the electrons
- $e = 1.6\ 10^{-19}$C

This frequency is the resonance frequency of the free electron gas around the equilibrium state. For common metals, it is located in deep UV and is the frontier between two regions:

- $\omega < \omega_p$ (IR-visible area): the metal has a complex index and is highly absorbing and reflecting.
- $\omega > \omega_p$ (UV region): the index of the metal is almost real, $k \approx 0$: the metal is transparent.

In general, most of the **metals** are highly **absorbing in the IR region** and absorbs lesser and lesser as the photon energy approaches the UV region. However, even if most of the metals become transparent in the UV, the analysis and the modeling operations remain quite difficult.

In general, ellipsometers enable to measure film thickness of metal ranging from 0 to 500Å, depending on the absorption of the metal understudy.

Glasses and plastics

Glasses could be equally regarded as dielectric materials. Most of glasses are transparent over a large part of the spectral range but some of them have an absorption edge in the UV when wavelength gets below 300nm or so. Colored glasses have absorptions in the visible area caused by dopants in the glass matrix. Float glass can be absorbing even in the whole spectral range.

For measurements of thin layers on glass it is always advantageous to determine the dispersion of the pure glass substrate in advance. The dispersion of the substrate must be known very precisely because usually the “optical contrast” (difference in dispersions) between deposited layer and glass substrate is very low.

Plastics are similar to glasses in terms of transparent regions, however, their characterization is much more complicated because they can be highly anisotropic.

Transparent conducting oxides

Transparent conducting oxides like ITO (indium tin oxides) show **absorption in the UV** due to interband optical transitions and also **in the IR** due to free carrier absorption. The modelling of the dispersion is rather complicated near these absorption bands. However, there is a transparent region in the visible part of the spectrum (400nm-760nm) where modelling is relatively straight forward.

Carbon-based materials

Carbon can bond in both, planar (sp^2) and tetrahedral (sp^3) configuration leading to graphite or diamond form. Diamond-like-carbon (DLC) is mainly used as protective coating due to its hardness and low-friction. **Diamond itself has a high energy band gap of ca. 7.1eV whereas the energy band gap of graphite is much lower.** Annealing in DLC deposition processes causes a decrease of the band gap so that it approaches more and more the one of graphic-like-carbon (GLC). For both, DLC and GLC, a strong absorption occurs at the energy bang gap and transparency is found only well below the band gap energy.

Summary:

MATERIALS	TYPES	SPECTRAL RANGE
Dielectrics	High-k	IR to deep UV
	Low-k	IR to near UV
Semiconductors	Crystalline	Below band gap Low absorption
	Amorphous	Below band gap broad band of absorption
Metals	$\omega<\omega_p$	Highly absorbing in IR and VIS
	$\omega>\omega_p$	Less absorptive in UV
Glasses	Normal	IR to visible
	Float glasses	Absorbing
Plastics	PET, PEN, PP, PC	Transparent VIS
Transparent conducting oxides		Transparent in Vis
Carbon	Diamond	IR to UV
	DLC	Transparent Below band gap: IR to UV
	GLC	Transparent Below band gap: IR to VIS

5.4.2 Choice of optimal step size

2 *Set step size*

After the setting of the spectral range, the user must adjust the step size. **The step size must be low enough to resolve spectral features like sharp absorption peaks or interference patterns in thick layers and large enough to make the acquisition as fast as possible.**

Step size commonly ranges between 0.1 eV to 0.005 eV depending on the measured sample.

In chapter 1 it was shown that the separation of maxima and minima of the interference pattern decreases with increasing film thickness. This means that with increasing thickness the step size has to be decreased to resolve properly the interference pattern and thus determine unambiguously the film thickness.

The chart below shows typical step size values for different thickness ranges:

Film thickness	Step size (eV)	Step size (nm)
0nm to 200nm	0.1eV	20nm
200nm to 500nm	0.05eV	10nm
500nm to 800nm	0.025eV	5nm, well resolved for wavelengths > 300nm

800nm to 1.2µm	0.02eV	5nm, well resolved for wavelengths > 800nm
1.2µm to 2µm	0.01eV	2nm, well resolved for wavelengths > 400nm
2µm to 30µm	0.005eV	2nm, well resolved for wavelengths > 500nm

5.4.3 Choice of optimal range units

We gave step size values in nanometers for the wavelength scale and in electron-Volts as an equivalent for the photon energy scale. However, keep in mind that acquisition of data with a spectral range in nanometers and acquisition of data with a spectral range in eV do not provide the same spectrum shape and the same distribution of points along the spectrum.

The conversion from wavelength to energy is expressed by:

$$E(eV) = \frac{1240}{\lambda(nm)}$$

Note that this conversion formula can only be applied to the endpoints of the spectral range but not to the step size! The following example shows that this would not make sense:

From: 1eV	↘	From:248nm
To: 5eV	↗	To: 1240nm
Every:0.025eV	→	Every:49600nm !!!

The software applies the conversion formula automatically only to the endpoints of the spectral range and not to the increments.

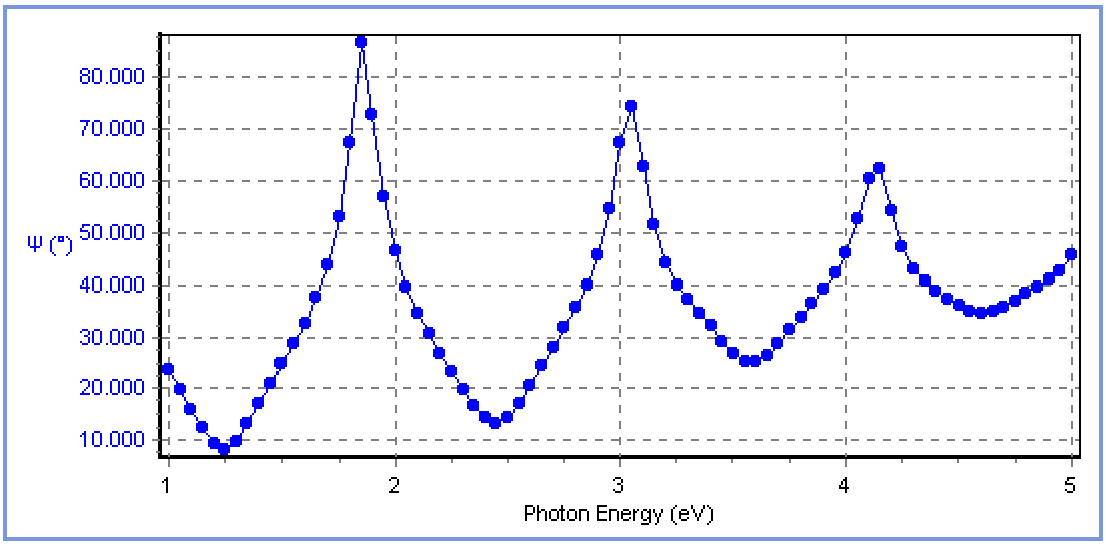
To pass from a spectrum in eV to a spectrum in nanometers, or the contrary, the software converts the range bounds and calculates the increments so that the number of points is kept constant, for example:

From: 1eV	↘	From:248nm
To: 5eV	↗	To: 1240nm
Every:0.025eV	→	Every:6.2nm

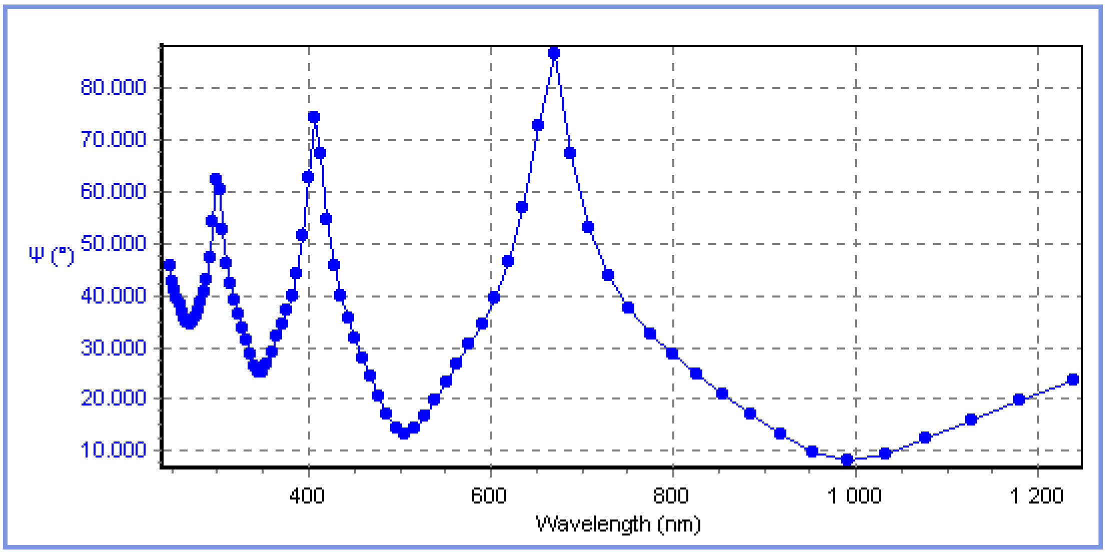
This gives 161 data points in both cases.

Note that for thick layers the interference pattern cannot be resolved for short wavelengths when data is collected in nanometers but they can be resolved for corresponding high energies when collected in photon energies because there the minima and maxima are separated nearly equally over the whole spectral range.

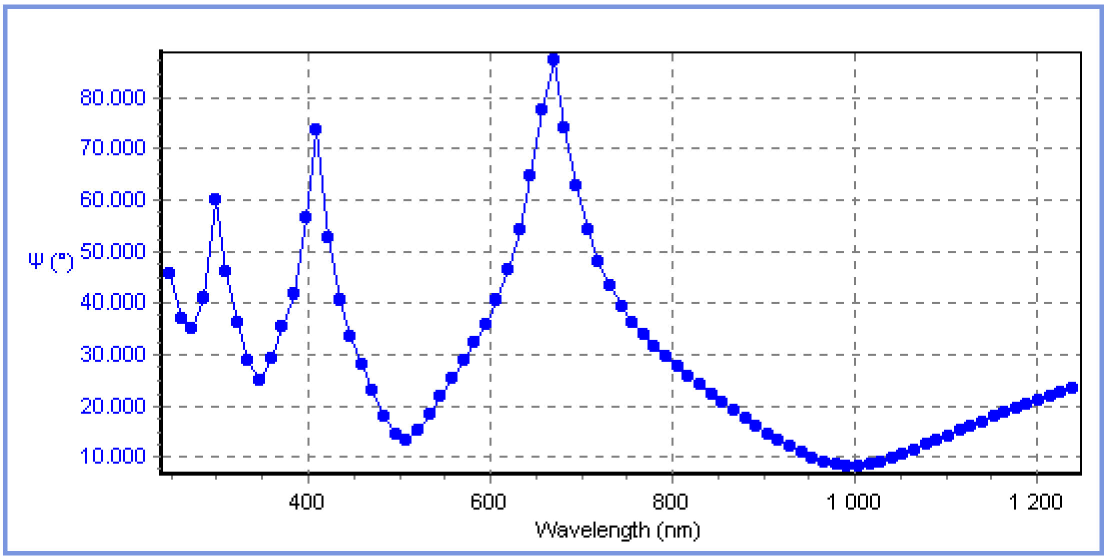
As an example of a 450nm thick sample of SiO_2/Si is shown in the energy range 1eV to 5eV corresponding to a wavelength range of 248nm to 1240nm (data collected in photon energies with increments of 0.05eV. This gives 81 points):



Then converted into wavelength scale, the points still remain equally spread over the interference structure:

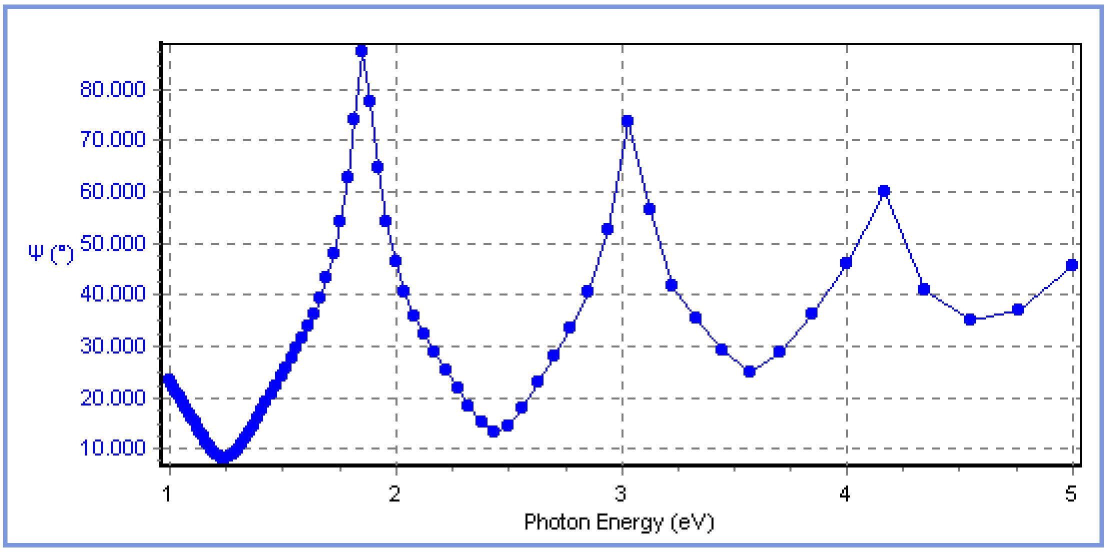


Data collected in wavelengths with increments of 12.4nm. This gives again 81 points:



It is obvious that data collected in nanometers does not resolve features in the short wavelength range.

Then converted into a photon energy scale, the points are not equally spread over the interference structure:



Wavelengths or photon energies?

In the following chart, we suggest which scale to use depending on the type of sample:

Sample	Features	Optimal units choice
Thick, transparent films	Rapidly changing features in Ψ and Δ at short wavelengths	Best to measure in terms of eV
Thick, UV absorbing films	Data features flat at short wavelengths.	Best to measure in terms of nm
Very thick and transparent films	Difficult to resolve short wavelength features	Measure only long wavelengths in terms of nm

5.4.4 Choice of optimal angles of incidence

3 *Set angle of incidence*

highest sensitivity around the Brewster angle

The goal is to work as close as possible to the Brewster angle (BA) of the substrate because there the highest sensitivity can be achieved.

The BA can be determined by calculation tan(BA) = $n_{substrate}$ or by monitoring Ψ as a function of the AOI because $\Psi = 0$ at the BA!

Note that you do not need to be exactly at the Brewster angle to perform the acquisition, being near the Brewster angle is sufficient to enhance sensitivity.

In the following chart, we provide reasonable angle of incidence combinations for different types of samples:

Samples	Combinations
Thin films on Si	65°, **70°**, 75°
Thick films on Si	60°, **70°**, 75° or 55°, 65°, 75°
Other films on glass	**55°**, 65°, 75°
Films on metals	**70°**, 80°
Anisotropic and graded films	55°, **65°**, 75° or 45°, **60°**, 75°

Variable angles of incidence

The variable angles coupled with spectroscopic ellipsometry are used to collect a great quantity of data. However the user must take these informations with a certain care, especially in the case of samples with an overlayer or a roughness layer, because acquisition with **variable angles does not always produce completely independent information**.

The advantages of this mode are:

- for a given wavelength, the acquisitions at different angles of incidence can give independent information and allow to reduce the measurement noise (improve of S/N).
- additional data statistically improves the determination of confidence limits
- the variation of the angle allows the determination of the angle for which the values of Ψ and Δ are the most sensitive.

5.4.5 Configurations (Azimuth setting of modulator and analyzer)

The UVISEL can acquire data for various azimuth settings of the modulator M and the analyzer A. The two most important configurations are described in the following table:

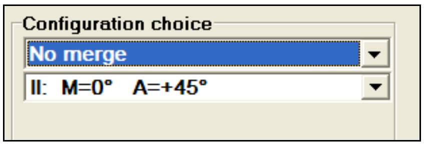
Configurations	Modulator M	Analyzer A
II	0° or 90°	±45°
III	±45°	±45°

- **configuration II:** allows accurate determination of Δ in the whole range but cannot be determined precisely at ca. 45°.
- **configuration III:** allows accurate determination of Ψ in the whole range but cannot determine Δ precisely at around 90° and 270°.

5.4.6 Configuration modes

In general we recommend to measure only in configuration II and use (Is,Ic) as fitting parameters.

The DP2 software allows automatic measurements in one or more configurations to get the optimal set of data.



Configuration choice

No merge

II: M=0° A=+45°

No merge

This is the standard mode of acquisition. The user can select configuration II or III. As a result one file is obtained either from configuration II or from configuration III. Note that the fit for an anisotropic material can only be done in configuration II (with A=45° and M=0°).

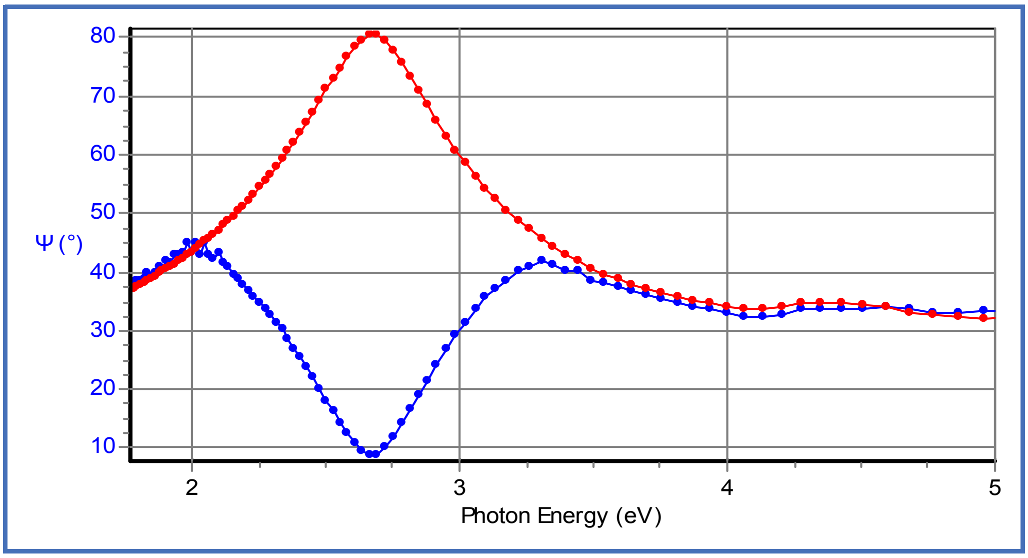
The merge function

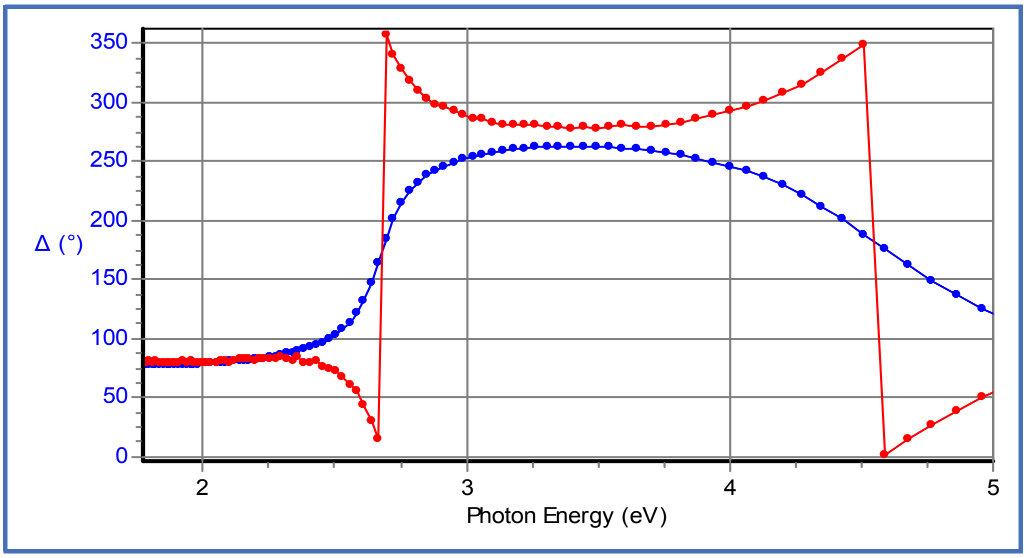
There are three types of merge: Standard merge, High accuracy merge and Smart merge which provide an acquisition in two scans. The principle of these merges is to measure in configuration II & III and calculate the best Ψ and Δ values using both acquisitions.

Standard merge

The standard merge function automatically generates three result files: xxx-CII.spe, xxx-CIII.spe and xxx-STM.spe.

For the example, a measurement of thermal oxide on a Si substrate gives the following and for configuration II (blue) and III (red):





There are obviously mirror effects for around 45° and for around 90° and 270°. The cause of these effects occurs in the last step of acquisition, the recreation of Ψ and Δ from Is and Ic:

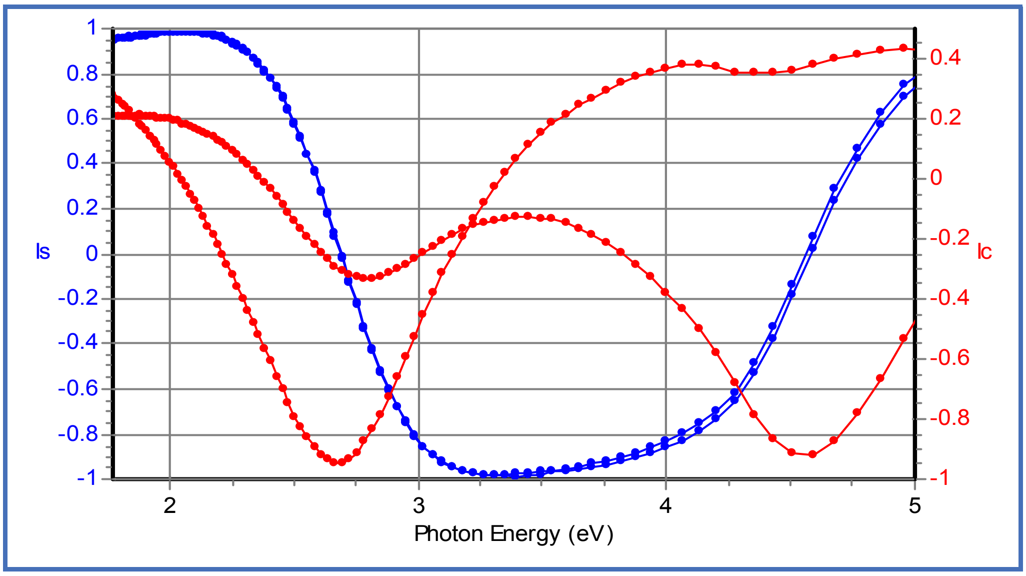
- in configuration II:

$$Is = \sin 2\Psi \sin \Delta \qquad Ic = \sin 2\Psi \cos \Delta$$

- in configuration III:

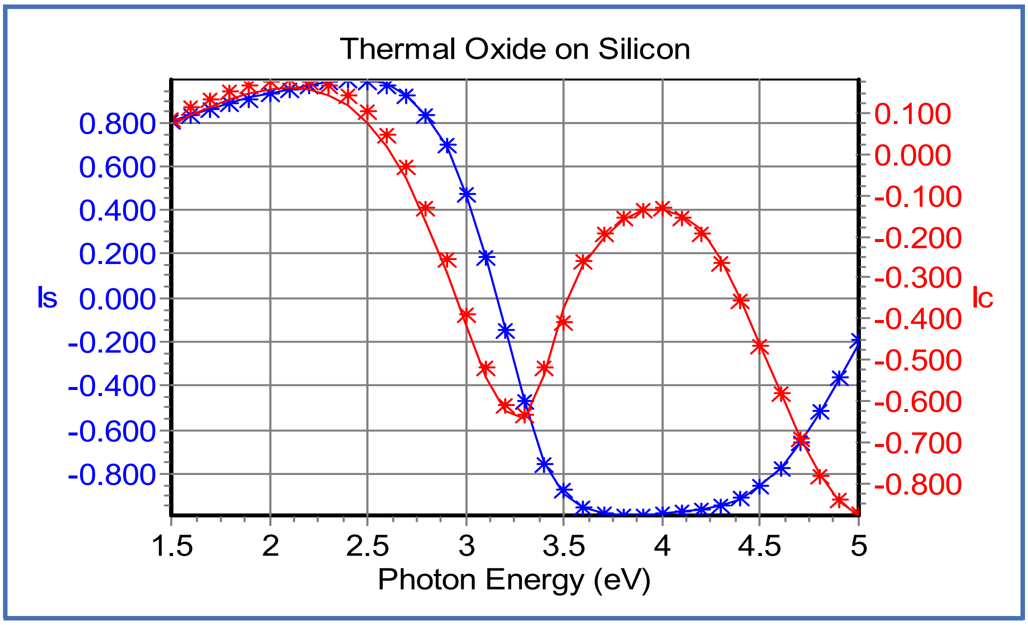
$$Is = \sin 2\Psi \sin \Delta \qquad Ic = \cos 2\Psi$$

The two couples (Is,Ic) are shown below; notice Is does not depend on the chosen configuration.



- in configuration II only sin(2Ψ) is known. It only defines Ψ in the interval [0,45], the values above are flipped down around the line Ψ=45°. On the other hand, in configuration III, the term cos(2Ψ) allows determination of Ψ over the complete domain.
- in configuration III only sinΔ is known. It defines Δ on the right half of the trigonometric circle, the left-side values are flipped right around the vertical axis. On the other hand, in configuration II, the terms sinΔ and cosΔ allow determination of over the complete domain.

That is why the resulting standard merge file xxx-STM.spe contains Δ from configuration II file and Ψ from configuration III file.



High accuracy merge

Like the standard merge, this one includes two scans. The final spectrum is composed of:

- Δ taken from configuration II
- Ψ is calculated with Is and Ic from configuration III and Δ from configuration II

  with the following formula: $\Psi = \frac{1}{2}\arctan\left(\frac{Is^{III}}{Ic^{III}\sin\Delta^{II}}\right)$

Smart merge

Again the first scan is in configuration II and the second in configuration III. The final spectrum is then composed of:

- Δ taken from configuration II
- Ψ is composed of several segments: the limits of the segments are determined by specified Ψ threshold values. The segments with Ψ less than this threshold give Ψ from configuration II and the segments with Ψ greater than the threshold give Ψ from configuration III.

Remarks

A fit can give a bad result after a merge acquisition when:

- configuration II gives wrong Ψ values: it is not possible then to fit on Ψ and Δ
- configuration III gives wrong Δ values: it is not possible then to fit on Ψ and Δ
- configuration III gives wrong Ic values: it is not possible then to fit on Is and Ic

In general we recommend to measure only in configuration II and use (Is,Ic) as fitting parameters.

The only interest of the merge method is to extract exact values for Ψ and Δ but does not improve the fitting itself.

5.4.7 Detector settings

5.4.7.1 Integration time

The integration time is the amount of time allowed for the signal to be acquired for each measurement point. In general select the shortest integration time that will give sufficient S/N in the interesting spectral range. Greater integration time provides better S/N but longer acquisition time.

For standard acquisition we use an integration time of 200ms, for measurements of samples with low reflectivity we recommend a value of 2000ms.

5.4.7.2 Background

Background off: does not take care of the background signal.

Background on: two acquisitions are carried out for each data point. The system closes the shutter located on the light source path and performs an acquisition. A signal plus dark acquisition are performed with the shutter open. The dark acquisition is then subtracted from the signal plus the dark acquisition; this technique minimizes the effects of any drift that may occur.

Automatic background: if the offsets calibration was performed, a results file (background.ini) was saved on the hard disc. If an acquisition is launched using this mode, the [$S0_{\text{background noise}}$ (HV)] will be then subtracted from the acquisition data.

5.4.7.3 High voltage

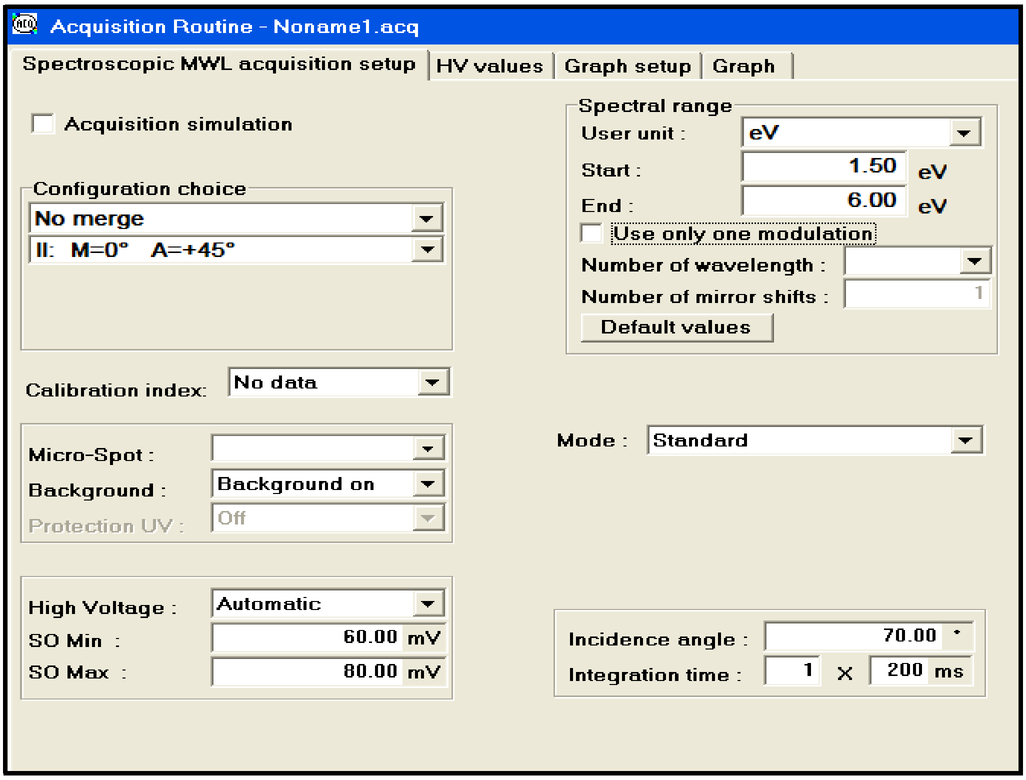
The high voltage box contains the value the user has to set to optimize the gain; this is the voltage applied to the photomultiplier tube (PMT). If you do not know what value to put notice that before launching an acquisition, the user has to acquire the signal in real time through the **VIEWS** window and make some settings described further so as to be in optimal conditions of acquisition. Then by clicking on **S0 adjustment** button, the high voltage value will be **automatically** adjusted.

5.4.7.4 Measurement spot size

The Micro-spot feature allows the user to set the size of the incident beam diameter. The choices are 1200, 250, 120 and 60µm. By reducing the spot size, the signal will decrease, though small spot size may be needed for small or structured samples.

5.5 Spectroscopic MWL acquisition mode

The following figure shows the DP2 page for setting the acquisition parameters:



☐ Acquisition simulation

Configuration choice
No merge
II: M=0° A=+45°

Calibration index: No data

Micro-Spot :
Background : Background on
Protection UV : Off

High Voltage : Automatic
SO Min : 60.00 mV
SO Max : 80.00 mV

Spectral range
User unit : eV
Start : 1.50 eV
End : 6.00 eV
☐ Use only one modulation
Number of wavelength :
Number of mirror shifts : 1

Mode : Standard

Incidence angle : 70.00 °
Integration time : 1 X 200 ms

Most of the parameters are identical to the Spectroscopic Mono mode. However some additional parameters have to be set:

Number of wavelengths:

A limited number of wavelength points can be selected.

Number of mirror shifts:

This is the minimum number of shifts necessary to cover the selected wavelength range.

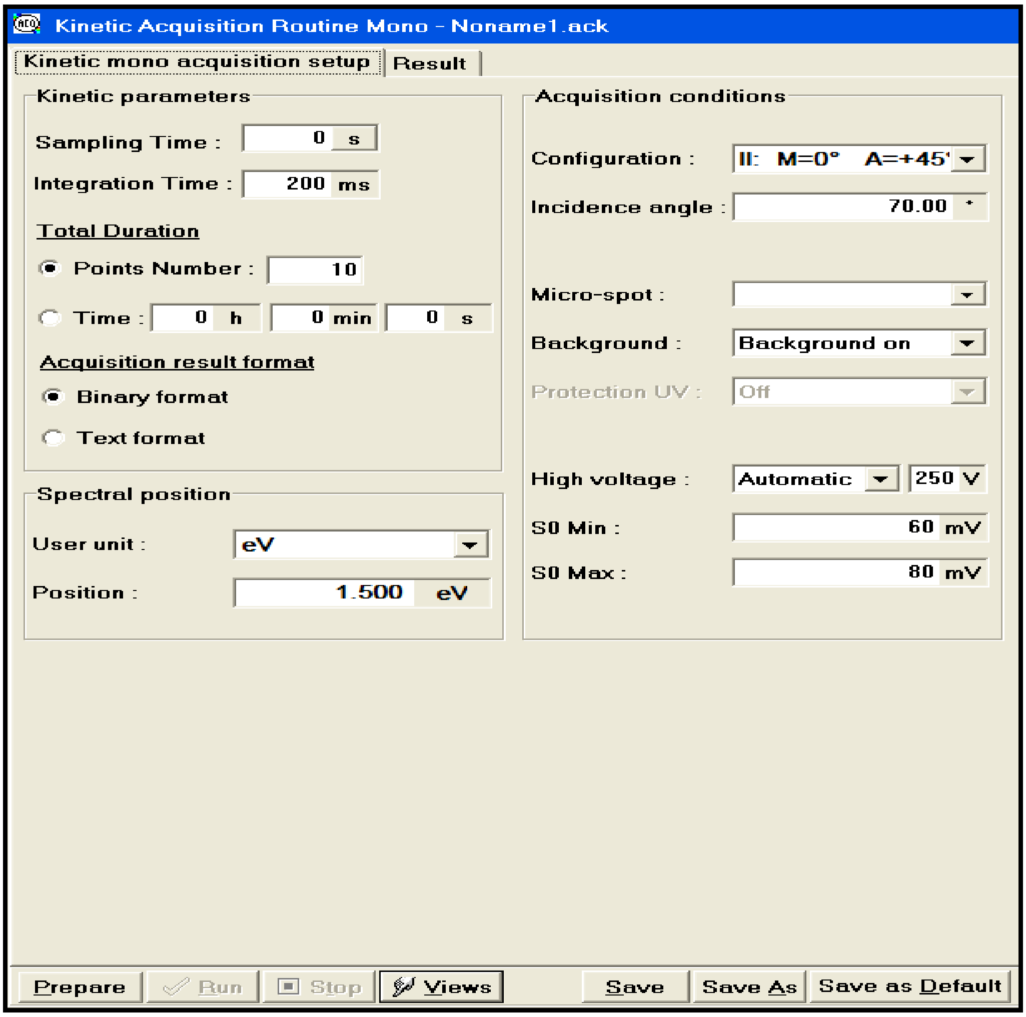
Use only one modulation:

A fixed modulation amplitude is used: the measurement is faster but the precision decreases in the IR.

5.6 Kinetic Mono acquisition mode

This mode allows the user to follow the growth of a material, in a reactor, in real time and for a given wavelength. This acquisition mode is very appropriate for industrial applications like process control. Usually this mode is used to determine thickness of the layer as a function of time.

The following figure shows the DP2 page for setting the acquisition parameters:



Kinetic parameters

Sampling Time : 0 s

Integration Time : 200 ms

Total Duration

● Points Number : 10

○ Time : 0 h 0 min 0 s

Acquisition result format

● Binary format

○ Text format

Spectral position

User unit : eV

Position : 1.500 eV

Acquisition conditions

Configuration : II: M=0° A=+45°

Incidence angle : 70.00 °

Micro-spot :

Background : Background on

Protection UV : Off

High voltage : Automatic 250 V

S0 Min : 60 mV

S0 Max : 80 mV

Sampling time:

Select here the time interval between measurement points.

Integration time:

Set integration time according to S/N.

Total duration:

Defined either by the number of points or by the total time of the experiment.

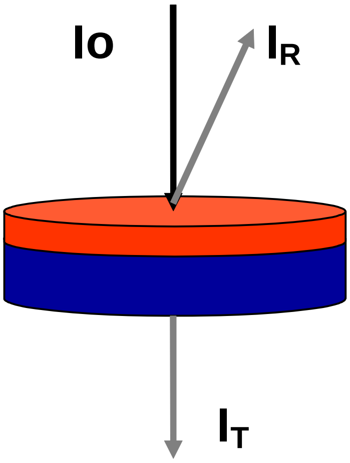
Spectral position:

Choose the wavelength (energy) where the data are taken.

5.7 R&T Mono acquisition mode

This acquisition mode measures the intensity of a transmitted or a reflected beam:

- in transmission I_T/I_0
- in reflection I_R/I_0



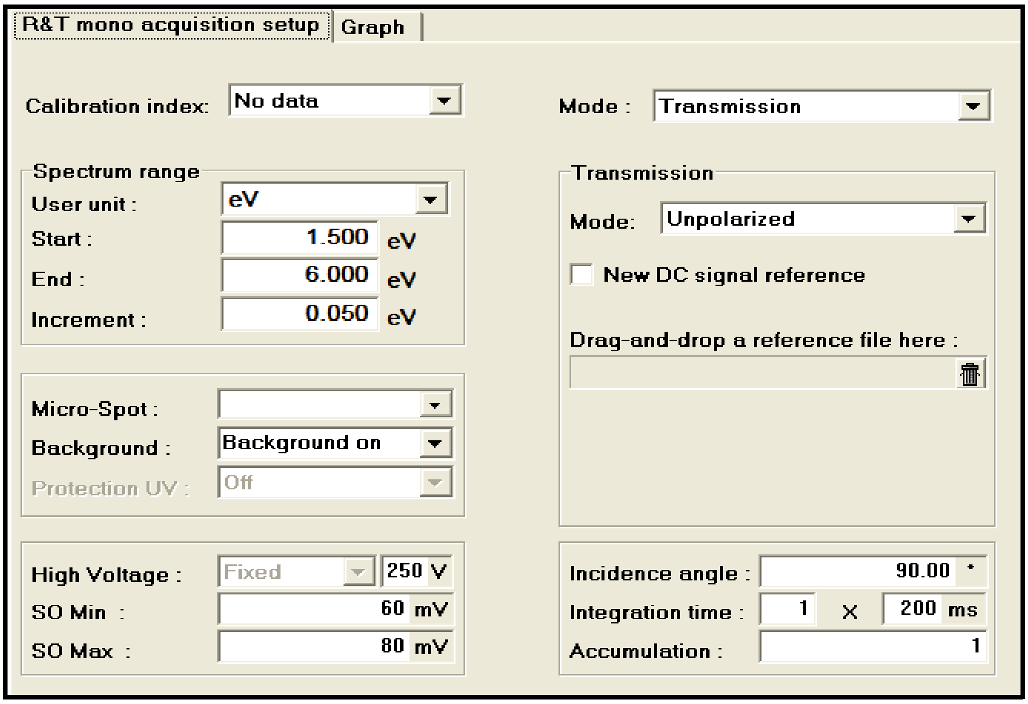
The transmission mode is very useful to decorrelate the analysis of thin absorbing films on transparent substrates or multilayers on transparent substrates.

The measurement in transmission requires several conditions:

- the sample must be placed perpendicular to the normal incident light beam
- The user must pay attention that the transmission measurement of a thick sample (>2mm) may not provide accurate data.
- in this acquisition mode the user must pay attention that fluctuations in lamp intensity or bad light collection may introduce errors in the measurement.
- for both, the reflectance and transmission mode, the user has to create a reference file for each wavelength.

Nevertheless, this measurement type is very important since it can be applied to glass substrates, which are of course very important in display technology etc.

The following figure shows the DP2 page for setting the acquisition parameters:



Calibration index: No data

Mode : Transmission

Spectrum range

User unit : eV

Start : 1.500 eV

End : 6.000 eV

Increment : 0.050 eV

Transmission

Mode: Unpolarized

☐ New DC signal reference

Drag-and-drop a reference file here :

Micro-Spot :

Background : Background on

Protection UV : Off

High Voltage : Fixed 250 V

SO Min : 60 mV

SO Max : 80 mV

Incidence angle : 90.00 °

Integration time : 1 × 200 ms

Accumulation : 1

Note that the High Voltage must be fixed during the whole experiment because we want to compare absolute intensities.

Mode:

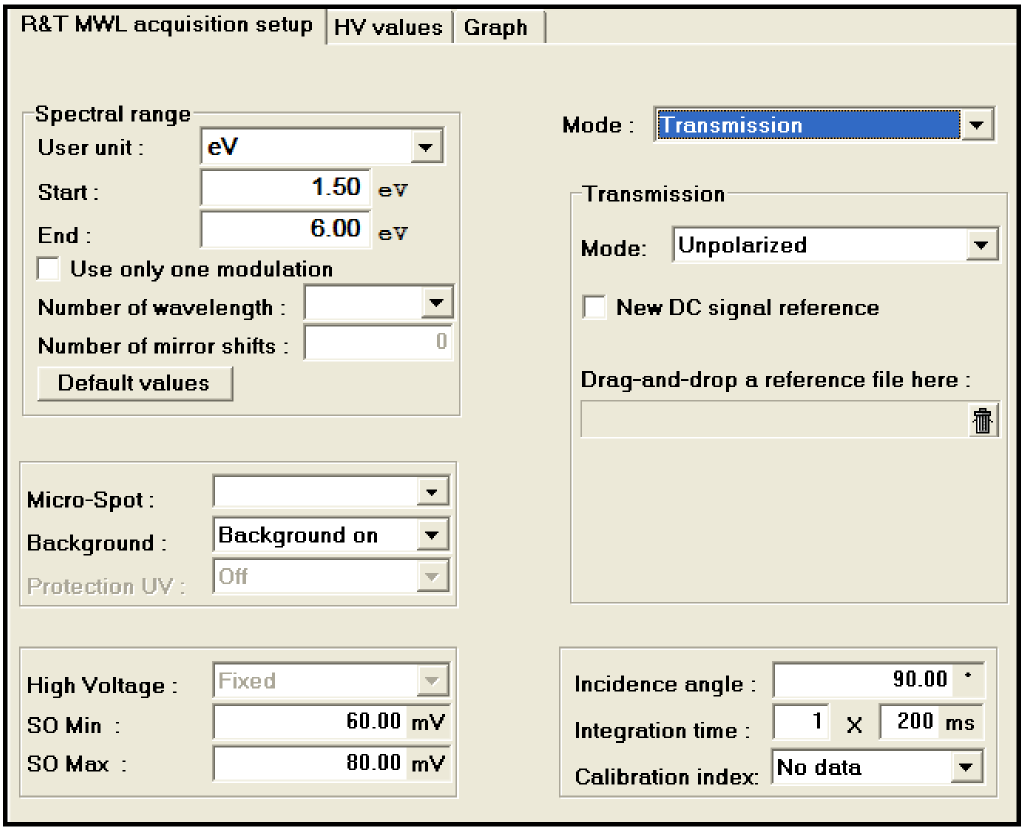
Choose transmission or reflection mode. Both can be performed in polarized or unpolarized mode.

Reference file:

Transmission and reflection experiments need a reference measurement of a known sample. This can be simply air (transmission) or Si (reflection). Choose whether you want to acquire a new DC signal reference or use an already existing measurement (Drag-and-Drop).

5.8 R&T MWL acquisition mode

The following figure shows the DP2 page for setting the acquisition parameters:



User unit : eV
Start : 1.50 eV
End : 6.00 eV
☐ Use only one modulation
Number of wavelength :
Number of mirror shifts : 0
Micro-Spot :
Background : Background on
Protection UV : Off
High Voltage : Fixed
SO Min : 60.00 mV
SO Max : 80.00 mV
Mode : Transmission
Mode: Unpolarized
☐ New DC signal reference
Drag-and-drop a reference file here :
Incidence angle : 90.00 °
Integration time : 1 X 200 ms
Calibration index: No data

Most of the parameters are identical to the R & T Mono mode. However some additional parameters have to be set:

Number of wavelengths:

A limited number of wavelength points can be selected.

Number of mirror shifts:

This is the minimum number of shifts necessary to cover the selected wavelength range.

5.9 Summary: measurement strategies

The following table shows typical settings for important applications:

Sample type	Spectral range/ Step size	AOI	General settings	Additional measurements
Thin transparent layer/Si	UV-VIS/0.1eV	70°	IT = 200ms	
Thick transparent layer/Si	VIS-IR/0.005eV	70°	IT = 200ms	
Absorbing layer/Si	Transparent region	70°	IT = 200ms	

Multilayer/Si	UV-VIS/0.05eV	70°	IT = 200ms	VASE: 65°, 75° R
Organic layer/Si	UV-VIS-IR/0.05eV	70°	IT = 200ms	VASE: 65°, 75° R
Glass substrate	UV-VIS-IR/0.1eV	ca. 55° (BA)	IT = 1000ms	
Thin layer/glass	UV-VIS/0.1eV	ca. 55° (BA)	IT = 1000ms	
Multilayer/glass	UV-VIS-IR/0.05eV	ca. 55° (BA)	IT = 1000ms	VASE: 60°, 65° T
Organic layer/glass	UV-VIS-IR/0.05eV	ca. 55° (BA)	IT = 1000ms	VASE: 60°, 65° T
Metal substrate	UV-VIS/0.05eV	70°	IT = 200ms	VASE: 65°, 75°
Thin Transparent layer/metal	UV-VIS/0.05eV	70°	IT = 200ms	VASE: 65°, 75°
Thick Transparent layer/metal	VIS-IR/0.005eV	70°	IT = 200ms	
Plastic substrate	UV-VIS/0.05eV	ca. 62° (BA)	IT = 1000ms Config. II	VASE: 60°, 65° T
Polymer/plastic	UV-VIS/0.05eV	ca. 62° (BA)	IT = 1000ms Config. II	VASE: 60°, 65° T

6 QuickStart Modeling

6.1 Introduction

The collected data of an ellipsometry measurement are the intensities of the harmonics of the reflected or transmitted signal in a predefined spectral range. These harmonics are mathematically treated to extract values of Is and Ic for each selected wavelength thus providing spectra Is = f(λ) and Ic = f(λ). **These values are not material parameters or thicknesses thus ellipsometry is an indirect technique of measurement.**

Starting from the values Is and Ic, the software can calculate quantities of interest such as Ψ and Δ .

To extract parameters of interest like optical constants and thickness from the measurement a model has to be set up that allows theoretical calculation of Is and Ic (or Ψ and Δ etc.). **The parameters of interest are determined by comparison of theoretical and experimental data (fitting: detail in chapter 6), the true optical constant values of the different parts composing the sample structure.**

A layer model can includes:

- layer structure: bare substrate, mono- or multilayer, super lattices…
- optical dispersions for each material: literature values, dispersion formulae, alloys, effective media
- thickness of the different layers
- optical anisotropy, index gradients,…

This abundance of modeling parameters is provided in order to match the experimental data as close as possible. Once the unique best fit is obtained the given model is considered the most sensible representation of reality. Thus the values for the modeling parameters (thickness, optical constants,…) obtained by the fitting operation will be considered as being the real ones.

Obviously, ellipsometry does not provide 100% exact values but which technique does? However, despite of errors due to modeling or measurement, ellipsometry is still an incredibly accurate, reproducible and precise optical technique of measurement. Furthermore, the present thin film calculation software has been designed to fulfil the analysis requirements for a great variety of users: the DP2 software can be used just as well by thin films research workers and by operators in semiconductor fabs.

Never forget that you have in hand a tool that is sample sensitive down to the atomic scale, just by putting your sample under light, in air environment without destroying.

6.2 Pre-requirements for modeling

Before starting the modeling step, there are some questions the user should answer to correctly proceed through this fundamental step of ellipsometric data analysis. Indeed, to build a model the user has to know the maximum of information about:

- the substrate, its composition, its historic (cleaning, annealing,…), its surface state (roughness, native oxide,…)
- the coating material(s) composing the sample, the number of films, deposition method, the type(s) of interface(s), post-treatment(s) like annealing
- homogeneity of the sample, isotropy or anisotropy (birefringent material, preferential polarization,…), index gradient
- presence of overlayer(s) like thin oxide film or roughness layer

The user has to keep in mind that all ellipsometric analyses are model dependent because it is not possible to measure physical and optical quantities directly. The desired parameters such as dielectric functions, refractive indices, material compositions, and film thicknesses are determined by reference to a model that is an idealized mathematical representation of the sample. So, the model must be physical and note that any inaccuracies in the fixed parameters will lead to inaccuracies in the final results.

Ellipsometric modeling provides a real challenge and is the part of job that is the most stimulating to the user of ellipsometry. The technique has a reputation of time sharing 10% for measurement and 90% for analysis. This is partly true but the pleasure or benefit consecutively obtained afterward just gets consecutively higher.

6.3 DeltaPsi2 software environment – Modeling Interface

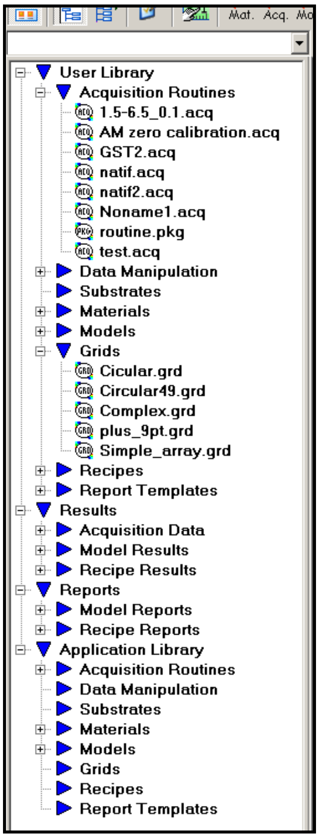
In this section we review a number of important software concepts or menus which are used during data analysis with DP2. You should be familiar with all of these environments as they are used throughout the analysis examples of this document. Discover each element of modeling software environment before proceeding onward.

6.3.1 Configurate and discover the working environment: User Profile

DP2 is a multi-user working platform. Thanks to the ***user's profile*** feature, all files to work with remain in a local environment. Consequently you can chose to create a profile for each user, for a group of users, for a specific application…To create a profile click on *software options* button and *create a new profile…*

There are no limits to the number of defined profiles. Once a new profile is created or an existing one is selected, the central node for handling analysis is the TreeView. Its general overview is detailed in the *DP2 reference manual* and its functionalities are similar to those of windows explorer.

6.3.2 TreeView folders



There are 4 main folders in this tree. They are visible directly when you launch the software. Two of these are libraries and two others are for data:

- User library
- Results
- Reports
- Application library

The secondary folders are visible or hidden according to a selection made in “software option/file explorer”.

- **Application library and User library have the same sub-structure**. The first one is the pre-set HORIBA Jobin Yvon library containing model examples, reference files, material dispersion files delivered with the installation disk. The latter should be the result of your work. It starts containing empty folders every time you create a new profile.

We suggest your work to be saved in the User library. Copy from the application library files of interest in your user library.

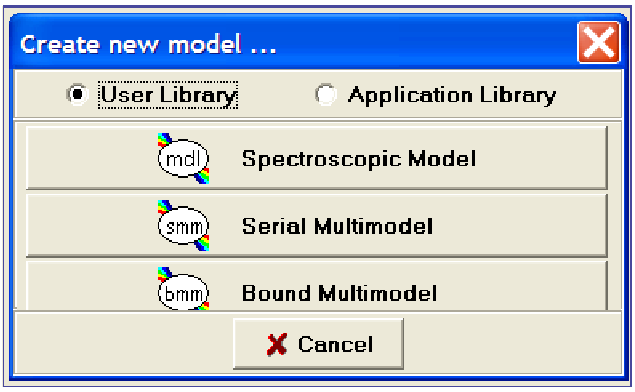
- **Results folder is the place where raw data are saved. These are either measured data or modeling result data.**

- Reports folder is the place where formatted data are saved. Modeling results or recipe results are saved here following a template format for printing or displaying HTML or microsoft word DOC documents.

6.3.3 Creation of a new model

Create a new model by clicking on the Mod. tab.:

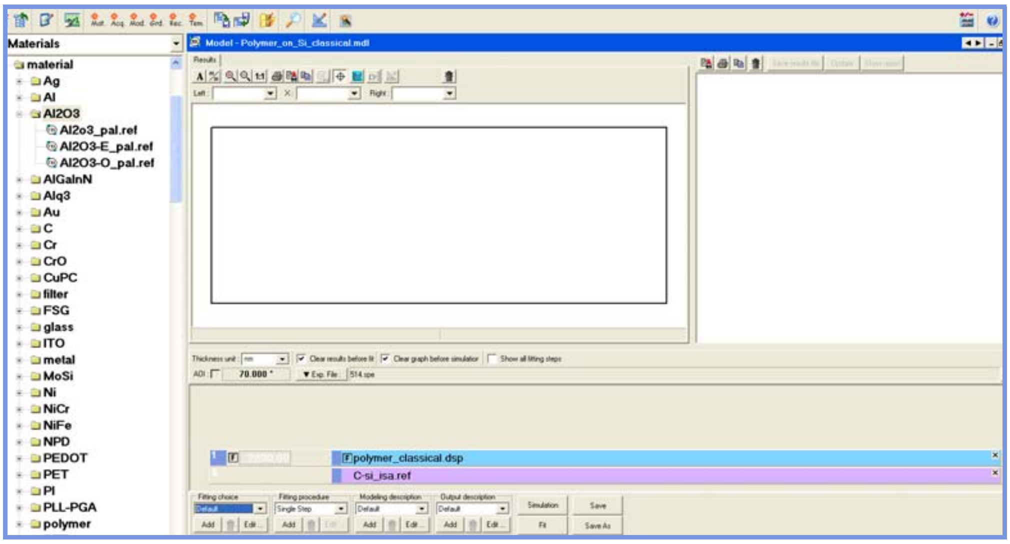
Make sure «User Library» is selected and then click on the «Spectroscopic Model» button.



6.3.3.1 Built your model using layers for each material

Drag acquisition data, reference, dispersion, etc. files from the tree view selection menu and drop it into the sample structure

Drag the experimental measurement file from the directory ***results – acquisition data*** to the grey bar “Exp file”.



A default angle of incidence of 70° is given. You can change it by clicking on “70°”. Generally do not fit the angle of incidence.

From “Modeling description” menu, click “Edit...”. From the “Modeling conditions” tab, the “Experimental file spectral range” fits your model to the spectral range of the used experimental file. However, if you want to use a smaller range, you can use a “User defined spectral range”. Click “Ok”.

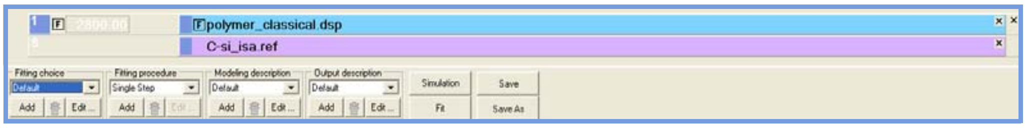
6.3.3.2 Set the unknown properties of the sample as model fit parameters

Check the boxes in the sample structure, and an “F” will appear

6.3.3.3 Launch the fitting process

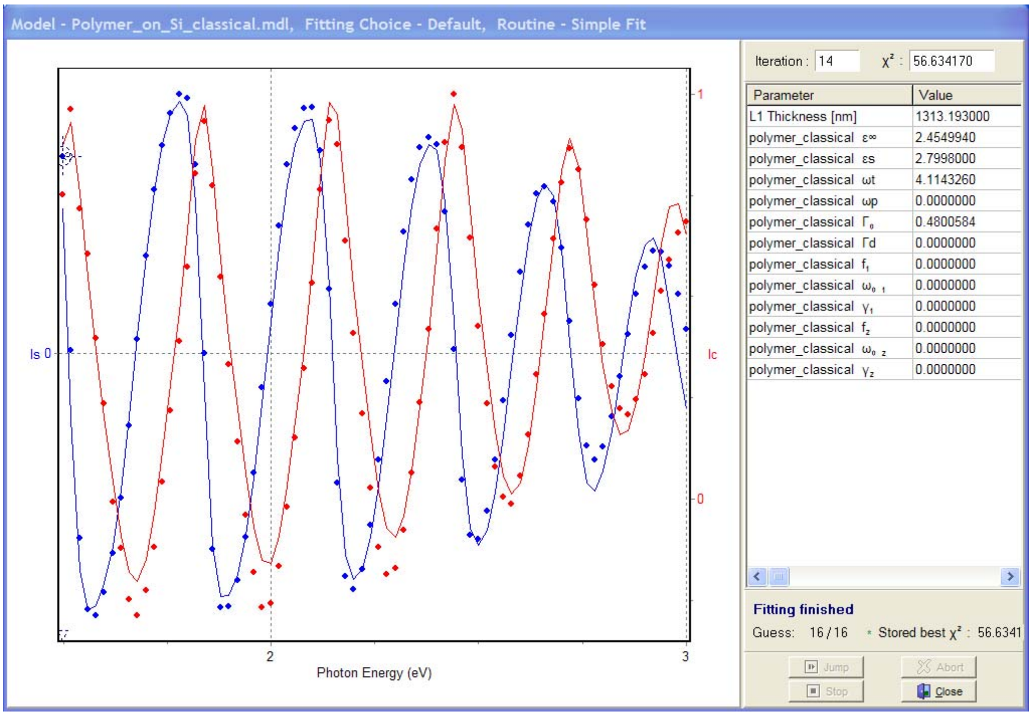
Now the fitting process can be launched. The software will automatically adjust the selected fit parameters to improve the agreement between the measured and the model-generated data.

Click on the “Fit” tab



6.3.3.4 The results are displayed graphically and in numbers.

The fit quality can be checked with the value of χ^2 (a smaller value indicates a better fit to the experimental data) and visually compare the measured experimental data and the final best-fit calculated data.



Iteration : 14 χ^2 : 56.634170

Parameter	Value
L1 Thickness [nm]	1313.193000
polymer_classical $\varepsilon\infty$	2.4549940
polymer_classical εs	2.7998000
polymer_classical ωt	4.1143260
polymer_classical ωp	0.0000000
polymer_classical Γ_0	0.4800584
polymer_classical Γd	0.0000000
polymer_classical f_1	0.0000000
polymer_classical $\omega_{0\ 1}$	0.0000000
polymer_classical γ_1	0.0000000
polymer_classical f_2	0.0000000
polymer_classical $\omega_{0\ 2}$	0.0000000
polymer_classical γ_2	0.0000000

Fitting finished

Guess: 16 / 16 Stored best χ^2 : 56.6341

6.4 Materials files

In both the application and the user library there is a folder called ***materials***. The folder contains files that represent the optical properties materials. These optical properties can be either expressed as complex refractive indices $N = n + ik$ or as dielectric functions $\varepsilon = \varepsilon_1 + i\varepsilon_2$. The two expressions are related according to $\varepsilon = N^2$.

Note that optical properties for a material are physically meaningful if $k \geq 0$ and $\varepsilon_2 \geq 0$ and that these optical properties are given only for a limited spectral range.

DP2 offers different "file" possibilities to handle optical properties. Here is a short overview.

6.4.1 Material file types

6.4.1.1 Reference (*.ref)

A reference file contains tabulated values of optical constants (n,k) as a function of wavelengths taken from literature.

These files have text format in a structure similar to all deltapsi2 experimental data files. They contain a table with 3 columns, wavelength or energy, real part then imaginary part of optical properties. Most of Application library files are from this type and contain energy and dielectric function. We will often mention these files as reference files. One can already keep in mind that **optical properties in such files are fixed and consequently cannot be adjusted**. A complete list of application library available reference files is given in the appendix.

Example:

SiO2_wor.ref

Access:

In the left-hand selection menu, expand «Application Library» «Materials»

Modelling Strategy:

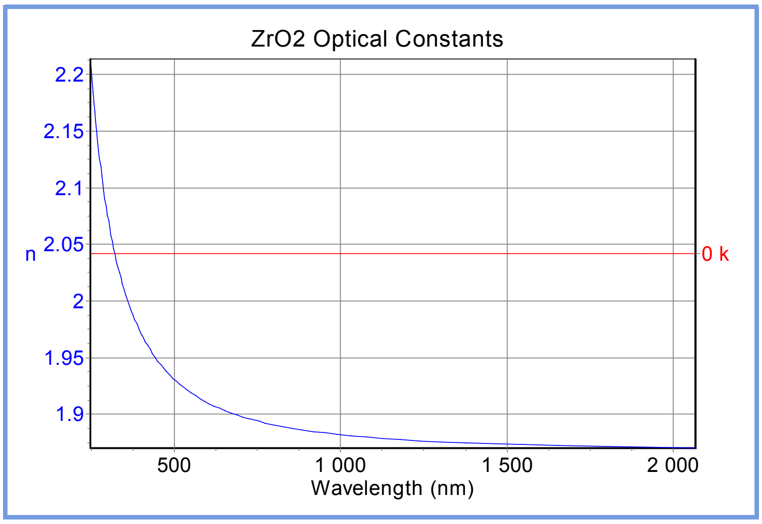
Using reference files means that the optical constants are fixed values. The advantage is that only the thickness will vary during the fitting process. The disadvantage is that it may not exactly represent the real optical constants of your material.

When to use it ?

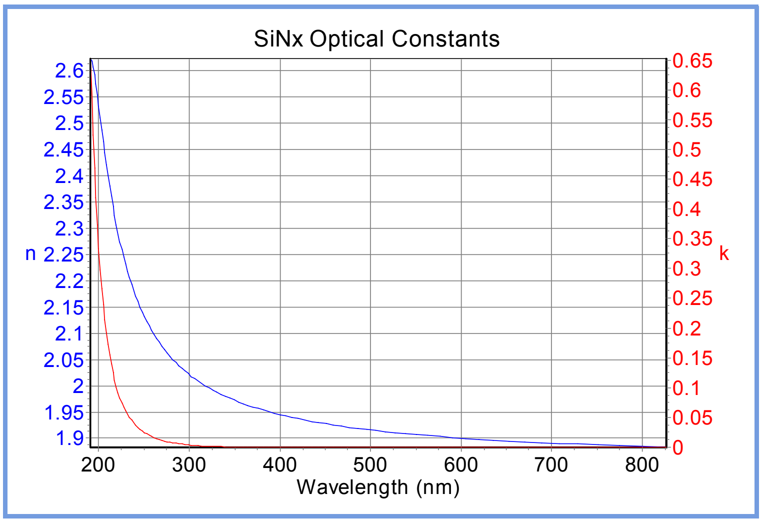
Often used materials like c-Si, SiO_2, Al, Al_2O_3, etc. are present in the application library. Use them as a starting step for modelling. A low value of the χ^2 implies a good representation of the optical constants and thickness of your sample under analysis. In the contrary case modify your model or your fit parameters until the best description is found.

Examples:

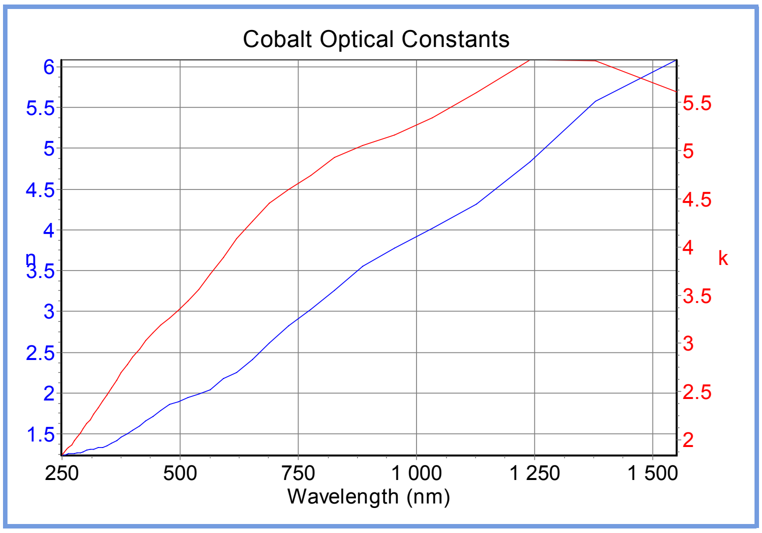
Transparent Dielectric



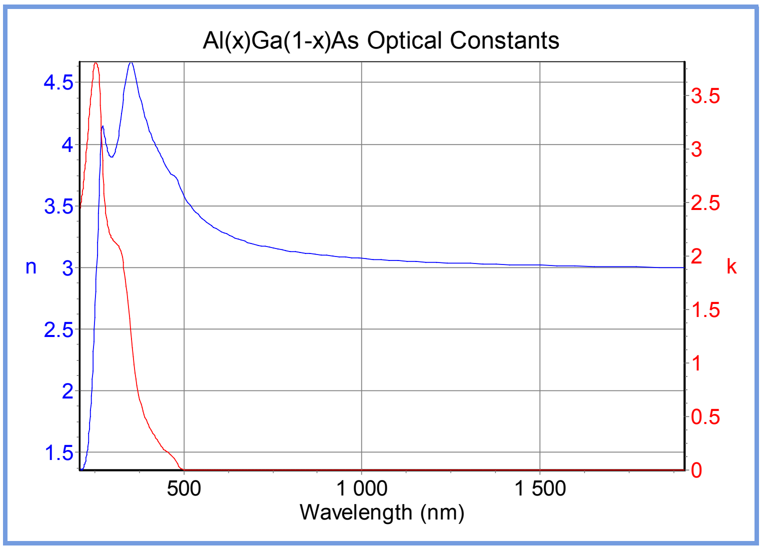
Absorbing Dielectric



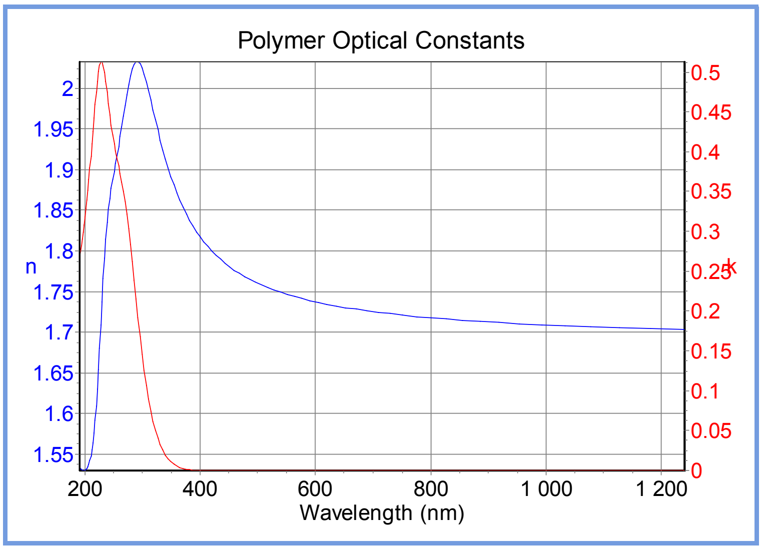
Metal



Semiconductor



Organics, polymers: Transparent at longer wavelengths, absorbing in FUV



6.4.1.2 Dispersion Formula (*.dsp)

Optical dispersion means dependence of optical properties on wavelength or photon energy. Sometimes this dependence can follow an explicit analytical formula, called dispersion formula. These dispersion formulae mostly are **physically** related to optical transitions in materials, however, they also can be purely **empirical** without any physical meaning.

DP2 offers pre-defined dispersion models which can be used straight forward. A legitimate question is "which one should I use?". Chapter 6 will explain in detail the most important dispersions. Appendix A give the theoretical background of all dispersions.

Note that a dispersion file contains the following information:

- the type of dispersion equation
- the dispersion parameters, real numbers
- the dispersion parameters boundaries: an optional constraint when fitting these parameters. When min = max = 0, the fitting routine considers no boundaries.

Example:

SiNx.dsp

Access:

Click on the "Mat" tab to access the dispersion files.

Examples for often used dispersions:

Main dispersion formula	**Materials family**	**Materials examples**
Lorentz oscillator	Transparent and weakly absorbing dielectrics	Oxides (SiO_2, SiON, Al_2O_3, HfO_2, MgO, ZrO_2), polymers, organics
Drude oscillator	Metals	Al, Ag, Cr, Cu, Ti
New amorphous, Tauc Lorentz	Semi-absorbing dielectrics and semiconductors	SiN, a-C, oxides (TiO_2, Ta_2O_5, ZnO), AlN, photoresist
Kato-Adachi, Adachi-New Forouhi	Crystalline semiconductors	AsGa, InP, InAs, HgCdTe, InGaP, ZnTe, CdTe

A dispersion file is used when a reference file for the material is not available or if the reference file does not lead to good fitting results (high χ^2 value).

Comment:

Weigh the benefit gained (goodness of fit) when using a dispersion based model instead of a reference file against the added complication (more regression parameters). As a rule of thumb the χ^2 should be improved by an order of magnitude when using a dispersion file.

6.4.1.3 *.ALY files

In Deltapsi2, the optical properties of four families of semiconductor materials can be described by an alloy modeling. These families are:

- **$Al_xGa_{1-x}As$**
- **$Hg_{1-x}Cd_xTe$**
- **$Si_{1-x}Ge_x$**
- **$In_{1-x}Ga_xAs_yP_{1-y}$**

The three first are ternary alloys, the last one is a quaternary alloy. For the three first, the composition is defined by the stoechiometry x, a value that can vary between 0 and 1. The fourth family of alloy is the quaternary material $In_{1-x}Ga_xAs_yP_{1-y}$. Its optical properties are given for the case of $x = 0.47\ y$. This stoechiometry relation restricts this family to the alloys that are lattice matched to InP. For this case, composition is defined by stoechiometry y, also between 0 and 1. For example:

$y = 0$ corresponds to the material InP

$y = 1$ corresponds to the material $In_{0.53}Ga_{0.47}As$.

For a given family of alloys, the modeling is based on existing reference files of known composition between 0 and 1. The software applies an appropriate interpolation procedure to generate optical properties for intermediate compositions within the interval [0, 1].

Note that an alloy file contains the following information:

- the type of alloy
- its composition

Using this type of material file illustrates how ellipsometry can give access to the composition of materials.

.PPC files

PPC means **point-by-point calculation**. This kind of material file is devoted to cases where fitting extracts the optical properties directly from experimental data at each wavelength. Assumptions are made regarding all other parameters that are kept constant.

Modeling with PPC file types will be illustrated in detail later in this manual.

.SPE or *.CLC files

SPE files are directly generated by **acquisition routines**. **CLC** files are **calculated files** that can be generated in the simulation environment. These two types of files are text files with standard DP2 data format. We consider in the following explanation ellipsometric data (remember DP2 also handles Reflectance or Transmittance data).

It is known from ellipsometry basic theory that angles Ψ and Δ for a sample are related to the “pseudo-index” of a sample according to the following equation:

$$\rho = \tan\psi e^{i\Delta}$$

$$\varepsilon = n^2 = \sin^2\theta_0\left[1 + \tan^2\theta_0\frac{(1-\rho)^2}{(1+\rho)^2}\right]$$

with θ_0 as the angle of incidence.

When the sample is a bulk material, its pseudo-index is simply the complex index of refraction of the material.

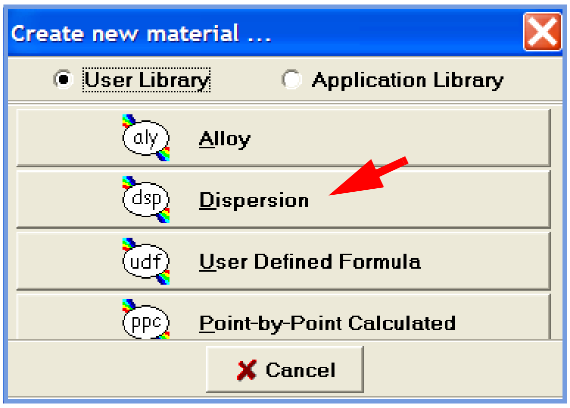
An ellipsometric data file can be seen as a material file, both, SPE and CLC files, can be used in the materials folder. and consequently in the model.

6.4.2 Creation of a dispersion file in the DeltaPsi2 software

For the creation of a dispersion Click on ***Mat*** in the top bar:

6.4.2.1 Creation of a dispersion file with a pre-defined dispersion formula

Select *Dispersion* in the following window if you want to use a given dispersion formula to describe your material dispersion:



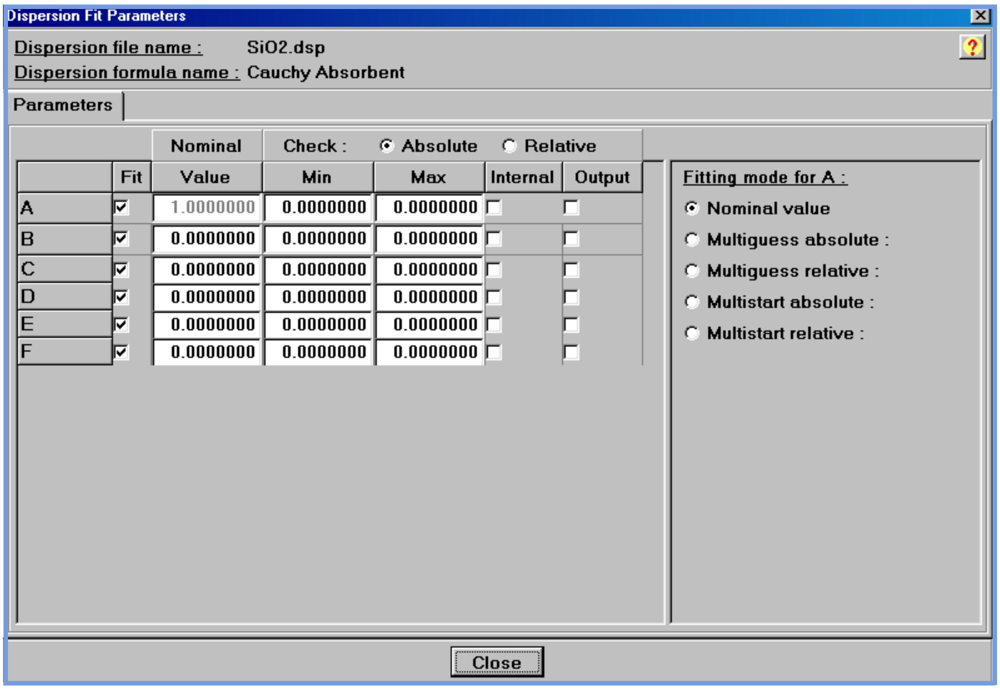
A dispersion window is displayed with a rolling menu to select a dispersion among the 32 existing, a list of adjustable fitting parameters and a graph that plots the dielectric function or other optical parameters (n, k,….) as a function of photon energy or wavelength.

Adjust the fitting parameters to your convenience and *save as* your dispersion.

The *.dsp file will be placed in the *materials* folder in the *User Library* of the TreeView. You can then drag and drop it in the layer model.

Each dispersion formula is an adjustable function. The parameters of the function are fitted when the corresponding check box in the model window is activated as shown below:

A fitting window appears by clicking twice on the check box allowing you to select the parameter(s) to fit. An example is shown below for the dispersion formula “Classical” that takes into account only the single lorentz (transparent) oscillator set fot the SiO_2 material.



Dispersion file name : SiO2.dsp
Dispersion formula name : Cauchy Absorbent

Check : ● Absolute ○ Relative

	Fit	Nominal Value	Min	Max	Internal	Output
A	☑	1.0000000	0.0000000	0.0000000	☐	☐
B	☑	0.0000000	0.0000000	0.0000000	☐	☐
C	☑	0.0000000	0.0000000	0.0000000	☐	☐
D	☑	0.0000000	0.0000000	0.0000000	☐	☐
E	☑	0.0000000	0.0000000	0.0000000	☐	☐
F	☑	0.0000000	0.0000000	0.0000000	☐	☐

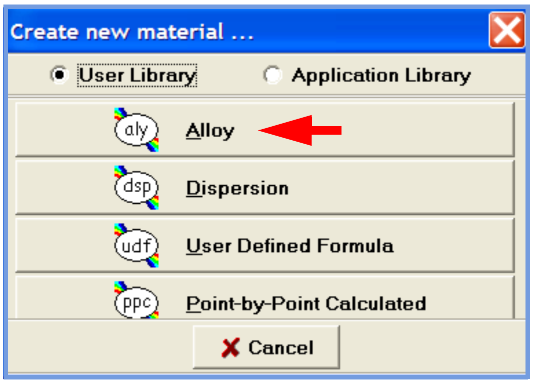
Fitting mode for A :
- ● Nominal value
- ○ Multiguess absolute :
- ○ Multiguess relative :
- ○ Multistart absolute :
- ○ Multistart relative :

6.4.2.2 Creation of a dispersion file with an alloy function

The dispersion for alloyed materials is created by an interpolation technique. The interpolation is based on real measurements that were performed for a series of compositions for the four alloy types of the library: $Al_xGa_{1-x}As$, $Hg_{1-x}Cd_xTe$, $Si_{1-x}Ge_x$ and $In_{1-x}Ga_xAs_yP_{1-y}$.

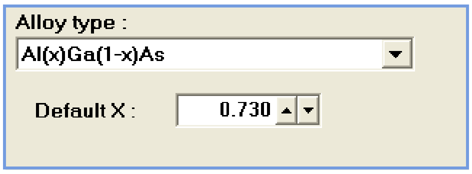
To create an alloy material with the Alloy feature of DP2, perform the following steps:

In the model window, go to ***mat*** and select ***Alloy***



● User Library ○ Application Library

In the Alloy window, select the alloy type. According to the x value the user set, the software will generate a spectrum of the given alloy by interpolation between the existing spectra of this alloy measured for well defined compositions.



Alloy type : Al(x)Ga(1-x)As
Default X : 0.730

Save the material in the *material* folder of the *User Library* with the extension *.aly.

You can drag and drop it in your model, like the other material files in DP2

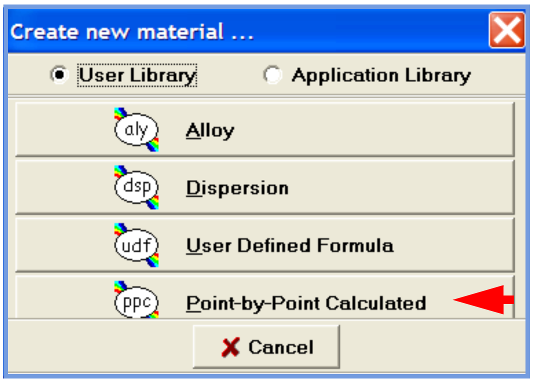
6.4.2.3 Creation of a dispersion file with the PPC feature

The Point-by-Point Calculated feature (also called NK fitting routine) fits n and k on a point-by-point basis. NK fitting does not use dispersion equations for the optical constants but it requires the exact knowledge of the film thickness.

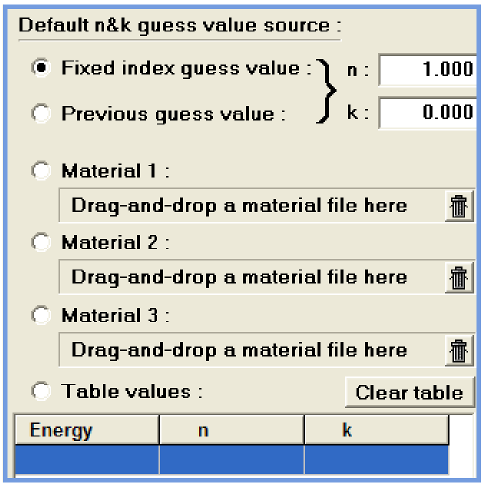
It was shown that spectroscopic ellipsometry measures two parameters, and as a function of wavelength. The optical properties of a sample (n, k) vary with wavelength, but the thickness (d) is of course independent of wavelength. If the thickness is known then a point-by-point calculation can invert the ellipsometric equations and give n and k for the sample at each wavelength.

The DeltaPsi software achieves this by performing the following steps:

From the main menu, select ***Mat***. choose ***Point-by-Point Calculated***.



Then the following options appear:


Default n&k guess value source :

● Fixed index guess value :
○ Previous guess value :
n : 1.000
k : 0.000

The ***fixed index guess value*** feature uses fixed optical constants, n and k, as the guess for each point.

The ***previous guess value*** feature uses the previous NK fit as the new guess for each point.

The ***material 1, 2 & 3*** feature uses one or several materials created by dispersion as starting point for the guess at each point. To perform this, drag and drop the material(s) to the appropriate box and check the box that contains the material you want to fit with.

When you save your PPC material you create a *.ppc file in the ***material*** folder of the ***User Library***.

For the use of the ***material 1, 2 & 3*** feature we recommend to have one (or several) dispersions that provide a good fit in order to have the best starting point for the guess.

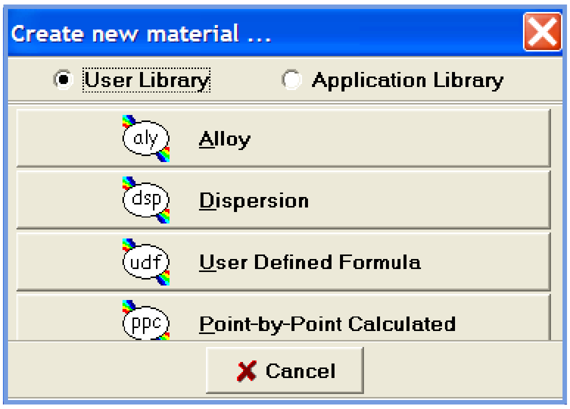
If you want n and k over all the spectral range or over one specified region, you will surely notice that, for most materials there are regions of the spectral range where the fit is not perfect. That is why we recommend to decompose the spectrum:

- for each region of interest, create a different *.ppc file
- for region(s) of the spectral range where the fit is good, use your current dispersion as starting point for the guess and be sure to perform the fit only over the specified region. To do this go to ***Modeling description > edit > Modeling conditions*** then check the box ***User defined spectral range***, here you can select the interval and the increment; we recommend to set the same increment you used during acquisition.
- for region(s) of the spectral range where the fit is not satisfying try another dispersion which provides a better fit over the specified region(s), then use it as starting point for the guess and fit over the specified region(s).
- in the fitting step, fit only on the PPC material; don't fit the thickness (it is supposed to be constant)
- fit only using the Marquardt algorithm: go to ***Modeling description > edit >fitting params***, choose ***Marquardt*** in ***Minimization algorithm***.
- after each fit, click on ***Update*** above the graphic displayed in the model window: it updates your *.ppc file, so when you open your PPC material, you get access to the optical constants for each photon energy or wavelength. If you created a *.ppc file for each region you can have n and k over the complete range of acquisition.
- to see if you performed correctly the entire process, you should obtain a χ^2 equal to zero.

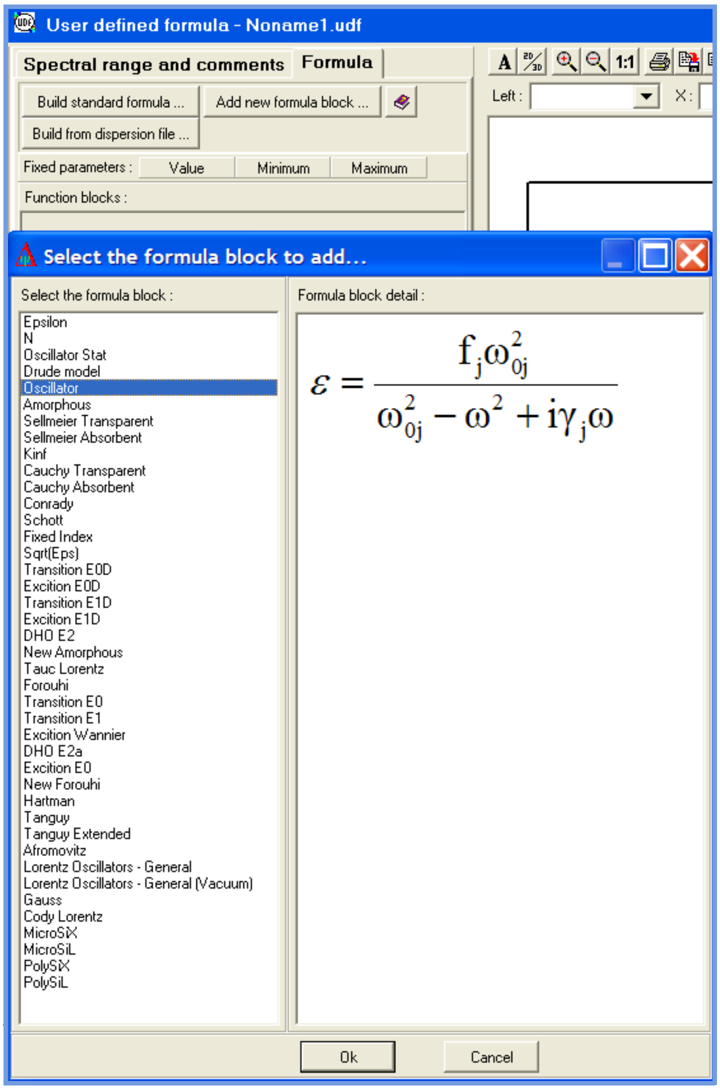
6.4.2.4 Creation of a dispersion file from analytical expressions

Select *User Defined Formula* in the following window if you want to compose your dispersion formula from analytical expressions to describe your material dispersion:

This function is dedicated to advanced users

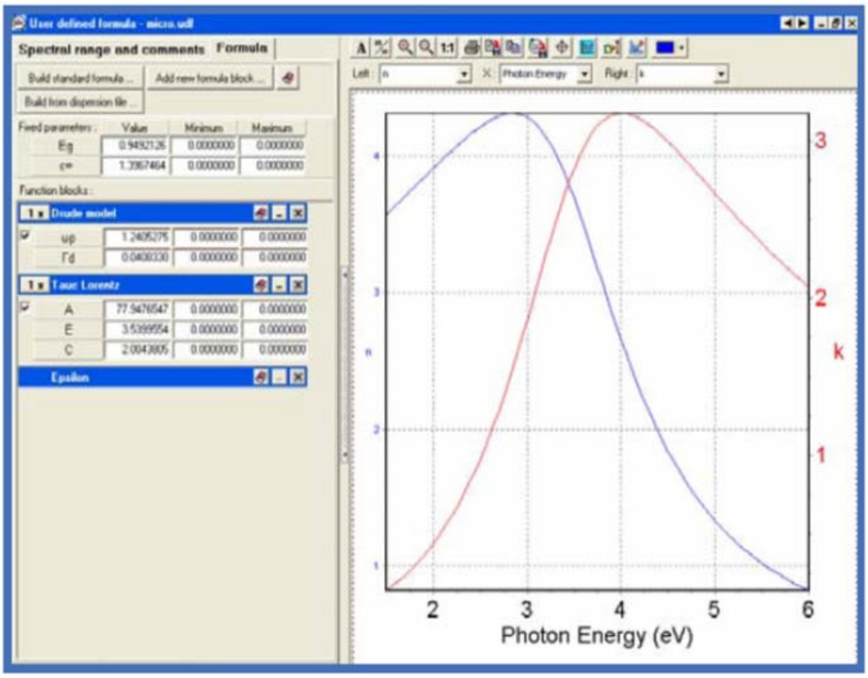


A window is displayed that allows to compose the dispersion formula from pre-defined blocks:



$$\varepsilon = \frac{f_j \omega_{0j}^2}{\omega_{0j}^2 - \omega^2 + i\gamma_j \omega}$$

The example below shows a new dispersion formula composed of two blocks, a Drude and a Tauc Lorentz term to represent micro-crystalline silicon:



Fixed parameters :	Value	Minimum	Maximum
Eg	0.9492126	0.0000000	0.0000000
ε∞	1.3967464	0.0000000	0.0000000

Drude model

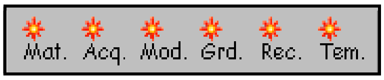
ωp	1.2405275	0.0000000	0.0000000
Γd	0.0400330	0.0000000	0.0000000

Tauc Lorentz

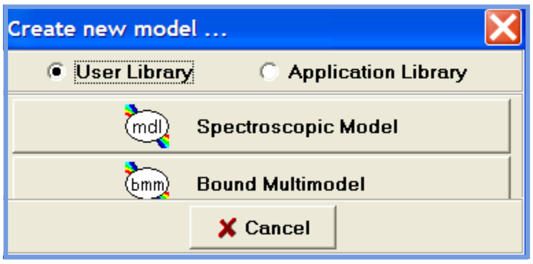
A	77.9476547	0.0000000	0.0000000
E	3.5399554	0.0000000	0.0000000
C	2.0043805	0.0000000	0.0000000

6.5 Creation of a Layer Model

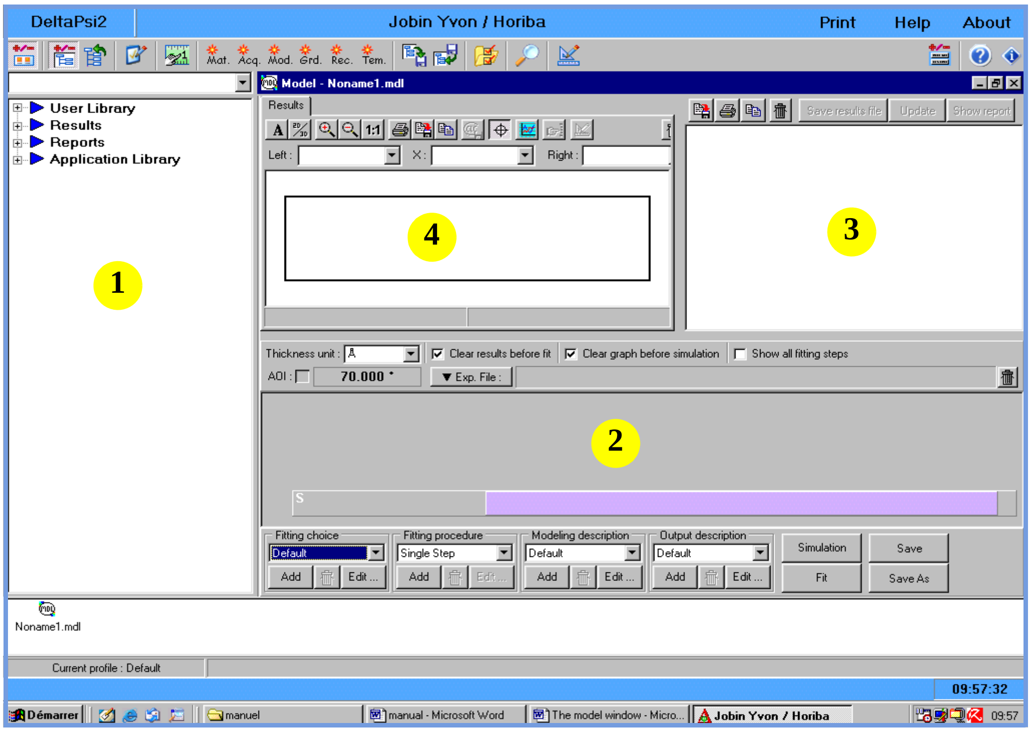
Model files are kept in model folder with the extension: *.MDL. In the main window of DP2, click on ***Mod*** button



and select ***Spectroscopic Model***:



The following window is displayed:



Thickness unit : Å
☑ Clear results before fit
☑ Clear graph before simulation
☐ Show all fitting steps
AOI : ☐ 70.000 °
Fitting choice: Default
Fitting procedure: Single Step
Modeling description: Default
Output description: Default
Current profile : Default

with:

1 **TreeView**
2 **model part**
3 **result window**
4 **fit/simulation graph window**

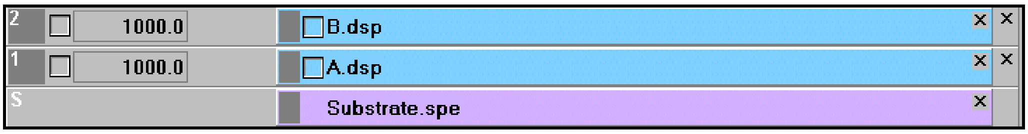
In the TreeView go to the Results/Acquisition data folder and drag and drop the experimental file in the Exp. File box.

Then go in the TreeView to the materials folder of the User Library (for created materials) or of the Application Library (for reference materials) and select the material(s) for the substrate layer (S).

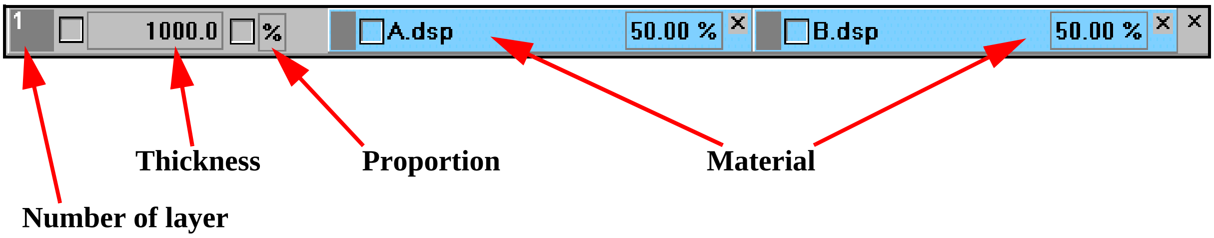
Drag and drop the material(s) from the TreeView window to the substrate layer

To create layers on top of the substrate layer just drag and drop a material file above the substrate layer.

For example a two-layer model look like this:



For all layers a mixture (effective medium approximation: EMA – details in chapter 5) of maximum three materials per layer can be created. For example a layer consisting of material A and B would look like this:



In the grey fields, you can:

- set thickness and/or composition values. A click on these values allows to open the "Fitting Choice Properties" window where you can set the fitting conditions.
- delete a layer by clicking the cross in the grey part on the right side.
- create/delete a layer repetition by a right click in the grey part
- change the type of layer by a right click in the grey part (gradient layer, anisotropic uniaxial/biaxial layer or gradient anisotropic uniaxial/biaxial layer).

In the coloured fields you can find all that concerns the material(s) and:

- access the material file by a double click on the material name in the layer. This possibility allows the user to see and/or modify the optical properties of the material. The modification of optical properties is not possible with reference files, you can only modify *.dsp, *.aly and *.ppc files. Remember to save your material file after modifications!
- delete a material by clicking on the cross in the colored parts
- set "Fitting parameters" by opening the "Fitting Choice Properties" window by a right click on the colored fields.

The modeling step and the fitting step are connected: some of the actions made in the modeling step are part of the fitting step. The fitting of a model to data is explained in detail in the corresponding chapter.

6.6 Thin Film Layer Structures

6.6.1 Modelling Strategy for Substrate

A film free substrate is characterized by: **0 < Ψ < 45° and 0 < Δ < 180°**. A measured value of greater than 45° implies that the sample is not a simple substrate, but has at least one film on it.

6.6.1.1 Opaque Substrate

The ellipsometric measurement of an opaque bulk substrate provides directly its optical constants (n,k) (assuming that the substrate is uniform and isotropic). An unknown surface film or roughness will cause the (n,k) values to be slightly different from the true ones.

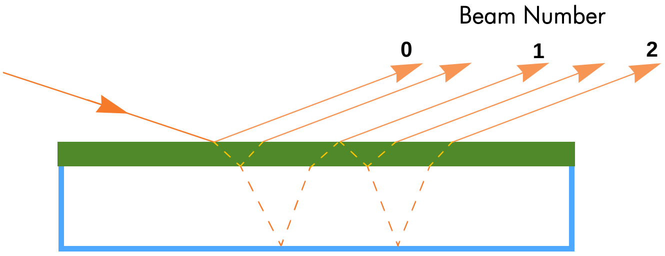
The ellipsometric measurement of the substrate can be used as a reference file. Just drag and drop the ellipsometric measurement (.spe) inside the substrate.


1 F 6000.0 F sio2-osabs.dsp
S substrat lah 66.spe

6.6.1.2 Transparent Substrate

A transparent substrate exhibits basckside reflections.

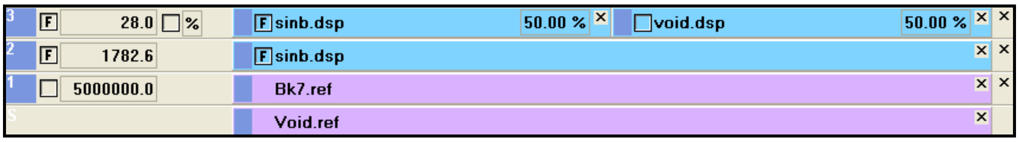
Case1: The substrate was measured with its backside reflections.



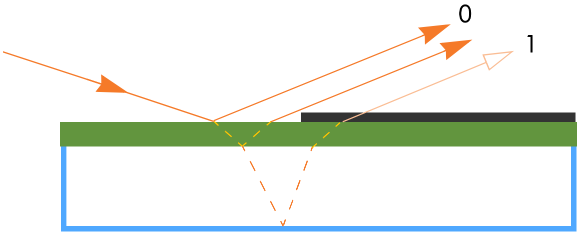
Use the «**backside reflection**» model. This model allows the optical treatment of the backside reflections collected during the measurement.

It consists in the use of void in the substrate, then add a layer that represents the transparent substrate (do not forget to mention its thickness), then continue your sample structure under analysis. In the example below, thicknesses are in Å.

Backside Reflection model


3 F 28.0 ☐ % F sinb.dsp 50.00 % ☐ void.dsp 50.00 %
2 F 1782.6 F sinb.dsp
1 ☐ 5000000.0 Bk7.ref
S Void.ref

Case2: The substrate was measured without backside reflections (the surface at the bottom of the substrate can be roughened: the light is scattered or the backside reflections are spatially separated from the first reflection and masked).

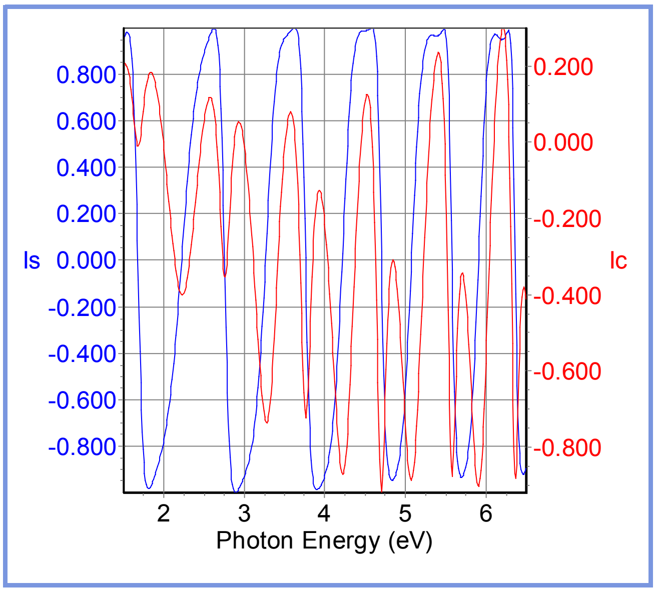


Sample with a mask

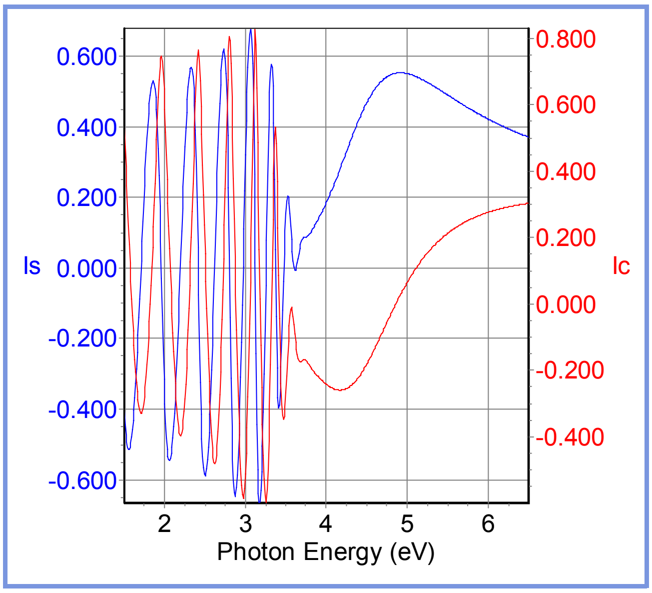
Use a simple substrate containing the reference or dispersion of your transparent material substrate.

6.6.2 Modelling Strategy for Single Layer

If the layer consists of a transparent material then we see interference fringes over the whole spectral range:

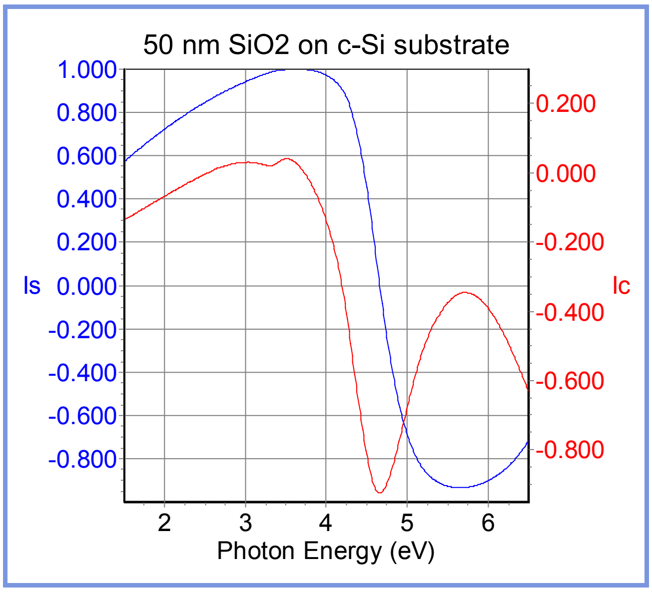


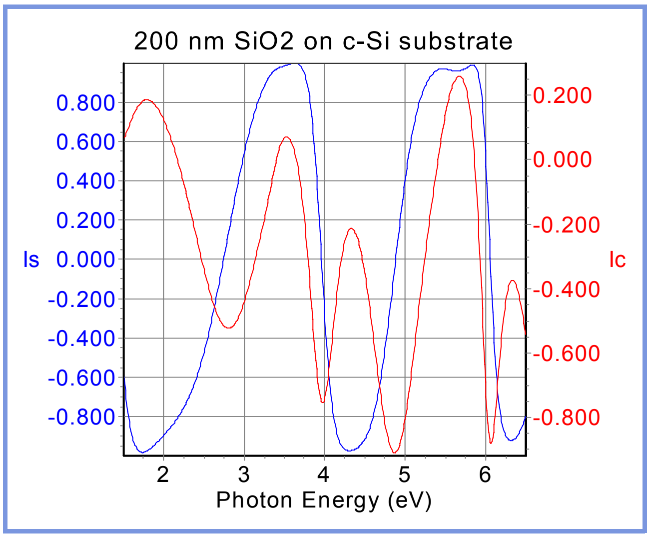
A Semi-absorbing material would show damping of the oscillations in a part of the spectrum. The following example shows a layer that is transparent from 1.5-3.5 eV and absorbing for energies above 3.5 eV:

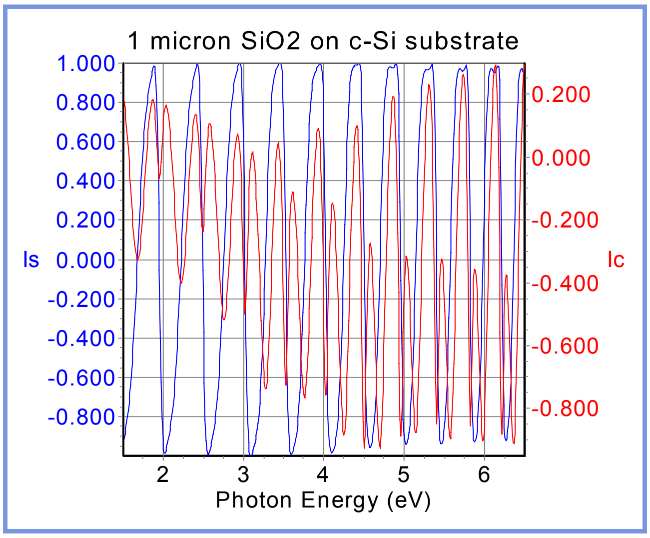


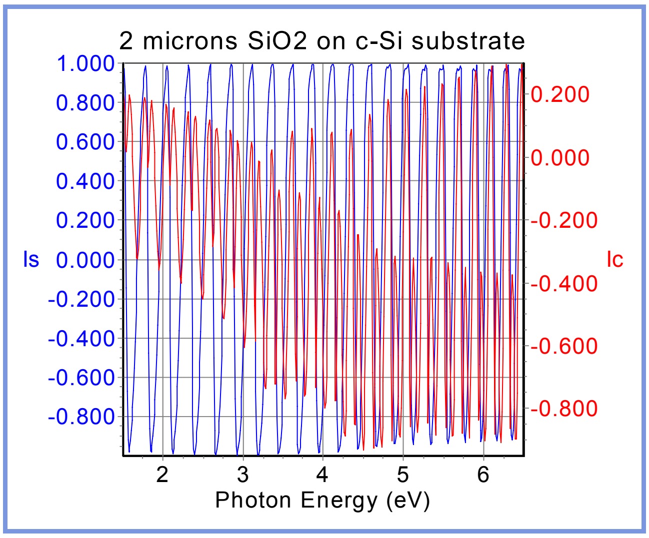
In the absorbing region the film behaves like a substrate. Light must penetrate the film to determine its thickness. In the example of the semi-absorbing material, you can determine the thickness in the spectral range 1.5 – 3.5 eV.

The thicker the transparent films is the closer the interference fringes are:

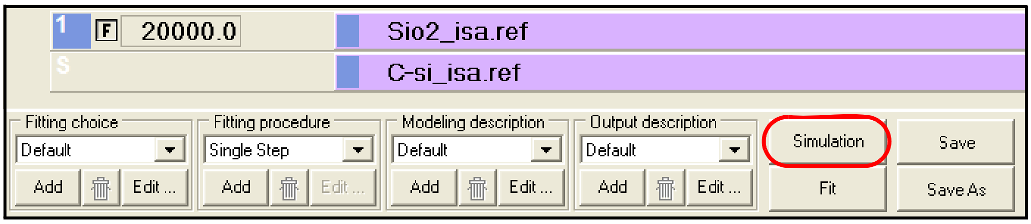








To get a first guess of the thickness, change the thickness of the layer and press the simulation button to see whether the calculated interference period matches the measured one:



1 F 20000.0 Sio2_isa.ref

S C-si_isa.ref

Fitting choice: Default

Fitting procedure: Single Step

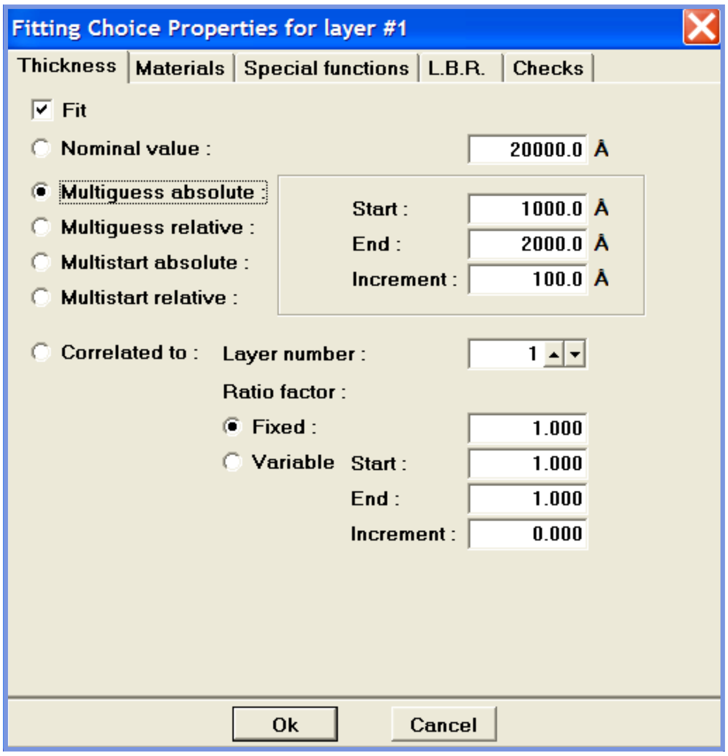
Modeling description: Default

Output description: Default

Alternatively multiguess or multistart functions allow to vary automatically the initial fitting values of thickness in a range defined by the user.

Click on the thickness value of the layer. The fitting choice properties screen will appear, then select the multiguess or multistart options available in the thickness tab. The larger the range and the smaller the increment, the longer the model calculation will take.

Activate Multiguess or Multistart functions



Fitting Choice Properties for layer #1

☑ Fit

○ Nominal value : 20000.0 Å

● Multiguess absolute :

○ Multiguess relative :

○ Multistart absolute :

○ Multistart relative :

Start : 1000.0 Å

End : 2000.0 Å

Increment : 100.0 Å

○ Correlated to : Layer number : 1

Ratio factor :

● Fixed : 1.000

○ Variable Start : 1.000

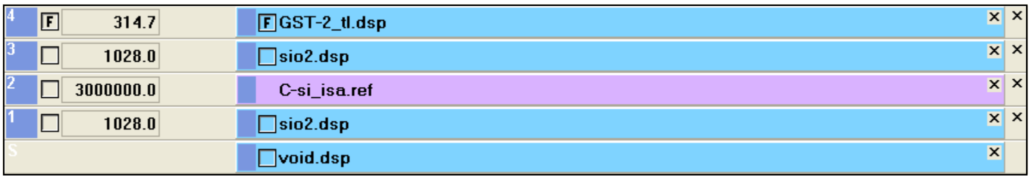
End : 1.000

Increment : 0.000

6.6.3 Modeling Strategy for a Layer Deposited on both Sides of the Substrate

This case often happens when a dip coating technique is used to deposit the layer.

If the substrate is transparent (like glass in the visible or c-Si in the NIR) and the backside reflections are collected during the measurement (that is there is no mask that hides the backside reflections, or the surface at the bottom of the substrate is not roughened) then the layer model has a structure as shown below:



4	F	314.7	F GST-2_tl.dsp
3	☐	1028.0	☐ sio2.dsp
2	☐	3000000.0	C-si_isa.ref
1	☐	1028.0	☐ sio2.dsp
S			☐ void.dsp

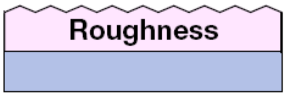
The model is based on the backside reflection model, so it implies void as the substrate. In this example, there is on both sides of c-Si a SiO_2 layer.

6.6.4 Modeling Strategy for Multilayers

It is good to know the approximate thicknesses of the individual layers. If this information is not available the multiguess or multistart options can help, but this might be very time-consuming for more than two layers.

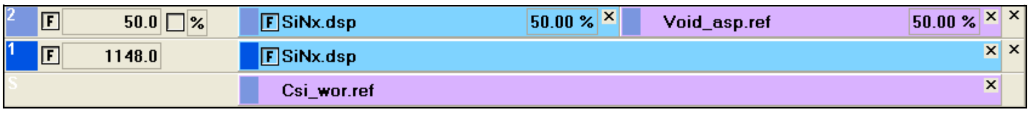
6.6.5 Roughness

Roughness is a small-scale variation in the height of the sample surface. It is often due to the thin film deposition technique or sample preparation.



Surface roughness is described as a discrete thin film at the surface. This layer can be described with the effective medium approximation (EMA) as a mixture of the material of the layer below with void (air) in a 50:50 ratio.

For this purpose add another layer and drag and drop the void reference file and the material of the layer below in this new layer. The default composition for a two-material layer is 50:50.



2	F	50.0 ☐ %	F SiNx.dsp	50.00 %	Void_asp.ref	50.00 %
1	F	1148.0	F SiNx.dsp			
S			Csi_wor.ref			

Modelling Strategy:

For small roughness thickness starting value is ca. 50Å. Generally do not adjust the composition. For large roughness the thickness starting values might be 150 – 500 Å. The EMA that is mainly used is the Bruggeman model (it is set by default and called EMA in DP2).

Thick roughness layers might scatter and depolarize light. Compare the χ^2 achieved with a fixed composition of 50:50 and a fitted composition parameter. Does the result make physically sense (for example 100% void: 0% material does not)?

Always begin with a simple model and increase complexity step by step. Add a rough overlayer on top of the structure and see whether the goodness of fit (χ^2) improves significantly.

Thin film deposition techniques that often produces a rough overlayer are sol-gel, anodizing, evaporation, sputtering, etc.

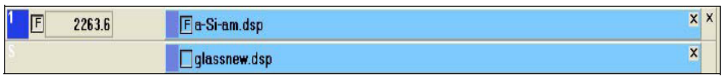
The oxidation (oxide layer < 100Å) of a surface can show the same effect as a roughness layer on top of the sample.

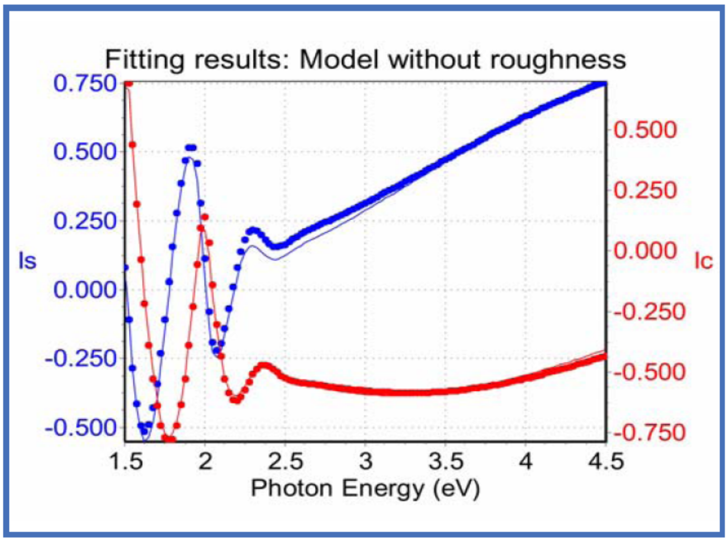
The use of a roughness layer can improve drastically the goodness of fit (χ^2) in a model. Typical examples give a goodness of fit of $1.5 < \chi^2 < 10$ without roughness layer for a film thickness < 5000Å. Adding a roughness layer can lead to $\chi^2 < 1$.

Note that surface roughness extracted by spectroscopic ellipsometry correlates with roughness measured by other techniques, such as AFM.

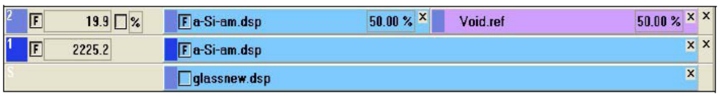
The example below shows how adding a roughness layer can improve the fit:

- Model without roughness: $\chi^2=6.23$

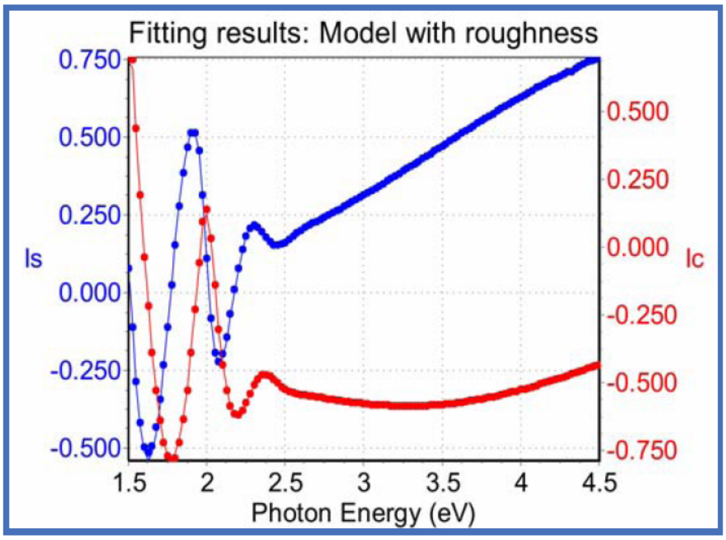




- Model with roughness: $\chi^2=0.46$



2	F 19.9 ☐ %	F a-Si-am.dsp 50.00 %	Void.ref 50.00 %
1	F 2225.2	F a-Si-am.dsp	
		☐ glassnew.dsp	

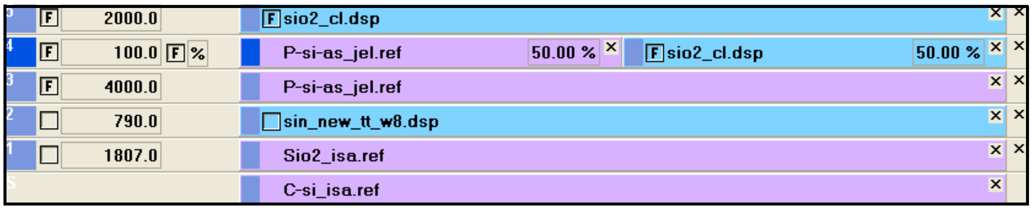


6.6.6 Interfacial Regions

An interface describes the common boundary of two layers. In a thin film structure a mixture of the material below and above the interface is assumed (using the Effective Medium Approximation EMA theory).

In the example below we want to create an interface layer between layer 3 (P-si-as) and the top layer (sio2_cl):

In the blue area of layer 3 click right and select copy layer to clipboard and then paste layer to clipboard. Another layer will be inserted above the layer 3 that contains the material of this layer. Then drag and drop the material of the layer 5 inside this new layer. A default composition of 50:50 is set:



5	F	2000.0	F sio2_cl.dsp	
4	F	100.0 F %	P-si-as_jel.ref 50.00 %	F sio2_cl.dsp 50.00 %
3	F	4000.0	P-si-as_jel.ref	
2	☐	790.0	☐ sin_new_tt_w8.dsp	
1	☐	1807.0	Sio2_isa.ref	
			C-si_isa.ref	

A reasonable starting value for the thickness of the interface layer is: 100Å.

In a first step keep the composition fixed and adjust the thickness of the interface. It is possible to automatically vary the thickness by using the multiguess or multistart option.

In a second step fit on both, the thickness and the composition and see whether there is a significant improvement in the goodness of fit.

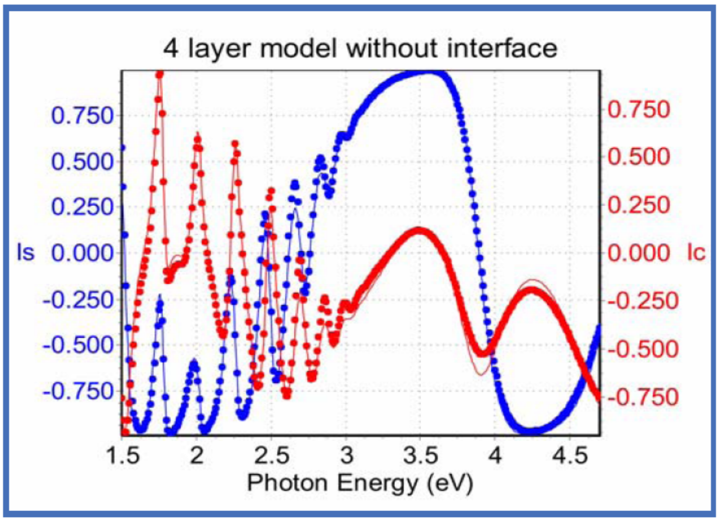
An interface layer is usually used when a homogeneous layer model gives a large χ^2 and adding a roughness layer still does not give a satisfactory χ^2.

Thin film deposition technique that produce inhomogenous coatings and thus interface layers are sol-gel, anodizing, evaporation, sputtering, etc.

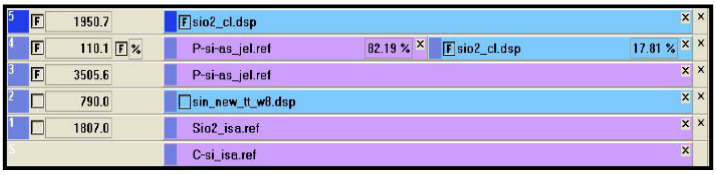
The example below shows how an interface layer can improve the fit:

- 4 layer model without interface: $\chi^2=24.5$

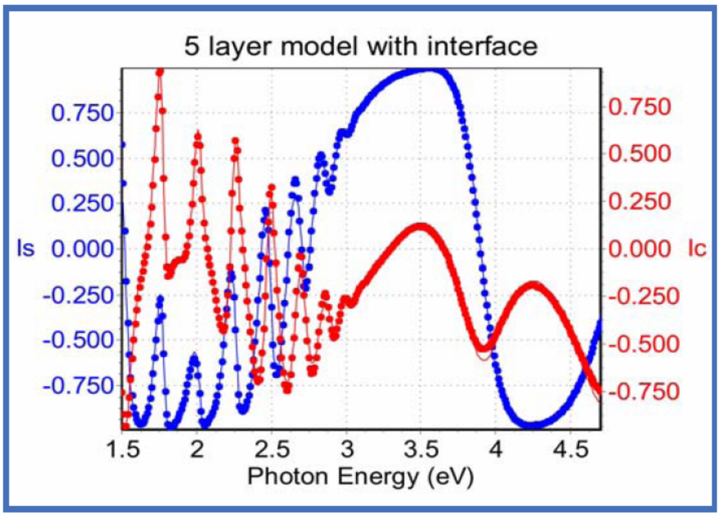
4	F	1904.4	F sio2_cl.dsp
3	F	3591.7	P-si-as_jel.ref
2	☐	790.0	☐ sin_new_tt_w8.dsp
1	☐	1807.0	Sio2_isa.ref
S			C-si_isa.ref



- 5 layer model with interface: $\chi^2=8.7$



5	F	1950.7	F sio2_cl.dsp	
4	F	110.1 F %	P-si-as_jel.ref 82.19 %	F sio2_cl.dsp 17.81 %
3	F	3505.6	P-si-as_jel.ref	
2	☐	790.0	☐ sin_new_tt_w8.dsp	
1	☐	1807.0	Sio2_isa.ref	
S			C-si_isa.ref	



7 Advanced Modeling

7.1 The most important dispersion formulae

As already said the real and imaginary parts of the optical properties of solids are wavelength / energy dependent. This dependency can be described by so-called dispersion formulae. These dispersion formulae can be classified in the following groups:

- empirical formulae
- classical oscillator models
- amorphous and multiple oscillator models
- transition based models (excitons,…)

The dependency of the optical properties on wavelength is due to different types of optical absorption processes in the materials. The most important are:

- interband absorption

This type of absorption occurs when a bound electron absorbs a photon from the light beam and is transferred to a higher energy level of the material. This absorption process appears in the range from NIR to UV. This process is typical for nearly all semiconductors and dielectric materials. Metals also show interband absorption, but additionally a strong absorption of photons by free carriers.

- intraband absorption

This is the second most important type of absorption process in which an electron absorbs a photon from the light beam and is transferred to a different energy state within the same band.

- free carrier absorption

Conducting materials such as metals contain free electrons which are not bound to any specific atom of the material. The absorption is usually proportional to the concentration of carriers. Because such materials have no bandgap, as Fermi energy for a metal lies within one of the electron energy band, the free carrier absorption is an intraband absorption phenomenon.

7.1.1 Empirical Formulae

These formulae are mostly based on polynoms. The most important examples are Cauchy, Sellmeier, Conrady and Briot. They can be used in the case that the refractive index changes simply with wavelength. Note that they are not Kramers-Kronig consistent (Appendix A).

7.1.1.1 Cauchy dispersion

Usually the Cauchy dispersion is only used for transparent materials. The refractive index is then given by (transparent Cauchy):

$$n(\lambda) = A + \frac{B \cdot 10^4}{\lambda^2} + \frac{C \cdot 10^9}{\lambda^4}$$

$$k(\lambda) = 0$$

However, the DeltaPsi2 software allows to take a small absorption into account (absorbent Cauchy):

$$n(\lambda) = A + \frac{B \cdot 10^4}{\lambda^2} + \frac{C \cdot 10^9}{\lambda^4}$$

$$k(\lambda) = D.10^{-5} + \frac{E \cdot 10^4}{\lambda^2} + \frac{F \cdot 10^9}{\lambda^4}$$

A, B, C, D, E and F are the fitting parameters.

These formulae can provide reasonable description of simple materials, but complicated dispersions cannot be determined and sometimes fitting of the coefficients does not converge to a good solution.

7.1.1.2 Sellmeier dispersion

This dispersion is very similar to the Cauchy dispersion. The expressions are:

$$\varepsilon = n^2(\lambda) = A + B \cdot \frac{\lambda^2}{\lambda^2 - \lambda_0^2} \quad \textbf{and} \quad k(\lambda) = 0 \quad \textbf{(transparent)}$$

or

$$\varepsilon = n^2(\lambda) = \frac{1 + A}{1 + \frac{B \cdot 10^4}{\lambda^2}} \quad \textbf{and} \quad k(\lambda) = \frac{C}{n \cdot D \cdot 10^{-2} \cdot \lambda + \frac{E \cdot 10^2}{\lambda} + \frac{1}{\lambda^3}} \quad \textbf{(absorbent)}$$

7.1.1.3 Conrady

The Conrady dispersion is a variation of the Cauchy Transparent dispersion and can also be applied to transparent and simple materials:

$$n(\lambda) = A + \frac{B \cdot 10^2}{\lambda} + \frac{C \cdot 10^9}{\lambda^{3,5}} \quad \textbf{and} \quad k(\lambda) = 0$$

7.1.1.4 Briot (Schott)

This dispersion formula is based on mathematics of Abelian and elliptic functions:

$$n(\lambda) = A_0 + A_1 \cdot 10^{-2} \cdot \lambda^2 + \frac{A_2 \cdot 10^{-2}}{\lambda^2} + \frac{A_3 \cdot 10^{-4}}{\lambda^4} + \frac{A_4 \cdot 10^{-6}}{\lambda^6} + \frac{A_5 \cdot 10^{-7}}{\lambda^8}$$

$$k(\lambda) = 0$$

Note that empirical dispersion relations such as Sellmeier, Cauchy, Conrady and Briot (Shott) have been widely used to describe transparent substrates and thin films till now. The constants in these formulae have no physical meaning.

7.1.1.5 Haltman

A further empirical model is described by the Haltman formula:

$$n(E) = A + \frac{C}{\lambda(E) - B}$$

$$k(E) = 0$$

$$\lambda(E) = \frac{h \cdot c}{E}$$

7.1.1.6 Fixed index

This model is mainly used to describe the dispersion of the ambient (air, liquid,…):

$$n(E) = \text{const}$$

$$k(E) = \text{const}$$

7.1.2 Classical oscillator models

Classical oscillator models are derived from the equation of motion of a bound charge. In the DP2 software the classical oscillator model contains:

- Lorentz oscillator
- Drude oscillator
- high frequency constant
- and additional oscillators

7.1.2.1 Lorentz oscillator

A Lorentz oscillator describes an electron bound to a heavy ion by a “spring” with a restoring force.

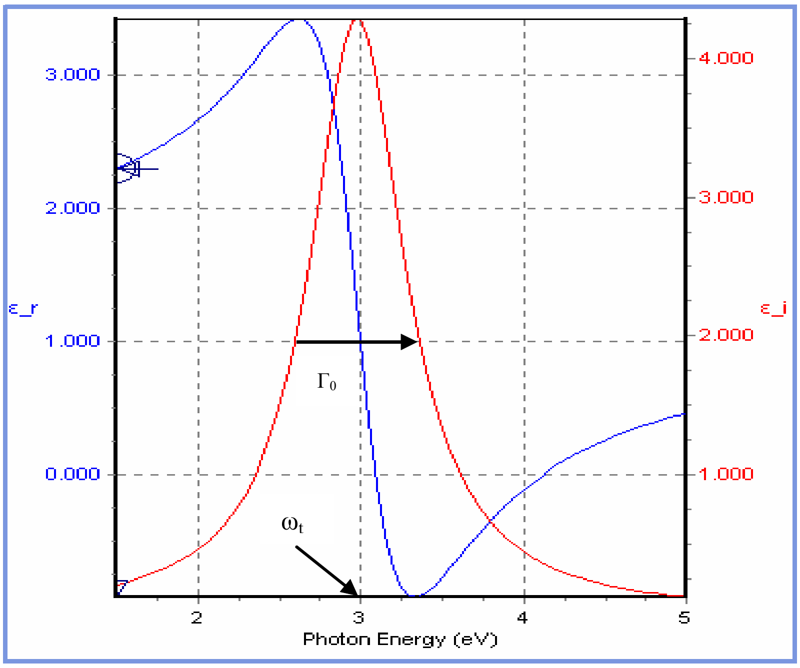
The single Lorentz oscillator is mostly used to describe transparent dielectric materials ($\Gamma_0=0$) such as SiO_2, SiON, Al_2O_3, HfO_2, MgO or weakly absorbing materials ($\Gamma_0 \neq 0$).

The formula for the Lorentz oscillator is:

$$\frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\omega}$$

where is the light energy (eV), ε_∞ is the dielectric constant for high frequencies, ε_s is the static dielectric constant, ω_t is the transition energy of the absorption process and Γ_0 is the damping constant.

For example in the next graph a Lorentz oscillator with $\varepsilon_\infty=1$, $\varepsilon_s=2$, $\varepsilon_t=3$eV and $\Gamma_0=0.7$ is shown (Im(ε) in red and Re(ε) in blue):



7.1.2.2 Drude term

The Drude free electron model is used mainly for metals. It can be derived from the Lorentz oscillator model by assuming that the restoring force is zero ($\omega_t = 0$). That means that all electrons are free to move throughout the material. The equation for the Drude oscillator is given by:

$$\frac{\omega_p^{\ 2}}{-\omega^2 + i\Gamma_D\omega}$$

where is the light energy (eV), ω_p is the plasma energy of the free electron gas and Γ_D is the damping constant. The damping force describes the scattering of the electrons associated with electrical resistivity.

7.1.2.3 Additional oscillators

Sometimes it is necessary to use additional oscillators for example in the case of materials that have several absorption bands such as organic polymers.

These additional oscillators have the form of Lorentz oscillators and are given by:

$$\sum_{j=1}^{2} \frac{f_j \omega_{0j}^{\ 2}}{\omega_{0j}^{\ 2} - \omega^2 + i\tau_j\omega}$$

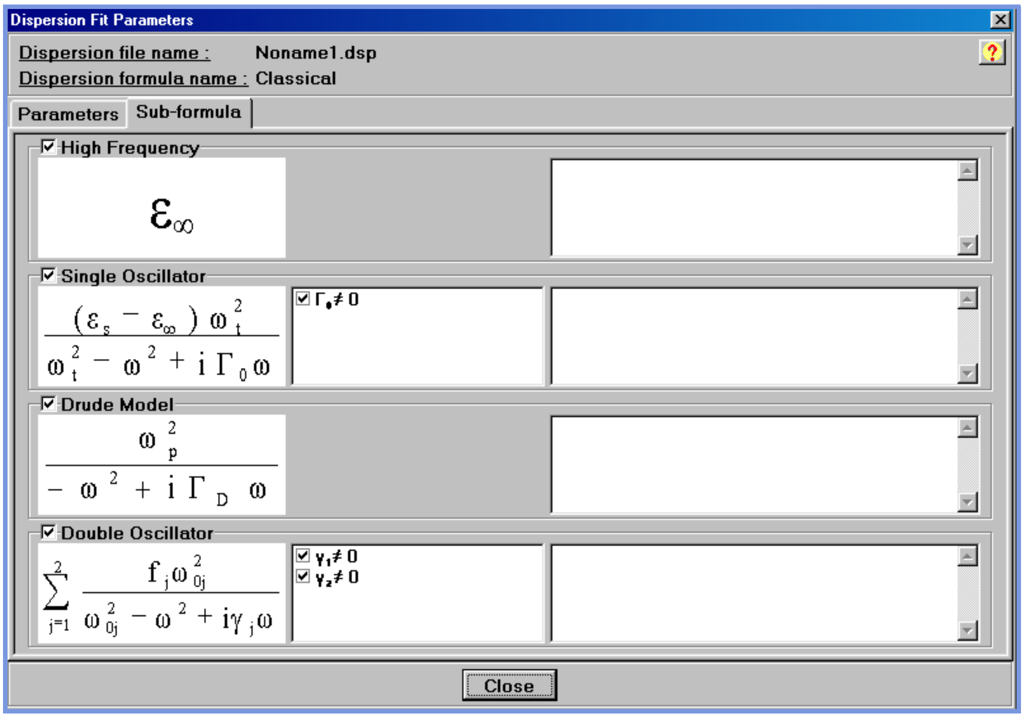
where ω is the light energy (eV), f is the oscillator strength, ω_0 is the transition energy of the absorption process and is the damping constant.

7.1.2.4 Summary: classical formula

The equation of the classical formula in the DP2 software is therefore given by:

$$\varepsilon = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\omega} + \frac{\omega_p^2}{-\omega^2 + i\Gamma_D\omega} + \sum_{j=1}^{2} \frac{f_j\omega_{0j}^2}{\omega_{0j}^2 - \omega^2 + i\tau_j\omega}$$

When the user checks the fitting box of the classical dispersion in the Model window, the software will ask the user to select the type(s) of oscillator:



Dispersion file name : Noname1.dsp

Dispersion formula name : Classical

☑ High Frequency

ε_∞

☑ Single Oscillator

$\frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\omega}$

☑ $\Gamma_0 \neq 0$

☑ Drude Model

$\frac{\omega_p^2}{-\omega^2 + i\Gamma_D\omega}$

☑ Double Oscillator

$\sum_{j=1}^{2} \frac{f_j\omega_{0j}^2}{\omega_{0j}^2 - \omega^2 + i\gamma_j\omega}$

☑ $\gamma_1 \neq 0$

☑ $\gamma_2 \neq 0$

7.1.2.5 Quatre Oscillators

This dispersion formula is just an extension of the double oscillator formula of the classical dispersion and is used for materials with several absorption bands such as polymers.

$$\varepsilon(\omega) = \varepsilon_\infty + \sum_{j=1}^{4} \frac{f_j\omega_{0j}^2}{\omega_{0j}^2 - \omega^2 + i\gamma_j\omega}$$

7.1.3 Oscillator models for amorphous materials

In thin film technologies a lot of materials exist in an amorphous or nearly amorphous structure. The optical properties of these materials can depend strongly on the growth conditions so that there can be a great variation of optical parameters. In the following we describe the most important dispersion models for this type of materials.

Common to these models is that there is an energy band gap below which there is no absorption.

7.1.3.1 New Amorphous

Probably the most commonly used dispersion formula for amorphous materials is based on a parameterization introduced by Forouhi & Bloomer:

$$n(\omega) = n_\infty + \frac{B(\omega - \omega_j) + C}{(\omega - \omega_j) + \Gamma_j^2}$$

$$k(\omega) = \begin{cases} \dfrac{f_j(\omega - \omega_g)^2}{(\omega - \omega_j) + \Gamma_j^2} & \omega > \omega_g \\ 0 & \omega < \omega_g \end{cases}$$

where

$$B = \frac{f_j}{\Gamma_j}\left[\Gamma_j^2 - (\omega_j - \omega_g)^2\right]$$

$$C = 2f_j \cdot \Gamma_j(\omega_j - \omega_g)$$

with the following fitting parameters:

- n_∞ the long wavelength (low energy) refractive index
- ω_j the energy of maximum absorption
- fj the oscillator strength
- ω_g the band gap energy
- Γ_j the broadening factor

The New Amorphous dispersion formula, which can be regarded as a single oscillator above a certain energy band gap below which there is no absorption, can be extended to allow 2 or 3 oscillators above the band gap:

- Double New Amorphous
- Triple New Amorphous

The fitting parameters are thus n_∞, ω_g, f_j, ω_j, Γ_j with $1 \leq j \leq 3$.

This is necessary if there are additional absorption bands present in the material.

7.1.3.2 Amorphous

This dispersion is based on an earlier parametrization found by Forouhi & Bloomer:

$$n(E) = \sqrt{\varepsilon_\infty} + \frac{B_0 \cdot E + C_0}{E^2 - B \cdot E + C'}$$

$$k(E) = \begin{cases} \dfrac{A(E - E_g)^2}{E^2 - B \cdot E + C} & E > E_g \\ 0 & E < E_g \end{cases}$$

where

$$B_0 = \frac{A}{Q}\left(-\frac{B^2}{2} + E_g \cdot B + C\right)$$

$$C_0 = \frac{A}{Q}\left[\left(E_g{}^2 + C\right)\frac{B}{2} - 2 \cdot E_g \cdot C\right]$$

$$Q = \frac{1}{2}\sqrt{4 \cdot C - B^2}$$

The fitting parameters are: ε_∞, E_g, A, B and C. The formulae can be extended to use up to 4 oscillators (Double-, Triple- and Quadruple Amorphous).

The drawback is that not all parameters have a proper physical meaning. ε_∞ is the high frequency dielectric constant and E_g is the energy band gap. A is simply a factor but B and C are expressions of physical parameters:

$B = 2E_0$ and $C = E_0{}^2 + \Gamma^2$

This makes it very difficult to guess proper start values for the dispersion.

The recommendation is to use the New Amorphous formula which is much more intuitive.
Although the Amorphous or New Amorphous parameterization works for a lot of materials and is very useful for spectroscopic ellipsometry there are some physical problems:

- the approximation $k(E) = 0$ for $E < E_g$ is not physically realistic
- for $E >> E_g$ the (New) Amorphous formula predicts $k(E)$ = constant which of course cannot be true for a real material.

A consequence is that these dispersions are not Kramers-Kronig consistent.

7.1.3.3 Tauc Lorentz formula

The Tauc Lorentz dispersion formula corrects the unphysical problems of the (New) Amorphous dispersion. This formula is based on the Tauc expression and Lorentz oscillator model. The imaginary part of the dielectric function near the band edge is given by:

$$\varepsilon_2(E) = 2n(E)k(E) = \begin{cases} \dfrac{1}{E} \cdot \dfrac{A \cdot E_0 \cdot C(E - Eg)^2}{\left(E^2 - E_0{}^2\right)^2 + C^2 \cdot E^2} & E > E_g \\ 0 & E < E_g \end{cases}$$

There are 5 fitting parameters: the energy band gap E_g, the peak in the joint density of states E_0, the high frequency dielectric constant ε_∞ in the ε_1 expression (see below), the factor *A*, which includes the optical transition matrix elements, and *C* the broadening factor.

The real part ε_1 is determined from ε_2 with the Kramers-Kronig relation:

$$\varepsilon_1(E) = \varepsilon_\infty + \frac{2}{\pi} \cdot P\int_{E_g}^{\infty} \frac{\xi\varepsilon_2(\xi)}{\xi^2 - E^2} d\xi$$

For details on this calculation refer to appendix A.

The Tauc Lorentz expression is consistent with known physical phenomena and is obviously Kramers-Kronig consistent.

7.1.4 Transition based dispersion models

These dispersion models are mainly used to describe transitions near the band gap in semiconductors. These are mostly band-to-band and excitonic transitions.

7.1.4.1 Adachi Model Dielectric Function (MDF)

The dielectric function of a material is composed by contributions from all transitions between the valence band and the conduction band.

The Adachi-MDF is mainly applied to transitions appearing in semiconductors near the band gap, namely E_0, E_0+_0, E_1, E_1+_1.

The complex dielectric function of the MDF model is composed of different terms corresponding to these transitions:

$$\varepsilon = \varepsilon_\infty + \varepsilon_1 + \varepsilon_2 + \varepsilon_3$$

The assumption is again that for energies lower than the fundamental band gap the absorption is zero: Im $(\varepsilon) = 0$ for $E < E_0$

For the transitions at E_0 and at $E_0 + \Delta_0$ we get:

$$\varepsilon_1 = A_0\left(\frac{f(\chi_0)}{E_0^{\ 3/2}} + \frac{f(\chi_{s0})}{2(E_0+\Delta_0)^{3/2}}\right)$$

with

$$f(\chi) = \frac{2-\sqrt{1+\chi}-\sqrt{1-\chi}}{\chi^2}$$

$$\chi_0 = \frac{E+i\Gamma_0}{E_0}$$

$$\chi_{s0} = \frac{E+i\Gamma_0}{E_0+\Delta_0}$$

The contribution of the excitonic transitions is described by:

$$\varepsilon_2 = \sum_{n=1}^{3}\frac{A_{0x}}{n^3}\left(\frac{1}{E_0-\left(\frac{G_0}{n^2}\right)-E-i\Gamma_0}\right)$$

In theory, the sum is done for an infinite number of excitonic states, but most of the time, only the first excitonic states are observable. The others are included in the band to band contribution due to their proximity.

For transitions E_1 and $E_1 + {}_1$ the contribution is:

$$\varepsilon_3 = -\frac{B_1}{\xi^2}\cdot\ln\left(1-\xi^2\right)$$

with

$$\xi = \frac{E + i\Gamma_1}{E_1}$$

The fitting parameters are A_0, A_{0x}, B_1, G_0, E_0, E_1, Γ_0, Γ_1, Δ_0 and ε_∞.

7.1.4.2 Excitonic model

This model describes the contribution of excitons at the transitions E_0, $E_0+\Delta_0$, E_1 and $E_1+\Delta_1$.

$$\varepsilon = \varepsilon_{ex,0} + \varepsilon_{ex,1}$$

$$\varepsilon_{ex,0} = \sum_{n=1}^{\infty}\frac{A_{0x}}{n^3}\left[\frac{1}{E_0 - \left(\frac{G_0}{n^2}\right) - E - i\Gamma_0} + \frac{1}{2}\left(\frac{1}{E_0 + \Delta_0 - \left(\frac{G_0}{n^2}\right) - E - i\Gamma_0}\right)\right]$$

$$\varepsilon_{ex,1} = \sum_{n=1}^{\infty}\frac{1}{(2n-1)^3}\left[\begin{array}{c}\dfrac{B_{1x}}{E_1 - \left[\dfrac{G_1}{(2n-1)^2}\right] - E - i\Gamma_0} \\ \\ +\dfrac{B_{2x}}{E_1 + \Delta_1 - \left[\dfrac{G_{1s}}{(2n-1)^2}\right] - E - i\Gamma_0}\end{array}\right]$$

With the following parameters:

ε_∞	High frequency
E_0	E_0 transition
D_0, also called Δ_0	E_0+D_0 transition
G_0	Broadening parameter
A_0	Strength parameter
A_{0x}	Exciton strength parameter
G_0	Exciton binding parameter
E_1	E_1 transition
D_1, also called Δ_1	E_1+D_1 transition
G_1	Broadening parameter
B_1	Strength parameter
B_2	Strength parameter
B_{1x}	Exciton strength parameter (E_1)
B_{2x}	Exciton strength parameter (E_1+D_1)
G_1	Exciton binding parameter
G_{1s}	Exciton binding parameter
E_2	E2 transition
C_0	Strength parameter
G_2	Broadening parameter

7.1.4.3 Tanguy model

The tanguy dispersion formula is used for alloyed III-V-semiconductors such as InGaAsP to describe the transitions near the band gap energy. The formula of the Tanguy model is:

$$\varepsilon(E) = \varepsilon_0 + \frac{a}{b-(E-i\Gamma)^2} + \frac{A\sqrt{R}}{E+i\Gamma}\left[\begin{array}{l} \ln\dfrac{E_g{}^2}{E_g{}^2-(E-i\Gamma)^2} + 2\sqrt{\dfrac{E_g}{R}} - -\sqrt{\dfrac{E_g+E+i\Gamma}{R}} - \sqrt{\dfrac{E_g-E-i\Gamma}{R}} \\ + 2\displaystyle\sum_{k=1}^{\infty}\left(\dfrac{2}{\sqrt{\dfrac{R}{E_g}}-k} - \dfrac{1}{\sqrt{\dfrac{R}{E_g+E+i\Gamma}}-k} - \dfrac{1}{\sqrt{\dfrac{R}{E_g-E-i\Gamma}}-k}\right) \end{array}\right]$$

The fitting parameters are:

- ε_0: low frequency dielectric constant
- E_g: band gap energy
- Γ: broadening parameter
- a, b: dispersion parameters for $E < E_g$
- c, d: dispersion parameters for k at E > Eg
- R: energy of exciton
- A: coefficient proportional to the square of the Kane momentum

7.1.4.4 Tanguy Extended Model

The Tanguy Extended dispersion formula is used as the Tanguy formula, however, it is mainly applied in the near-IR spectral region. The formula is:

$$\varepsilon(E) = 1 + \frac{a}{b - E^2} + \frac{A\sqrt{R}}{E + i\Gamma}\left[g[\zeta(E + i\Gamma)] + g[\zeta(-E - i\Gamma)] - 2g[\zeta(0)] \right]$$

with

$$g(\zeta) = 2\ln(\zeta) - 2\pi \cdot \cot(\pi\zeta) - 2\Psi(\zeta) - \frac{1}{\zeta}$$

$$\Psi(z) = \frac{d}{dz}\ln[\Gamma(z)]$$

$$\zeta(z) = \sqrt{\frac{R}{E_g - z}}$$

so that we obtain:

$$n = \mathrm{Re}\left(\sqrt{\varepsilon}\right)$$

$$k = \begin{cases} \mathrm{Im}\left(\sqrt{\varepsilon}\right) & E < E_g \\ \mathrm{Im}\left(\sqrt{\varepsilon}\right) + c\left(E - E_g\right) + d\left(E - E_g\right)^2 & E > E_g \end{cases}$$

The fitting parameters are the same as the one from Tanguy formula

- ε_0: low frequency dielectric constant
- E_g: band gap energy
- Γ: broadening parameter
- a, b: dispersion parameters for $E < E_g$
- c, d: dispersion parameters for k at E > Eg
- R: energy of exciton
- A: coefficient proportional to the square of the Kane momentum

7.1.5 Further models and combination of previous models

There are further dispersion models implemented in the DP2 software. Some are extensions or combinations of already discussed models. The most important are:

- Afromowitz
- Kato-Adachi
- Kato-Adachi IR
- Adachi-n Forouhi
- Adachi-New Forouhi

They are all described in detail in appendix A!

7.1.6 Summary

The following table summarizes again the discussed dispersion models and their applications:

Dispersion type	**Dispersion**	**Materials**	**Fitting parameter**
Classical oscillators	classical	Transparent or weakly absorbent materials: SiO_2, SiON, Al_2O_3, HfO_2, MgO, ZrO_2. Metals with Drude Oscillator	4 up to12
	Quatre oscillators	Polymers,TPD materials	9
Polynomial	Cauchy	Transparent or weakly absorbent thin materials: glass, thin SiO_2 films..	3 up to 6
	Sellmeier		3 up to 5
	Conrady	Transparent and simple materials	3
	Briot		6
	Haltman		3
Amorphous	New Amorphous	Al_2O_3, TiO_2,Ta_2O_5	5 up to 11
	Amorphous	Transparent or complex absorbent materials, Alq3, AlN, pentacene	5 up to 14
	Tauc Lorentz	a-Si_xN_y:H,	5 up to 11
Transition-based	Excitonic		19
	Adachi-MDF	Semiconductors II-VI, ZnTe, HgCdTe	8
	Tanguy	Semiconductors III-V, InGaP near band gap energy	7
	Tanguy Extended	Semiconductors III-V in the IR region of the spectra	8
	Afromovitz	Semiconductors III-V	6

Combination of previous dispersion	Kato-Adachi	Semiconductors III-V till 3eV	11
	Kato-Adachi IR		8
	Adachi n Fourouhi	PZT: lead zirconate titanate,	8 up to 14
	Adachi-New Fourouhi		8

7.1.7 Dispersion parameter manual adjustment - Examples

During the fitting process the DP2 software automatically adjusts dispersion parameters to obtain the best fit. In complex cases the solution of the fitting process might be far from the best solution. Therefore it is crucial to set the starting parameters for the dispersion models as close to reality as possible.

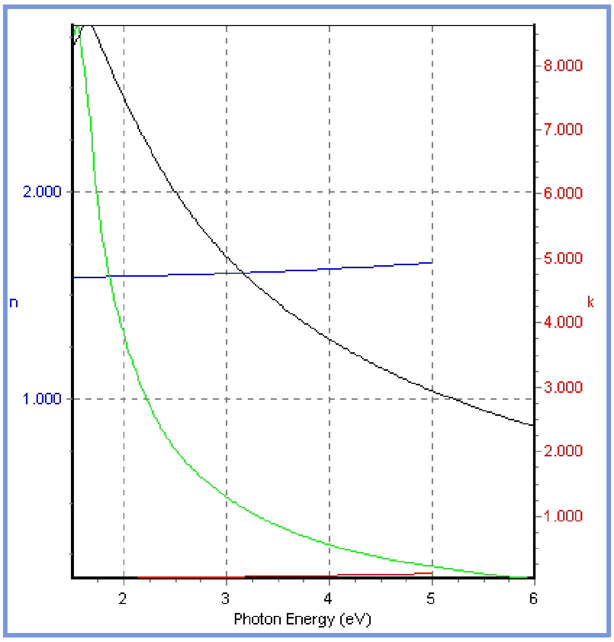
For this reason it is important to get the maximum of information of the optical properties of the material to be modelled by consulting literature values and/or the reference files of the DP2 software.

In the next chapters dispersion models and corresponding start values for various materials are discussed.

7.1.7.1 Classical/Drude Oscillator dispersion for Aluminium

The following graph shows in the dispersion window:

- n of the Drude Oscillator in blue
- k of the Drude Oscillator in red
- n of the Aluminium reference file in green
- k of the Aluminium reference file in black



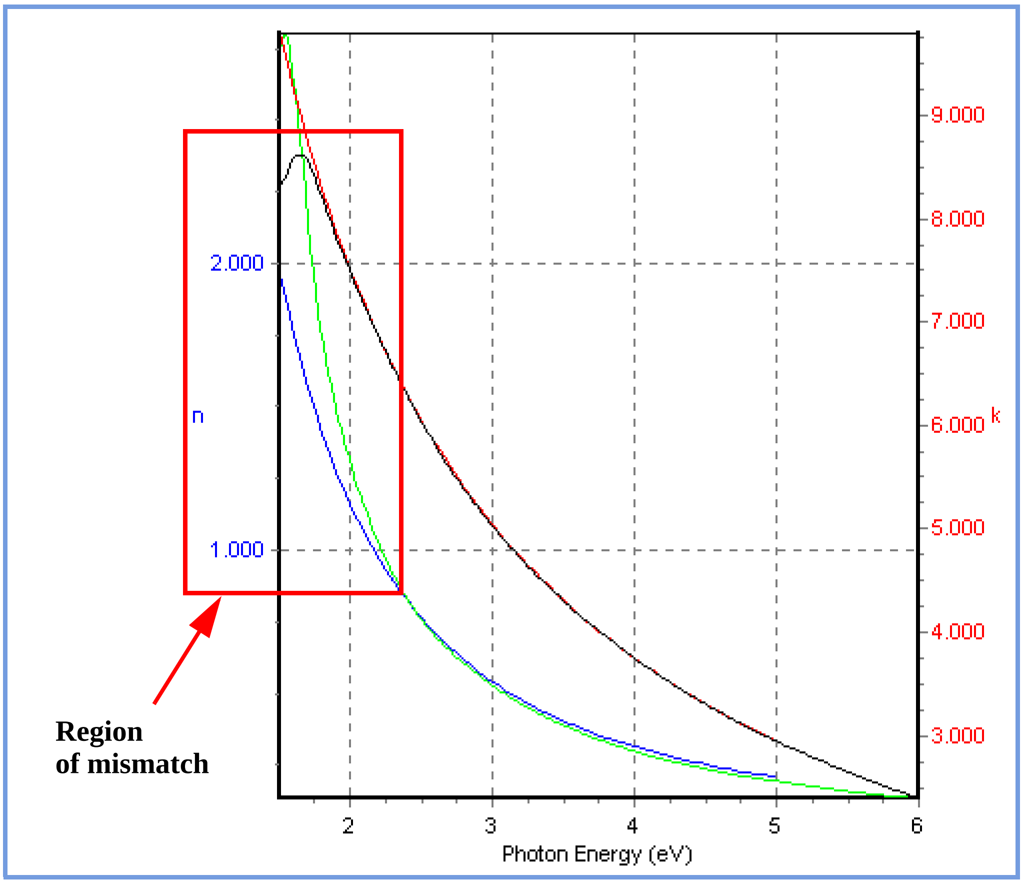
The above graph is obtained when you open a classical dispersion with the aluminium reference superposed on it. The starting fitting parameters are:

E_∞	1.0000000
ε_s	2.5000000
ω_t	12.0000000
ω_p	0.0000000
Γ_0	5.0000000
Γ_d	0.0000000
F_1	0.0000000
ω_{01}	0.0000000
y_1	0.0000000
F_2	0.0000000
ω_{02}	0.0000000
Y_2	0.0000000

Aluminium is a metal, so we use the Drude Oscillator dispersion whose parameters are the plasma frequency ω_p and the damping constant Γ_d. ε_∞ is generally set to 1 and we do not fit on it. All other parameters, except for ω_p, Γ_d and ε_∞ are set to 0.

ω_p and Γ_d are now adjusted to match the reference curve. The following set of parameters is a good guess for matching the dispersion with the reference from 2.5eV to 6eV:

ε_∞	1.0000000
ω_p	15.6500000
Γ_d	0.6200000

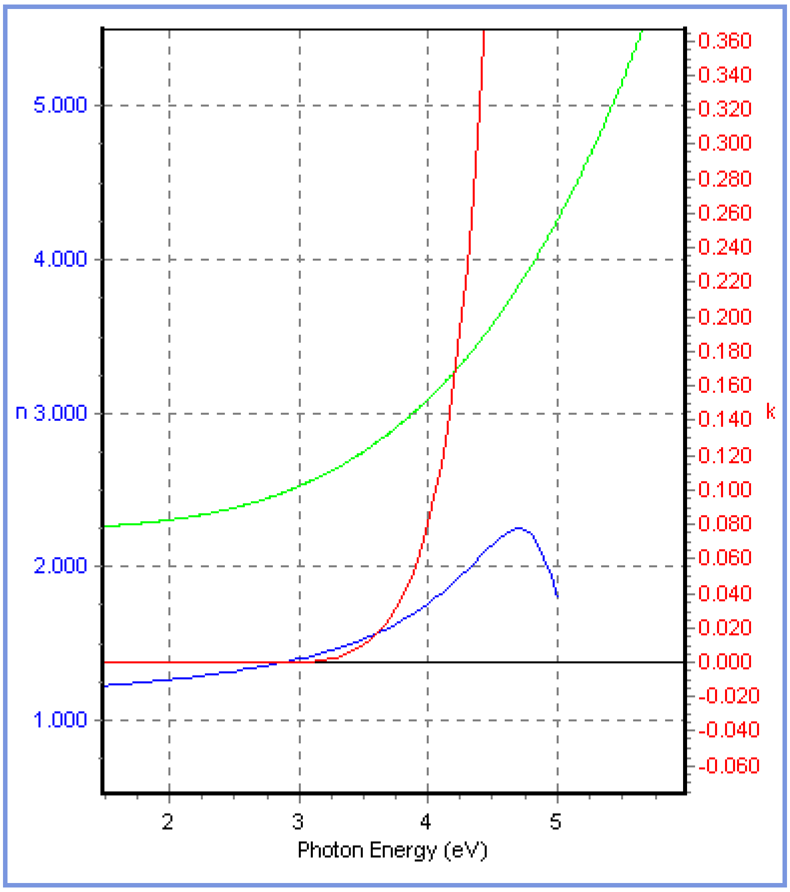


Aluminium, like all metals, is strongly absorbent in the IR. Usually it does not matter if the dispersion is not appropriate in the IR region, because most of time the visible and UV region are of interest. However, if the IR region is important a more sophisticated dispersion formula is necessary.

7.1.7.2 New Amorphous dispersion for TiO_2

The following graph shows in the dispersion window:

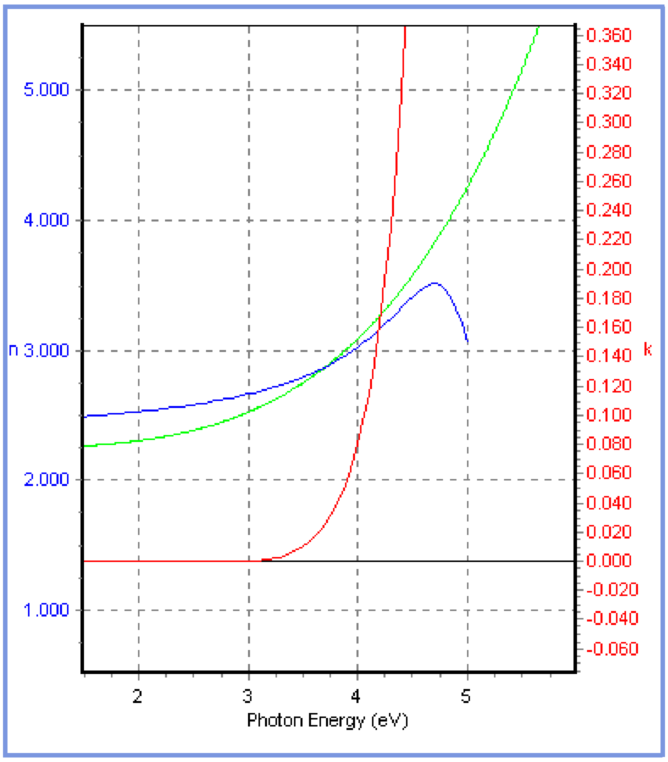
- n of New Amorphous in blue
- k of New Amorphous in red
- n of TiO_2 reference file in green
- k of TiO_2 reference file in black



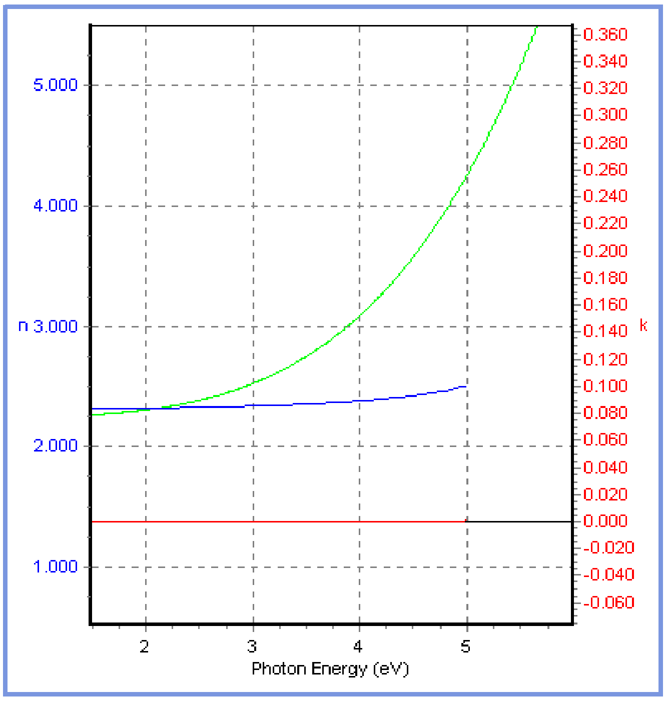
The goal is to adjust parameters so that the dispersion matches the reference. Initial parameters of the New Amorphous dispersion are for example:

n_∞= 1.0000000
ω_g= 3.0000000
f_j = 0.1000000
ω_j = 5.0000000
Γ_j = 0.5000000

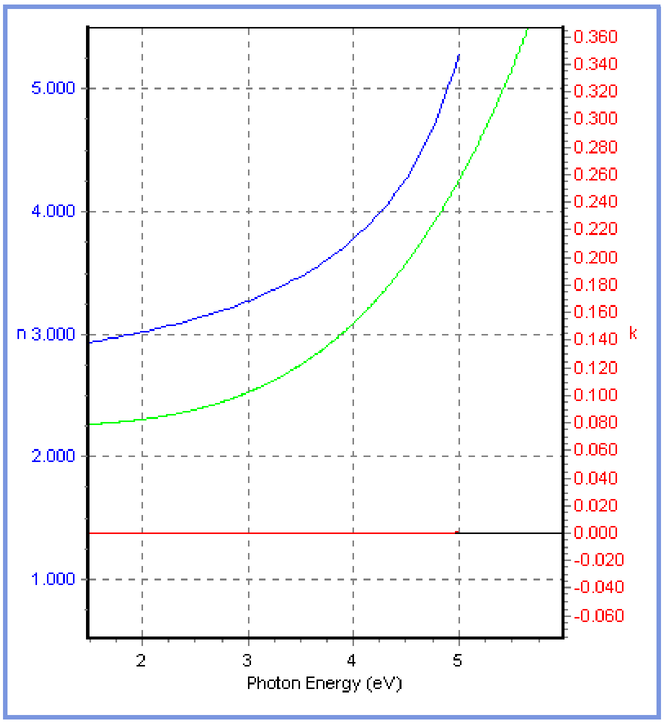
Look at n of the reference file near the lowest energy: n(1.5eV) = 2.265. We can put this value to n_∞.



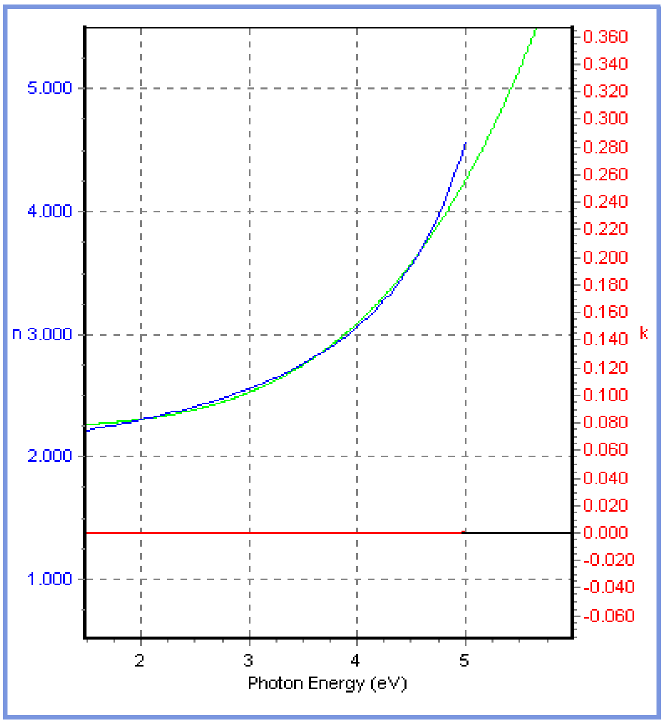
According to the reference there is no absorption (k = 0); That means that we have to set ω_j and ω_g high enough so that there is no absorption in the given spectral range. For example set $\omega_g = 4.9$eV and $\omega_j = 6$eV; by definition $\omega_g < \omega_j$. You will obtain:



Then adjust the strength and the broadening parameter. An increasing oscillator strength leads to a higher value of n. A decreasing broadening parameter leads to a steeper increase of n with energy. Set for example $f_j = 0.25$ and $\Gamma_j = 0.10$eV thus we obtain a correct curve profile:



Finally we adjust again the value of n. For example set n = 1.55:



The final start values in this case are then:

n_∞ = 1.5500000

ω_g = 4.9000000

f_j = 0.2500000

ω_j = 6.0000000

Γ_j **= 0.1000000**

It does not matter if the starting parameters lead to a dispersion that does not exactly match the reference values because they will be adjusted in the fitting process. Real TiO_2 samples can show different optical properties for example they can show absorption for lower energies which means lower values for ω_g and ω_j. For example for one of our samples we found after the fitting process the following parameters:

n_∞ **= 1.9922565**

ω_g **= 3.0720084**

f_j **= 0.1764574**

ω_j **= 4.2158175**

Γ_j **= 0.4805436**

7.1.8 Effective medium approximation

Effective medium approximations (EMAs) are used to describe the optical constants of mixtures of materials of known optical constants.

EMAs are applied successfully when inhomogeneities are at scale somewhere in between atomic distances and the wavelength. The most important applications are:

- surface roughness layers
- interface layers
- porous materials
- mixture of materials

7.1.8.1 The effective medium models

The DP2 software uses several models of effective medium, according to the phase proportions in the mixture:

- *MG* for Maxwell-Garnett model
- *EMA* for Bruggeman model
- *EMAMG* for Maxwell-Garnett & Bruggeman model
- *SSC* for Sen, Scala & Cohen model

Maxwell-Garnett model

This model is based on the Clausius-Mosetti relationship which describes the dielectric function of a set of spheres that are at a certain distance to each other and homogeneously immerged in a host medium. This model defines the dielectric function ε of the effective medium according to the following formula:

$$\varepsilon = \varepsilon_0 \frac{\varepsilon_1 (1 + 2f) + 2\varepsilon_0 (1 - f)}{\varepsilon_1 (1 - f) + \varepsilon_0 (2 + f)}$$

With the dielectric constant of spherical particles ε_1 immerged in a host medium whose dielectric constant is ε_0. f is the volume fraction of the spheres.

The Maxwell-Garnett model is valid in cases where there are inhomogeneities in granular form. It is only valid for a two-component mixture. It is for example very useful for certain nanocrystals embedded in hosts and for cermats. However, the proportion of the inclusions in the host medium must be low, otherwise the Bruggeman model, which is discussed next, must be used.

EMA-Bruggeman model

In this model the different components of the mixture are treated equivalently, without preliminary assumption on the relative proportions. This model is self-consistent: the mixture of the different materials forms the host medium, which means that the dielectric function of the host medium is the EMA-Bruggeman dielectric function.

In this model the number of phases can exceed 2. The dielectric functions of the different materials are ε_i (with i=1,2,3,…) with corresponding volume fractions f_i. The dielectric function of the effective medium fulfills the following equation:

$$\sum_i f_i \frac{\varepsilon_i - \varepsilon}{\varepsilon_i + 2\varepsilon} = 0$$

This polynomial equation has a degree equal to the number of material components. For example, in the case where i = 2, $f_2 = 1 - f_1$ and the following equation has to be solved:

$$-2\varepsilon^2 + [3f_1(\varepsilon_1 - \varepsilon_2) + 2\varepsilon_2 - \varepsilon_1]\varepsilon + \varepsilon_1\varepsilon_2 = 0$$

In the DP2 software the number of components per layer is limited to three to avoid complicated calculi and eventual correlations between the different parameters.

This model is very useful for modelling surface roughness consisting of 50% void and 50% material of the layer below.

EMAMG

The EMAMG model is a combination of the Maxwell-Garnett model and the Bruggeman model.

SSC model

Sen & al presented a self similar model based on the following equation:

$$\frac{\varepsilon - \varepsilon_0}{\varepsilon + 2\varepsilon_0} = f\,\frac{\varepsilon_1 - \varepsilon_0}{\varepsilon_1 + 2\varepsilon_0}$$

The derivation provided by Sen & al results in:

$$\left(\frac{\varepsilon_1 - \varepsilon}{\varepsilon_1 - \varepsilon_0}\right) \cdot \left(\frac{\varepsilon_0}{\varepsilon}\right)^{1/3} = \phi$$

with ϕ the proportion of the host medium

This model is applied to a fractal medium of infinitely wide particle size distribution. For example it is useful for modelling real porous systems, which show a wide size distribution of the void inclusions.

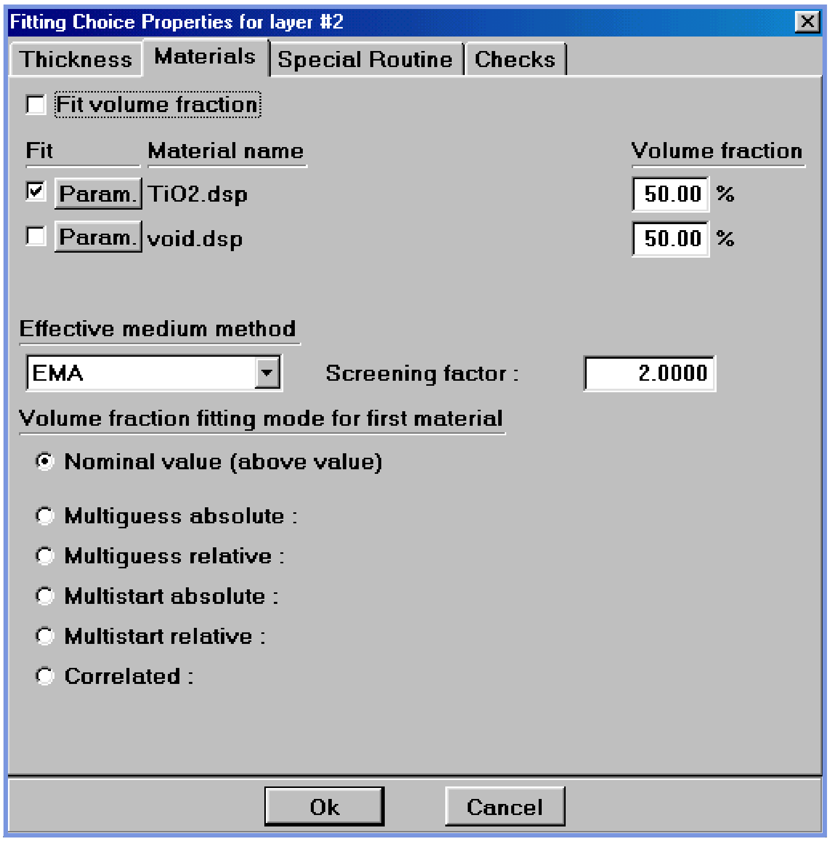
7.1.8.2 Effective medium approximations in DP2

To create an effective medium in DP2 a layer has to be created that contains the host medium and one or two additional materials. The materials can be assigned to the layer simply by “drag and drop” from the material folders in the User or Application library:

- ***User Library > Materials*** if materials are created by the user
- ***Application Library > Materials*** if already existing materials are used

If there are more than one material assigned to a layer there will be the additional fitting parameter “%”, which is the proportion of the different materials. By checking the proportion fit box this parameter will be adjusted during the fitting process.

By default, a mixture of two materials is set to 50% of material A and 50% of material B. To adjust the proportion click on any % symbol displayed on the layer and the following window appears ***Fitting choice Properties for layer # >Materials*** :



☐ Fit volume fraction

Fit		Material name	Volume fraction
☑	Param.	TiO2.dsp	50.00 %
☐	Param.	void.dsp	50.00 %

Effective medium method

EMA

Screening factor : 2.0000

Volume fraction fitting mode for first material

● Nominal value (above value)

○ Multiguess absolute :

○ Multiguess relative :

○ Multistart absolute :

○ Multistart relative :

○ Correlated :

Volume fraction: the proportions can be adjusted; for a three component mixture the same window with three values of proportion will appear.

Material name: the different materials that compose the layer are shown with their respective fit box.

Volume fraction fitting mode: the different fitting functions on the proportion can be chosen.

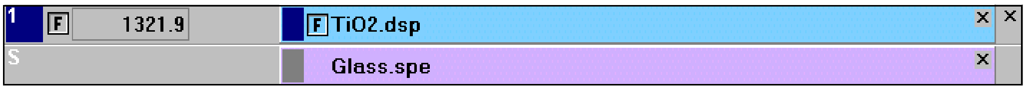
Effective medium method: the method for the effective medium approximation can be selected.

In the following sections some examples for the application of EMAs are shown.

7.1.8.3 Examples for EMA

Roughness layer

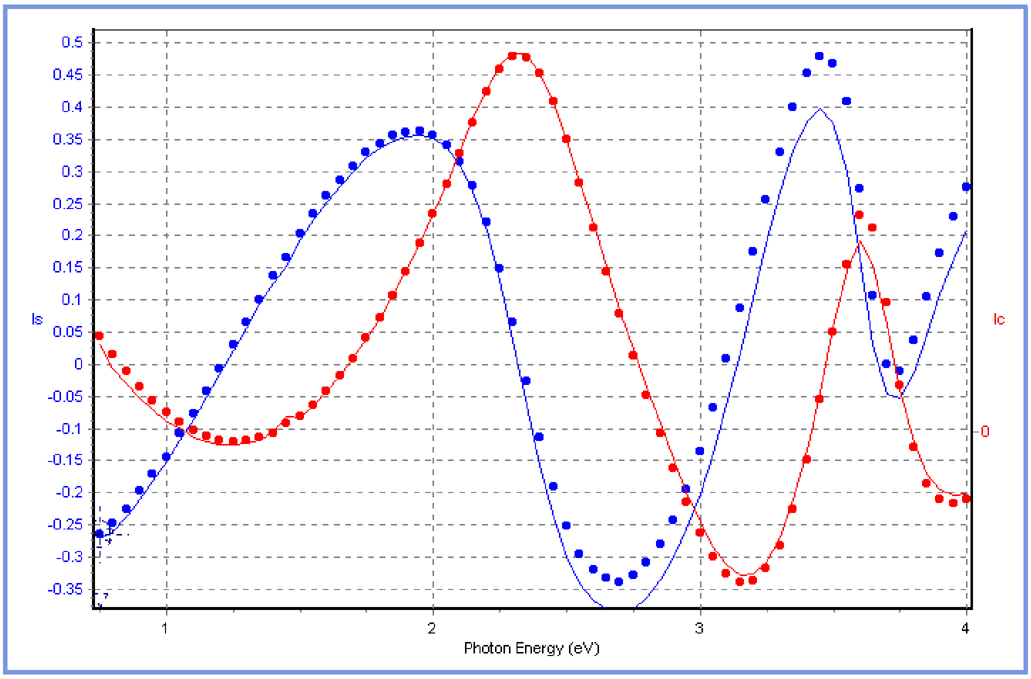
In the case of TiO_2 layer on a glass substrate we start with a simple model using a New Amorphous dispersion for the TiO_2 layer:



1 F 1321.9 F TiO2.dsp ✕ ✕

S Glass.spe ✕

The acquired spectra (dots) and the fit (lines) are shown in the graph below:

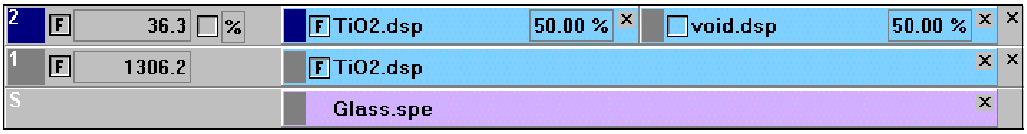


The results of the fit are:

d = 1321.9Å for the thickness and

$\chi^2 = 12.88$ for the goodness of fit

Now we add a roughness layer on top of the TiO_2 layer. This roughness layer is represented by a mixture of 50% TiO_2 and 50% void with a starting thickness of 30Å:

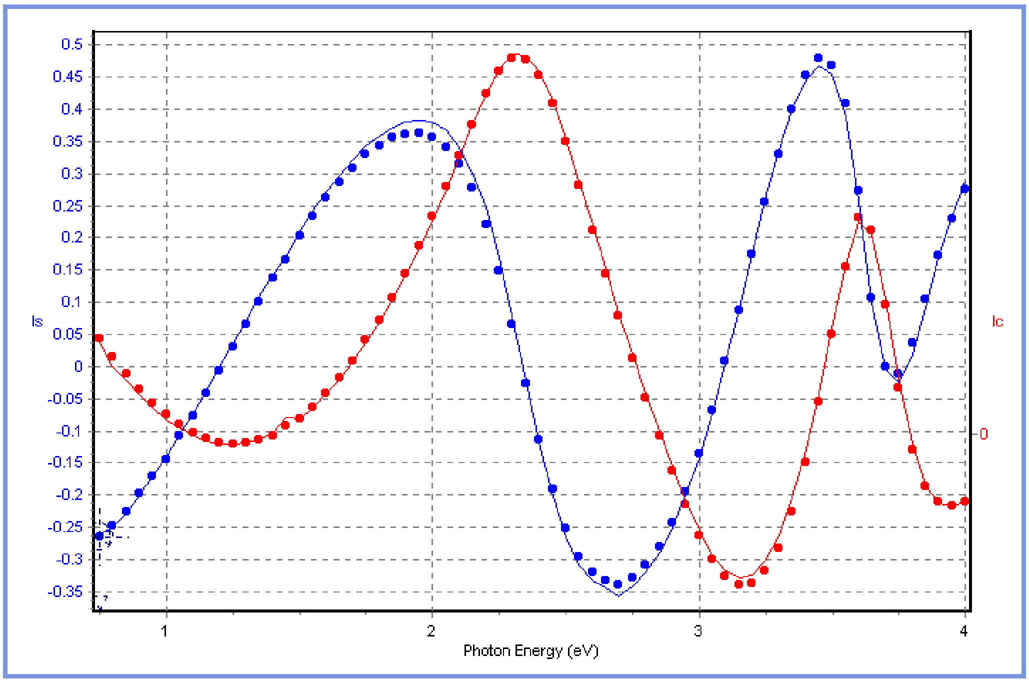


2 F 36.3 ☐ % F TiO2.dsp 50.00 % ✕ ☐ void.dsp 50.00 % ✕ ✕

1 F 1306.2 F TiO2.dsp ✕ ✕

S Glass.spe ✕

The acquired spectra (dots) and the fit (lines) are shown in the graph below:



The results are now:

d = 1306.2Å for the thickness of the TiO_2 layer,

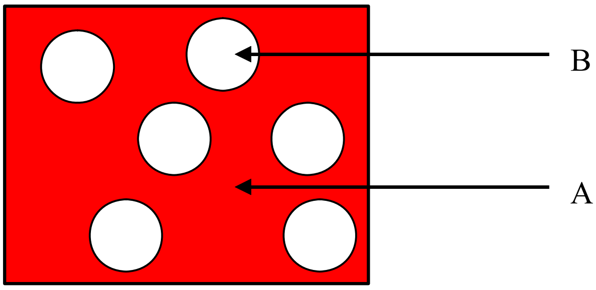
d = 36.3Å for the thickness of the roughness layer and

χ^2=1.23 for the goodness of fit (ten times better than without roughness layer!).

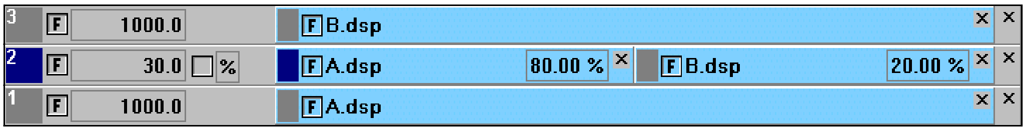
Interface layer

An interface layer may form between two layers for example by diffusion (mixture) or the given surface structure (hooking):

- material composite with portion of material B < portion of material A



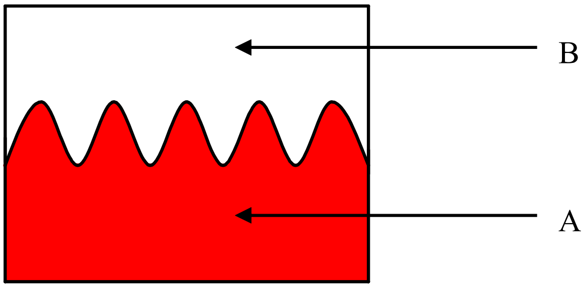
The layer model would in this case look like the following:

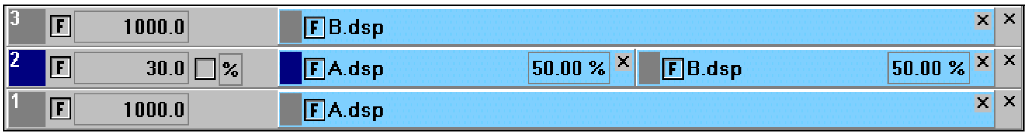


3	F	1000.0		F B.dsp		
2	F	30.0 ☐ %	F A.dsp	80.00 %	F B.dsp	20.00 %
1	F	1000.0		F A.dsp		

Once a good fit is obtained with a fixed proportion, one can try to fit on the proportion to further reduce the value of χ^2.

- hooking layer with portion of material B = portion of material A

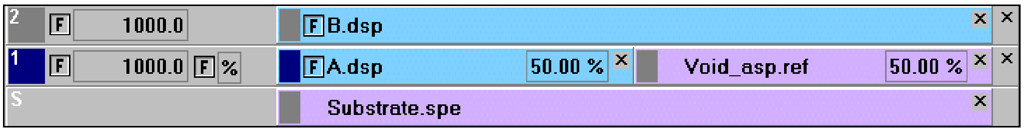



3 F 1000.0 | F B.dsp
2 F 30.0 ☐ % | F A.dsp 50.00 % | F B.dsp 50.00 %
1 F 1000.0 | F A.dsp

Also in this case one can try to fit on the proportion to further reduce the value of χ^2.

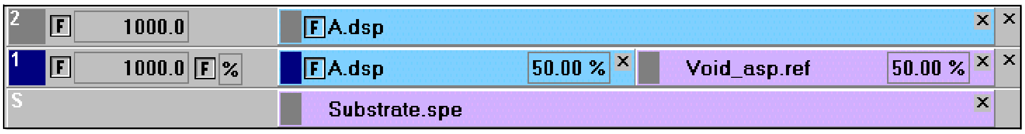
Porous layer

If the porous material A is embedded between the substrate and material B the model would look like:


2 F 1000.0 | F B.dsp
1 F 1000.0 F % | F A.dsp 50.00 % | Void_asp.ref 50.00 %
S | Substrate.spe

The layer with the porous material A is modelled by: material A & Void. It is recommended to set the proportion as fitting parameter.

The situation is similar for a material where the optical properties depend on thickness. A rigorous treatment of this case is done by choosing a "gradient layer" but mostly a 2 layer model is enough. For example if the optical index increase from bottom to top the model looks like:

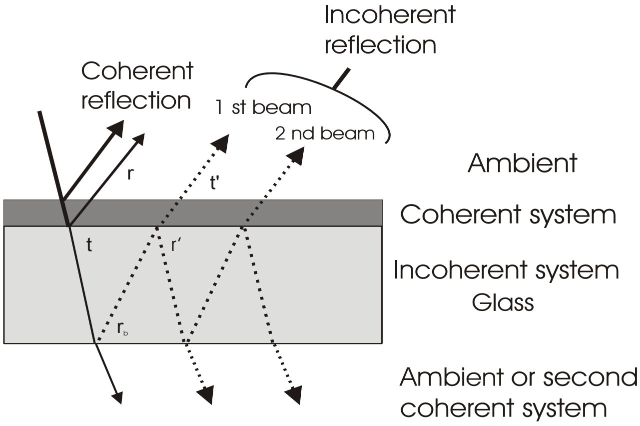

2 F 1000.0 | F A.dsp
1 F 1000.0 F % | F A.dsp 50.00 % | Void_asp.ref 50.00 %
S | Substrate.spe

The material is modelled by two layers: the normal layer and an effective medium layer with material A & Void. A fit on the proportion is also recommended. This model can equally be used for the inverse case by exchanging layer 1 and 2.

7.2 Back side reflections

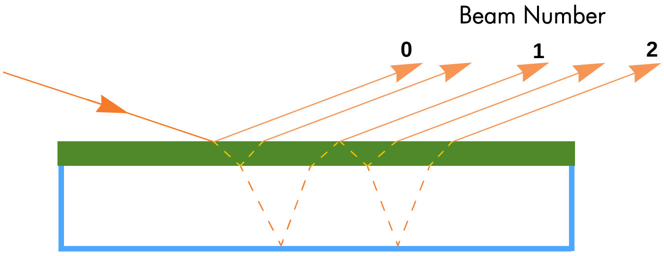
7.2.1 Transparent Substrate

In many cases the analyzed sample including the substrate is transparent for at least a part of the spectrum. If the backside of the sample is in addition polished then back side reflection phenomena can occur.



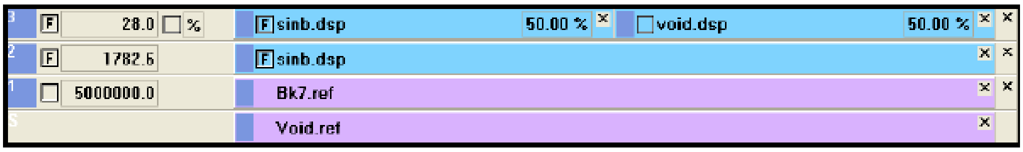
Assuming the optical properties of the transparent material are isotropic we can distinguish two cases:

Case 1: The substrate was measured with its backside reflections



Use the "backside reflection" model which allows the optical treatment of the backside reflections collected during the measurement:

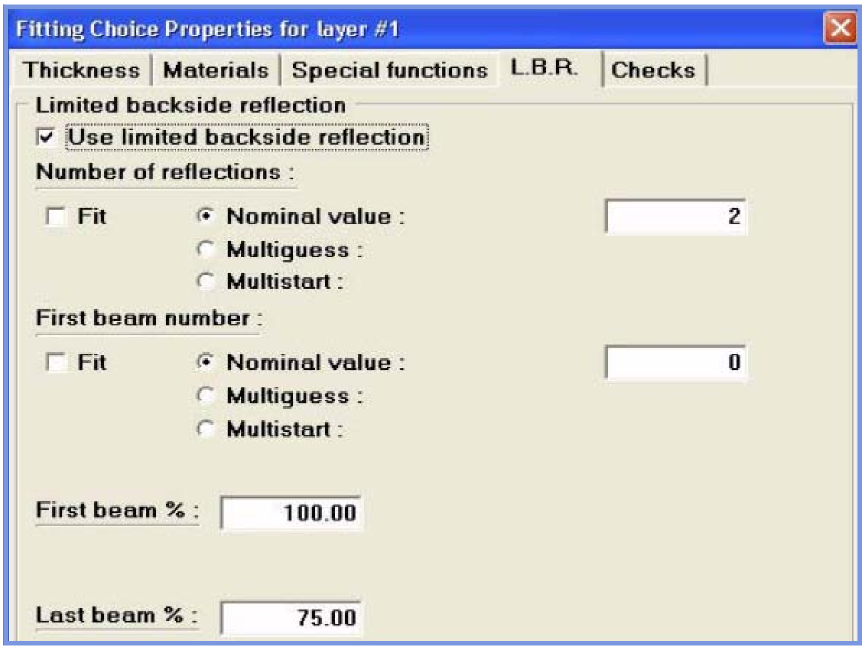
Use void as the substrate and then add a layer that represents the transparent substrate (assign the correct thickness to this layer!). Then add the layer structure as usual. An example is shown below:



3	F	28.0	☐ %	F sinb.dsp	50.00 %	☐ void.dsp	50.00 %
2	F	1782.6		F sinb.dsp			
1	☐	5000000.0		Bk7.ref			
S				Void.ref			

The backside reflection model can be optimized by setting the total number of backside reflected beams and the percentage of the first and the last collected beam with the ***limited backside reflection*** function.

This function can be accessed by clicking on the thickness of layer 1 and then from the fitting choice properties tab by clicking on L.B.R. Check the box "use limited backside reflection".



Limited backside reflection

☑ Use limited backside reflection

Number of reflections :

☐ Fit ● Nominal value : 2

○ Multiguess :

○ Multistart :

First beam number :

☐ Fit ● Nominal value : 0

○ Multiguess :

○ Multistart :

First beam % : 100.00

Last beam % : 75.00

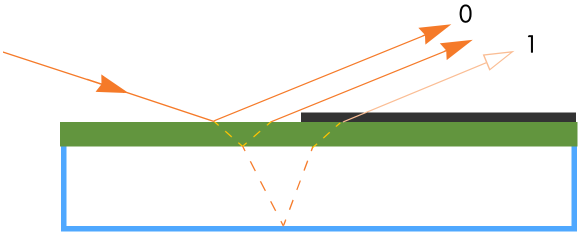
We advise to use the limited backside reflection function for thin transparent substrates of ca. 1mm thickness.

Reasonable values for the settings are:

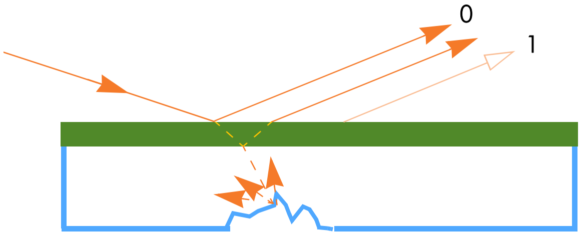
- Number of reflections: nominal values = 2
- First beam number: nominal value = 0
- This means that the beam reflected from the surface and the first beam reflected from the backside are collected. In general do not fit the number of reflections.
- First beam % = 100
- Last beam % = 75 (can be adjusted manually from ca. 70% to 80% to improve the fit)

Case 2: The substrate was measured without backside reflections

This can be achieved by roughening the backside surface or if the backside reflected beam is spatially separated from the first reflection by masking it.

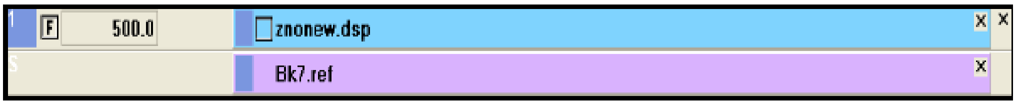


Sample with a mask



Sample where the bottom of the substrate is roughened

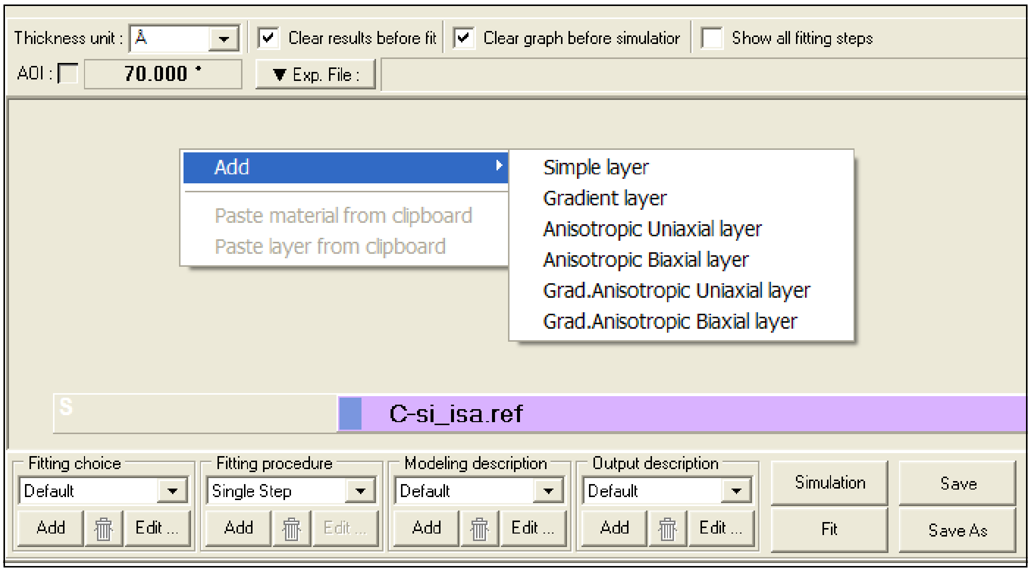
In this case a simple substrate containing the reference or dispersion file of the transparent material can be used as the substrate, for example:



7.3 Advanced layer structures

Until now only isotropic layers with constant optical dispersion through the layer were treated. These layers are called "simple layers". However, layers can be anisotropic or can show a dependency of optical parameters on depth.

A layer can be added to an existing layer model by clicking with the right mouse bottom above the existing layers. The DP2 software allows to choose between the following types of layers:


Thickness unit : Å
☑ Clear results before fit
☑ Clear graph before simulation
☐ Show all fitting steps
AOI : ☐ 70.000 °

- Simple layer: isotropic layer with homogeneous optical dispersion
- Gradient layer: isotropic layer with depth dependency of the optical dispersion
- Anisotropic Uniaxial layer: layer with uniaxial anisotropy and homogeneous optical dispersion
- Anisotropic Biaxial layer: layer with biaxial anisotropy and homogeneous optical dispersion
- Gradient Anisotropic Uniaxial layer: layer with uniaxial anisotropy and depth dependency of the optical dispersion
- Gradient Anisotropic Biaxial layer: layer with biaxial anisotropy and depth dependency of the optical dispersion

7.3.1 Graded Optical Constants

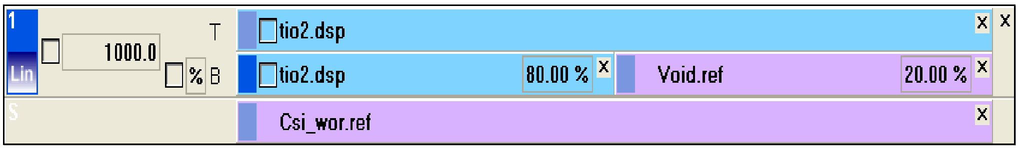
Graded optical constants are used to describe a gradual variation of optical constants (n and k) through a film. The refractive index at the top of the layer can thereby be larger or smaller than the index at the bottom of the layer. The index profile can be linear or exponential.

To add a gradient layer click right in the model area and then ***add Gradient layer***.

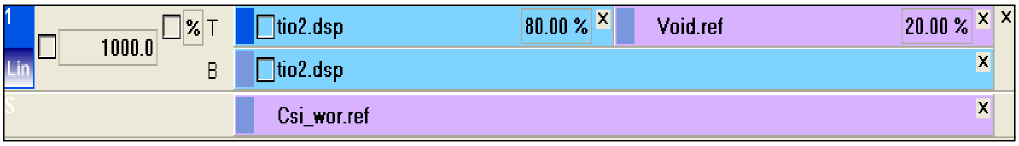
The example below describes a TiO_2 layer as a gradient layer.

First we use “void” inside one of the two layers (top & bottom) to vary the index of refraction. It can be used with reference or dispersion materials.

The index at the top of the layer is higher than the one at the bottom:



The index at the bottom of the layer is larger than the one at the bottom:



Alternatively the same dispersion formula can be used as a starting point but with two different names allowing the fitting process to provide two different dispersions, one at the top and the other one at the bottom of the layer:

A gradient layer can be used if a homogeneous layer model provides a large χ^2 and adding a roughness layer is not enough to provide a satisfactory χ^2.

The example below (TiO_2 layer on a glass substrate) shows how χ^2 can be successively improved by adding a gradient and a roughness layer:

Results with a single layer model:

$\chi^2 = 13.24$; d= 1317 Å

Results with a single layer + roughness layer:

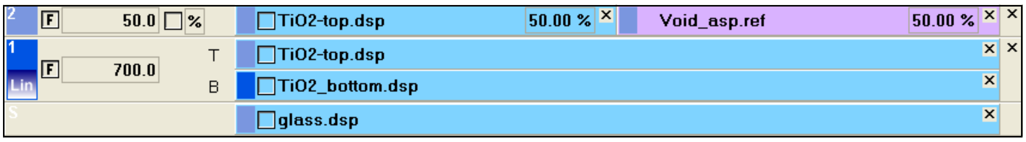
$\chi^2 = 2.31$; thickness (TiO_2) = 1297Å; thickness (roughness) = 34Å

Results with a graded layer:

$\chi^2 = 4.1$; thickness = 1293Å

Results with a graded layer + roughness layer:

$\chi^2 = 0.94$; thickness (graded layer) = 1304Å; thickness (roughness) = 34Å

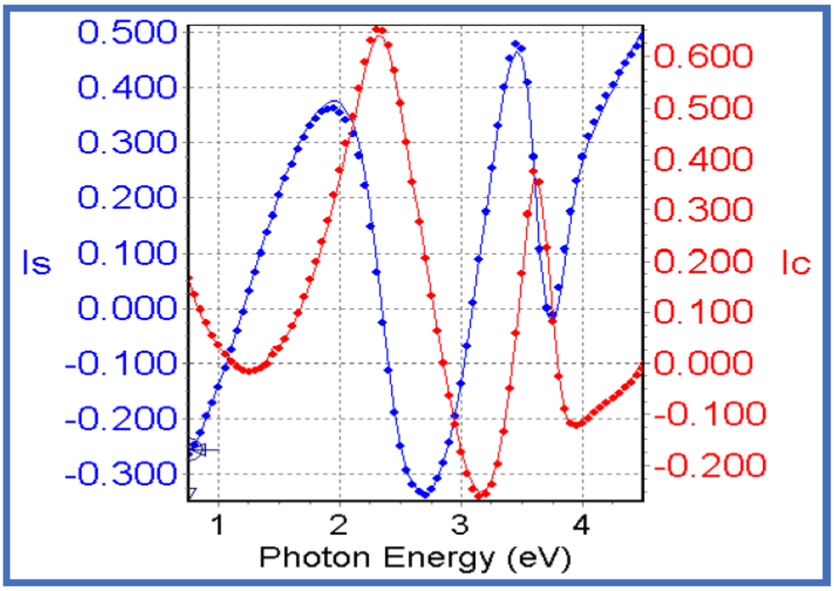

2 F 50.0 ☐ % ☐TiO2-top.dsp 50.00 % ✕ Void_asp.ref 50.00 % ✕ ✕

1 F 700.0 T ☐TiO2-top.dsp ✕ ✕

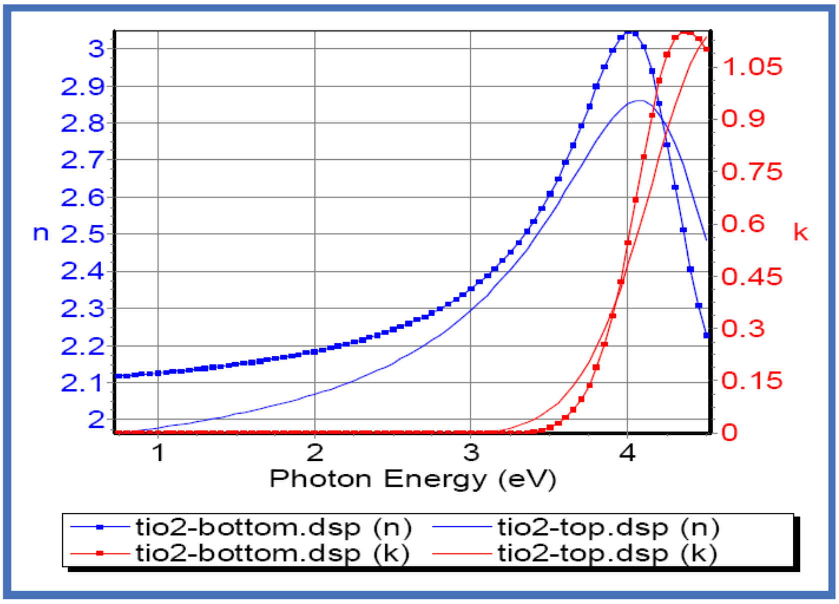
Lin B ☐TiO2_bottom.dsp ✕

S ☐glass.dsp ✕

The final model leads to a nearly perfect fit as can be seen in the graph below:



With the following “graded” optical constants for TiO_2:



7.3.2 Optical Anisotropy

A material that is anisotropic has different optical properties in different directions. At the opposite an isotropic material has the same optical properties in all directions.

In the most general case the dielectric tensor is a rank-2 tensor (3 x 3 matrix) in eigenaxes coordinates. This tensor is diagonal. The three distinct refractive indices are n_x, n_y and n_z.

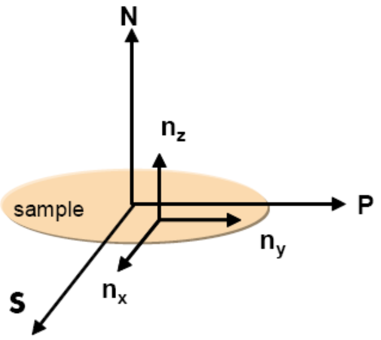
$$\varepsilon = \begin{bmatrix} n_x^{\ 2} & 0 & 0 \\ 0 & n_y^{\ 2} & 0 \\ 0 & 0 & n_z^{\ 2} \end{bmatrix}$$

Anisotropy is an intrinsic material property. Reasons are non-symmetric atomic or molecular structures of long range order throughout the material. Common anisotropic materials are non-cubic crystals such as sapphire, rutile, calcite, lithium niobate and ordered polymers or organic materials like liquid crystal films.

A sign of anisotropy is asymmetric interference fringes in the spectra.

In DP2 we define the laboratory coordinates by (N, S, P): N describing the direction of anisotropy perpendicular to the sample surface, S perpendicular to the plane of incidence and P parallel to the plane of incidence.

The ***Euler angles*** , and are used to describe the relative orientation of the two coordinate systems (n_x, n_y, n_z) and (N, S, P).



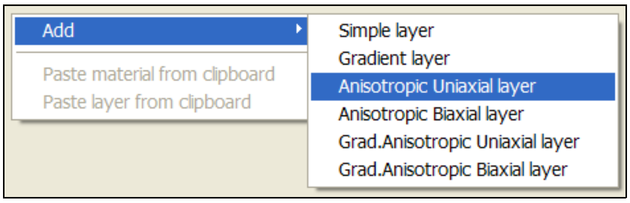
An ***axis of anisotropy*** is defined as the axis along which isotropy is broken (or an axis of symmetry such as normal to crystalline layers). Anisotropic materials can have one or two such optical axes.

An ***uniaxial material*** has 2 different optical constants ($n_x = n_y \; n_z$) which are also called extraordinary (E) or ordinary (O). The birefringence magnitude is then defined by $n = n_e – n_o$.

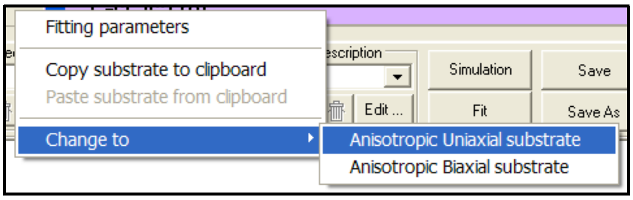
A ***biaxial material*** has 2 axes of anisotropy and thus 3 different optical constants ($n_x \; n_y \; n_z$).

There are three simple cases of uniaxial anisotropy in DP2 when the optical axis (i.e. n_e) is parallel to N, S or P. In all other cases (ne not aligned with one laboratory axis N, S or P or for biaxial anisotropy) the Euler angles have to be set.

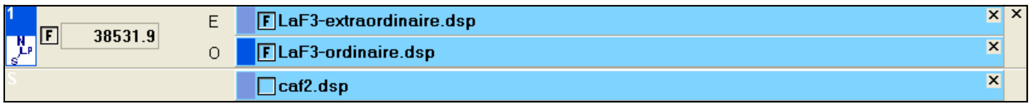
To add an anisotropic layer into your model click right in the model area, and then ***add Anisotropic uniaxial*** or ***biaxial layer***.



Note that the anisotropic material can be used also as a substrate:



A uniaxial anisotropic layer model would look like this then:



1 F 38531.9
E LaF3-extraordinaire.dsp
O LaF3-ordinaire.dsp
caf2.dsp

Modeling an uniaxial anisotropic layer

Modeling an anisotropic layer or substrate mostly relies on the identification of the direction of the axis of anisotropy from “pre-measurements”:

- if two measurements at the same point on the sample rotated by 90° around its normal provide the same results the axis of anisotropy is N.
- if two measurements at the same point on the sample rotated by 90° provide different results the axis of anisotropy perpendicular to N (in-plane anisotropy).

There are 3 methods to identify the direction of the axis of anisotropy in the case of in-plane anisotropy in order to uncouple S and P directions.

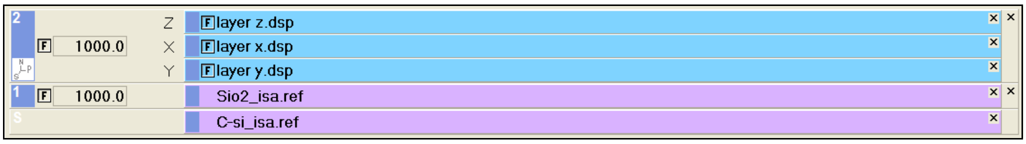
1. using the MM-16 rotate the sample to annul the off-diagonal elements of the Mueller Matrix: mij = 0

$$\begin{bmatrix} M_{11} & M_{12} & m_{13} & m_{14} \\ M_{21} & M_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & M_{33} & M_{34} \\ m_{41} & m_{42} & M_{43} & M_{44} \end{bmatrix}$$

2. using the UVISEL in the configuration M = 0 and A = 0 rotate the sample to annul R and R_2 ($R = R_2 = 0$).
3. if the sample is transparent a birefringent sample will affect the light extinction between crossed polarizers.

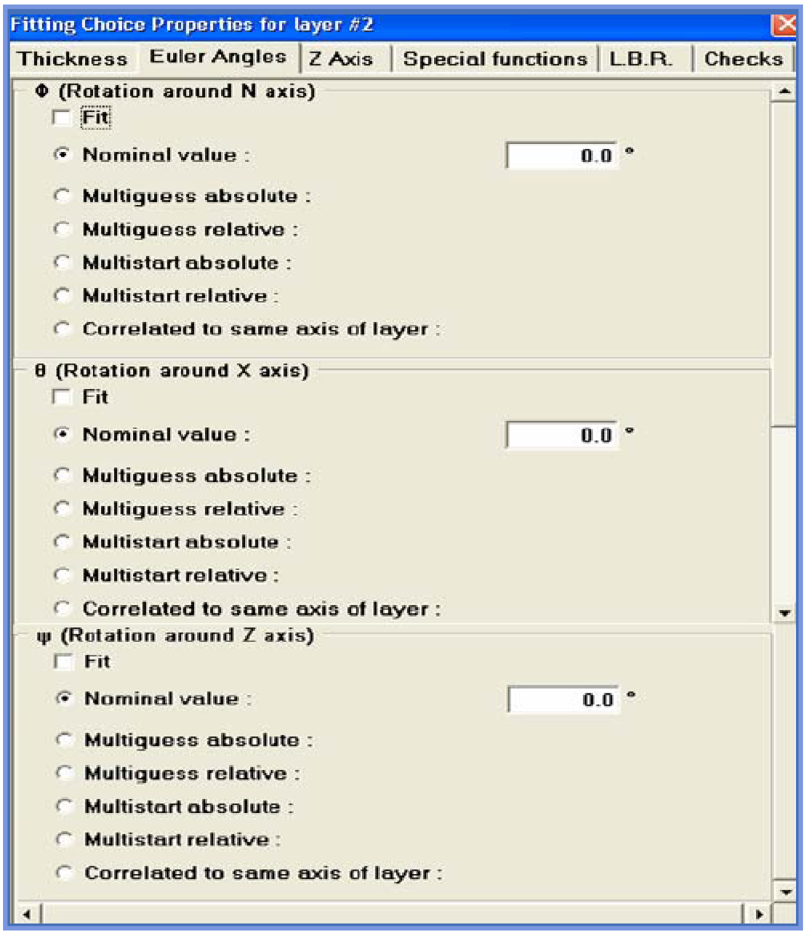
Modeling an biaxial anisotropic layer

In DP2 an biaxial anisotropic layer can be described by 3 orthogonal optical properties:



2 F 1000.0
Z layer z.dsp
X layer x.dsp
Y layer y.dsp
1 F 1000.0 Sio2_isa.ref
C-si_isa.ref

The orientation of (nx, ny, nz) in the laboratory coordinates (N, S, P) is expressed by the Euler angles. Click on the thickness of the biaxial anisotropic layer. In the fitting choice properties tab select Euler angles:



Fitting Choice Properties for layer #2

Φ (Rotation around N axis)

☐ Fit

● Nominal value : 0.0 °

○ Multiguess absolute :

○ Multiguess relative :

○ Multistart absolute :

○ Multistart relative :

○ Correlated to same axis of layer :

θ (Rotation around X axis)

☐ Fit

● Nominal value : 0.0 °

○ Multiguess absolute :

○ Multiguess relative :

○ Multistart absolute :

○ Multistart relative :

○ Correlated to same axis of layer :

ψ (Rotation around Z axis)

☐ Fit

● Nominal value : 0.0 °

○ Multiguess absolute :

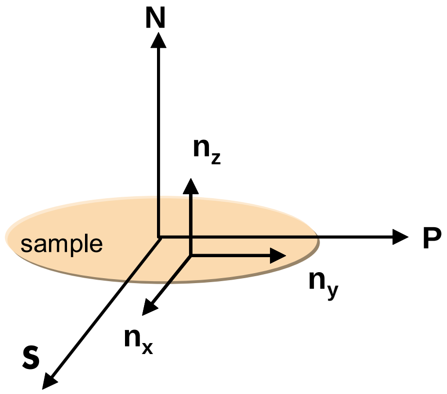
○ Multiguess relative :

○ Multistart absolute :

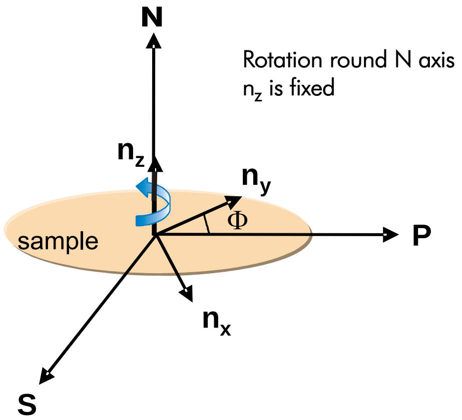
○ Multistart relative :

○ Correlated to same axis of layer :

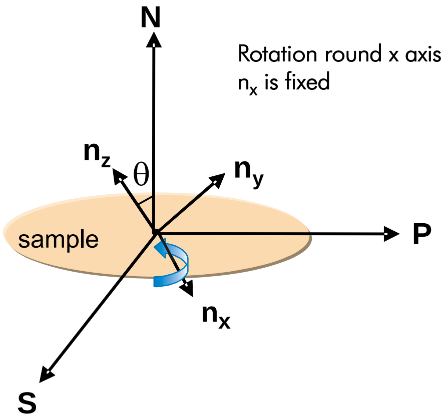
For simplicity try to describe the material with the first two Euler angles Φ and Θ.



Φ rotates the in-plane orientation around the sample normal:



Θ tips the Z-direction away from the sample normal:



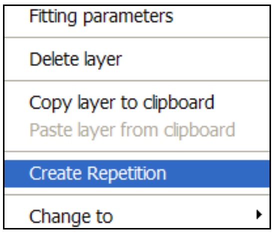
7.3.3 Periodic structure

A periodic structure is a repetition of one to x layers.

For example if there is 20 times the layer stack (SiO_2/TiO_2) on Si it is not necessary to fit the thickness of the 40 individual layers. One can assume that the all SiO_2 and all TiO_2 have the same thickness and thus reduce the number of unknown parameters drastically.

The most important applications are mirrors, anti-reflective coatings (ARC) and multi-quantum wells.

To model a periodic structure click on the blue number of the layer and select ***Create repetition***. A default repetition value of 2 appears in the selected layer. You can change it by clicking twice on it. By using the horizontal lines of the repetition feature you are able to select the layers involved in the periodic structure.

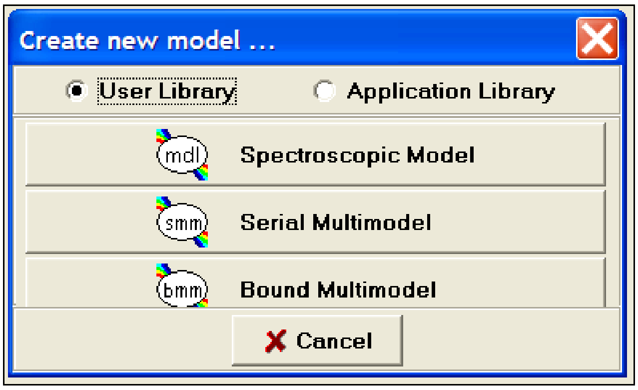


A typical periodic structure would look like:

7.4 Bound Multimodels

A bound multimodel is useful to bind several experimental data types from the same sample or different samples that exhibit at least one common physical property. Combining data provides generally the advantage to reduce strong parameter correlation in the optical modeling process.

To create a bound multimodel click on «Create a new model...» tab. Make sure «User Library» is selected and then click on the «Bound MultiModel» button.



7.4.1 Multiple data for the same sample

It is generally advantageous to collect as much independent experimental data as possible. Reflectance, transmittance and ellipsometric data all provide complementary information.

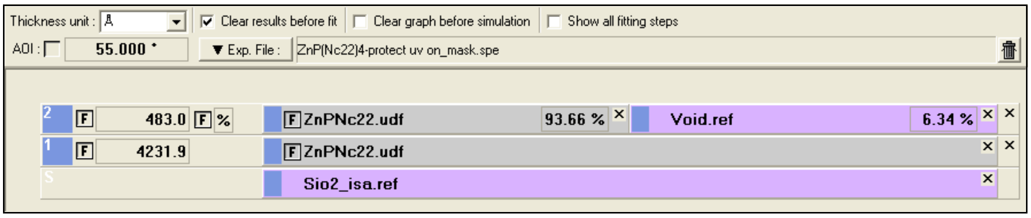
It is important to make sure that data were acquired from the same location on the sample under analysis.

As an example we show the combined analysis of transmittance and ellipsometric data:

Usually first a measurement is performed in the ellipsometric mode. Then both optical heads are moved to 90° to perform the second measurement in the transmittance mode.

Build one model for each measurement configuration and set the fitting parameters for each model.

The model for the ellipsometric mode has to contain the corresponding experimental file and the right angle of incidence. Make also sure that the right spectral range for the fitting and the right fitting parameters are chosen (Is, Ic) or (Ψ, Δ). By default, the experimental file full spectral range and (Is, Ic) data are selected.



Thickness unit : Å ☑ Clear results before fit ☐ Clear graph before simulation ☐ Show all fitting steps

AOI : ☐ 55.000 ° ▼ Exp. File : ZnP(Nc22)4-protect uv on_mask.spe

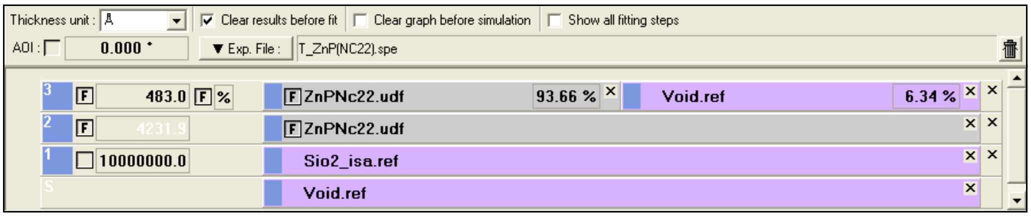
2 F 483.0 F % F ZnPNc22.udf 93.66 % Void.ref 6.34 %

1 F 4231.9 F ZnPNc22.udf

S Sio2_isa.ref

Note that in this example the ellipsometric measurement of the sample has been performed with a mask avoiding the measurements of backside reflections.

The model for the transmittance mode has to contain again the corresponding experimental file and the angle of incidence set to 0° (do not confuse with the 90° of the ellipsometer heads, here this is the angle of the sample in the plane of incidence!). Make also sure that the right spectral range for the fitting is chosen and that the fitting parameter is T.



Thickness unit : Å ☑ Clear results before fit ☐ Clear graph before simulation ☐ Show all fitting steps

AOI : ☐ 0.000 ° ▼ Exp. File : T_ZnP(NC22).spe

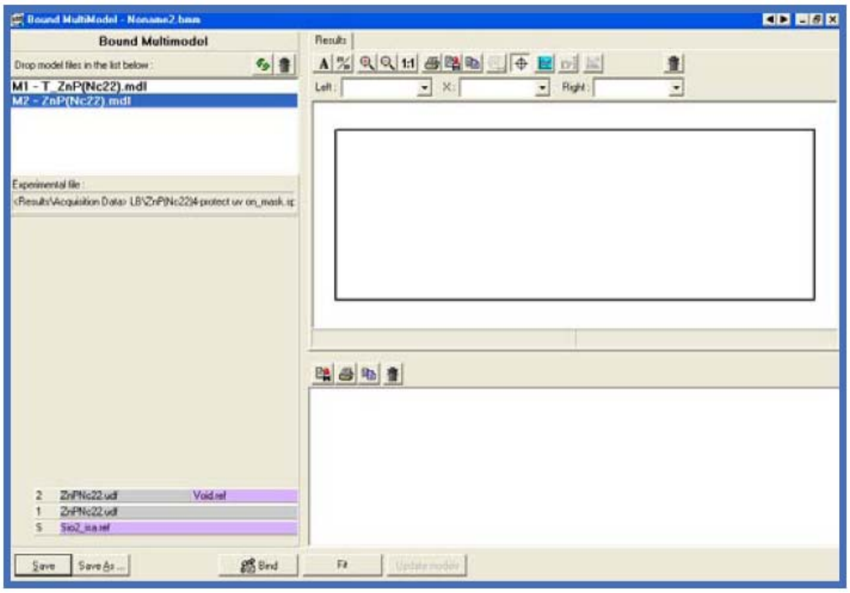
3 F 483.0 F % F ZnPNc22.udf 93.66 % Void.ref 6.34 %

2 F 4231.9 F ZnPNc22.udf

1 ☐ 10000000.0 Sio2_isa.ref

S Void.ref

Then create a bound multimodel and drag and drop the two model files in the blank area in the right of the window. The first model is called M1 and the second M2.



Drop model files in the list below :

M1 - T_ZnP(Nc22).mdl

M2 - ZnP(Nc22).mdl

Experimental file :

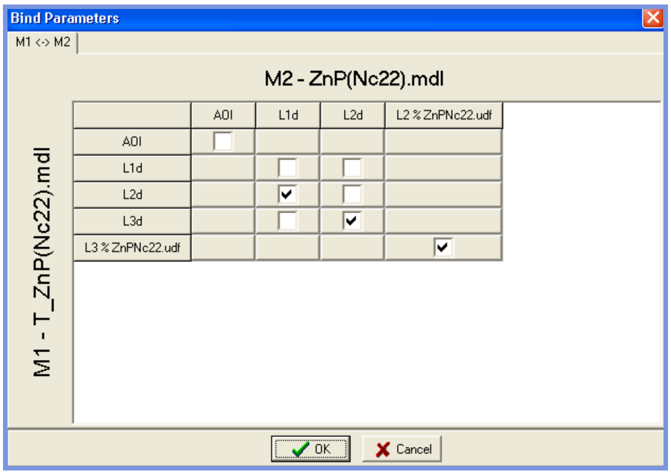
<Results\Acquisition Data> LB\ZnP(Nc22)4-protect uv on_mask.sp

2 ZnPNc22.udf Void.ref

1 ZnPNc22.udf

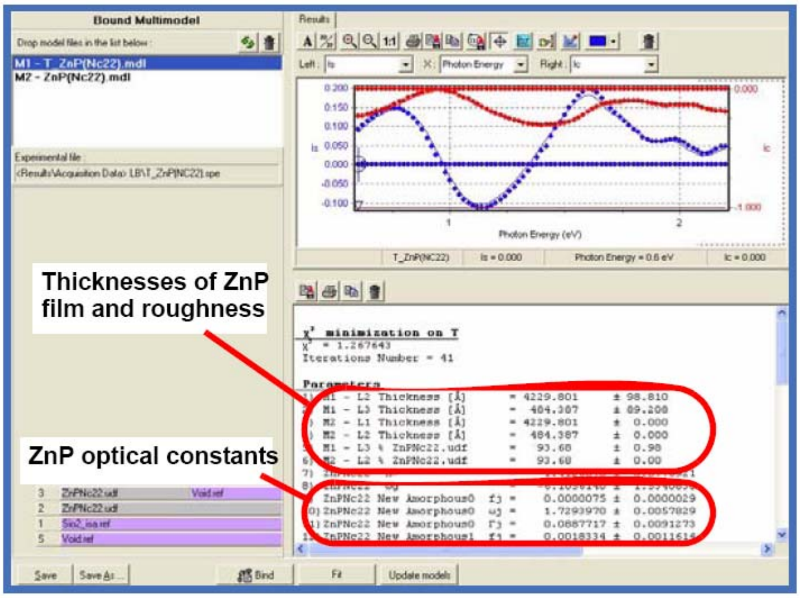
S Sio2_isa.ref

Click on bind. For this example the layer of ZnP and the roughness are coupled for the two models. It means that layer 2 and 3 of model M2 measured in transmission and layer 1 and 2 of model M1 measured in standard ellipsometry are coupled.



	AOI	L1d	L2d	L2 % ZnPNc22.udf
AOI	☐			
L1d		☐	☐	
L2d		☑	☐	
L3d		☐	☑	
L3 % ZnPNc22.udf				☑

Now the fit can be launched. The thickness and optical constants for ZnP as well as for the thickness of the roughness layer are forced to be identical for both models. The results are shown below:



```
χ² minimization on T
χ² = 1.267643
Iterations Number = 41

Parameters
1) M1 - L2 Thickness [Å]      = 4229.801    ± 98.810
   M1 - L3 Thickness [Å]      =  404.387    ± 89.200
)  M2 - L1 Thickness [Å]      = 4229.801    ±  0.000
)  M2 - L2 Thickness [Å]      =  404.387    ±  0.000
   M1 - L3 % ZnPNc22.udf      =   93.68     ±  0.98
6) M2 - L2 % ZnPNc22.udf      =   93.68     ±  0.00
7)
8)
   ZnPNc22 New Amorphous0  fj =   0.0000075 ± 0.0000029
0) ZnPNc22 New Amorphous0  ωj =   1.7293970 ± 0.0057829
1) ZnPNc22 New Amorphous0  Γj =   0.0887717 ± 0.0091273
   ZnPNc22 New Amorphous1  fj =   0.0018334 ± 0.0011614
```

This method is used for layers on transparent substrates (like thin layers on glass) when strong parameter correlation is present.

7.4.2 Multiple Sample Analysis

Any time two or more samples are known to have some physical property in common, the analysis of both (or all) samples may be performed simultaneously, with the common physical property coupled across the models for the different samples.

Simply perform the ellipsometric measurements of your the samples. Then build a model for each sample and set the right fitting parameters. The experimental variables are (Is, Ic) or (Ψ, Δ) for ellipsometric measurements.

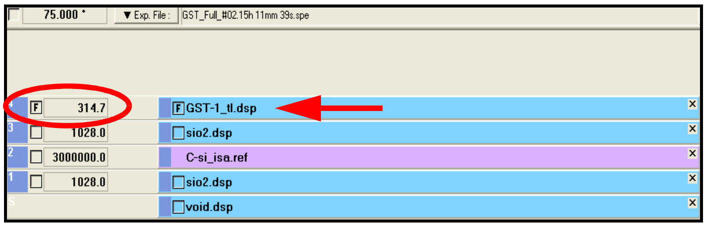
Example Combined analysis of two samples

•Measurement strategy

- Simply perform the ellipsometric measurements of your two samples.

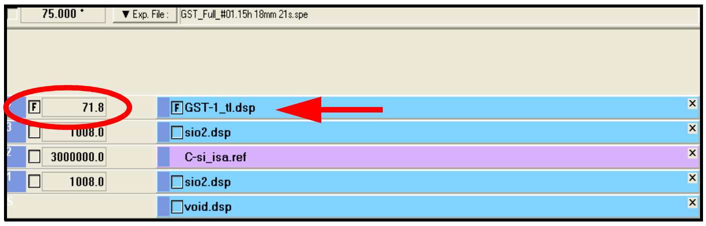
•Modelling features

- Build each model and register them. Make sure to set the fitting parameters for each model. The experimental variables are (Is, Ic) or (ψ, Δ).
- The two samples are composed of a GeSbTe alloys deposited onto a SiO_2 layer, the substrate is silicon. The GeSbTe films are nominally identical but of differing thickness.



75.000 ° ▼ Exp. File : GST_Full_#02.15h 11mm 39s.spe

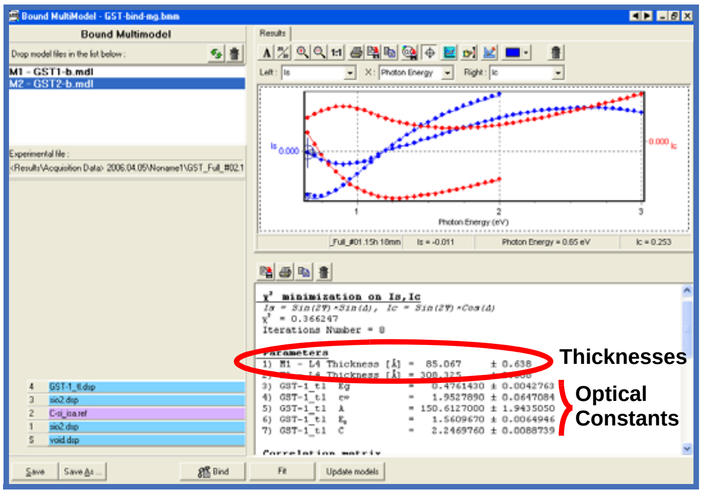
4 ☒ 314.7 ☒ GST-1_tl.dsp
3 ☐ 1028.0 ☐ sio2.dsp
2 ☐ 3000000.0 C-si_isa.ref
1 ☐ 1028.0 ☐ sio2.dsp
5 ☐ void.dsp



75.000 ° ▼ Exp. File : GST_Full_#01.15h 18mm 21s.spe

4 ☒ 71.8 ☒ GST-1_tl.dsp
3 ☐ 1008.0 ☐ sio2.dsp
2 ☐ 3000000.0 C-si_isa.ref
1 ☐ 1008.0 ☐ sio2.dsp
5 ☐ void.dsp

- A dispersion is used to represent the optical properties of the GeSbTe alloy. Note that you have to use the same name for both, «GST-1_tl.dsp» for this example. As the name is the same, the optical constants are bound by default.
- Then create a bound multimodel and drag and drop the two model files in the blank area in the left of the window. The first model is called M1 and the second M2.
- Launch your fit. The GeSbTe film thickness will vary on each sample and a single set of GeSbTe optical constants are forced to be identical for both films.



Bound MultiModel - GST-bind-mg.bmm

Bound Multimodel

Drop model files in the list below :

M1 - GST1-b.mdl
M2 - GST2-b.mdl

Experimental file :
<Results\Acquisition Data> 2006.04.05\Noname1\GST_Full_#02.1

Left : Is X : Photon Energy Right : Ic

Full#01.15h 18mm Is = -0.011 Photon Energy = 0.65 eV Ic = 0.253

```
χ² minimization on Is,Ic
Is = Sin(2Ψ)*Sin(Δ), Ic = Sin(2Ψ)*Cos(Δ)
χ² = 0.366247
Iterations Number = 8

Parameters
1) M1 - L4 Thickness [Å] =  85.067     ± 0.638
2) M2 - L4 Thickness [Å] = 308.325
3) GST-1_tl  Eg          =   0.4761430 ± 0.0042763
4) GST-1_tl  ε∞          =   1.9527890 ± 0.0647084
5) GST-1_tl  A           = 150.6127000 ± 1.9435050
6) GST-1_tl  E₀          =   1.5609670 ± 0.0064946
7) GST-1_tl  C           =   2.2469760 ± 0.0088739

Correlation matrix
```

Fitting results of combined analysis of two samples

When to use it ?

- Anytime, two or more samples have some physical property in common.
- It is very useful to characterize ultra-thin films like thin metal or organic films on opaque or glass substrate. These examples are well known to provide strong correlation between thickness and optical constants.

Results Accuracy

- The parameter correlations should be reduced.
- A unique solution should be obtained.

8 Fitting model to data

8.1 The fitting process

A spectroscopic ellipsometry measurements yields experimental data that have to be fitted to a model to determine the unknown sample parameters.

The goodness of fit (GOF) is determined by the χ^2 value which should be as low as possible. If we measure for example spectra of Ψ and Δ then the χ^2 value is a comparison of n theoretically calculated pairs (Ψ_{th}, Δ_{th}) and n experimental determined pairs (Ψ_{exp}, Δ_{exp}):

$$\chi^2 = \min \sum_{i=1}^{n} \left[\frac{\left(\Psi_{th} - \Psi_{exp}\right)_i^2}{\Gamma_{\Psi,i}} + \frac{\left(\Delta_{th} - \Delta_{exp}\right)_i^2}{\Gamma_{\Delta,i}} \right]$$

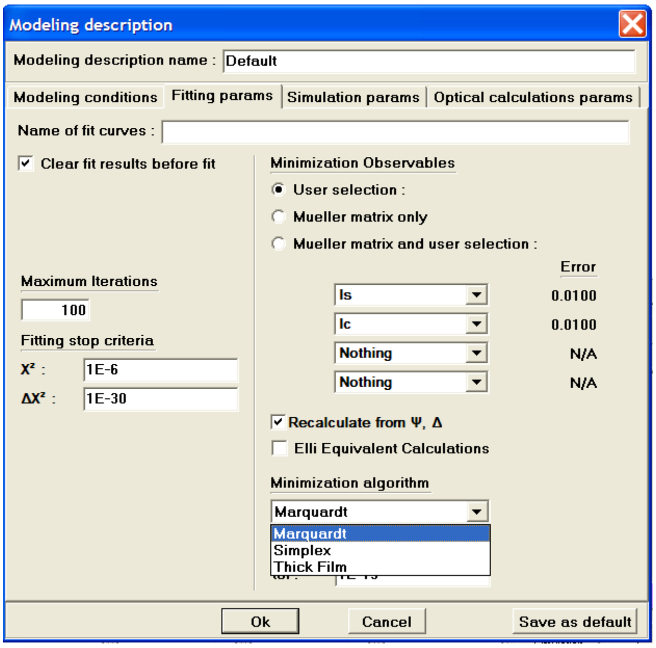
with Γ_i the standard deviation of each data point (generally set to 1).

One difficulty in such a process is to set optimal starting values for the unknown parameters in the model from which the theoretical pairs are calculated. The simulation option of the DP2 software is a fast way to check whether a model is approximately correct or not.

Another common problem of the fitting process is the correlation of different parameters of a model. In this case the solution might not be unique but might dependent on the initial set of starting parameters. The solution might then correspond to a local minimum and not as wanted to the absolute global minimum.

8.2 The iterative algorithms

In the bottom of the model window, the user can go to ***Modeling description > edit > fitting params*** and select the minimization algorithm: **Levenberg-Marquardt**, **Simplex** or **Thick Film**.



Modeling description name : Default

Name of fit curves :

☑ Clear fit results before fit

Maximum Iterations: 100

Fitting stop criteria

X² : 1E-6

ΔX² : 1E-30

Minimization Observables

● User selection :

○ Mueller matrix only

○ Mueller matrix and user selection :

	Error
Is	0.0100
Ic	0.0100
Nothing	N/A
Nothing	N/A

☑ Recalculate from Ψ, Δ

☐ Elli Equivalent Calculations

Minimization algorithm: Marquardt

Marquardt
Simplex
Thick Film

8.2.1 The Levenberg-Marquardt algorithm

This algorithm is a combination of the Inverse Hessian method and the steepest descent method. **It uses the calculus of partial derivatives**. The choice of starting parameters is here critical because the algorithm can converge easily to a local minimum. Therefore the starting values for the fitting parameters have to be set very cautiously to avoid this. However, if the starting fitting parameters are already close to the ideal solution, the Levenberg-Marquardt algorithm converges very rapidly.

Another advantage is that the algorithm provides a correlation matrix and an estimate of the uncertainty for each fitted parameter.

8.2.2 The Simplex algorithm

The Simplex algorithm is a **geometric minimization method** that does not use the calculus of partial derivatives. The big advantage is that it is able to “crawl out” of local minima to find the global minimum. The simplex is a geometrical figure in a n-dimension space that has n+1 vertices: n is the number of unknown parameters (adjustable parameters). The n+1 points in the n-dimension space form a triangle in 2D, and tetrahedron in 3D. This minimization method evaluates a function at each vertex and attempts to move it into a new minimum. Each new minimum of the function becomes a vertex of a new polyhedron. This is repeated until the absolute minimum is encountered. The simplex formed from the points should thereby be non-degenerate, thus it should have a non-zero volume.

With this method **the choice of initial values is not critical**, which is important when little information on the studied material is available. However, this algorithm is slow and fitting many parameters can be really time-consuming. Moreover, this algorithm is not always sensible to the global minimum we search: two consecutive fits do not lead necessarily to the same solution.

To conclude, the simplex algorithm is good for opening a path to the final solution. However, it is not the best method to find the final solution. Another disadvantage is that the user cannot get access to the measurement precision or a parameter correlation matrix with the simplex method.

8.2.3 The thick film algorithm

This algorithm is based on a **fast Fourier Transformation** and can therefore be applied only to spectra of thick layers that show at least some interference pattern.

8.2.4 Conclusion

The Simplex method and the Levenberg-Marquardt algorithm are complementary. However, with a high number of unknowns (more than 6), some difficulties might appear:

- the initial parameters may be critical for the solution
- the uniqueness of the solution

Keep in mind that the Simplex method is used to approach the solution and has to be used when little information about the sample is provided. The Levenberg-Marquardt algorithm is faster but it can be used only when the starting values are already close to the solution.

Most of the time, for simple samples (thin monolayer or thin bilayer) of well defined materials (reference or simple dispersion) the Levenberg-Marquardt algorithm will yield the best solution.

8.3 The fitting functions

Nominal value: this option is used to perform the fit for a given value of the parameter

Multiguess: this method allows the user to perform a fitting process with different initial/end values of the parameter. The retained fitted value is directly related to the best χ^2.

Multistart: this method allows the user to perform a fitting process with different constant values of the parameter. χ^2 is calculated for these fixed values. The retained value is directly related to the best χ^2.

Multiguess and ***Multistart*** have two options: ***absolute*** and ***relative***:

The option ***absolute*** allows the user to choose the guess range and the increment value; the defined interval of values is independent from the nominal value.

The option ***relative*** allows the user to define the guess range as a variation in percentage around the nominal value and not as an interval of values.

Correlated: this option allows to correlate a parameter from the current layer to a corresponding parameter of second layer. This ratio can be constant or variable. The fitting process will be performed only on the current layer and the retained value is the one which will reach the best χ^2.

8.4 How to perform a fit

8.4.1 1st STEP : Define and set the fitting parameters

Once the structure of the model is defined (type of layer, materials, succession of layers…), the user has to define the fitting parameters and set their values. The fitting parameters can be thickness, angle of incidence, proportion of an effective medium layer and parameters of an optical dispersion.

To define the fitting parameters, just check the appropriate fit box. Note: when the user checks the fit box of the material, a window appears: Dispersion Fit Parameters, Alloy Fit Parameters or PPC Fit Parameters in which the optical fitting parameters of the materials can be defined.

To set a value for the thickness, the angle of incidence or the proportion respectively click on thickness value, AOI value and proportion value. The Fitting Choice Properties window appears in which you can set the appropriate value.

The only way to set the value of the different optical fitting parameters, open the material by a double click on the material name (or by a right click on the material name, then select Open material). Then, set a value for each parameter and save your material; the displayed window is the same you obtain when you create a material.

An alternative way of defining the fitting parameters and their values is to right click on the layer and select Fitting parameters; the Fitting Choice Properties window appears. In this window, several tabs are displayed: Thickness, Materials…in which you can define and/or set the different fitting parameters.

8.4.2 2nd STEP : Fitting description

Once the parameters are defined and their values are set, the next step of the fitting process is to determine the way the fit will be performed. The user has to determine:

- the fitting functions
- the iterative algorithm
- the spectral range on which the fit will be performed
- the observables on the graph
- the ellipsometric configuration used to acquire the spectrum

The fitting functions apply for angle of incidence, thickness and proportion. A left click on these values (or right click + ***Fitting parameters*** on these values) allows to access to the ***Fitting Choice Properties*** window where the fitting functions are displayed:

- multiguess absolute
- multiguess relative
- multistart absolute
- multistart relative

The iterative algorithms can be determined in ***Modeling description*** by clicking ***edit***; these option are available in the ***Fitting params*** tab. The user has the choice between:

- the Levenberg-Marquardt algorithm
- the Simplex algorithm
- the Thick Film algorithm

and can also determine the maximum number of iterations. We suggest 100 iterations for simple cases of model, and 1000 iterations for complicated cases where the χ^2 does not cease to decrease.

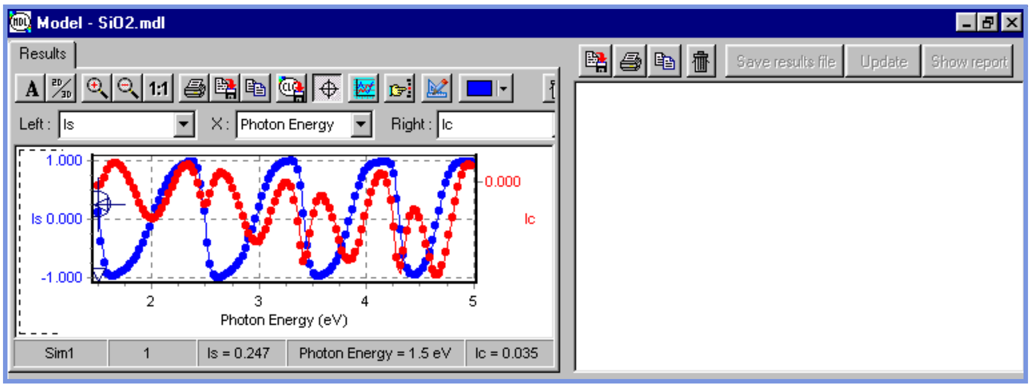
The spectral range, ellipsometric configuration and observables can be determined in ***Modeling description*** by clicking ***edit***; these option are available in the ***Modeling conditions*** tab. By default, the DP2 software uses the experimental spectral range and the experimental ellipsometric configuration. If you wish to modify the spectral range for the fitting process, we recommend you to take the same increment of wavelength or photon energies.

8.4.3 3rd STEP : To launch the fit

9/2/08

Once all the fitting requirements and fitting choices are done, the user can perform a simulation to rapidly see whether the starting parameters are reasonable. The other option is to launch the fit. Here are the simulation and fit buttons:

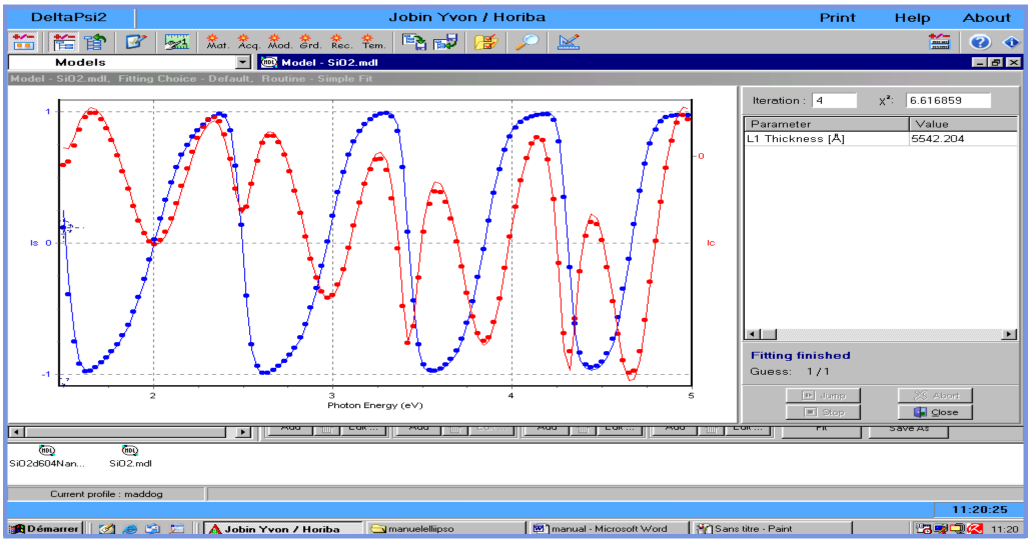
When a simulation is launched, the simulation appear together with the experimental results in the fit/simulation graph window:



Left : Is
X : Photon Energy
Right : Ic

Sim1 | 1 | Is = 0.247 | Photon Energy = 1.5 eV | Ic = 0.035

When a fit is launched, the fit window is displayed:



Model - SiO2.mdl, Fitting Choice - Default, Routine - Simple Fit

Iteration : 4
χ^2: 6.616859

Parameter	Value
L1 Thickness [Å]	5542.204

Fitting finished
Guess: 1 / 1

Current profile : maddog

Which shows the fit result (thickness in this case), the goodness of fit (χ^2) and the number of iteration needed to get the result.

In the fit window one can:

- Abort the fit: it stops immediately any fitting process and only the last χ^2 value displayed on screen is retained
- Jump to the next start value (available for Multiguess or Multistart fitting): this is used to pass to the next guess when the current guess seems to be not reasonable
- Stop the fit: this stops the fitting process, but the best χ^2 obtained so far is recalculated and retained
- Close: this is available when the fitting process is terminated and allows to return to the main window of DP2

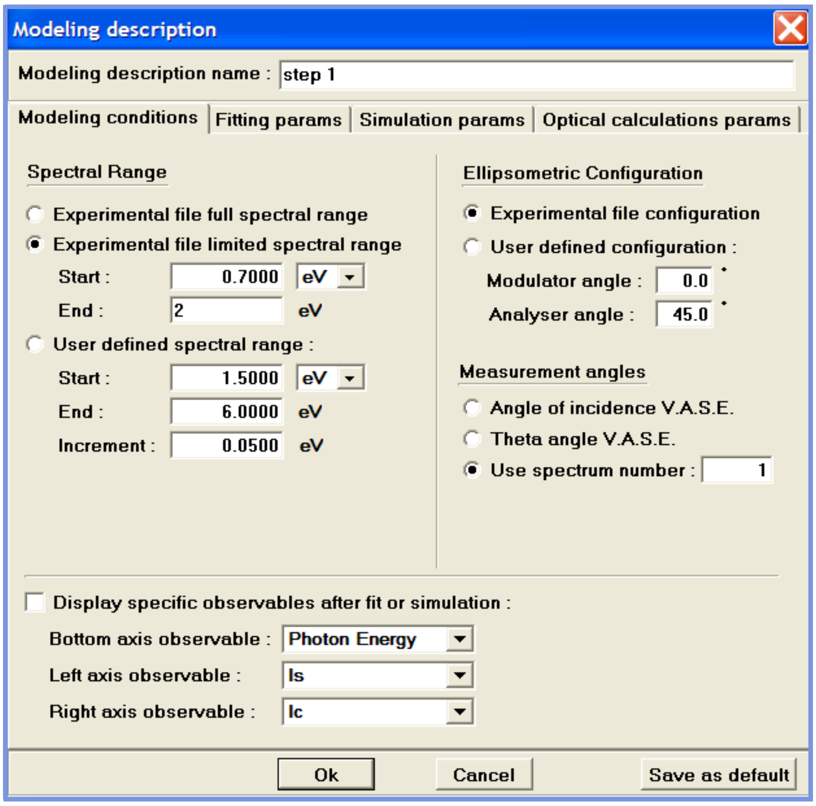
8.5 Fitting procedures

Sometimes it is necessary to perform a fit in separated steps.

For example polymers can have a very complicated optical dispersion in the UV but are mostly transparent in the visible and the IR. It can be advantageous to determine in a first fitting step the thickness in the visible-IR part of the spectrum and then determine in a second step the dispersion in the UV with the fixed thickness from the first fitting step:

First we define the model and fitting conditions for step 1:

In the ***model description*** we set the fitting range from 0.7 to 2eV and name it step 1.



Modeling description name : step 1

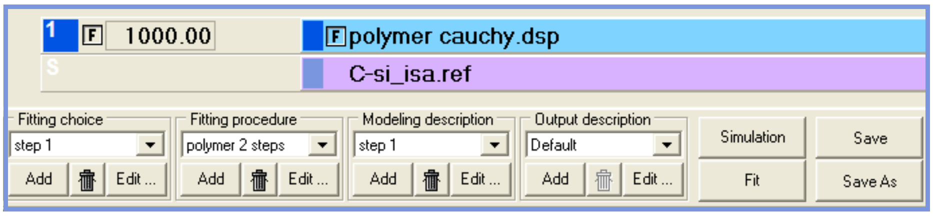
Spectral Range
○ Experimental file full spectral range
● Experimental file limited spectral range
Start : 0.7000 eV
End : 2 eV
○ User defined spectral range :
Start : 1.5000 eV
End : 6.0000 eV
Increment : 0.0500 eV

Ellipsometric Configuration
● Experimental file configuration
○ User defined configuration :
Modulator angle : 0.0 °
Analyser angle : 45.0 °

Measurement angles
○ Angle of incidence V.A.S.E.
○ Theta angle V.A.S.E.
● Use spectrum number : 1

☐ Display specific observables after fit or simulation :
Bottom axis observable : Photon Energy
Left axis observable : Is
Right axis observable : Ic

Then we define the fitting parameters thickness and Cauchy coefficients for the polymer in this spectral region:



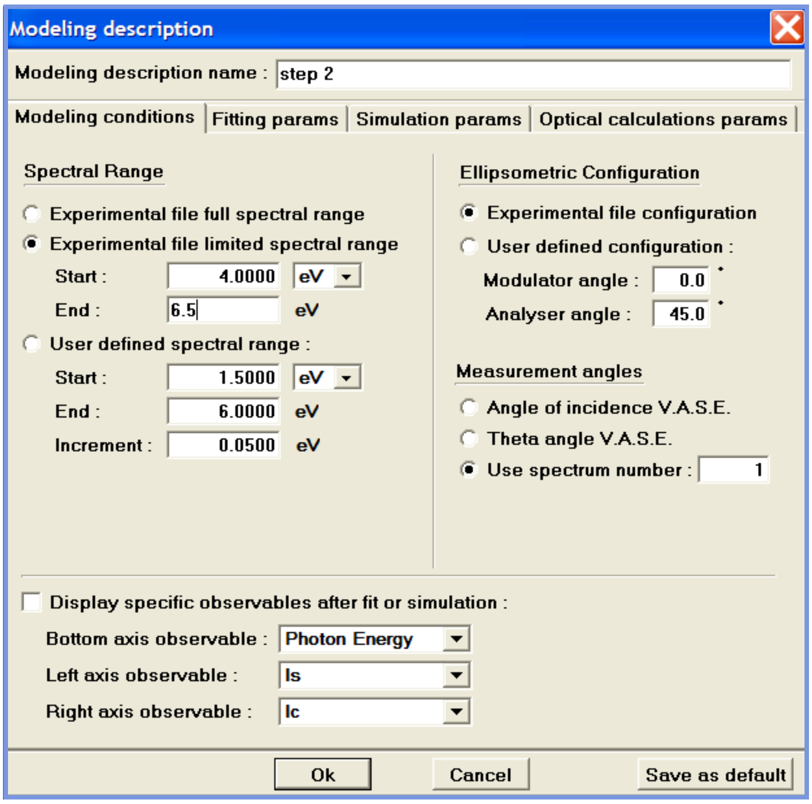
1 F 1000.00 F polymer cauchy.dsp
S C-si_isa.ref

Fitting choice: step 1
Fitting procedure: polymer 2 steps
Modeling description: step 1
Output description: Default

We name it step 1 in the ***Fitting choice*** menu.

Now we define the model and fitting conditions for step 2:

In the ***model description*** we set the fitting range from 4 to 6.5eV and name it step 2.



Modeling description

Modeling description name : step 2

Spectral Range

○ Experimental file full spectral range
● Experimental file limited spectral range
Start : 4.0000 eV
End : 6.5 eV
○ User defined spectral range :
Start : 1.5000 eV
End : 6.0000 eV
Increment : 0.0500 eV

Ellipsometric Configuration

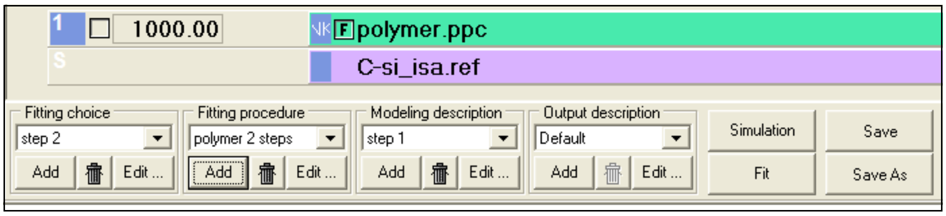
● Experimental file configuration
○ User defined configuration :
Modulator angle : 0.0 °
Analyser angle : 45.0 °

Measurement angles

○ Angle of incidence V.A.S.E.
○ Theta angle V.A.S.E.
● Use spectrum number : 1

☐ Display specific observables after fit or simulation :
Bottom axis observable : Photon Energy
Left axis observable : Is
Right axis observable : Ic

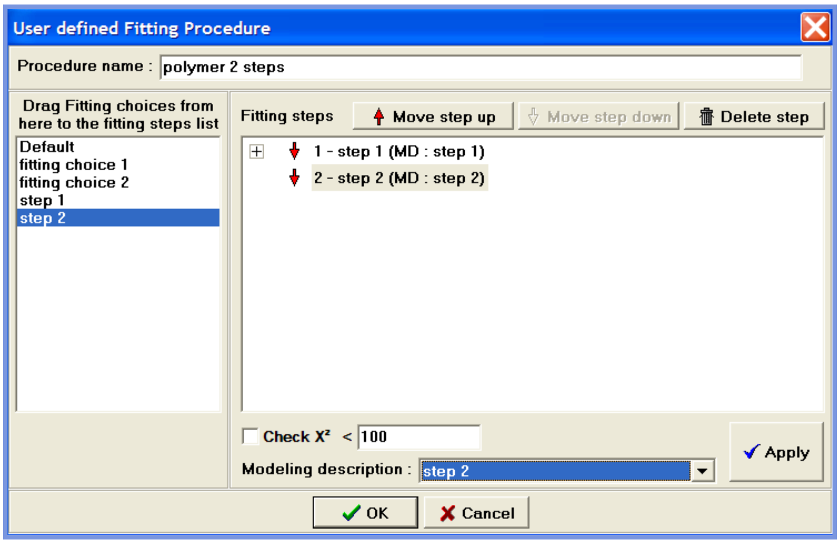
Then we define the fitting parameters polymer in the given spectral region: now it is only point-by-point calculation of the dispersion – the thickness is fixed to the value found in the first step:



1 ☐ 1000.00 polymer.ppc
S C-si_isa.ref

Fitting choice: step 2
Fitting procedure: polymer 2 steps
Modeling description: step 1
Output description: Default

Now we can set-up the fitting procedure that we call for example "polymer 2 steps" by assigning the fitting choice and corresponding model description (MD):



User defined Fitting Procedure

Procedure name : polymer 2 steps

Drag Fitting choices from here to the fitting steps list

Default
fitting choice 1
fitting choice 2
step 1
step 2

Fitting steps

1 - step 1 (MD : step 1)
2 - step 2 (MD : step 2)

☐ Check X² < 100
Modeling description : step 2

Now the complete fitting procedure can be launched.

8.6 Quality of Data - Goodness of fit (GOF)

When a model is used to describe experimental data the software always provides some sort of result. The user then has to decide whether the result is good or not. There are some techniques that help the user to evaluate the quality of the results. The first steps for an evaluation are:

- check the goodness of fit (GOF) value represented by χ^2
- compare visually the measured optical data and the final best-fit calculated data
- check whether results are physically reasonable boundaries % output check criteria

These issues are discussed in detail below.

8.6.1 χ^2 value

The χ^2 value is a direct measure of discrepancies between measured optical data and the final best-fit calculated data. High χ^2 values are usually indicative of a poor fit to the experimental data.

Note that what is a low and what is a high χ^2 value depends on the layer model and the fitting conditions. A high χ^2 value in one case can be a low value in another. Generally speaking, the more simple the model is the lower the χ^2 value should be.

For example, the χ^2 values for a spectroscopic ellipsometer measurement in the range 1.5eV-5eV should give the following values:

Samples	**χ2**
SiO_2 20Å on Si	**$\chi^2 < 0.20$**
SiO_2 2000Å on Si	**$\chi^2 < 2$**
PZT 5500Å on Pt	**$\chi^2 < 10$**
TiO_2 5500Å on Si	**$\chi^2 < 10$**
AlN 25000Å on Si	**$\chi^2 < 15$**

The following points have to be kept in mind when evaluating χ^2 values:

- the thicker the layer the more structure is in the spectra the higher χ^2 will be
- optical properties that enhance structural features in the spectra will lead to higher χ^2 values
- by reducing the fitting range, the χ^2 value generally decreases because the spectrum shape appears simpler on small wavelength intervals. However, reducing the fitting range reduces the precision because information is suppressed, so that generally the confidence limits increase.
- reducing the number of measurement points will lead to a lower χ^2 value because the spectra will have less features

8.6.2 Physically reasonable parameters

The determined parameters should of course make physically sense. Signs of failure are for example:

- negative thickness values
- negative dispersion values (peak energies, band gaps, damping,…)
- transparent materials: an index of refraction that increases with increasing wavelength

Unphysical optical constants are a sign for an inappropriate optical model. The optical constants may become unphysical in order to compensate the deficiencies of the model.

One way to avoid this problem is to fix the unphysical optical constants to reasonable values and to fit only the other parameters. If this does not work a more sophisticated model has to be chosen.

8.6.3 Confidence limits

The Marquardt Levenberg fitting algorithm provides confidence limits for each parameter.

If a confidence limitis of the same order of magnitude as the fitting parameter itself there is very likely a problem with the model. Even if the χ^2 value is good, the optical constants make physically sense the fit can still be bad if the confidence limits are high. The reasons can be:

- the experimental data are not sensitive to the fitted parameter of interest
- the model is incorrect and the final χ^2 value is large and thus bad. In this case, all the fitted parameters are affected by large confidence limits: the larger the χ^2 value the larger the confidence limits.
- parameters are strongly correlated. In this case their confidence limits will be very large.

8.7 Uniqueness of fit

The final thing the user has to do in the fitting process is to determine whether the best-fit result is unique or not.

Non-unique results can occur if:

- there are parameters that only weakly affect the fit: the best thing to do is to fix these parameters to reasonable values and to not fit them.
- there is strong correlation between parameters: reduce the parameter set in order to eliminate the correlations.

8.7.1 Parameter correlation

Parameter correlation occurs when:

- there are too many unknown parameters in the model
- the effects of one parameter compensates exactly the effects of another parameter

Correlations between parameters can be identified by the following symptoms:

- the Marquardt Levenberg fitting algorithm provides a correlation matrix. If the magnitude of any of the non-diagonal elements of the correlation matrix is close to unity then strong parameter correlation exists.
- the fitting process needs a lot of iterations and the χ^2 value is only slightly reduced during each iterations: the iterative algorithms are not capable of determining which of the correlated parameters needs to be adjusted.
- the fitting parameters take drastically different values at each iteration and the χ^2 value varies only slightly. In this case at least two parameters are correlated and compensate each other and/or the χ^2 value is not sensitive to the given parameter(s).
- static repeatability measurements: if the repeatability value of parameters is bad although χ^2 is reasonable then parameters are correlated
- profile scans across the sample: physically reasonable parameters should vary steadily across the sample. If there are "jumps" then there is most probably parameter correlation

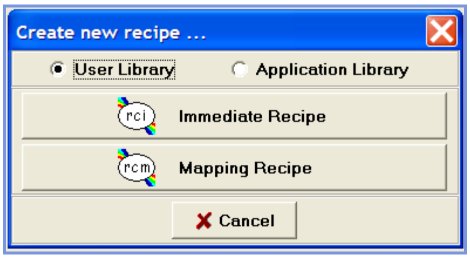
Parameter correlation can be of course also avoided by combining different optical data types like data from spectroscopic ellipsometry (at different angles of incidence), reflectometry and transmission measurements. The DP2 software can handle all these data types and all data can be fitted simultaneously.

9 Routine Measurements

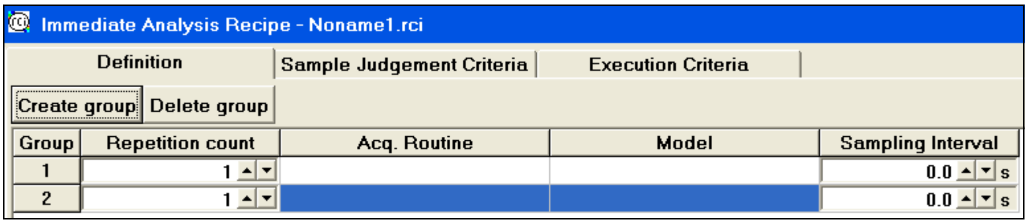
There are methods that allow the user to automate the measurements and the out-putting of the results. These methods will be described only shortly here because there is a detailed description in the DP2 user manual.

9.1 Recipes

With the help of recipes you can automate your measurements. Click on the recipe button Rec. and you see that there are two types of recipes:

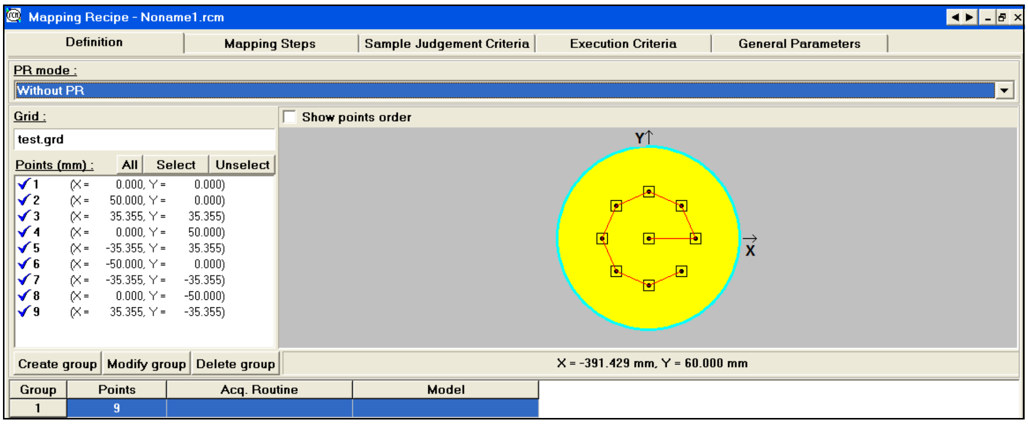


The main application of the ***immediate recipe*** is to measure repeatedly at the same spot with the same acquisition routine & model. However by defining groups you can also apply different acquisition routines & models repeatedly at the same spot:



Group	Repetition count	Acq. Routine	Model	Sampling Interval
1	1			0.0 s
2	1			0.0 s

The **mapping recipe** allows the application of acquisition routines & models to a series of different points on the sample (grid):



PR mode : Without PR

Grid : test.grd

Points (mm) :
✓1 (X = 0.000, Y = 0.000)
✓2 (X = 50.000, Y = 0.000)
✓3 (X = 35.355, Y = 35.355)
✓4 (X = 0.000, Y = 50.000)
✓5 (X = -35.355, Y = 35.355)
✓6 (X = -50.000, Y = 0.000)
✓7 (X = -35.355, Y = -35.355)
✓8 (X = 0.000, Y = -50.000)
✓9 (X = 35.355, Y = -35.355)

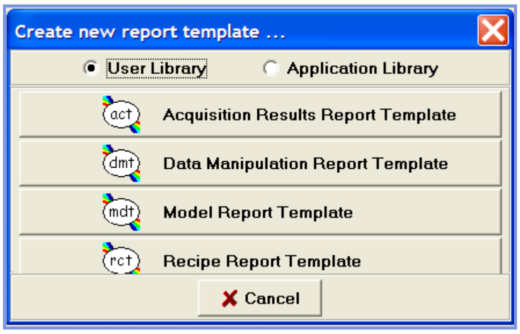
X = -391.429 mm, Y = 60.000 mm

Group	Points	Acq. Routine	Model
1	9		

The grid is set-up in the grid-menu that can be opened with the Grd. button.

9.2 Reports

With DP2 reports can be created automatically after the measurements. You can set-up a template for a report by clicking the Tem. button.

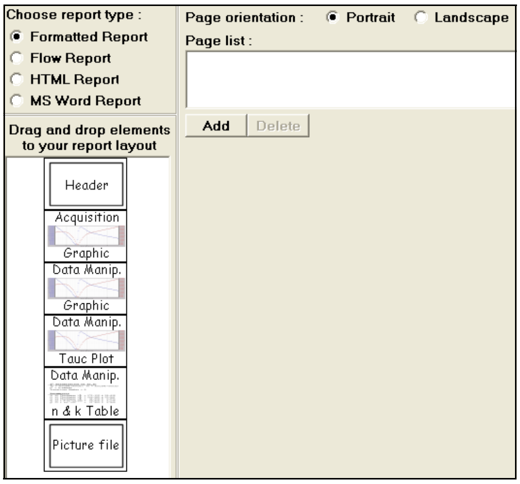


Create new report template ...

● User Library ○ Application Library

In the report templates you can activate features like headers, pictures of the layer model, acquisition data, results, etc.

As an example the options for the Acquisition Results Report Template are shown below:



Choose report type :
● Formatted Report
○ Flow Report
○ HTML Report
○ MS Word Report

Page orientation : ● Portrait ○ Landscape

Page list :

Drag and drop elements to your report layout

10 QuickStart

10.1 SiO_2/Si: HJY certified sample

In this chapter the basic steps are shown to perform the complete analysis of a very simple sample, the system test sample: native SiO_2/Si substrate.

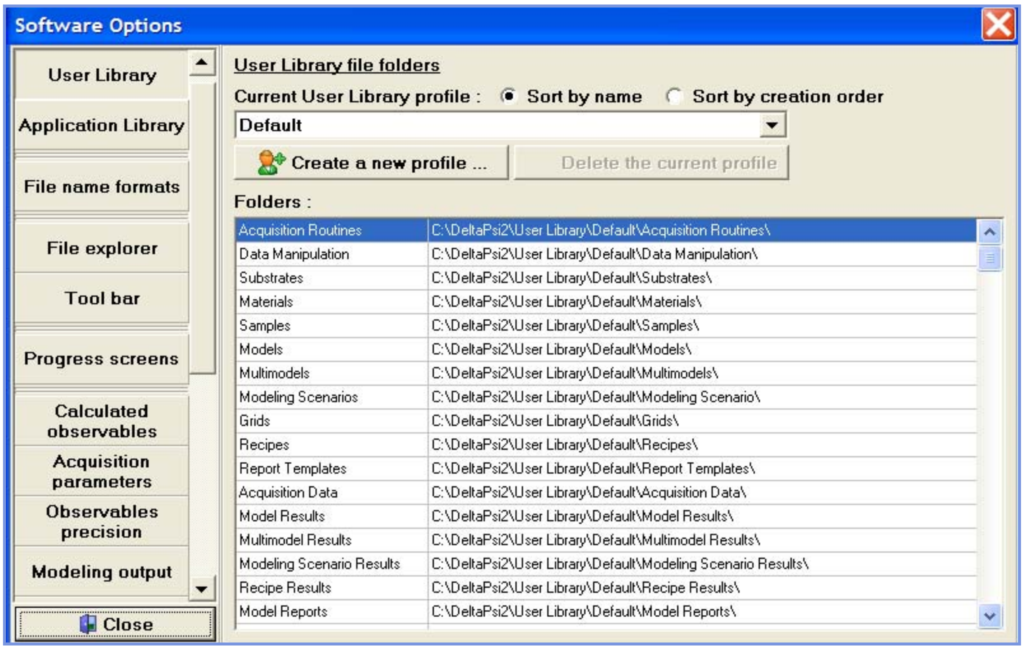
The idea is to begin with the analysis of a simple sample to get the automatisms that will be needed for analysis of more difficult samples. As already discussed, the main steps of any analysis are:

- system start
- sample positioning
- data acquisition
- modelling
- data fitting

System start

- Switch on the controller unit and the computer where the ***DeltaPsi2*** software is installed.
- Turn on the ***light source*** (usually a Xe arc lamp) and wait 15min to let it stabilize.
- Open the ***DeltaPsi2*** software and click on the "software options" tab:

The following window will appear:



Current User Library profile : ● Sort by name ○ Sort by creation order

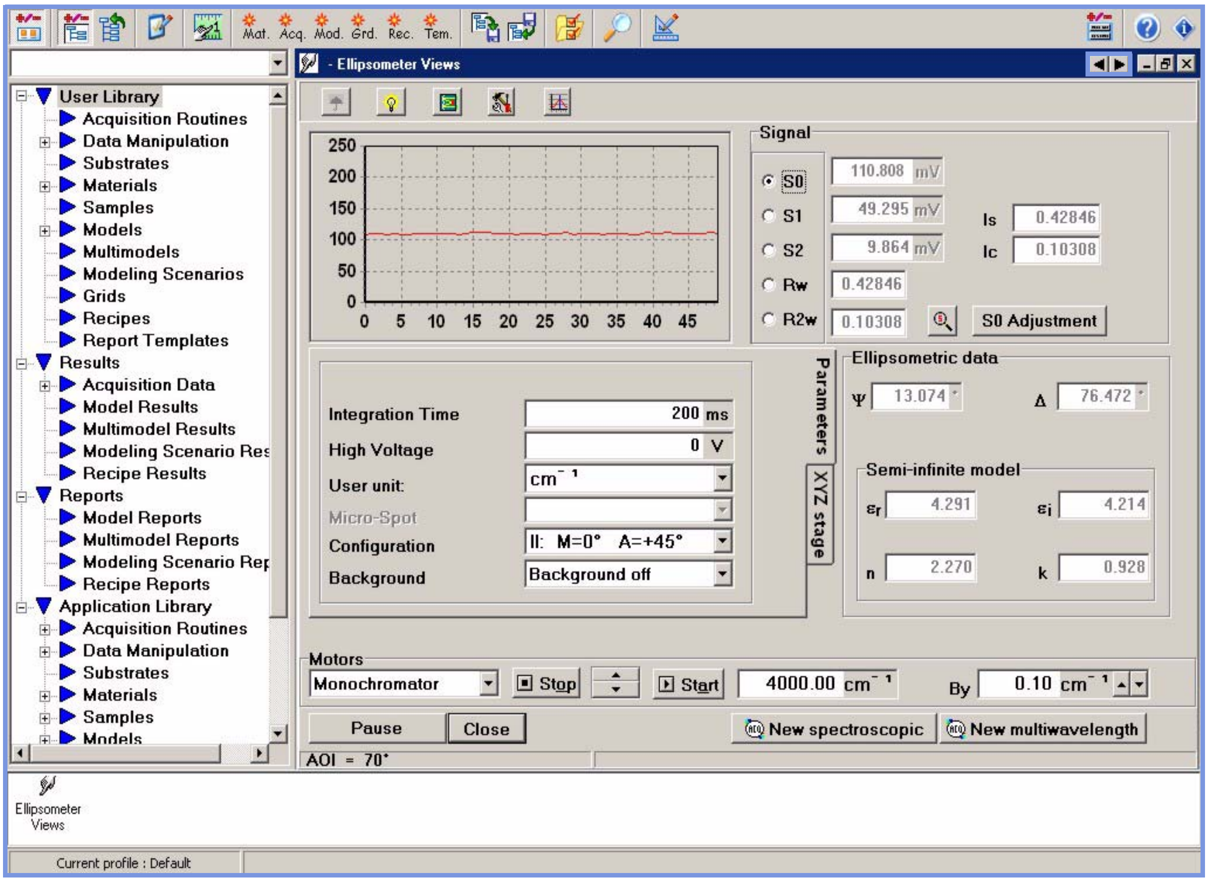
Default

Folders :

Acquisition Routines	C:\DeltaPsi2\User Library\Default\Acquisition Routines\
Data Manipulation	C:\DeltaPsi2\User Library\Default\Data Manipulation\
Substrates	C:\DeltaPsi2\User Library\Default\Substrates\
Materials	C:\DeltaPsi2\User Library\Default\Materials\
Samples	C:\DeltaPsi2\User Library\Default\Samples\
Models	C:\DeltaPsi2\User Library\Default\Models\
Multimodels	C:\DeltaPsi2\User Library\Default\Multimodels\
Modeling Scenarios	C:\DeltaPsi2\User Library\Default\Modeling Scenario\
Grids	C:\DeltaPsi2\User Library\Default\Grids\
Recipes	C:\DeltaPsi2\User Library\Default\Recipes\
Report Templates	C:\DeltaPsi2\User Library\Default\Report Templates\
Acquisition Data	C:\DeltaPsi2\User Library\Default\Acquisition Data\
Model Results	C:\DeltaPsi2\User Library\Default\Model Results\
Multimodel Results	C:\DeltaPsi2\User Library\Default\Multimodel Results\
Modeling Scenario Results	C:\DeltaPsi2\User Library\Default\Modeling Scenario Results\
Recipe Results	C:\DeltaPsi2\User Library\Default\Recipe Results\
Model Reports	C:\DeltaPsi2\User Library\Default\Model Reports\

- Choose "user library" and choose an existing user library profile in the drop-down menu or "Create a new profile…".
- Close the "software options" window and click the "manual measurement" tab to open the "Views" screen:

Views screen:



● S0 110.808 mV
○ S1 49.295 mV
○ S2 9.864 mV
○ Rw 0.42846
○ R2w 0.10308

Is 0.42846
Ic 0.10308

Integration Time 200 ms
High Voltage 0 V
User unit: cm^{-1}
Micro-Spot
Configuration II: M=0° A=+45°
Background Background off

Ψ 13.074 °
Δ 76.472 °

ε_r 4.291
ε_i 4.214
n 2.270
k 0.928

Monochromator 4000.00 cm^{-1} By 0.10 cm^{-1}

AOI = 70°

Current profile : Default

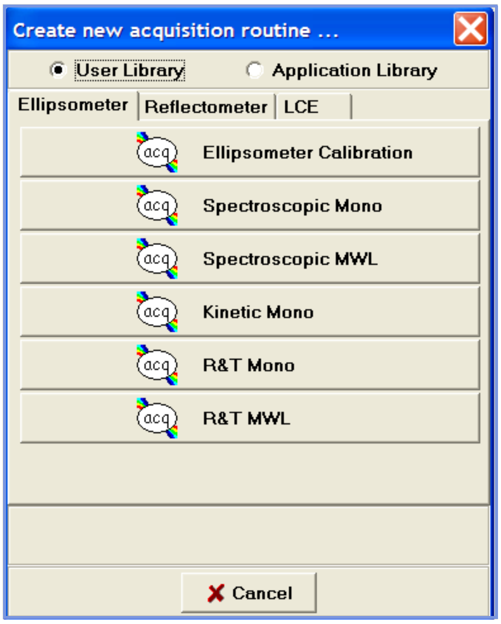
Sample positioning

- Place your ***sample*** on the ***stage*** and switch on the ***autocollimator illumination***.
- Look through the eyepiece of the autocollimator and align the crosshairs so that the centers overlap by adjusting the two knobs underneath the stage.
- In the views screen set the monochromator to 2.75eV (or 450nm if you prefer to work with wavelength).
- Adjust now the height of the stage by turning the corresponding knob underneath the stage. Try to find the position where S0 is at its maximum
- In the views screen click "S0 adjustment" or manually set the high voltage so that S0 is between 60 and 80mV.

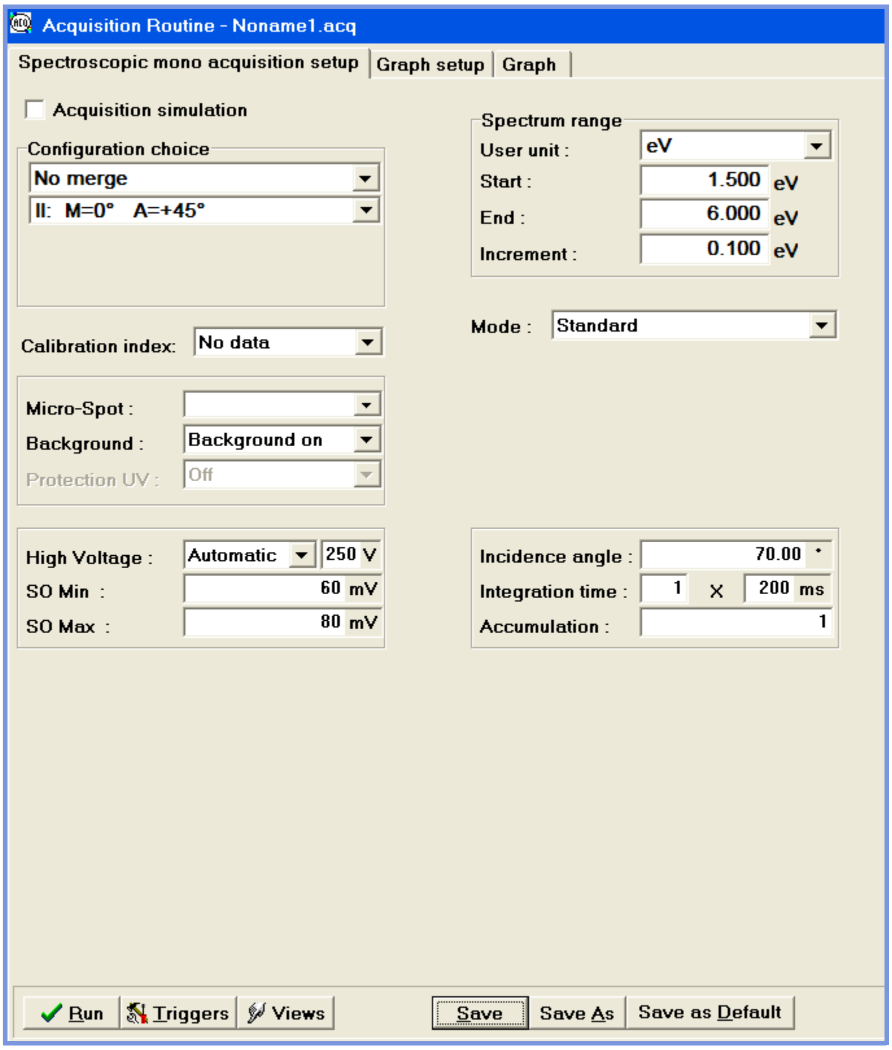
Data acquisition

For data acquisition click on the ***Acq.*** button:

The following window will appear:



Choose ***Spectroscopic Mono***:



☐ Acquisition simulation

Configuration choice: No merge; II: M=0° A=+45°

Calibration index: No data

Micro-Spot :

Background : Background on

Protection UV : Off

High Voltage : Automatic 250 V

SO Min : 60 mV

SO Max : 80 mV

Spectrum range

User unit : eV

Start : 1.500 eV

End : 6.000 eV

Increment : 0.100 eV

Mode : Standard

Incidence angle : 70.00 °

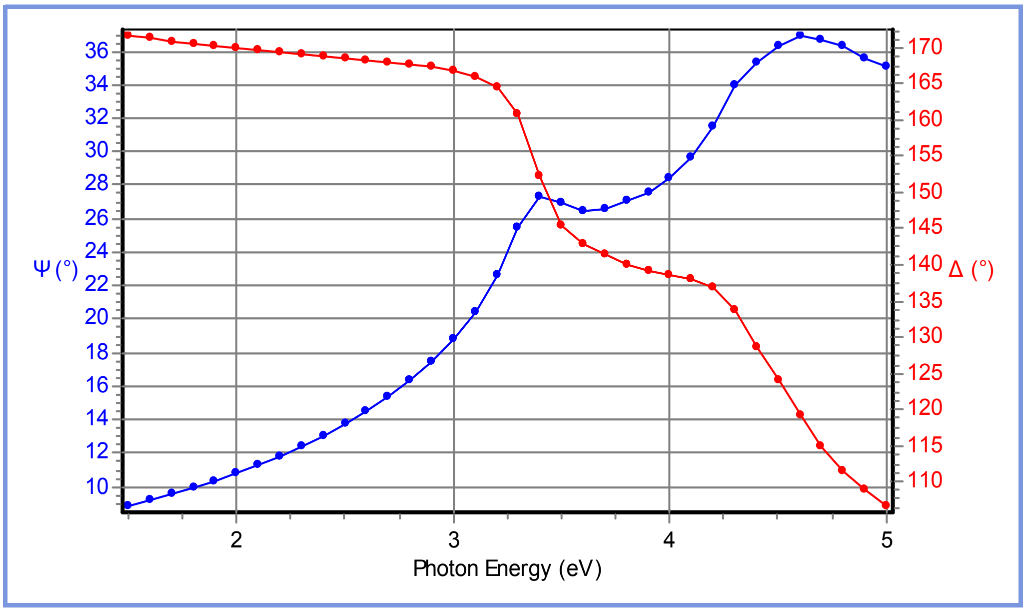
Integration time : 1 x 200 ms

Accumulation : 1

For a thin SiO_2/Si sample the acquisition parameters should be the following:

  - AOI: 70° (close to the Brewster angle of a pure Si substrate)
  - spectral range: in order to test the system the complete spectral range should be used
  - step size: 0.1eV: this allows the resolution of all spectral features of a thin SiO_2/Si sample
  - configuration II: you want to determine very accurately and do not expect to be close to 45°.
  - integration time: 200ms

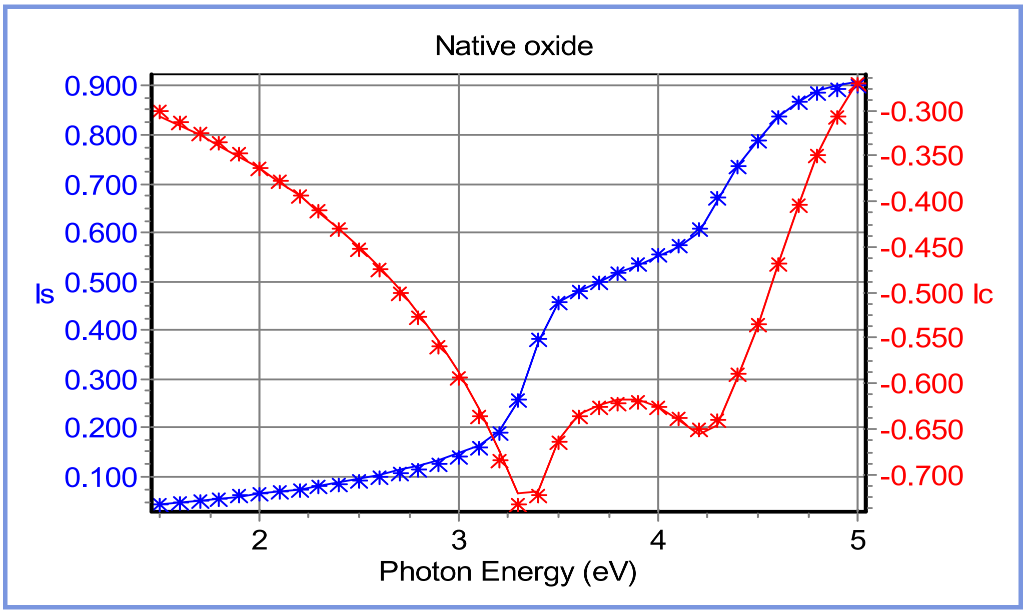
- Since the sample is already in the right position you can ***run*** the acquisition. Enter the sample name any comments if needed. Click "o.k.".
- After the measurement is run the acquired spectra are stored automatically in the folder ***Results\Acquisition data***. The spectra should look like the following:



Different parameters can be displayed as functions of the wavelength or photon energy:

  - Ψ and Δ: the ellipsometric angles known to a wide community and therefore used for publications, reports, etc.
  - I_s and I_c: these are the measured parameters of a phase modulated ellipsometer: they are usually used for the fitting process
  - n and k or ε_r and ε_i: optical constants: useful to see immediately the properties of a substrate or a "pseudo"-substrate

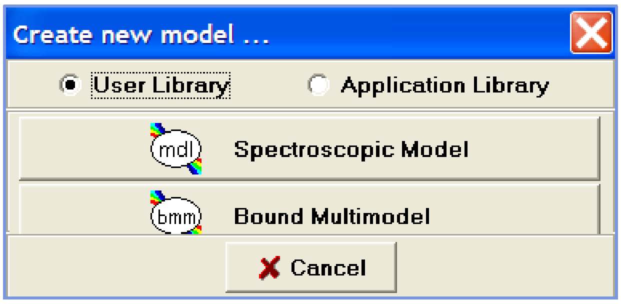
For example the graph from above looks in the $I_s(E)$ and $I_c(E)$ representation like this:



Modelling

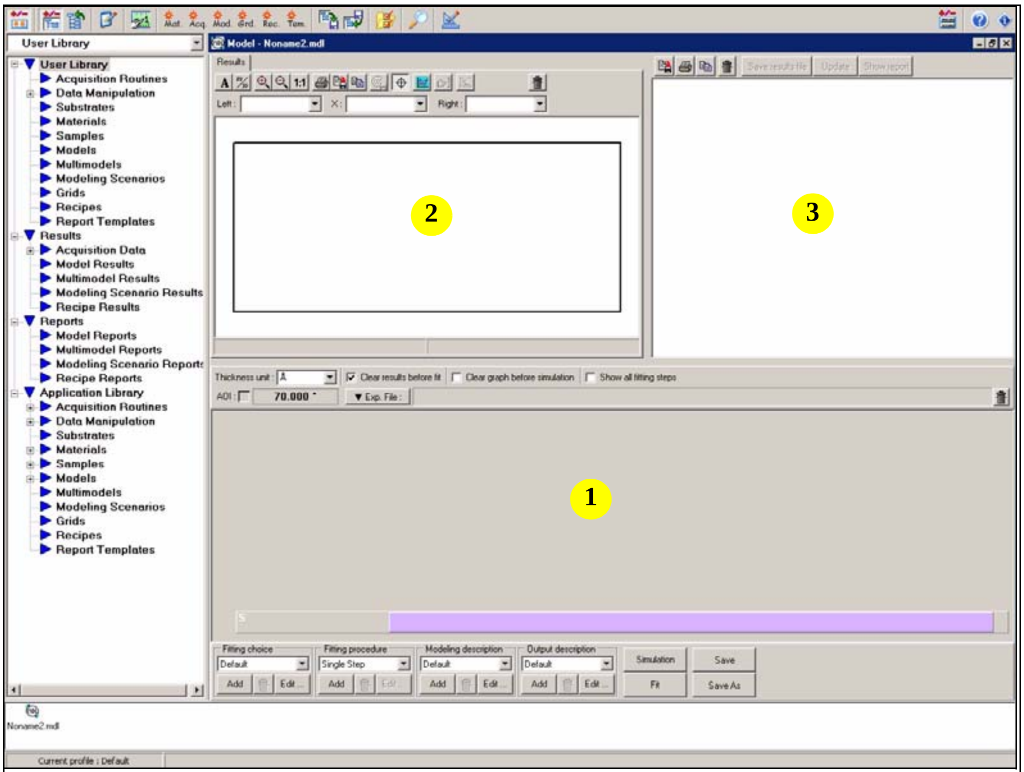
To create a new model click on the ***Mod.*** tab:

The following window appears:



● User Library ○ Application Library

You can choose the folder where you want to put the model file (User library or Application library). Click on ***Spectroscopic Model*** to access the model window:



1 **Sample Structure area**

2 **Results Graphics display area**

3 **Fitting Results area**

Modeling screen layout

Within ***Results\Acquisition data*** in the *TreeView*, select the acquired file ****.spe*** and drag and drop it to the corresponding area (***Exp.File)***.

Go to the ***Application Library\Materials*** folder and drag and drop the file ***C-si_isa.ref*** into the pink bar marked ***S*** for substrate. Then drag and drop the file ***Sio2_isa.ref*** from ***Application Library\Materials*** above the substrate:

1 ☐ 1000.0 Sio2_isa.ref ×

S C-si_isa.ref ×

The next step is to change the default value for the thickness (1000Å) to the approximate value of your sample (in this case 20Å): click on the displayed thickness value to open the window ***Fitting choice Properties for layer #1*** and adjust the thickness. Keep thereby the option ***nominative value***:

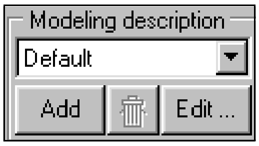
1 F 20.0 Sio2_isa.ref ×

S C-si_isa.ref ×

Now a simulation can be launched by clicking on the corresponding button to check whether the thickness start value is reasonable.

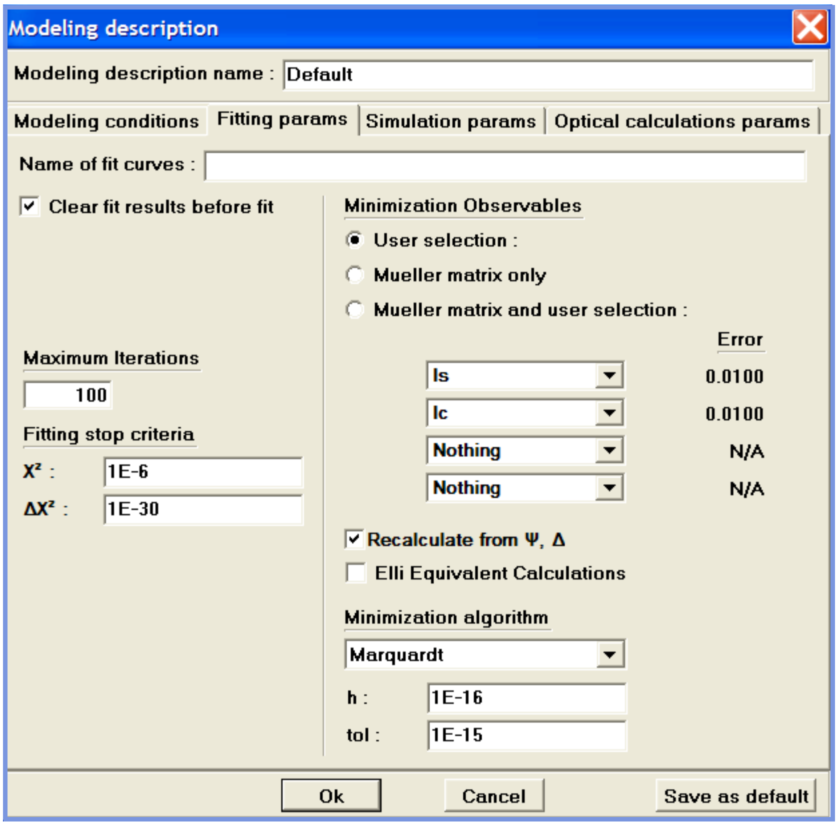
Data fitting

Now that the model is set-up the experimental data can be fitted. For that click on ***Edit*** in ***Modeling description*** on the bottom of the model window:



Modeling description: Default

Select ***fitting params*** and verify that I_s and I_c are the minimization observables. Choose ***Marquardt*** as ***Minimization algorithm***.



Modeling description name : Default

Name of fit curves :

☑ Clear fit results before fit

Maximum Iterations: 100

Fitting stop criteria

X^2 : 1E-6

ΔX^2 : 1E-30

Minimization Observables

● User selection :

○ Mueller matrix only

○ Mueller matrix and user selection :

	Error
Is	0.0100
Ic	0.0100
Nothing	N/A
Nothing	N/A

☑ Recalculate from Ψ, Δ

☐ Elli Equivalent Calculations

Minimization algorithm: Marquardt

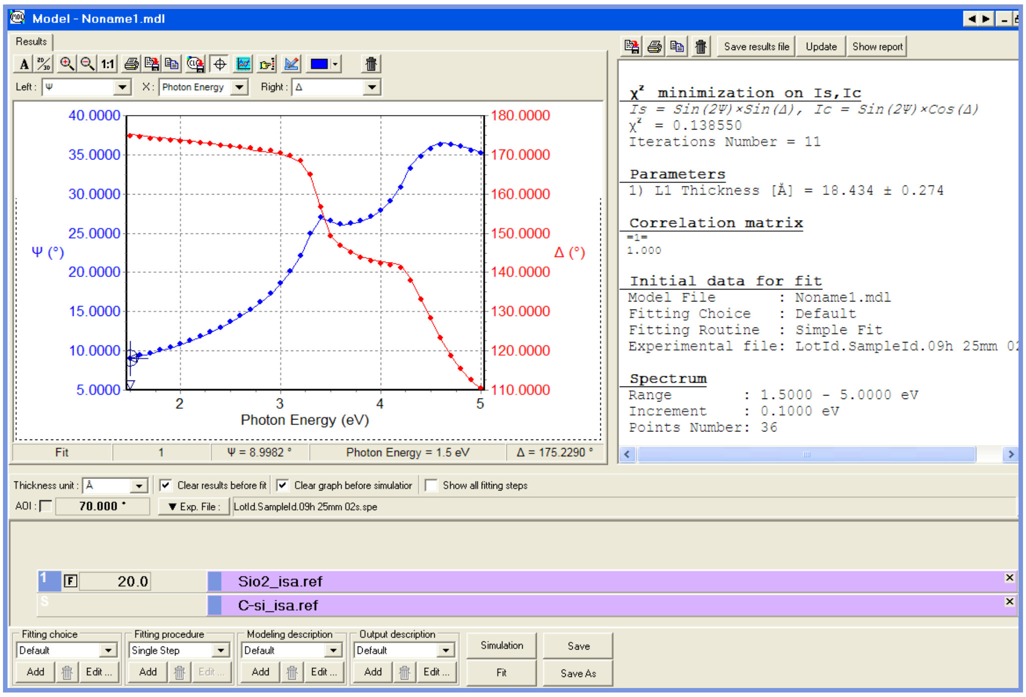
h : 1E-16

tol : 1E-15

Click "Ok", save the model and launch the fit with the appropriate button.

Results

The page displayed after the fit will be:



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 0.138550
Iterations Number = 11

Parameters
1) L1 Thickness [Å] = 18.434 ± 0.274

Correlation matrix
=1=
1.000

Initial data for fit
Model File        : Noname1.mdl
Fitting Choice    : Default
Fitting Routine   : Simple Fit
Experimental file: LotId.SampleId.09h 25mm 02

Spectrum
Range          : 1.5000 - 5.0000 eV
Increment      : 0.1000 eV
Points Number: 36
```

Fit | 1 | Ψ = 8.9982 ° | Photon Energy = 1.5 eV | Δ = 175.2290 °

Thickness unit : Å ☑ Clear results before fit ☑ Clear graph before simulation ☐ Show all fitting steps

AOI : ☐ 70.000 ° ▼ Exp. File : LotId.SampleId.09h 25mm 02s.spe

1 F 20.0 Sio2_isa.ref

C-si_isa.ref

Fitting choice: Default
Fitting procedure: Single Step
Modeling description: Default
Output description: Default

where you can see that:

thickness = 18.434Å ± 0.274 (confidence limits)

χ^2 = 0.13 (and thus < 0.20 as required)

You can try now to change the spectral range for this specific case. Click on ***Edit*** in ***Modeling description*** on the bottom of the model window, and check the box: ***User defined spectral range*** in ***Modeling conditions***. Try different settings. The result should stay more or less the same as shown in the table below:

	Thickness (Å)	**χ^2**
From: 1.5eV To: 5eV Increment: 0.1eV	18.434	0.13
From: 1.5eV To: 4.5eV Increment: 0.1eV	18.638	0.14
From: 1.5eV To: 4.0eV Increment: 0.1eV	18.341	0.11
From: 1.5eV To: 3.5eV Increment: 0.1eV	17.840	0.09
From: 1.5eV To: 3eV Increment: 0.1eV	18.350	0.09

This is due to the fact that the result for the thickness is nearly independent of the spectral range in the case of a transparent material. This is not necessarily the case if the deposited layer shows a complicated dispersion with absorption bands (examples in chapter 10).

11 Application Examples

11.1 Overview

The following table summarizes the examples discussed in this chapter:

Chapter	Task	Sample	Topic
11.2	Thickness of thin film	SiO_2/Si	UVISEL configurations
11.3	Thickness and dispersion	Si_3N_4/Si	Dispersion files
11.4.1	Transparent substrate	glass	Back side reflection
11.4.2	Film on transparent substrate	a-Si/glass	Back side reflection Amorphous dispersion
11.5	Composed materials	OPSL	EMA
11.6	Multilayers	$TiO_2/SiO_2/Si$	Layer repetition
11.7	Complicated dispersions	Organic layer	Nk-fit
11.8	Inhomogeneous layer	ITO/glass	Graded index layer
11.9	Correlated parameters	TiO_2/glass	Bound multimodel
11.10	Non-cubic crystals	Al_2O_3	Uniaxial anisotropy
11.11	Strained materials	polymers	Biaxial anisotropy

11.2 Thickness of a single film

11.2.1 Silicon Oxide on Silicon

11.2.1.1 Key points

- Influence of the measurement configurations
- How to use of the merge function

11.2.1.2 Typical settings of acquisition parameters:

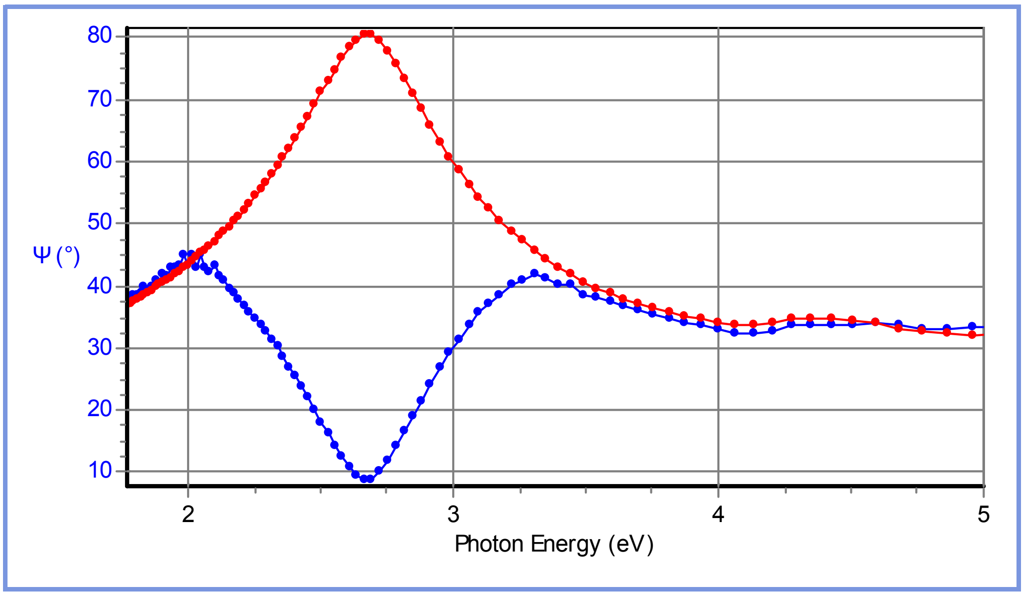
Sample	Thermal oxide layer
Spectral range	1.5 – 5eV
Increment	0.050eV

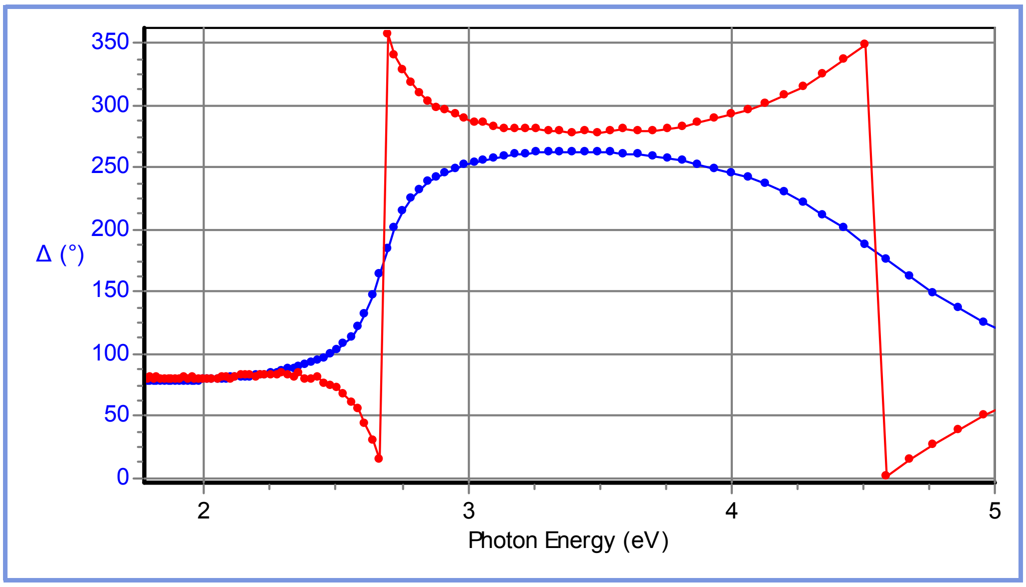
AOI	70°
Spot size	1mm x 3mm
Integration time	200ms
configuration	II & III in standard merge

11.2.1.3 Experiment

The standard merge (STM) acquisition function generates automatically 3 files:

one for the measurement in configuration II: xxx-CII.spe, one for the measurement in configuration III: xxx-CIII.spe and the "merged" file: xxx-STM.spe. The two next figures show Ψ and Δ spectra for configuration II (blue) and configuration III (red). Remember that from the definition of the ellipsometric angles ($\rho=\tan\Psi e^{i\Delta}$) the domains are [0, 90[for Ψ and [0, 360[for Δ.





There are obviously mirror effects on Ψ around 45° and on Δ around 90° and 270°. Explanation:

Ψ, Δ are calculated from Is and Ic in the last step of the acquisition flowchart, which starts by digital processing in the acquisition board (details in appendix C):

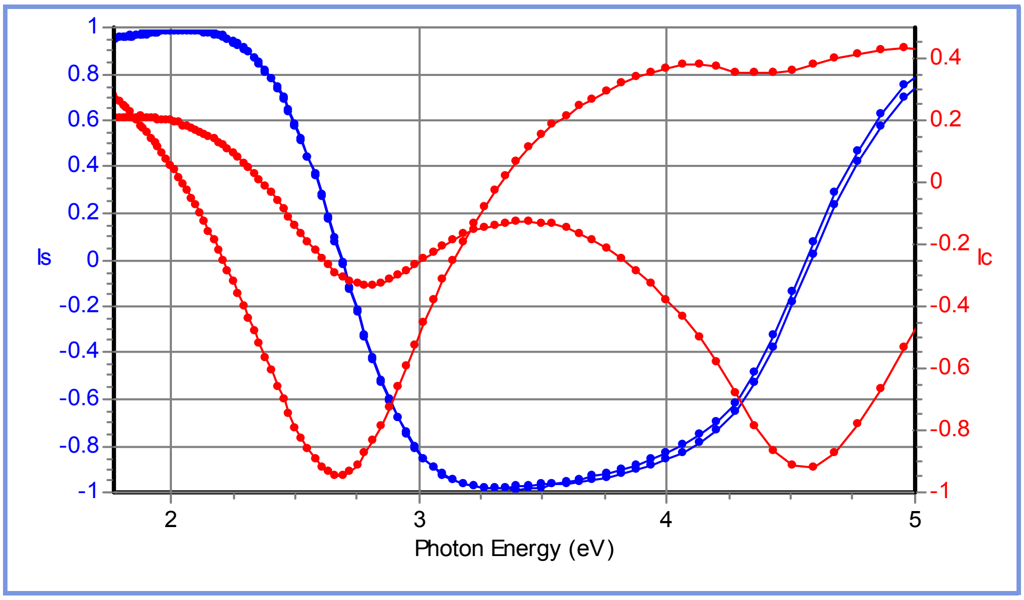
$$\begin{tikzcd}\begin{pmatrix} S_0 \\ S_1 \\ S_2 \end{pmatrix} \arrow[r] & \begin{pmatrix} S_\omega \\ S_{2\omega} \end{pmatrix} \arrow[r] & \begin{pmatrix} \mathrm{I}s \\ \mathrm{I}c \end{pmatrix} \arrow[r] & \begin{pmatrix} \Psi \\ \Delta \end{pmatrix}\end{tikzcd}$$

The deduction of Ψ and Δ from Is and Ic is according to the following relations:

Configuration II, for $M = 0$ and $A = 45°$: $Is = \sin 2\Psi \sin\Delta$ and $Ic = \sin 2\Psi \cos\Delta$

Configuration II, for $M = 45°$ and $A = 45°$: $Is = \sin 2\Psi \sin\Delta$ and $Ic = \cos 2\Psi$

The next graph shows Is and Icfor the two configurations (note that Is does not depend on the configuration):



A closer look at the trigonometric functions shows that:

	Ψ	Δ
Config. II	sin2Ψ defines Ψ in the interval [0, 45] only. Values above are flipped down around the line $\Psi = 45°$	knowing sinΔ and cosΔ allows determination of Δ over the complete domain
Config. III	cos2Ψ allows the determination of Ψ over the complete domain	sinΔ defines Δ in the interval [0, 90] only. Values above are flipped down around the line $\Delta = 90°$

The resulting standard merge file contains therefore Ψ from configuration III and Δ from configuration II.

The next table summarizes fitting results for the two configurations:

File	Thickness	χ^2	Fitting spec
Config. II	859	2	(Is, Ic)
Config. II	855	400	(Ψ, Δ)
Config. III	859	1000	(Is, Ic)
Config. III	860	2000	(Ψ, Δ)
STM	859	2	(Is, Ic)
STM	859	2	(Ψ, Δ)

The high χ^2 or a wrong thickness result from:

configuration II file has the wrong and cannot be fitted using (Ψ, Δ)

configuration III file has wrong and cannot be fitted using (Ψ, Δ)

configuration III file has wrong Ic and cannot be fitted using (Is, Ic)

Conclusion:

we recommend to restrict generally to configuration II and use (Is, Ic) as minimization observables. The only interest of STM is to extract exact values for Ψ and Δ but it does not improve the fitting process.

11.3 Thickness and dispersion of a single film

11.3.1 Silicon Nitride on Si

11.3.1.1 Key points

- Choice of dispersion
- Illustration of local minimum
- Fitting functions and algorithms

This example illustrates the determination of optical properties of the film by two different dispersion models.

It also emphasizes the behaviour of fitting algorithms and wrong mathematical solutions (local minima).

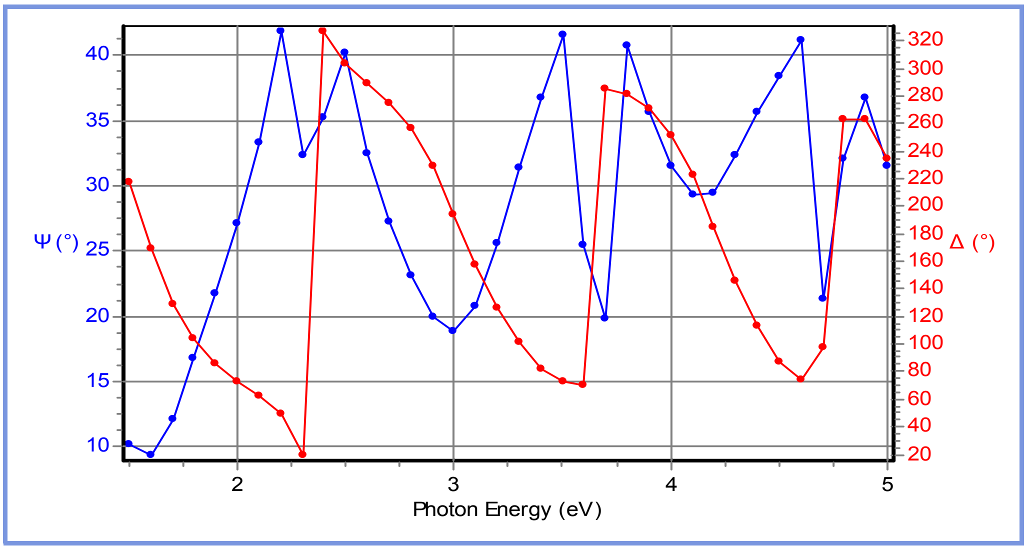
11.3.1.2 Typical settings of acquisition parameters:

Sample	Si3N4 layer
Spectral range	1.5 – 5eV
Increment	0.050eV
AOI	70°

Spot size	1mm x 3mm
Integration time	200ms
Configuration	II & III in standard merge

11.3.1.3 Experiment

The standard .spe file obtained in configuration II should look like that:



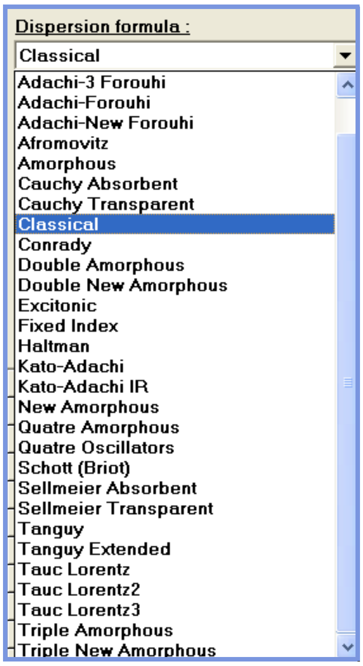
Note that Ψ is flipped for some parts of the curve. This is not important for modelling which is done on Is and Ic and not on Ψ and Δ.

11.3.1.4 Interpretation

Optical properties of a material can be described either with the dielectric function or with the complex index of refraction. The relation between the two complex values is:

$$\mathbf{re(\varepsilon) + i\, im(\varepsilon) = (n + ik)^2}$$

The first dispersion under study is called ***classical***. Classical, because it is not based on quantum mechanics.



Dispersion formula : Classical

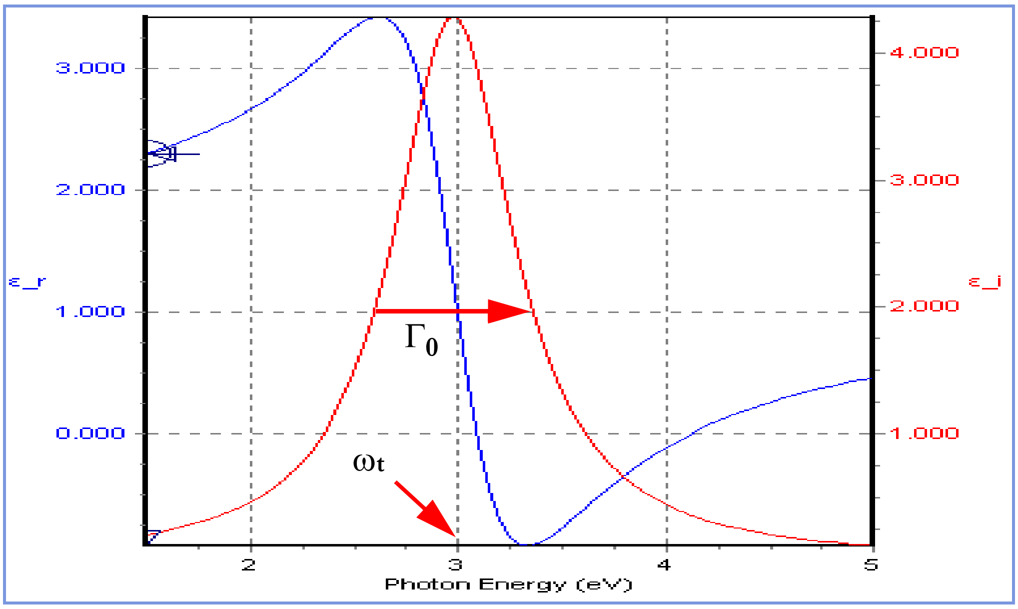
The complete expression is:

$$\varepsilon = \varepsilon_r + i\varepsilon_i = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\omega} + \frac{\omega_P^2}{-\omega^2 + i\Gamma_D\omega} + \sum_j \frac{f_j\omega_j^2}{\omega_j^2 - \omega^2 + i\Gamma_j\omega}$$

For Si_3N_4 we use only one Lorentzian oscillator, so that the dispersion can be written as:

$$\varepsilon = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\omega}$$

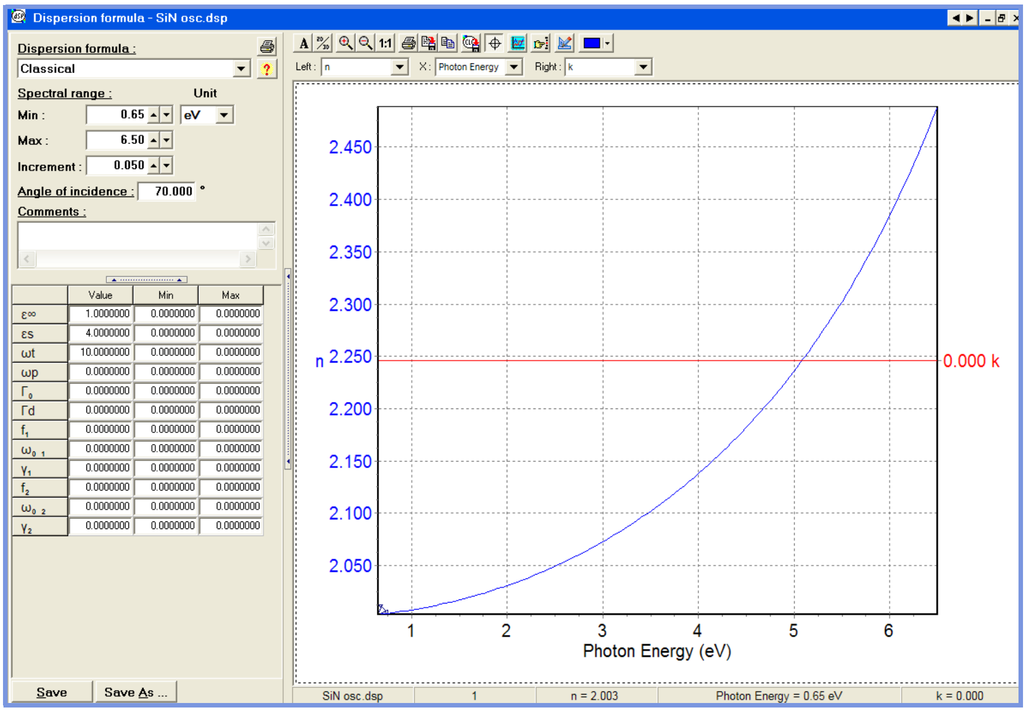
The graphical representation is:



Note that:

- if $\Gamma_0 = 0$: im(ε) = 0: the material is transparent.
- if $\Gamma_0 \geq 0$: im(ε) $\geq$ 0: the material shows absorption.
- im(ε) is small except around ω_t. The FWHM of this peak is equal to Γ_0.
- for $\omega \rightarrow 0$, re(ε) $\rightarrow \varepsilon_s$
- for $\omega \rightarrow \infty$, re($\varepsilon$) $\rightarrow \varepsilon_\infty$
- ε_∞ is usually equal to 1 unless otherwise specified.

If we enter the parameters ε_s=4 and ω_t=10 the following dispersion is generated:



Dispersion formula - SiN osc.dsp

Dispersion formula : Classical

Spectral range : Unit

Min : 0.65 eV

Max : 6.50

Increment : 0.050

Angle of incidence : 70.000 °

Comments :

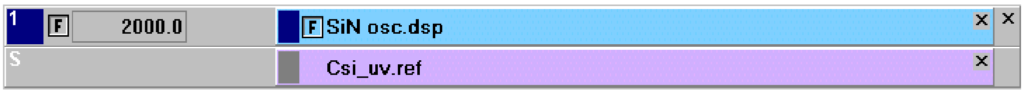
	Value	Min	Max
ε∞	1.0000000	0.0000000	0.0000000
εs	4.0000000	0.0000000	0.0000000
ωt	10.0000000	0.0000000	0.0000000
ωp	0.0000000	0.0000000	0.0000000
Γ_0	0.0000000	0.0000000	0.0000000
Γd	0.0000000	0.0000000	0.0000000
f_1	0.0000000	0.0000000	0.0000000
$\omega_{0\ 1}$	0.0000000	0.0000000	0.0000000
γ_1	0.0000000	0.0000000	0.0000000
f_2	0.0000000	0.0000000	0.0000000
$\omega_{0\ 2}$	0.0000000	0.0000000	0.0000000
γ_2	0.0000000	0.0000000	0.0000000

Left : n X : Photon Energy Right : k

SiN osc.dsp | 1 | n = 2.003 | Photon Energy = 0.65 eV | k = 0.000

We recognize ε_s = 4 in low energies ($n^2=\varepsilon_s$ for ω=0).

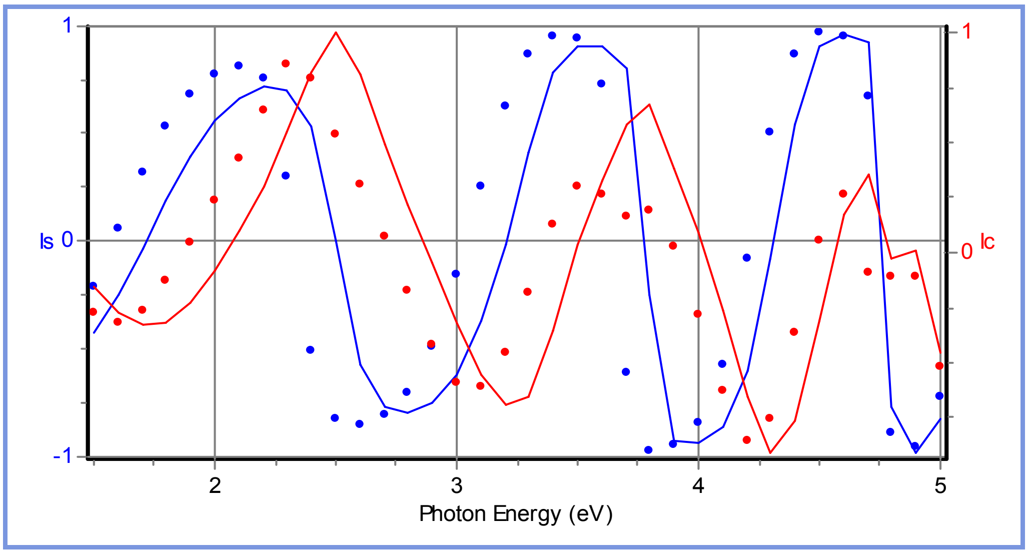
We use this material SiN osc.dsp into the mdl environment:



1 F 2000.0 F SiN osc.dsp

S Csi_uv.ref

Simulations with varying thickness show that 2000 Å will be a good guess :



Fitting thickness and two dispersion parameters leads to following results :

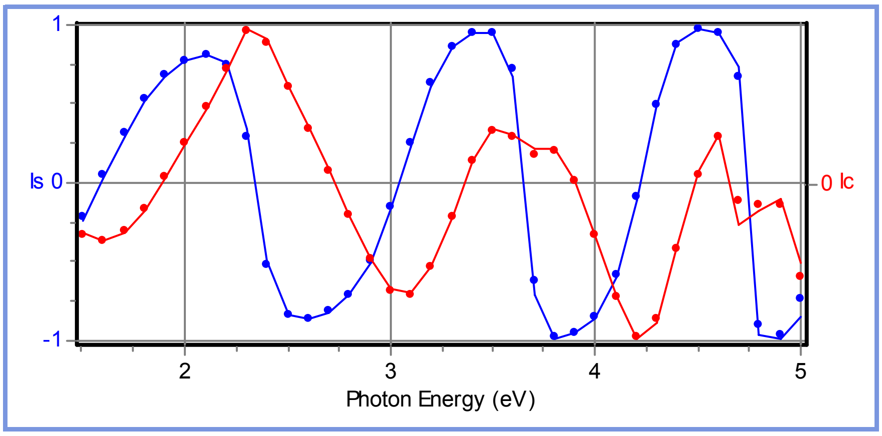
thickness : 2506 Å ± 26

$\varepsilon_s = 3.24 \pm 0.05$

$\omega_t = 9.28 \pm 0.06$

$\chi^2 = 11$

and an excellent graphic agreement :



We repeat fitting with different initial values for thickness in the range 500 to 5000Å:

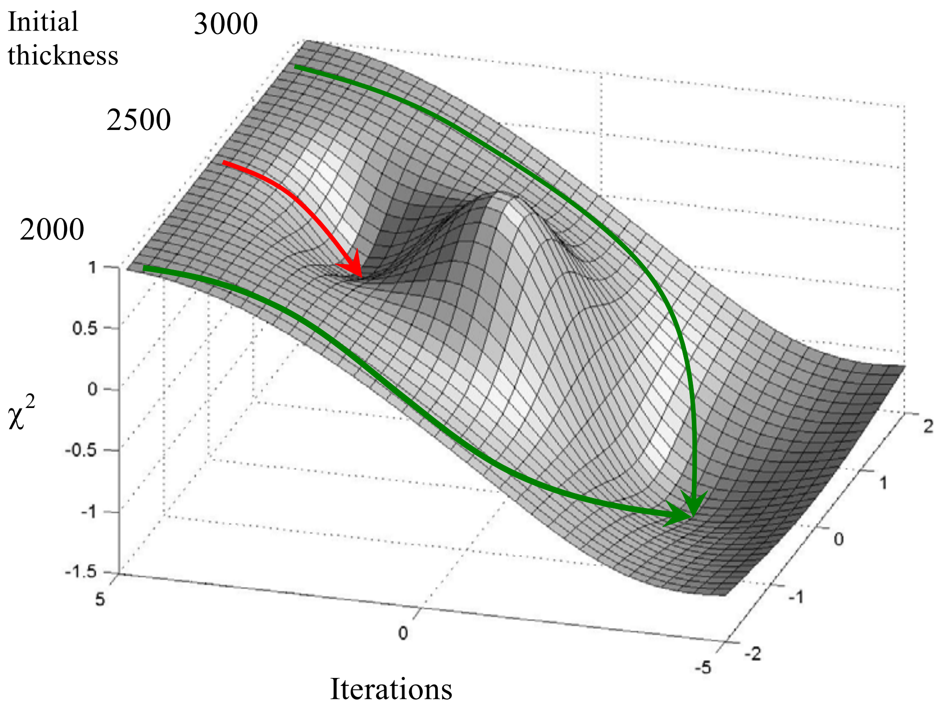
Initial thickness	χ^2	thickness result - comment
500	4100	169Å - Bad
1000	3300	550Å - Bad
1500	2400	639Å - Bad
2000	11	2500Å - Good
2500	3300	2500Å - Bad
3000	11	2500Å - Good

3500	5000	1327Å - Bad
4000	4300	2000Å - Bad
4500	5400	2000Å - Bad
5000	5200	2200Å - Bad

Obviously, only two thickness start values, 2000 and 3000Å give good solutions (lowest χ^2). For the other start values the Marquardt minimization algorithm falls into a local minimum where χ^2 is much higher.

Note that **starting from the right thickness (2500Å) leads to a bad solution**. This is due to the fact that we are fitting in addition to thickness also 2 dispersion parameters. This shows that permanent care has to be taken with multi-dimensional minimization routines.

The next figure shows the fitting function and local/global minima:



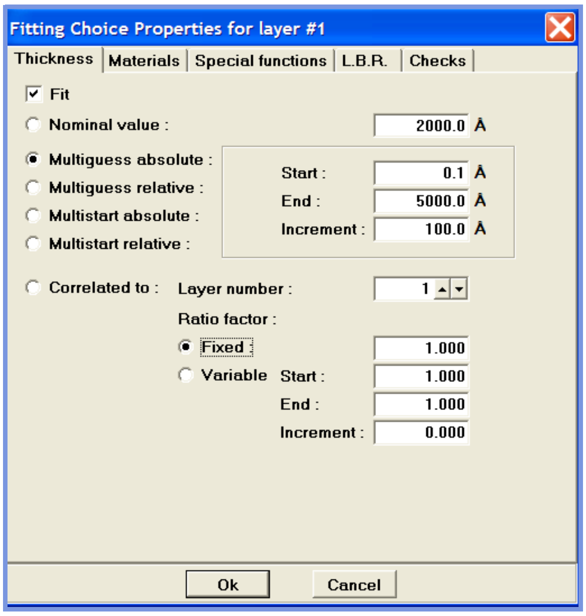
The red trajectory starting from the right thickness does not lead to the best (global) minimum. The minimization algorithm falls into a local minimum with correct thickness but a much too high χ value caused by the incorrect final dispersion parameters.

Two green trajectories starting from wrong thicknesses (2000 and 3000Å) follow the high slope of the χ surface, thus avoiding the local minima met above, and fall into the correct solution, which corresponds to the global minimum.

DP2 can handle these potential difficulties in two ways:

1. ***multiguess***

several fits are performed with different start values:



☑ Fit

○ Nominal value : 2000.0 Å

● Multiguess absolute :

○ Multiguess relative :

○ Multistart absolute :

○ Multistart relative :

Start : 0.1 Å

End : 5000.0 Å

Increment : 100.0 Å

○ Correlated to : Layer number : 1

Ratio factor :

● Fixed : 1.000

○ Variable Start : 1.000

End : 1.000

Increment : 0.000

In the present case we apply ***multiguess absolute***, starting from different thicknesses between 0 and 5000Å (increment100Å). We find the correct solution:

thickness: 2506Å ± 26Å

$\varepsilon_s = 3.24 \pm 0.05$

$\omega_t = 9.28\text{eV} \pm 0.06\text{eV}$

$\chi^2 = 11$

The multiguess method was applied here only for one variable (thickness), but of course it can be applied to every adjustable parameter.

The method is very reliable but can be very time consuming. For example if we choose in the case of m adjustable parameters 10 guesses for each parameter the number of fits will be 10^n!

2. *Simplex minimization method*

At the beginning the user should again set start values for the adjustable parameters. For example if m parameters are adjustable the Simplex method will generate randomly m additional sets of these m variables. The result is a polyhedron in a m-dimensional space. The Simplex method will then twist and scrunch this polyhedron around a neighborhood of “small” χ^2. This method is less sensitive to local minima than the Marquardt-Levenberg algorithm. Its drawbacks are speed and the fact that two successive attempts will never give the same solution. Therefore one should repeat the fit several times to make sure the method has really reached the best solution. Although DP2 allows it, we suggest not to combine this method with the multiguess option.

In the following table the results of 10 successive attempts (same initial values) are summarized for the present example.

Simplex	χ^2	Solution found, comment
1	8000	2500 Å – Bad

2	4200	1500 Å – Bad
3	4700	1100 Å – Bad
4	4200	1300 Å – Bad
5	3300	2500 Å – Bad
6	4000	2600 Å – Bad
7	64	2200 Å – Bad
8	4000	1400 Å – Bad
9	10	2500 Å – Good
10	2600	1600 Å – Bad

Unfortunately only attempt number 9 leads to the correct solution. This means that one has to repeat the fit many times to be sure about the correct solution.

Now we return to our initial problem, the properties of the nitride layer. The best solution for the moment gives $\chi^2 \approx 11$. If we set additional Γ_0 as unknown parameter we get:

thickness: 2564Å ± 31Å

$\varepsilon_s = 3.13 \pm 0.05$

$\omega_t = 9.25\text{eV} \pm 0.0\text{eV}$

$\Gamma_0 = 0.06\text{eV} \pm 0.02\text{eV}$

$\chi^2 \approx 8$

So χ^2 has decreased from 11 to 8 (thus 30 %) while the number of fitted parameters has increased from 3 to 4 (thus 33 %). This means that the introduction of one more parameter does not improve the fit significantly. The model using a Lorentz dispersion formula has reached its limit in this case. An alternative is the ***new amorphous*** formula, which corresponds to a rewriting of the original Forouhi-Bloomer formula:

$$n = n_\infty + \frac{B_i(\omega - \omega_i) + C_i}{(\omega - \omega_i)^2 + \Gamma_i^2}$$

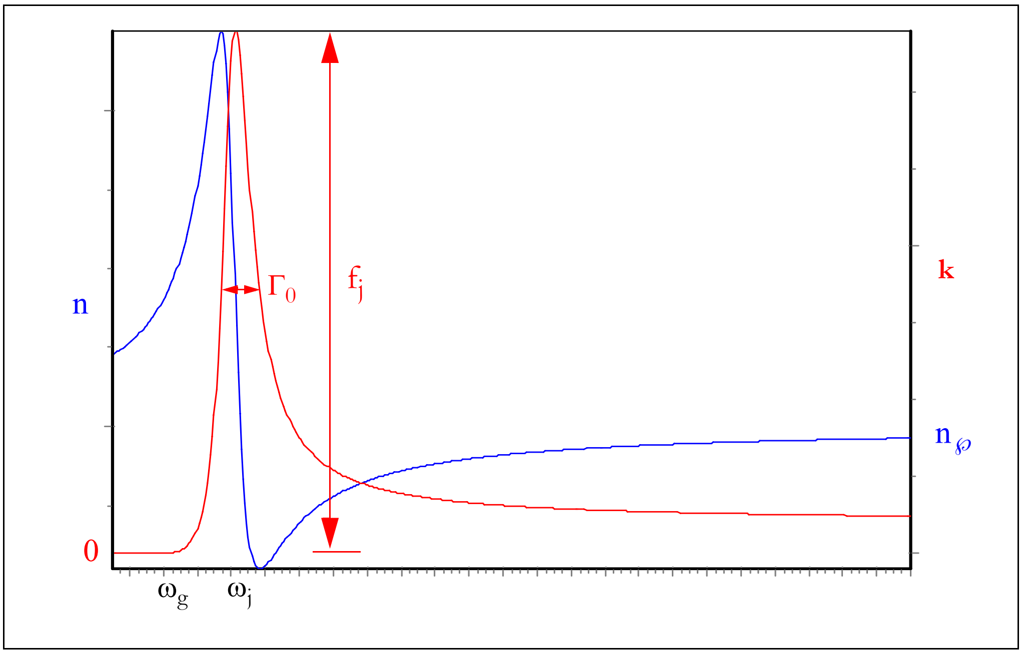
and

$$k(>g) = \frac{f_i(\omega - \omega_g)^2}{(\omega - \omega_i)^2 + \Gamma_i^2} \;;\; k(\omega g) = 0$$

;

where $B_i = \frac{f_i}{\Gamma_i}\left[\Gamma_i^2 - (\omega_i - \omega_g)^2\right]$ **and** $C_i = 2 f_i \Gamma_i (\omega_i - \omega_g)$

The following graph shows an example of this dispersion:



Note that for $\omega \leq \omega_g$: k = 0 that means the material is transparent below the band gap. We try the following start parameters for Si_3N_4:

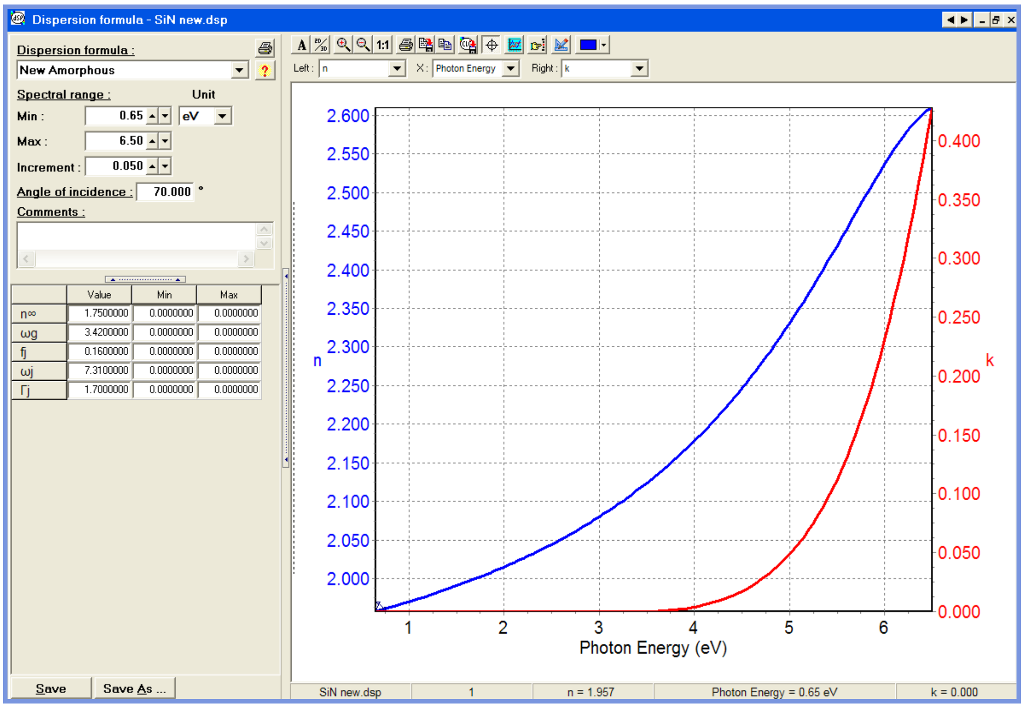
$n_\infty = 1.75$

$\omega_g = 3.42eV$

$fj = 0.16$

$\omega_j = 7.31eV$

$\Gamma_j = 1.7eV$



Dispersion formula : New Amorphous

Spectral range : Unit eV

Min : 0.65

Max : 6.50

Increment : 0.050

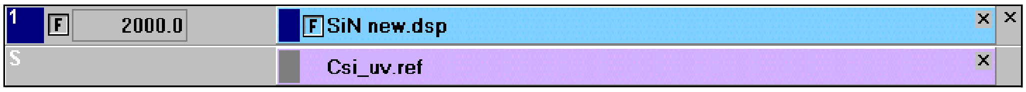
Angle of incidence : 70.000 °

Comments :

	Value	Min	Max
n∞	1.7500000	0.0000000	0.0000000
ωg	3.4200000	0.0000000	0.0000000
fj	0.1600000	0.0000000	0.0000000
ωj	7.3100000	0.0000000	0.0000000
Γj	1.7000000	0.0000000	0.0000000

SiN new.dsp | 1 | n = 1.957 | Photon Energy = 0.65 eV | k = 0.000

We use now the dispersion SiN new in the model instead of SiN osc:



1 F 2000.0 F SiN new.dsp

S Csi_uv.ref

and get:

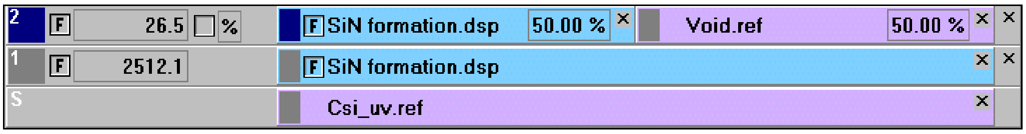
$\chi^2 = 4.95$

thickness = 2530Å ± 19Å

Thus χ^2 has decreased from 11 to 4 while the number of fitted parameters has increased from 3 to 6. This means that the New Amorphous formula should be used instead of the classical formula.

An additional reduction of χ^2 can often be achieved by adding a ***top layer*** in the layer model. This top layer is defined as an ***EMA*** (effective medium approximation) of 50% of the underlying material and 50% of void. A good start value for the thickness is in most cases 30Å. The volume fraction is usually kept fixed but thickness becomes an additional fitting parameter.

The new layer model would then look like:

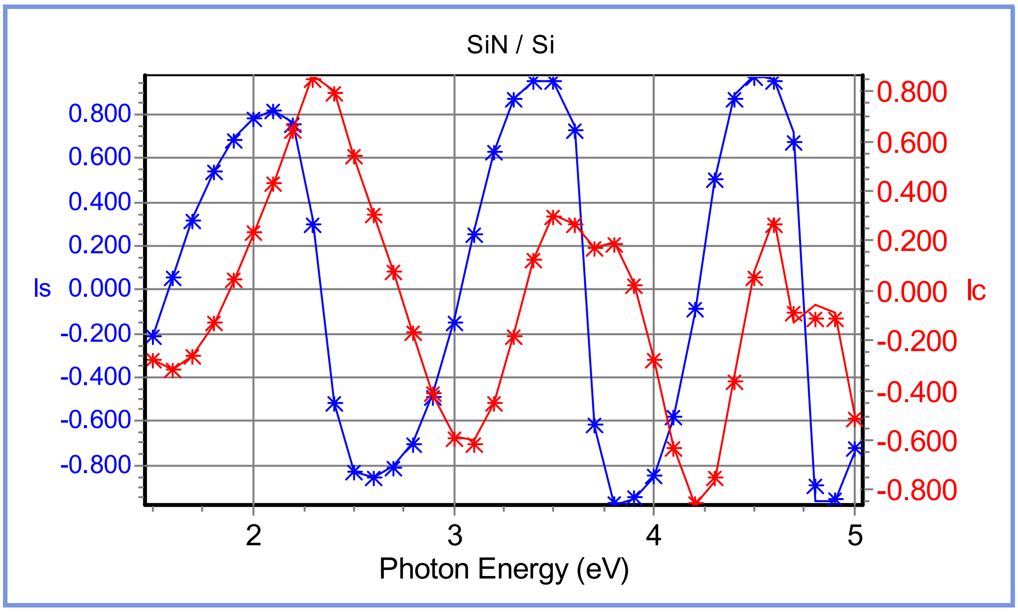


2 F 26.5 ☐ % F SiN formation.dsp 50.00 % Void.ref 50.00 %

1 F 2512.1 F SiN formation.dsp

S Csi_uv.ref

In the present case this overlayer improves the fit to = 2.8. The total thickness (layer + overlayer) is very close to the one layer model result.



The results of the dispersion parameters are then:

$$\mathbf{n_\infty = 1.679}$$

$$\mathbf{\omega_g = 4.226eV}$$

$f_j = 0.081$

$\omega_j = 7.074\text{eV}$

$\Gamma_j = 0.887\text{eV}$

11.4 Transparent substrates

11.4.1 Pure glass without film

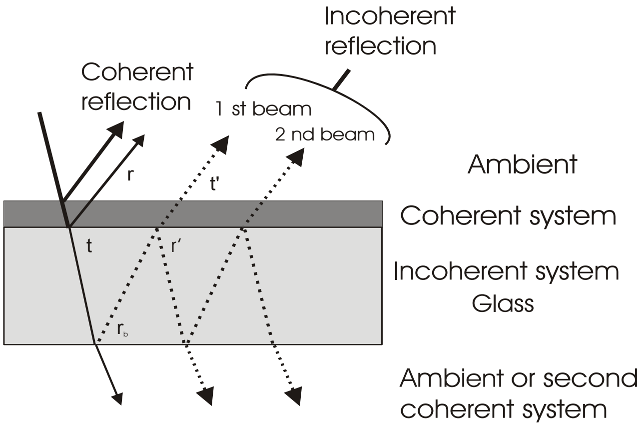
11.4.1.1 Key points

- Back side reflection
- Influence of substrate thickness
- Reflection & Transmission experiments

11.4.1.2 Typical settings of acquisition parameters:

Sample	Glass substrate
Spectral range	1.5 – 6.5eV (825 – 190nm)
Increment	0.050eV
AOI	55°- 60°
Spot size	1mm x 3mm
Integration time	1000ms
Configuration	II

For transparent materials that are polished on both sides we get effects due to the backside (BS) refection of the light beams:



In the case of a 1mm thick glass sample that is polished on both sides the detection head will collect several incoherent from the BS reflected beams. The exact number of collected incoherent beams is not critical as long as they are at least 2.

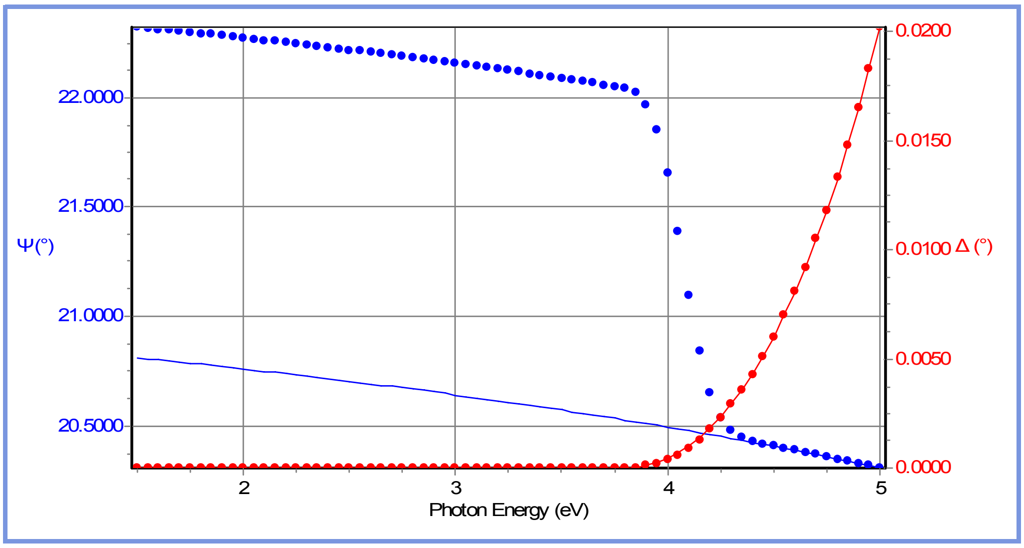
When the substrate thickness is bigger than 2mm the BS reflected beams are sufficiently separated from the front side reflected beams so that they can be masked and do not reach the detection head. This separation can be optimized by adjusting the spot size of the beam on the sample (beam diameter & angle of incidence).

The following table suggests solutions for different substrate thickness ranges:

thickness/mm	Solution
< 0.1	Measure as it is. Model calculations assume infinite number of coherent BS reflected beams.
0.1 – 1	Measure as it is. Model calculations assume infinite number of incoherent BS reflected beams.
1 – 2	Mask the BS reflected beams with appropriate spot size (beam diameter & angle of incidence).
> 2	Mask the BS reflected beams.

Note that BS reflection effects can be observed for all materials that are transparent in a part of the light spectrum. For glass the transparent region is in the visible, for other materials such as Si, InP, GaAs the transparent region is in the NIR.

The following graph shows calculated spectra for a 1mm thick glass sample, with (dots) and without (lines) BS reflected beams:

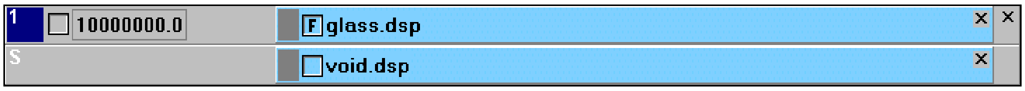


In the low energy range the two spectra are very different. That is the spectral range where the BS reflection affects the measurements. In the high energy range the glass is absorbing so that no light reflected from the BS reaches the detector. The absorption edge of the glass is around 4.2eV.

11.4.1.3 Experiment

Since glass has a reflectivity of only ca. 5% the integration time is increased to 1000ms to improve signal-to-noise ratio (S/N).

The BS reflected beams will be included in the model: we have a real substrate (void) underneath the 1mm thick glass layer:

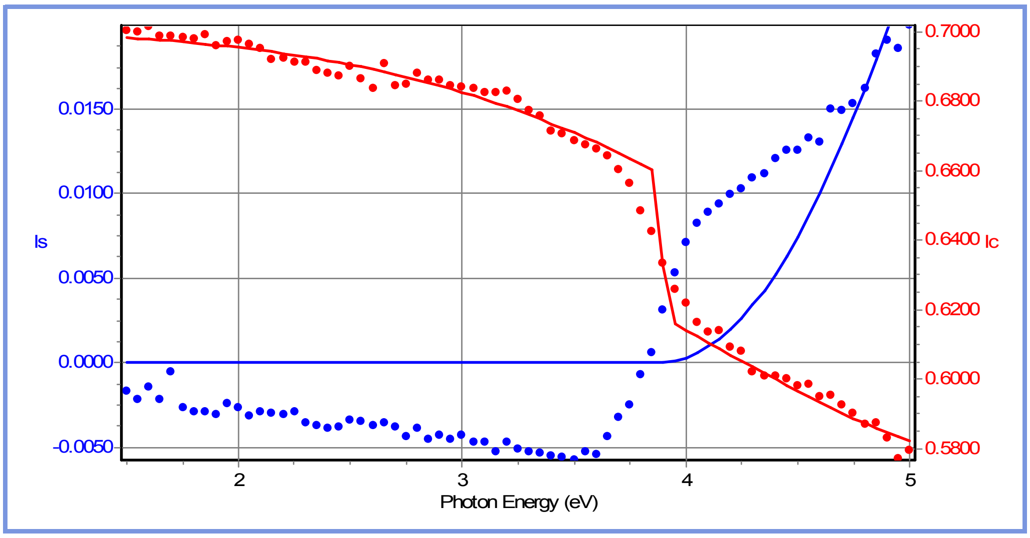


The optical properties of the void substrate are of fixed index type dispersion with n = 1 and k = 0 over the whole spectral range.

The optical properties of glass can be modelled by a New Amorphous dispersion. Start values are for example:

Parameter value	Comment
$n_\infty = 1.45$	Refractive index of glass at long wavelengths
$\omega_g = 3.8$	Absorption edge, optical bandgap
$f_j = 0.01$	Small value for small k
$\omega_j = 12$	Absorption peak, in far UV
$\Gamma j = 1.5$	Damping parameter: not critical as long as it is positive

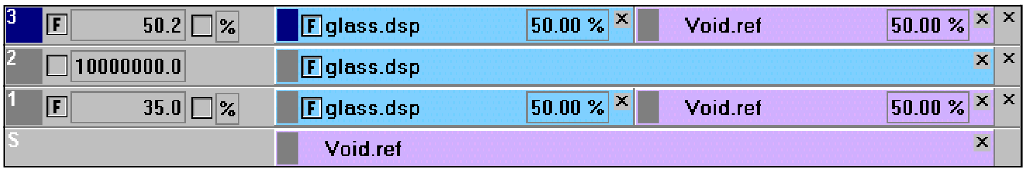
The following graph shows measurement (dots) and fit (lines):



The model described above did not given an excellent fit. For the transparent region of a material we would always expect Is = 0 (= 0) with or without BS reflection. The measurement does not give Is = 0. This is due to surface roughness on the glass.

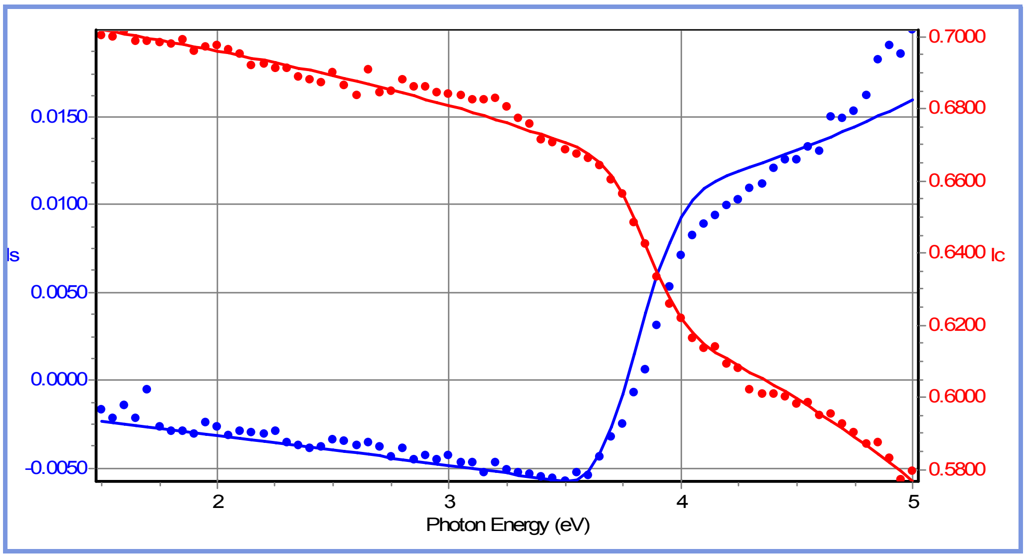
Assuming that the sample is symmetrical, we therefore add a standard roughness layer (30Å, EMA: 50% glass & 50% void) on both sides of the glass.

The final layer model would therefore be the following:



3	F 50.2 ☐ %	F glass.dsp	50.00 % ✕	Void.ref	50.00 % ✕ ✕
2	☐ 10000000.0	F glass.dsp			✕ ✕
1	F 35.0 ☐ %	F glass.dsp	50.00 % ✕	Void.ref	50.00 % ✕ ✕
S		Void.ref			✕

The fit is now much better:



We can derive the final dispersion parameters:

$n_\infty = 1.373$

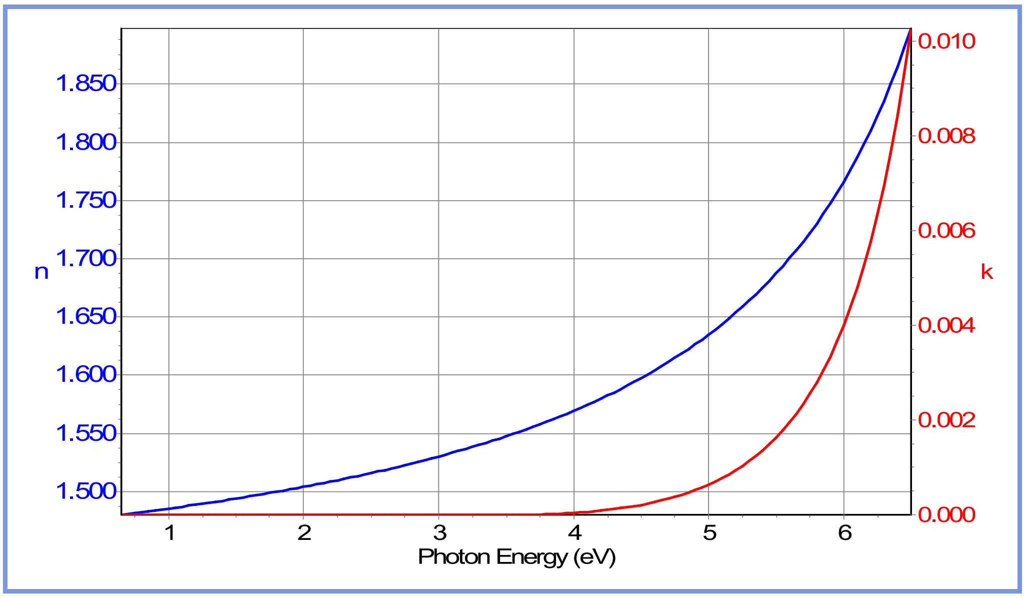
$\omega_g = 3.496\text{eV}$

$f_j = 0.002$

$\omega_j = 7.987\text{eV}$

$\Gamma_j = 0.063$

Leading to the following dispersion curves:



11.4.2 a-Si on glass

11.4.2.1 Key points

- New Amorphous and Tauc Lorentz dispersion
- spectral range for thickness determination
- importance of overlayer

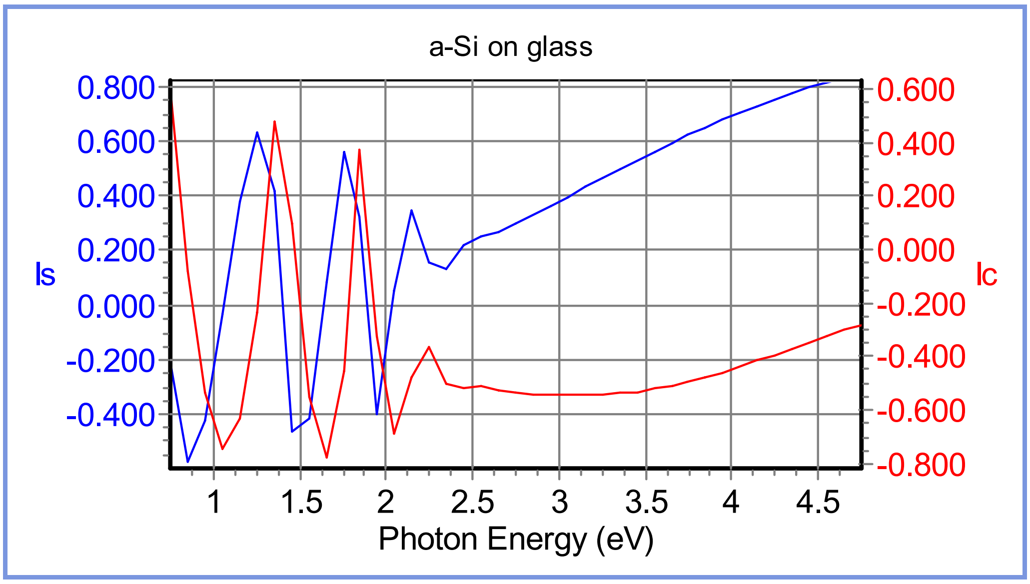
11.4.2.2 Typical settings of acquisition parameters:

Sample	a-Si on glass
Spectral range	1.5 – 6.5eV (825 – 190nm)
Increment	0.050eV
AOI	55° - 60°
Spot size	1mm x 3mm

Integration time	1000ms
Configuration	II

11.4.2.3 Experiment

The following graph shows a measurement of a-Si on a glass substrate:



The spectrum can be divided into two parts:

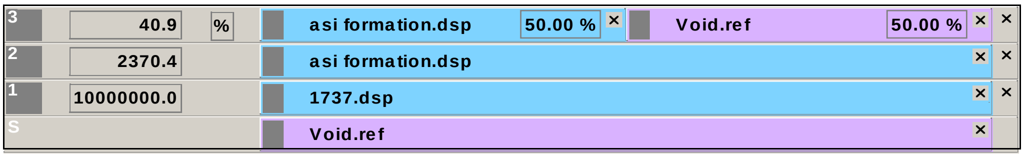
For energies < 2.5eV there are interference fringes indicating that the material a-Si is transparent in this spectral region. The thickness of the a-Si layer is basically determined in that spectral range.

For energies > 2.5eV the fringes disappear, a-Si is absorbing in this spectral range.

11.4.2.4 Analysis

A first attempt is to model a-Si as a single layer with two different dispersion formula: a single layer model with New Amorphous dispersion gives a fit value of $\chi^2 = 87$ while using a Tauc-Lorentz dispersion leads to $\chi^2 = 32$.

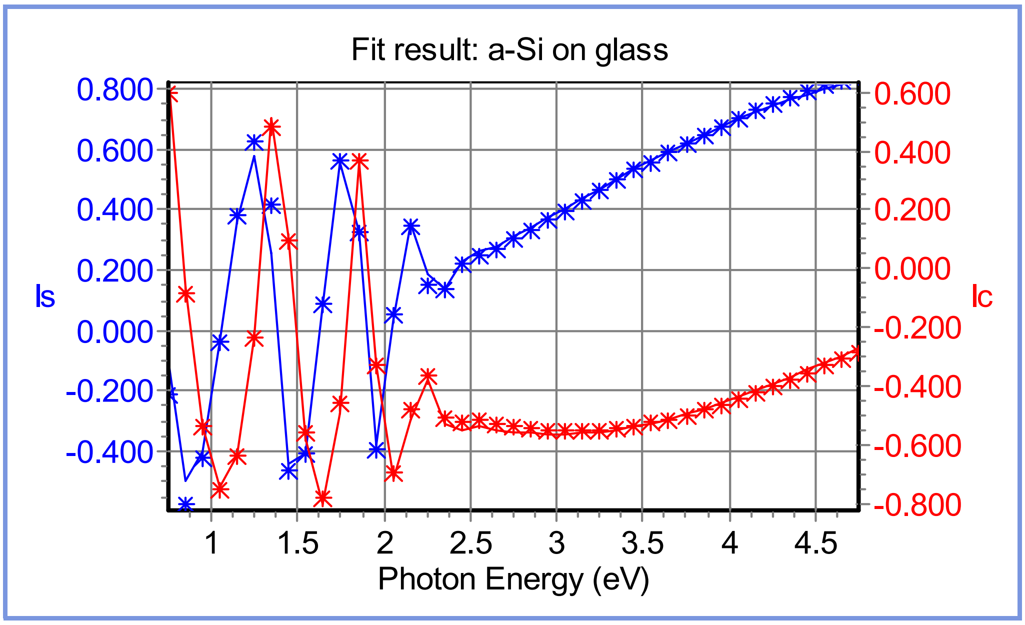
The fit result is better with the Tauc Lorentz formula. However, the fit can further be improved to $\chi^2 \approx 8$ when an overlayer is introduced to the layer model:



3	40.9	%	asi formation.dsp	50.00 %	Void.ref	50.00 %
2	2370.4		asi formation.dsp			
1	10000000.0		1737.dsp			
S			Void.ref			

This overlayer is an EMA of 50% a-Si and 50% void. Physically it corresponds to a roughness layer + a native oxide layer that forms on a-Si (as it does on c-Si and p-Si).

The following graph shows the experimental data (dots) and the final fit (lines):



The deduced dispersion parameters for a-Si are then:

E_g = 1.672eV

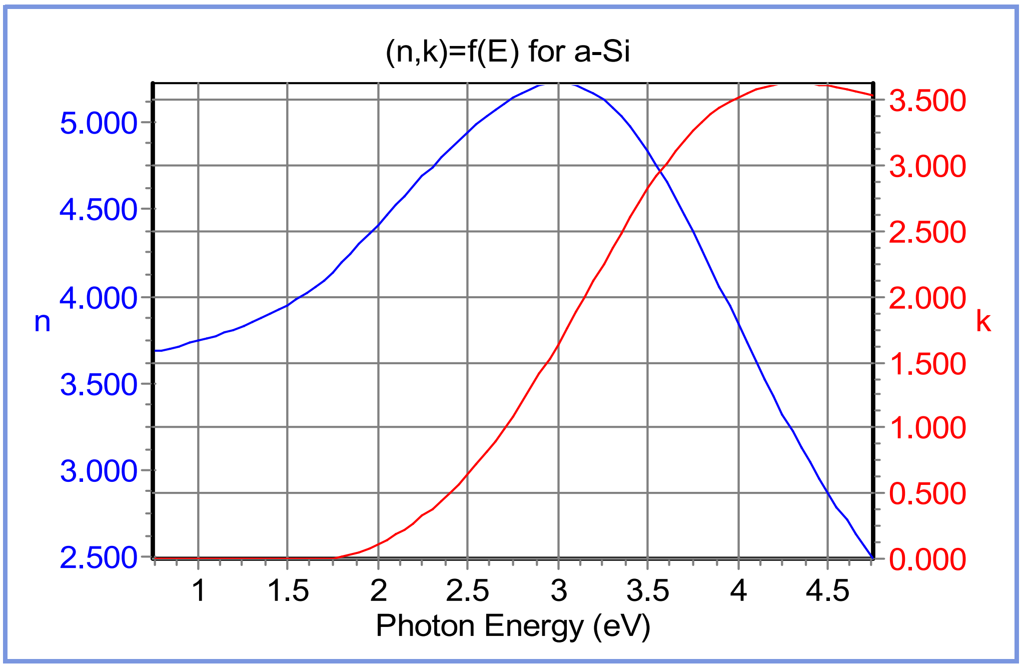
ε_∞ = 0.764

A = 222.674

E_0 = 3.609

χ^2 = 2.272

The corresponding dispersion is displayed in the graph below:



9/2/08

11.5 Composed Materials

11.5.1 Oxidized porous Silicon Layer (OPSL)

11.5.1.1 Key points

- inhomogeneity of OPSL
- EMA: composition of SiO_2 and c-Si (crystalline Si)
- Model improvement step by step
- Total thickness of OPSL layer

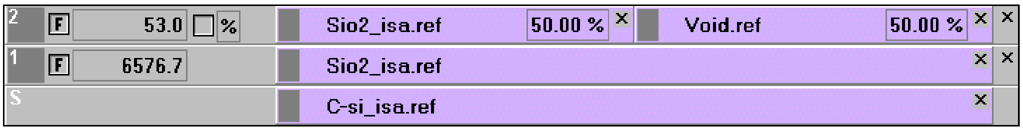
11.5.1.2 Typical settings of acquisition parameters:

Sample	10µm OPSL	Reference (0.5µm SiO_2)
Spectral range	0.75-4.5eV (1655-275nm)	0.75-4.5eV (1655-275nm)
Increment	0.005eV	0.050eV
AOI	70°	70°
Spot size	1mm x 3mm	1mm x 3mm
Integration time	200ms	200ms

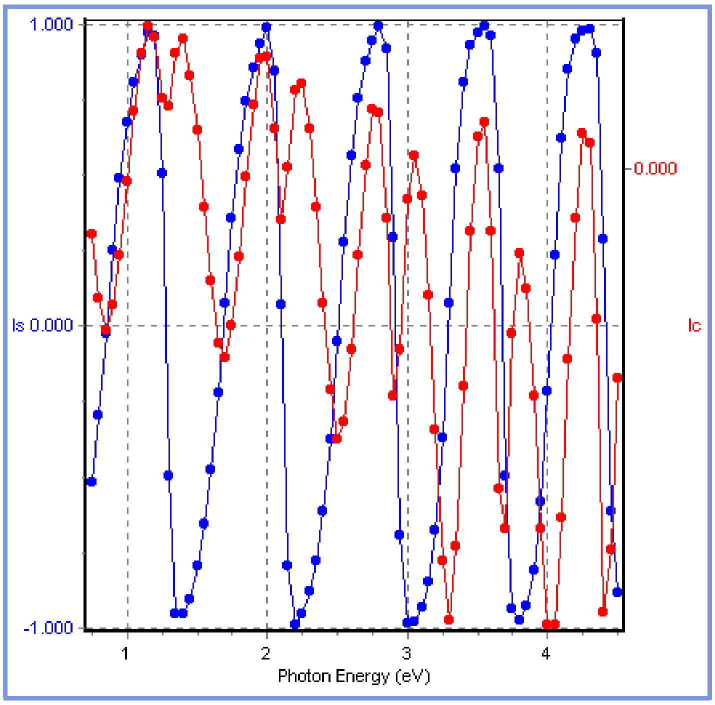
11.5.1.3 Measurement of the reference sample:

In this example we analyze a sample coated with a layer of silicon and OPSL (approximately 10µm thick) and a reference sample coated with a SiO_2 layer (approximately 0.5µm thick).

The reference is analyzed to determine the optical properties of the material in a simple layer structure. As a first step we use the reference file to model SiO_2 and introduce a roughness layer on top (EMA: 50% SiO_2 & 50% void):


2 F 53.0 ☐ % Sio2_isa.ref 50.00 % Void.ref 50.00 %
1 F 6576.7 Sio2_isa.ref
S C-si_isa.ref

Below the experimental (dots) and fit (lines) data:



As a result we get:

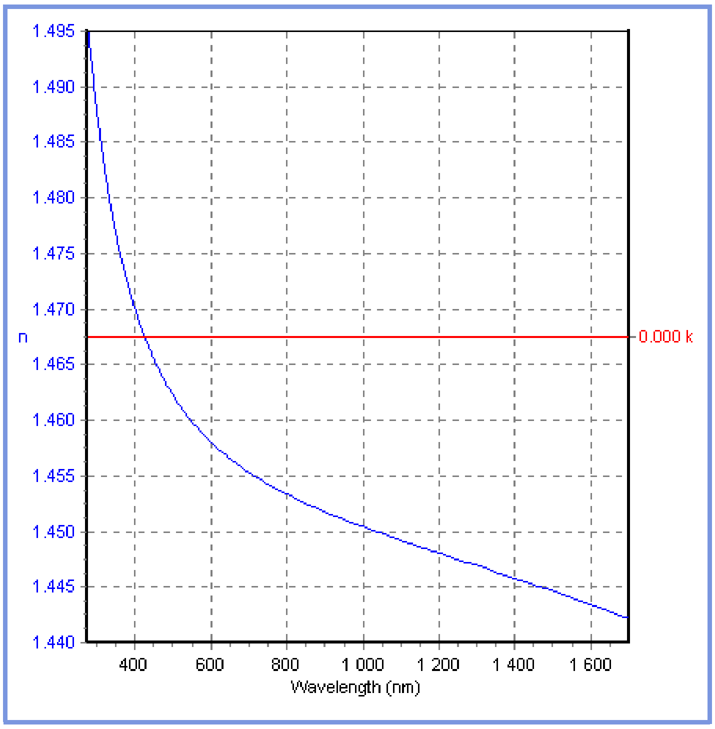
$\chi^2 = 3.82$

thickness SiO_2 = 6576.7Å

thickness roughness layer = 53Å

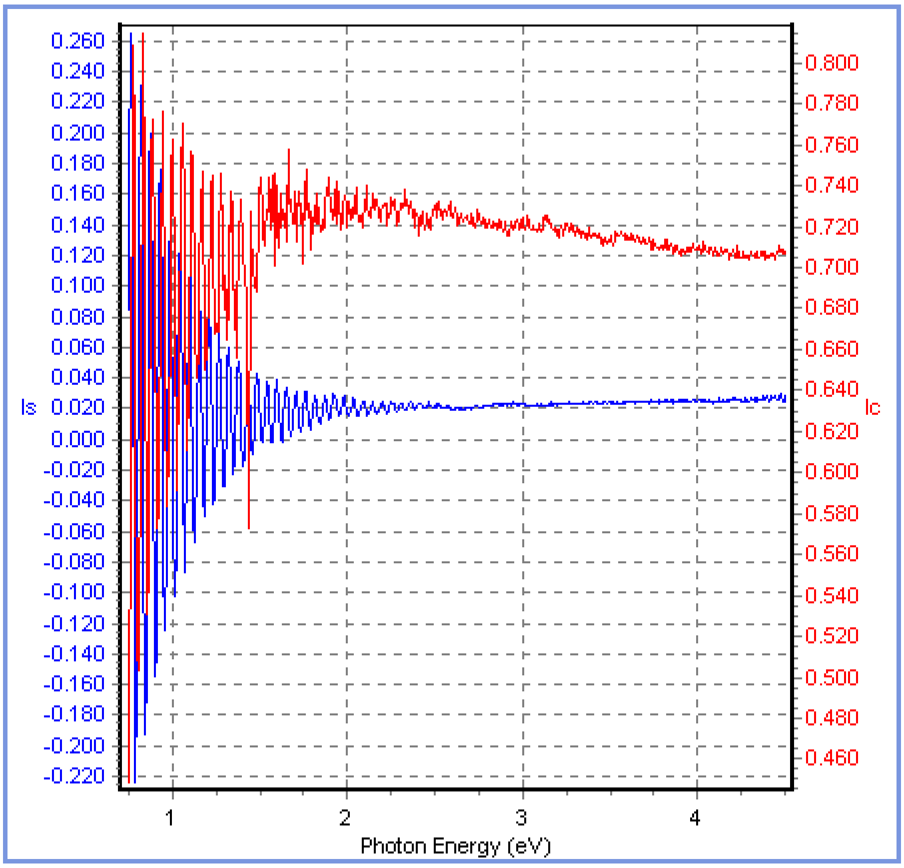
The fit is excellent so that the optical properties of SiO_2 correspond to the used reference file.

The dispersion of SiO_2 is displayed below:



11.5.1.4 Measurement of the OPSL sample:

Below the acquired spectrum:



The spectrum is acquired in the range 0.750 - 4.5eV (275-1700nm) which corresponds to the transparent region of SiO_2.

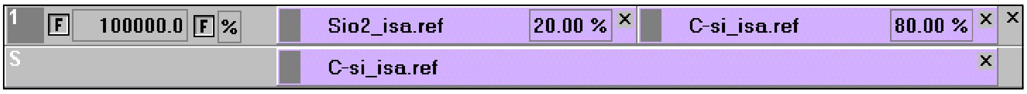
The amplitude of the interference fringes decreases fast around 1.5eV. We can ascribe this unexpected behaviour to the fact that the OPSL layer is a mixture of transparent SiO_2, void and c-Si. c-Si is already absorbent around 2 ~ 3eV.

Because of the absorption we better fit in the spectral range 0.75 - 1.40eV (885 - 1700nm) to determine the thickness of the OPSL layer.

11.5.1.5 OPSL results and comments

The OPSL layer should be a mixture of SiO_2, c-Si and void. Thus the layer is a mixture of a high index component (C-si) and two low index components (SiO_2 and void). The index of void and SiO_2 are close compared to the index of c-Si so that we actually cannot distinguish between SiO_2 and SiO_2 + void. There would be strong correlation between these two components.

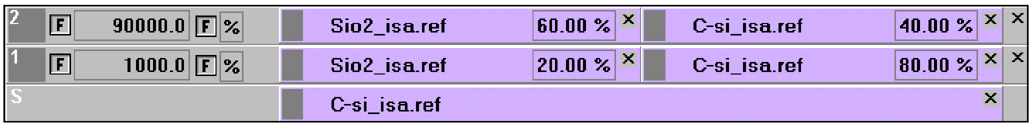
Therefore we can start with the following model: one layer which is composed of c-Si with inclusions of SiO_2:



1 F 100000.0 F % Sio2_isa.ref 20.00 % C-si_isa.ref 80.00 %
S C-si_isa.ref

This first attempt provides a very bad fit with $\chi^2 \approx 2500$ so that we have to improve the model.

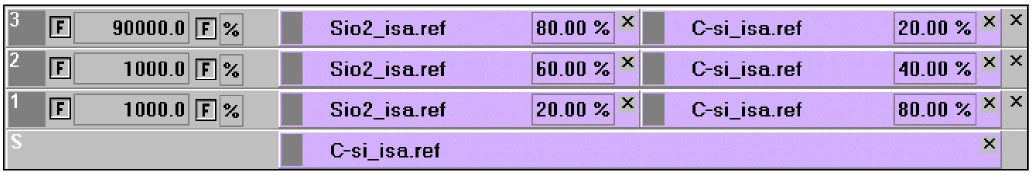
The process of OPSL deposition suggests a dependency of SiO_2 proportion on depth within the film. So that we create a succession of EMA layers with increasing SiO_2 content from bottom to top:



2 F 90000.0 F % Sio2_isa.ref 60.00 % C-si_isa.ref 40.00 %
1 F 1000.0 F % Sio2_isa.ref 20.00 % C-si_isa.ref 80.00 %
S C-si_isa.ref

We choose 90000Å for the top layer and 1000 Å for the bottom layer. The total thickness of the layers should be around 100000Å. Then there are two possible approaches: the top layer has a high index (higher c-Si content than SiO_2) or a low index (lower c-Si content than SiO_2). Both approaches lead to bad fit results with χ^2 values around 500 ~ 570. However, fits are already better than in the previous model.

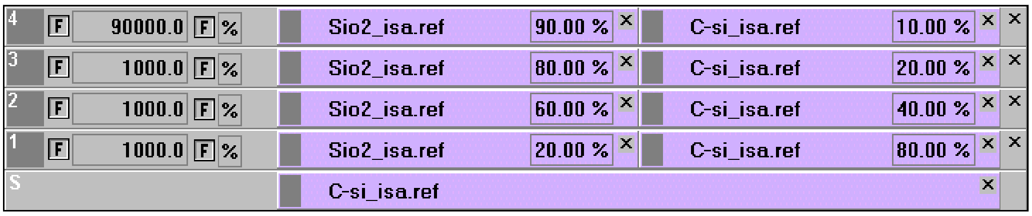
We continue adding layers:



3 F 90000.0 F % Sio2_isa.ref 80.00 % C-si_isa.ref 20.00 %
2 F 1000.0 F % Sio2_isa.ref 60.00 % C-si_isa.ref 40.00 %
1 F 1000.0 F % Sio2_isa.ref 20.00 % C-si_isa.ref 80.00 %
S C-si_isa.ref

The χ^2 value drops now sharply to 80 ~ 90.

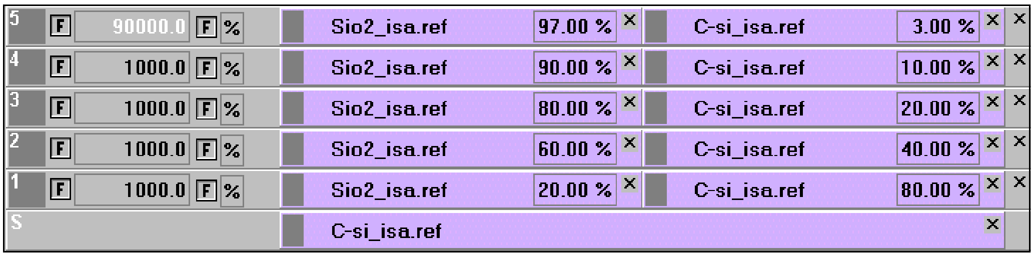
We continue adding layers:



4	F	90000.0	F	%	Sio2_isa.ref	90.00 %	C-si_isa.ref	10.00 %
3	F	1000.0	F	%	Sio2_isa.ref	80.00 %	C-si_isa.ref	20.00 %
2	F	1000.0	F	%	Sio2_isa.ref	60.00 %	C-si_isa.ref	40.00 %
1	F	1000.0	F	%	Sio2_isa.ref	20.00 %	C-si_isa.ref	80.00 %
S					C-si_isa.ref			

The χ^2 value drops to ~10.

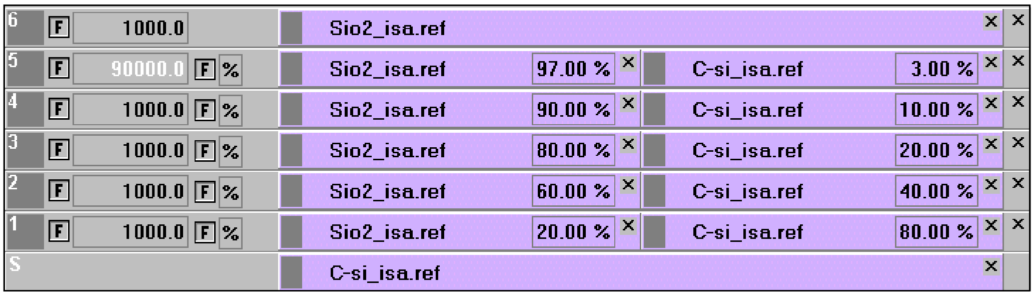
We add now a final layer close to 100% SiO_2 on top. We suppose that this layer is the thickest, however, we try now different thickness start values by using the ***multiguess absolute*** function. We try start values in the interval 80000 - 110000Å (increment 5000Å) and get the following final result:



5	F	90000.0	F	%	Sio2_isa.ref	97.00 %	C-si_isa.ref	3.00 %
4	F	1000.0	F	%	Sio2_isa.ref	90.00 %	C-si_isa.ref	10.00 %
3	F	1000.0	F	%	Sio2_isa.ref	80.00 %	C-si_isa.ref	20.00 %
2	F	1000.0	F	%	Sio2_isa.ref	60.00 %	C-si_isa.ref	40.00 %
1	F	1000.0	F	%	Sio2_isa.ref	20.00 %	C-si_isa.ref	80.00 %
S					C-si_isa.ref			

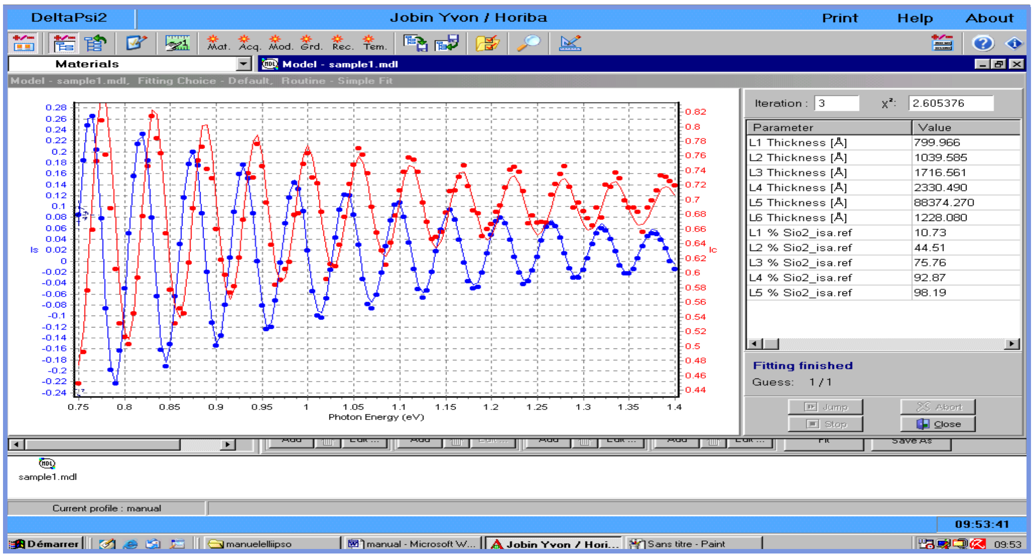
We get a χ^2 value of 4.73.

Physically the top layer should be 100% SiO_2. So we add a “thin” layer of pure SiO_2 on top:



6	F	1000.0			Sio2_isa.ref			
5	F	90000.0	F	%	Sio2_isa.ref	97.00 %	C-si_isa.ref	3.00 %
4	F	1000.0	F	%	Sio2_isa.ref	90.00 %	C-si_isa.ref	10.00 %
3	F	1000.0	F	%	Sio2_isa.ref	80.00 %	C-si_isa.ref	20.00 %
2	F	1000.0	F	%	Sio2_isa.ref	60.00 %	C-si_isa.ref	40.00 %
1	F	1000.0	F	%	Sio2_isa.ref	20.00 %	C-si_isa.ref	80.00 %
S					C-si_isa.ref			

The experimental (dots) and fit (lines) data are shown below:

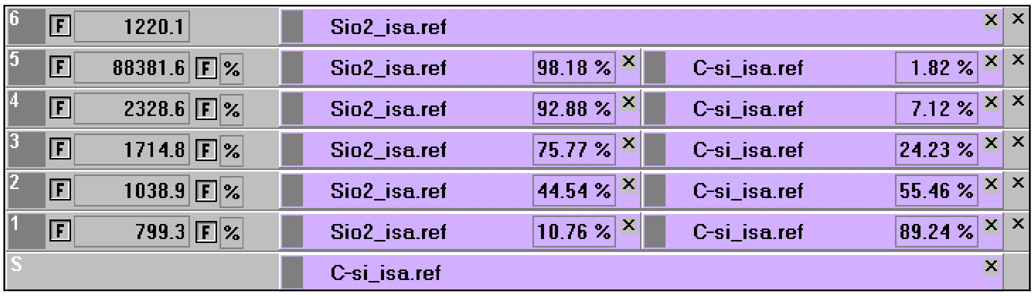


Iteration : 3 χ²: 2.605376

Parameter	Value
L1 Thickness [Å]	799.966
L2 Thickness [Å]	1039.585
L3 Thickness [Å]	1716.561
L4 Thickness [Å]	2330.490
L5 Thickness [Å]	88374.270
L6 Thickness [Å]	1228.080
L1 % Sio2_isa.ref	10.73
L2 % Sio2_isa.ref	44.51
L3 % Sio2_isa.ref	75.76
L4 % Sio2_isa.ref	92.87
L5 % Sio2_isa.ref	98.19

Fitting finished
Guess: 1 / 1

The results for thickness and composition of each individual layer can be seen in the next figure:



6	F	1220.1			Sio2_isa.ref			
5	F	88381.6	F	%	Sio2_isa.ref	98.18 %	C-si_isa.ref	1.82 %
4	F	2328.6	F	%	Sio2_isa.ref	92.88 %	C-si_isa.ref	7.12 %
3	F	1714.8	F	%	Sio2_isa.ref	75.77 %	C-si_isa.ref	24.23 %
2	F	1038.9	F	%	Sio2_isa.ref	44.54 %	C-si_isa.ref	55.46 %
1	F	799.3	F	%	Sio2_isa.ref	10.76 %	C-si_isa.ref	89.24 %
S					C-si_isa.ref			

The best χ^2 value is 2.60 with a total OPSL layer thickness of 95483.3Å.

11.6 Multilayers

11.6.1 Eight layer High-Low Stack on Silicon

11.6.1.1 Key points

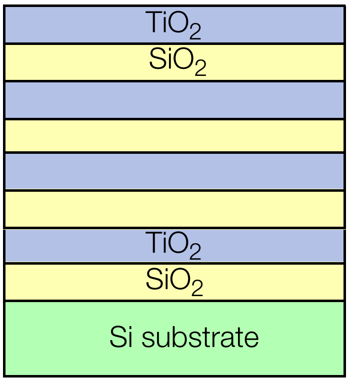
- layer repetition
- layer correlation

11.6.1.2 Typical settings of acquisition parameters:

Sample	4 repetitions of TiO_2/SiO_2 on Si
Spectral range	1.5 – 6.5eV (825 – 190nm)
Increment	0.050eV
AOI	70°

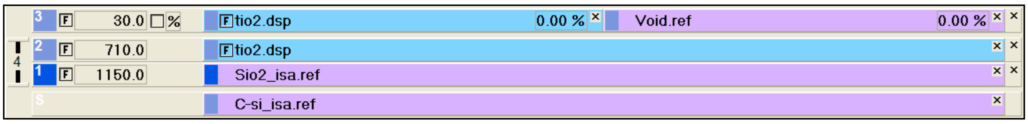
Spot size	1mm x 3mm
Integration time	200ms
Configuration	II

In this example we will fit ellipsometric data from a eight layer high-low index stack deposited on silicon substrate to determine the refractive indexes and thicknesses of all eight layers. The sample structure is approximately 4 x (1150Å TiO_2 / 710 Å SiO_2) / Si:



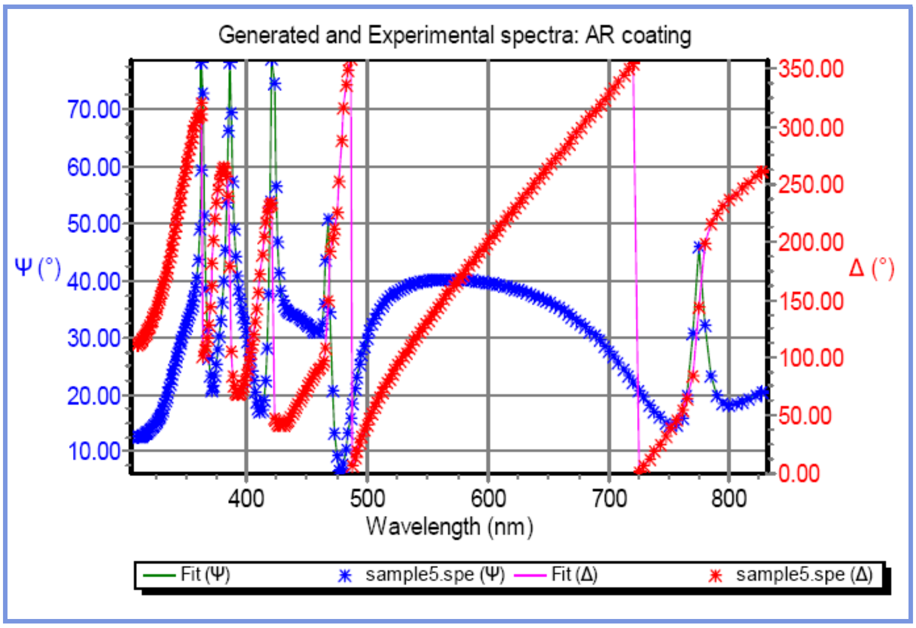
11.6.1.3 Experiment

The corresponding Layer model is the following::



3	F	30.0 ☐ %	F tio2.dsp	0.00 %	Void.ref	0.00 %
2	F	710.0	F tio2.dsp			
1	F	1150.0	Sio2_isa.ref			
S			C-si_isa.ref			

It consists of a repetition (4x) of the SiO_2/TiO_2 stack and a roughness layer on top. The measurements and the fit with this model is shown below.



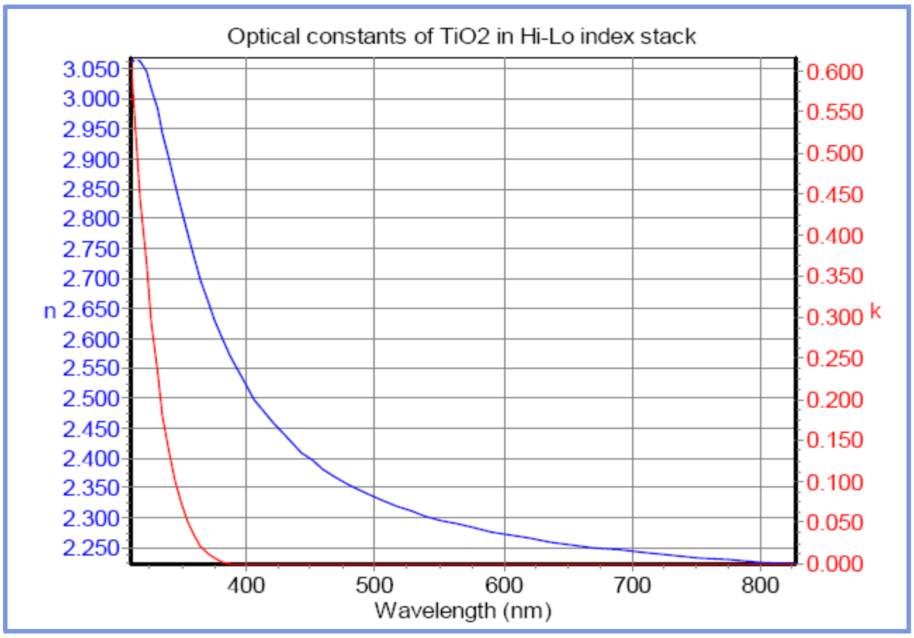
We get the average thickness of the SiO_2 and the TiO_2 layer as well as the average dispersion of the TiO_2 layer. Additionally we get of course the thickness of the roughness layer:

Average thickness SiO_2: 1162Å

Average thickness TiO_2: Å

Thickness roughness:

Dispersion of TiO_2:



11.7 Complicated dispersions

11.7.1 NK-fit for an organic layer

11.7.1.1 Key points

- Performing a NK-fit
- Creation of calculated files *.clc
- Refractive index /dielectric constant extension to a higher range

11.7.1.2 Typical settings of acquisition parameters:

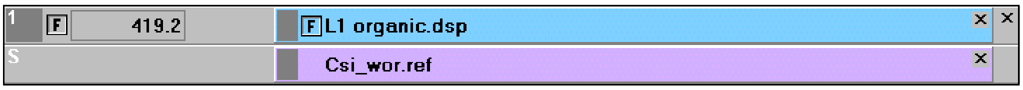
Sample	Organic layer
Spectral range	1.5 – 6.5eV
Increment	0.050eV

AOI	70°
Spot size	1mm x 3mm
Integration time	200ms
Configuration	II

This analysis is performed on an unknown organic layer of ca. 400Å thickness. The difficulty here is that none of the dispersion models is able to provide a good fit over the entire measurement range of 1.5 - 6.5eV. A good fit can only be obtained in the reduced spectral range of 1.5 - 5eV.

Thickness and optical properties can be determined from 1.5 – 5eV. To get the optical constant also from 5eV to 6.5eV with the same precision that we have for the reduced range 1.5-5eV we can use the ***NK-fit*** function. This function allows direct calculation of n and k in the spectral region of interest if all other parameters including thickness are well known and fixed.

The model for the reduced range of 1.5 - 5eV is a single layer model with a multiple oscillator dispersion. In this case we use ***Triple New Amorphous*** (classical dispersion would provide similar results). For the substrate we use the material file Csi_wor.ref that provides data points in the UV region, which we need later:



1 F 419.2 F L1 organic.dsp

S Csi_wor.ref

It is not straight forward to find the set of parameters for this kind of dispersion.

The method we suggest is to begin with simple or double oscillators and to launch a fit on the interval 1.5 - 3.5eV or 1.5 - 4eV. Try different start values for the dispersion parameters until the χ^2 value cannot be improved anymore.

Select now a dispersion of the same type with a higher number of oscillators (for example New Amorphous → Double New Amorphous) and launch the fit on the same interval (using the previously found parameters as start values).

If there is an improvement of the fit try to extend the range, for example: 1.5 – 4eV or 1.5 – 4.5eV.

Carry on adding oscillators and extending the range as long as the χ^2 value can be improved.

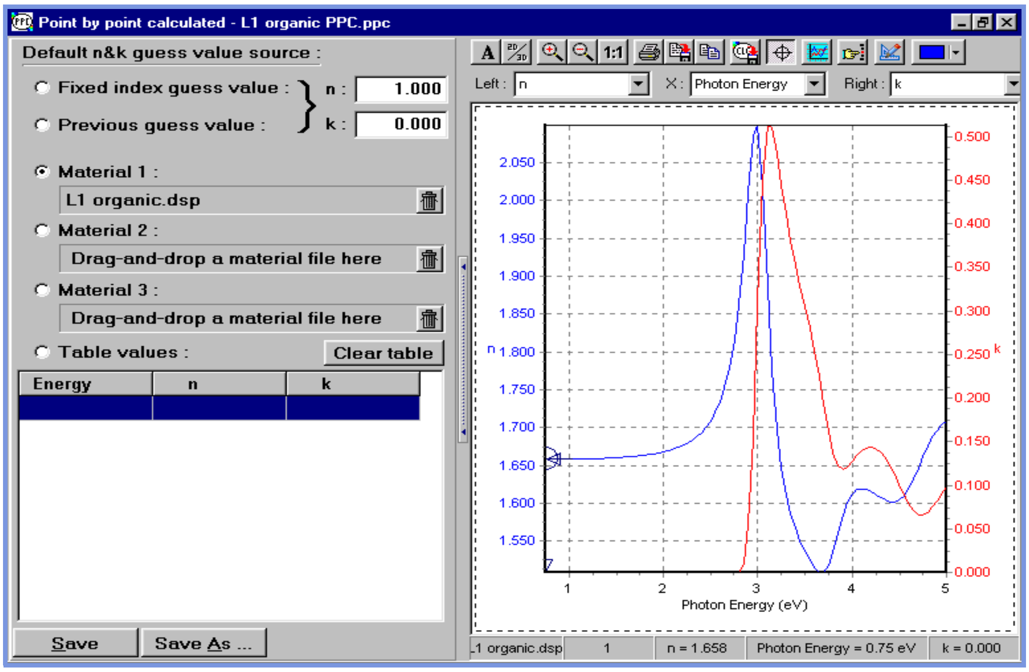
With Triple New Amorphous we get a χ^2 value of 2 and a thickness of 419.2Å in the range 1.5 - 5eV. The dispersion parameters are displayed below. Once we exceed 5eV the fit starts to deteriorate and the χ^2 value increases. That is the point where we better use the NK-fit function to obtain *n* and *k* until 6.5eV.

The dispersion parameters (triple new amorphous) for the reduced range 1.5 – 5eV are:

n_∞	1.6658216
ω_g	2.7930357
F_1	-0.0048616
ω_1	4.6567426
Γ_1	0.3770423

F_2	0.1749506
ω_2	3.0110691
Γ_2	0.1551019
F_3	-0.0077110
ω_3	3.8020499
Γ_3	0.2434855

To use the NK-fit function click on ***Mat***. and select ***Point by Point Calculated***. Drag and drop the dispersion that was found in the reduced range to the material 1 box and activate the box:



Point by point calculated - L1 organic PPC.ppc

Default n&k guess value source :

○ Fixed index guess value : n : 1.000

○ Previous guess value : k : 0.000

● Material 1 : L1 organic.dsp

○ Material 2 : Drag-and-drop a material file here

○ Material 3 : Drag-and-drop a material file here

○ Table values :

Energy	n	k

Left : n X : Photon Energy Right : k

L1 organic.dsp | 1 | n = 1.658 | Photon Energy = 0.75 eV | k = 0.000

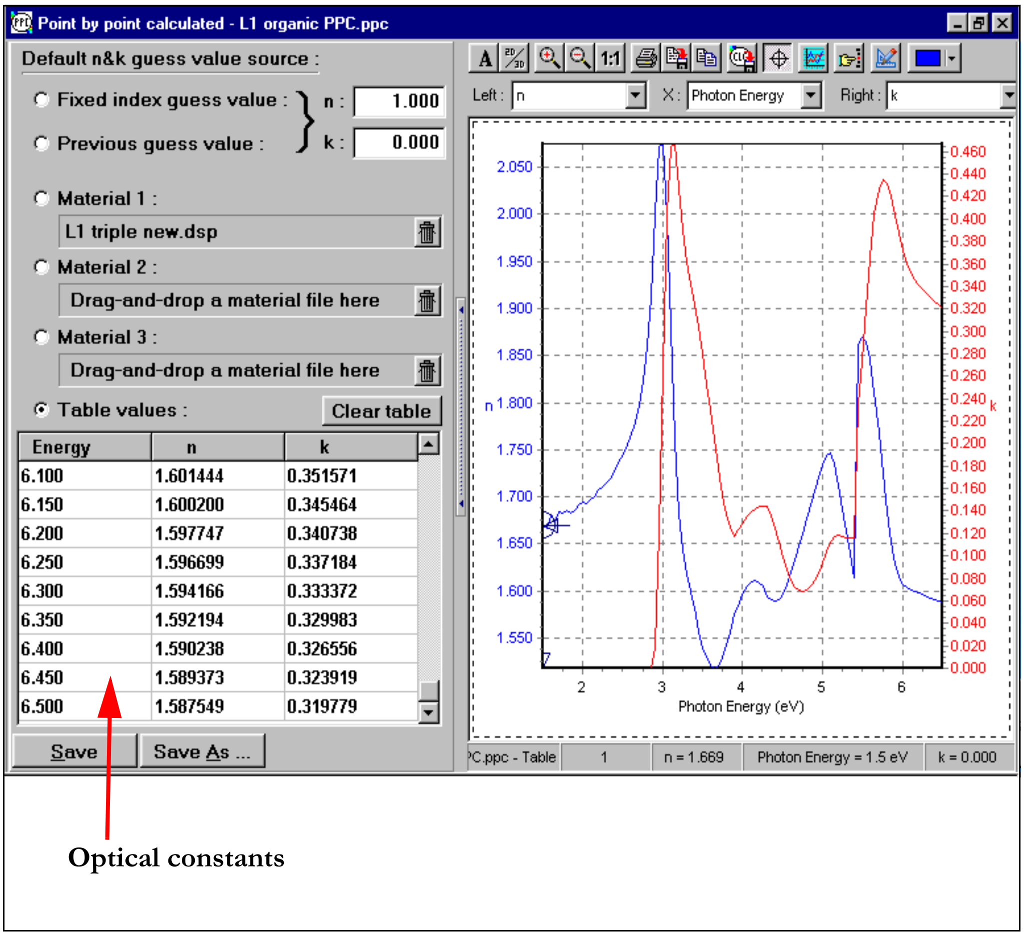
Then replace the dispersion layer of your model by the PPC layer you just created:

1	419.2	NK F	L1 organic PPC.ppc
S			Csi_wor.ref

The dispersion of the layer is now fitted at a fixed layer thickness (obtained by fitting in the reduced range).

Launch the fit in the spectral region 1.5 - 6.5eV (using the Levenberg-Marquardt algorithm). The fit should give a χ^2 value of 0. Update the model and the PPC file to get the dispersion of the layer in the complete spectral range.

Opening the PPC file in the material folder to get access to the optical constants:



Point by point calculated - L1 organic PPC.ppc

Default n&k guess value source :

○ Fixed index guess value : n : 1.000

○ Previous guess value : k : 0.000

○ Material 1 : L1 triple new.dsp

○ Material 2 : Drag-and-drop a material file here

○ Material 3 : Drag-and-drop a material file here

● Table values :

Energy	n	k
6.100	1.601444	0.351571
6.150	1.600200	0.345464
6.200	1.597747	0.340738
6.250	1.596699	0.337184
6.300	1.594166	0.333372
6.350	1.592194	0.329983
6.400	1.590238	0.326556
6.450	1.589373	0.323919
6.500	1.587549	0.319779

Left : n X : Photon Energy Right : k

C.ppc - Table | 1 | n = 1.669 | Photon Energy = 1.5 eV | k = 0.000

Optical constants

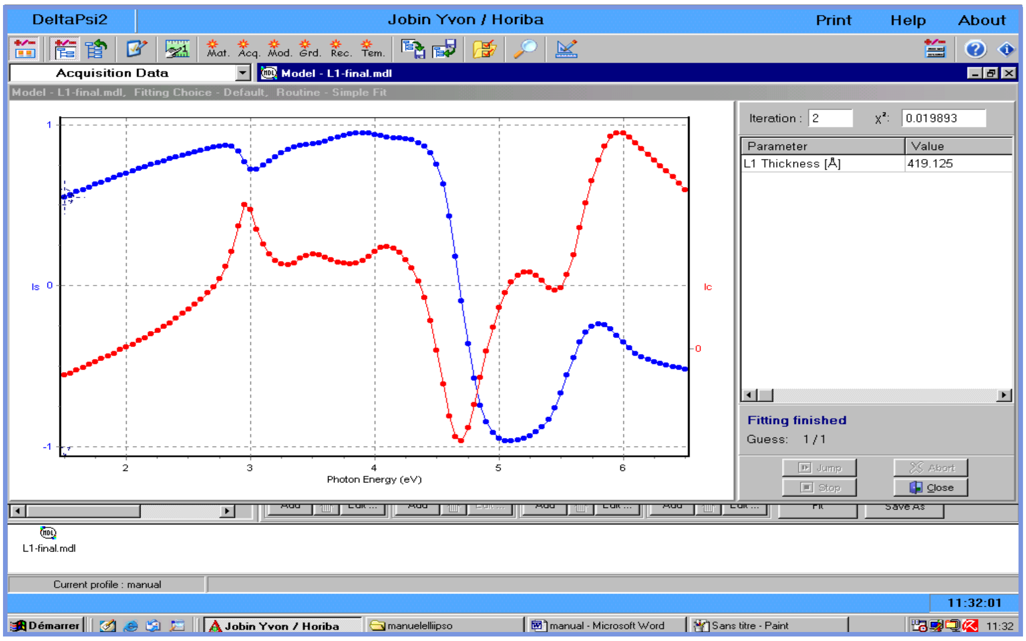
You can also create a *.clc file which can be used as a reference file of the organic layer by activating the box ***Table values*** and clicking on the icon CLC .

Now we can use the PPC file in the model:

1 F 419.1 L1 organic CLC.clc

S Csi_wor.ref

and fit the thickness over the entire spectral range:



Model - L1-final.mdl, Fitting Choice - Default, Routine - Simple Fit

Iteration : 2 χ^2: 0.019893

Parameter	Value
L1 Thickness [Å]	419.125

Fitting finished

Guess: 1 / 1

Current profile : manual

11:32:01

The result is:

thickness = 419.125Å

χ^2 **= 0.019893**

Note that χ^2 value is not exactly 0. This is due to the fact that for the PPC calculation we used start values (thickness of 419.2Å) that are not 100% exact. Hence, the calculated material contains little imperfections but is still very close to reality.

11.7.1.3 Interpretation

The starting point of the NK-fit is to obtain the best fit possible in a reduced spectral range (here for example 1.5 - 5eV instead of 1.5 - 6.5eV) to determine the thickness and dispersion of the layer.

Then these values are fixed and the optical constants *n* and *k* are calculated in the complete spectral range.

However, keep in mind the NK-fit provides results from a calculation and not from a measurement. The quality of the results depends directly on the quality of the model. Important is to obtain a very good fit in the reduced spectral range.

11.7.2 Quaternary semiconductor material

11.7.2.1 Key points

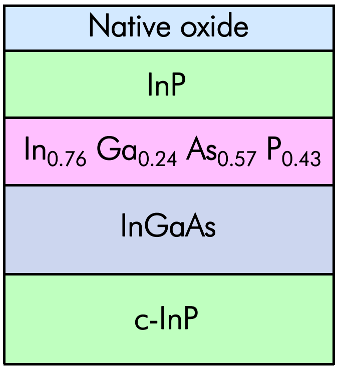
- Alloy function

9/2/08

11.7.2.2 Typical settings of acquisition parameters:

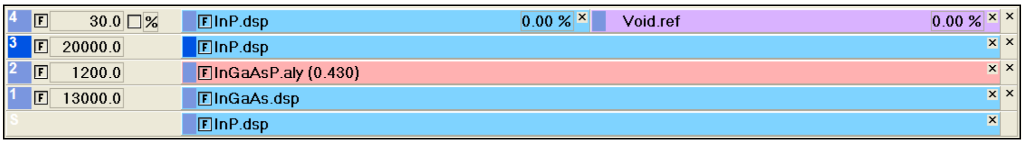
Sample	**Photodiode structure**
Spectral range	1.5 – 6.5eV
Increment	0.050eV
AOI	70°
Spot size	1mm x 3mm
Integration time	200ms
Configuration	II

Sample structure:



11.7.2.3 Experiment

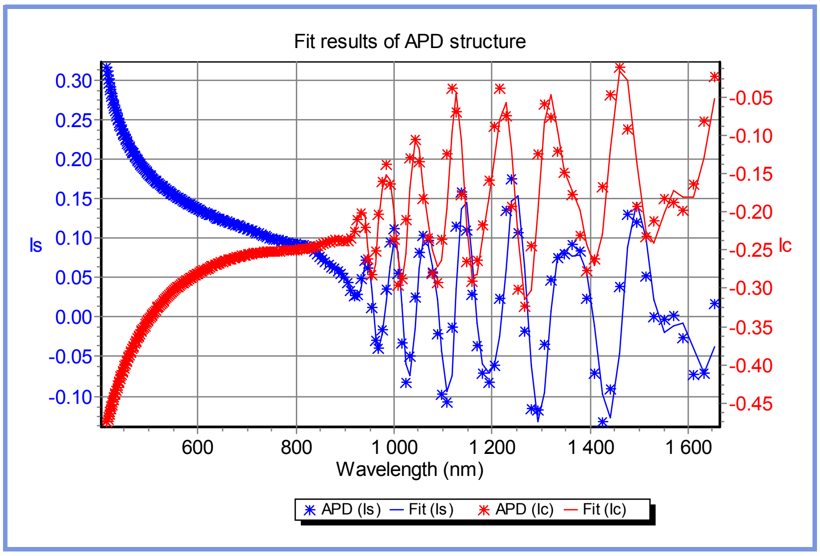
The corresponding layer model is the following:



```
4  F     30.0 ☐%   F InP.dsp              0.00 % ×   Void.ref   0.00 % × ×
3  F  20000.0      F InP.dsp                                           × ×
2  F   1200.0      F InGaAsP.aly (0.430)                               × ×
1  F  13000.0      F InGaAs.dsp                                        × ×
S                  F InP.dsp                                           ×
```

It consists of a InP substrate, a InGaAs, InGaAsP and InP layer with an overlayer on top. The dispersion of InP and InGaAs was modeled with the Kato-Adachi dispersion formula. For the quaternary material the alloy function was used.

The measurements and the fit with this model is shown below.



As a result we get the thickness of each individual layer and the dispersion of the materials. For the quaternary material we also can derive the composition:

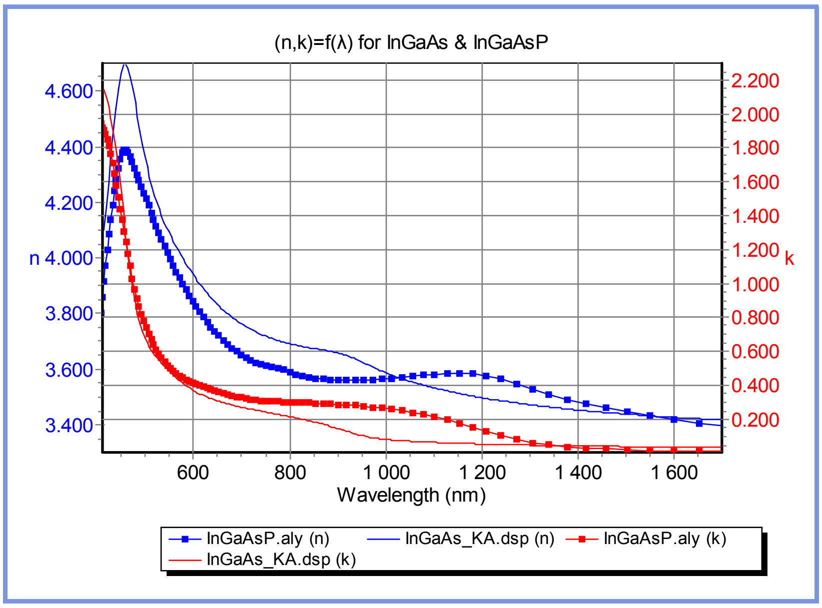
Thickness InGaAs: 13095Å

Thickness $In_{0.76}Ga_{0.24}As_{0.57}P_{0.43}$: 1192Å

Thickness InP: 20525Å

Thickness overlayer: 21Å

Dispersions:



11.8 Inhomogeneous layers

11.8.1 Polymer / ITO on glass substrate

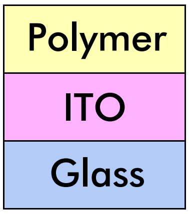
11.8.1.1 Key points

- graded index layer

11.8.1.2 Typical settings of acquisition parameters:

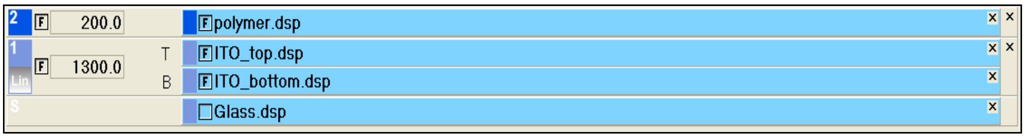
Sample	Polymer / ITO on glass
Spectral range	1.5-6.5eV (825-190nm)
Increment	0.050eV
A.O.I	58°
Spot size	1mm
Integration time	200ms

The measurements and the fit with this model is shown below.



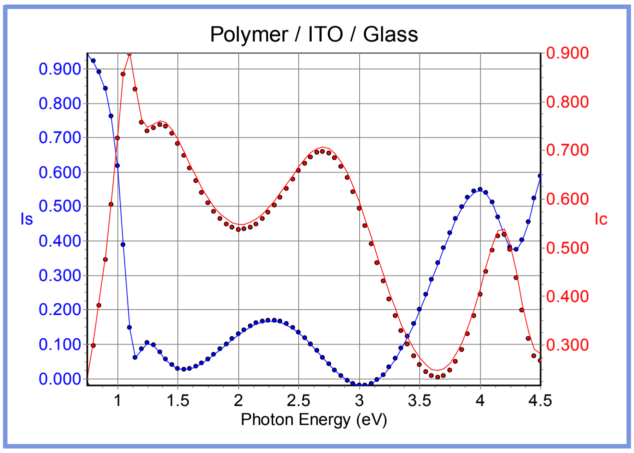
11.8.1.3 Experiment

ITO is a semi-transparent conducting material that exhibits absorption in the FUV and NIR. It is known to be inhomogeneous due to deposition methods and post-treatments. A graded layer model has therefore to be taken into account:


2 F 200.0 F polymer.dsp
1 F 1300.0 T F ITO_top.dsp
Lin B F ITO_bottom.dsp
S ☐Glass.dsp

For both the polymer and the ITO we use the classical oscillator model for the dispersion.

The experimental data and the fit are shown below:

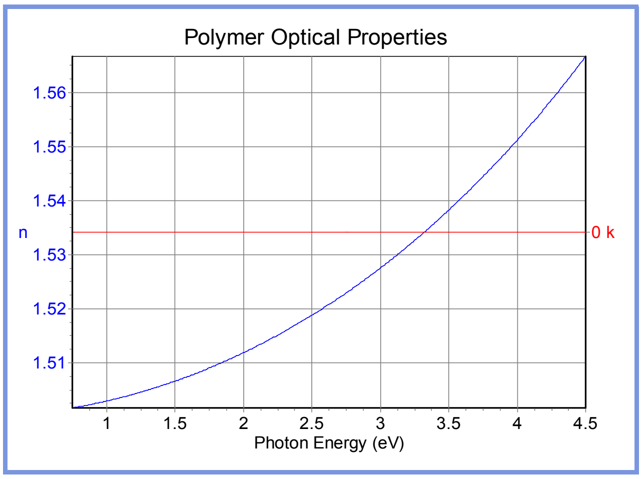


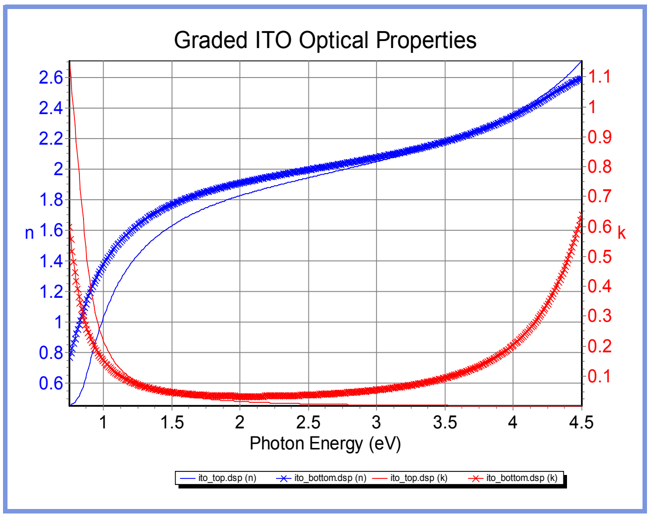
As a result we get the thickness of both layers and the optical constants:

Thickness ITO layer: 1280Å

Thickness Polymer layer: 210Å

Dispersions:





11.9 Parameter correlation

11.9.1 TiO_2 on Glass: Bound Multimodel

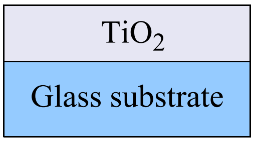
11.9.1.1 Key points

- Bound Multimodel
- Transparent substrate
- Reflection and Transmission data

11.9.1.2 Typical settings of acquisition parameters:

Sample	TiO_2 on glass
Spectral range	1.5 – 6.5eV (190 – 825nm)
Increment	0.050eV
AOI (SE)	70°
Spot size	1mm x 3mm
Integration time	200ms
Configuration	II

Sample structure:

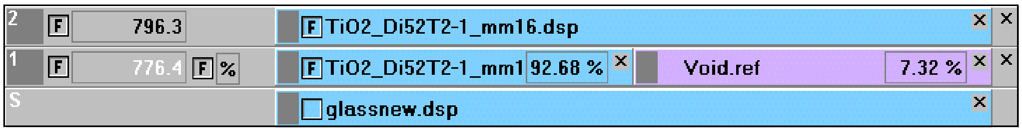


In this example we analyze a TiO_2 layer on a glass substrate. The TiO_2 layer is not homogeneous in depth. Therefore we model the TiO_2 layer with two layers:

A top layer of TiO_2 modelled by an appropriate dispersion formula and a bottom layer described by an EMA of TiO_2 and Void.

The sample is equally coated on both sides. Measurements are performed in transmission and in reflection.

The model for the reflection measurement is the following:



2 796.3 TiO2_Di52T2-1_mm16.dsp

1 776.4 TiO2_Di52T2-1_mm1 92.68 % Void.ref 7.32 %

S glassnew.dsp

On layer 1 the thickness is fitted in the multiguess absolute mode (range: 0.1 to 1000Å/ increment: 200Å).

The model for the transmission measurement is the following:

5	F	796.3		F TiO2_Di52T2-1_mm16.dsp			
4	F	776.4	F %	F TiO2_Di52T2-1_mm1	92.68 %	Void.ref	7.32 %
3	☐	10000000.0		☐ glassnew.dsp			
2	☐	L4*1.000	☐ %	F TiO2_Di52T2-1_mm1	92.68 %	Void.ref	7.32 %
1	☐	L5*1.000		F TiO2_Di52T2-1_mm16.dsp			
S				Void.ref			

Here the multiguess absolute mode (range: 0.1 to 1000Å / increment: 200Å) for fitting the thickness is applied to layer 4.

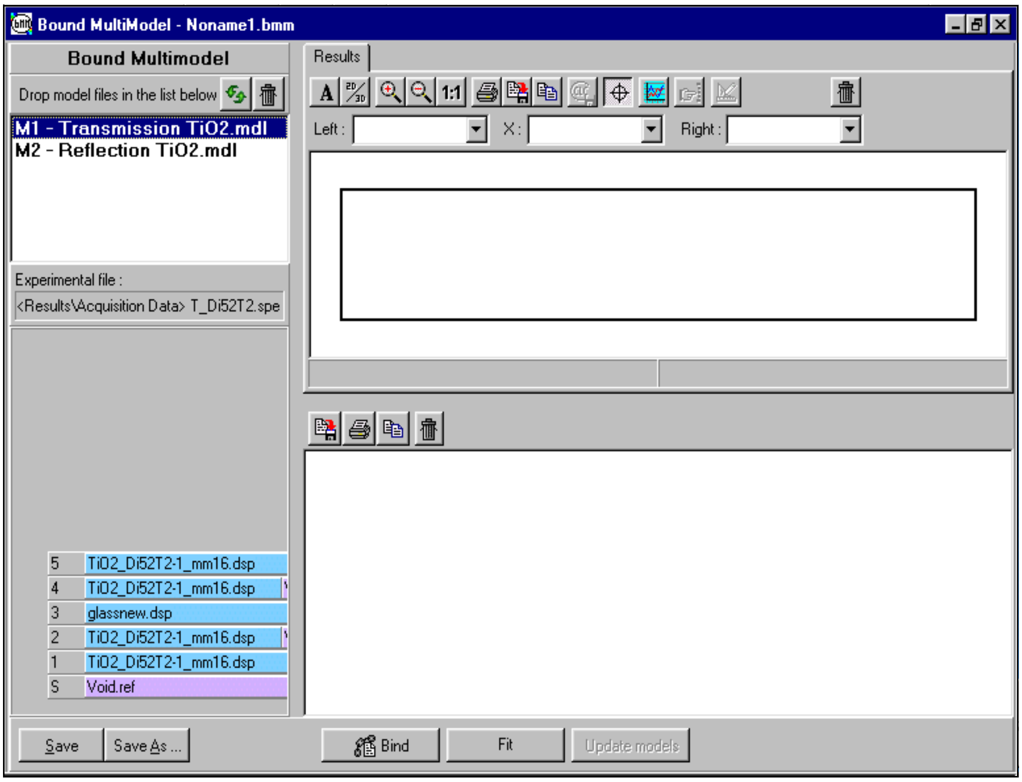
We set a correlation between layer 2 and 4, between layer 1 and 5 and between the proportions of layer 2 and 4. The "***Correlated to***" feature can be selected by left-clicking on the thickness/proportion value of the layer of interest.

In transmission the light beam goes through the entire sample. Therefore we set the Void.ref file as the substrate in the layer model.

Now we can combine the two different measurements and two different models for the sample. The dispersion that is used for TiO_2 must be of course the same for the two models. Also, the thickness of the corresponding layers must be the same.

To meet these requirements we use the Bound Multimodel feature of the DP2 software. This feature allows to bind parameters of different models.

Click on ***Mod.*** and choose ***Bound Multimodel***. The following window appears:



M1 - Transmission TiO2.mdl
M2 - Reflection TiO2.mdl

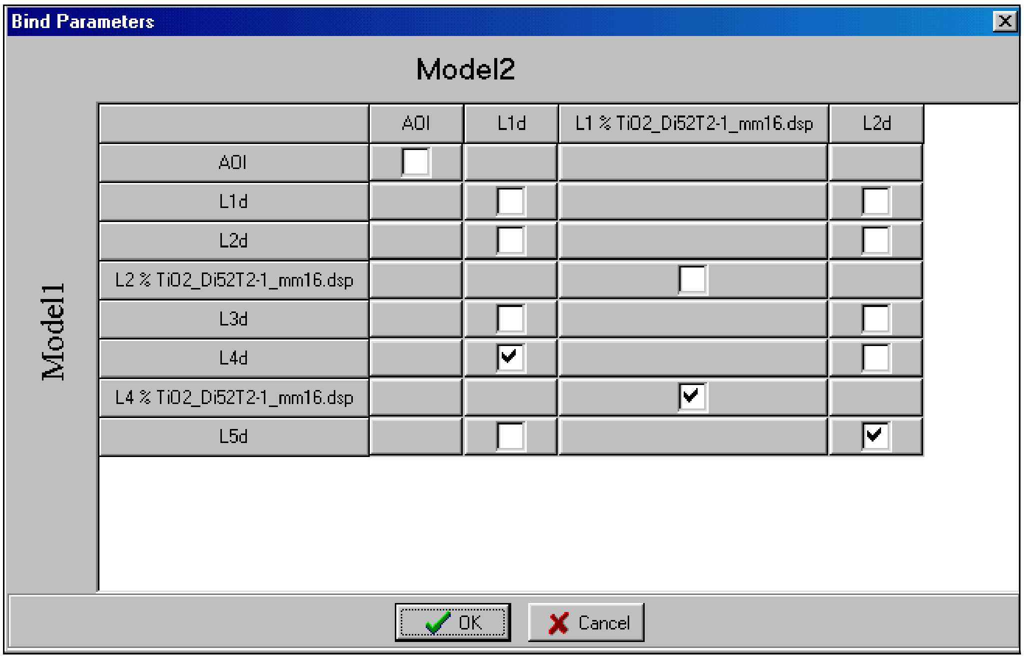
Experimental file :
<Results\Acquisition Data> T_Di52T2.spe

5	TiO2_Di52T2-1_mm16.dsp
4	TiO2_Di52T2-1_mm16.dsp
3	glassnew.dsp
2	TiO2_Di52T2-1_mm16.dsp
1	TiO2_Di52T2-1_mm16.dsp
S	Void.ref

Drop the model files of the transmission and reflection measurements in the upper left box of the Bound Multimodel window. To display one of the models, just click on it.

Binding the parameters:

Click on bind at the bottom of the window. The following window appears:



	AOI	L1d	L1 % TiO2_Di52T2-1_mm16.dsp	L2d
AOI	☐			
L1d		☐		☐
L2d		☐		☐
L2 % TiO2_Di52T2-1_mm16.dsp			☐	
L3d		☐		☐
L4d		☑		☐
L4 % TiO2_Di52T2-1_mm16.dsp			☑	
L5d		☐		☑

In this case model 1 is the model for the transmission measurement and model 2 is the model for the reflection measurement.

Now we activate the boxes to bind the following parameters:

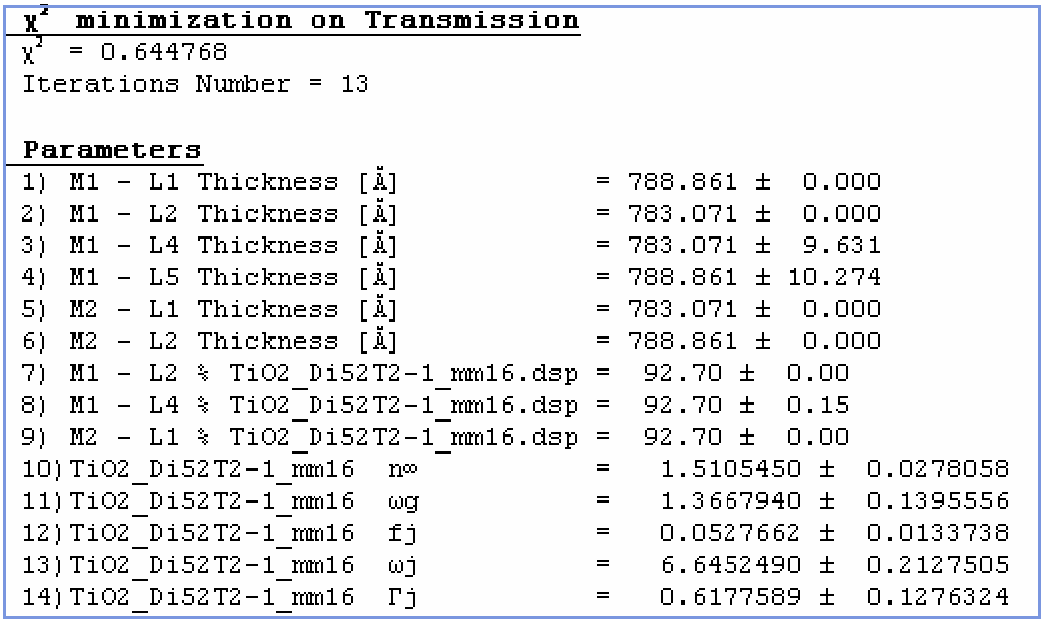
- thickness of layer 4 of model 1 with thickness of layer 1 of model 2
- thickness of layer 5 of model 1with thickness of layer 2 of model 2
- composition of layer 4 of model 1with the composition of layer 1 of model 2.

Now we can launch the fit.

11.9.1.3 Results and Comments

The following two graphs show the experimental results and fits.

We obtain the following set of parameters with a χ^2 value of 0.644768:

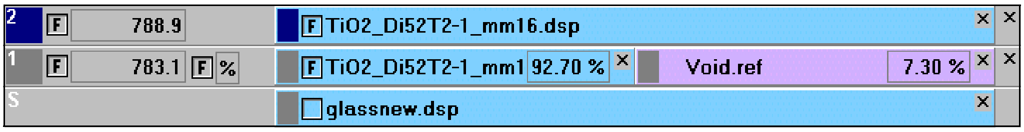


```
χ²  minimization on Transmission
χ²  = 0.644768
Iterations Number = 13

Parameters
1) M1 - L1 Thickness [Å]           = 788.861 ±  0.000
2) M1 - L2 Thickness [Å]           = 783.071 ±  0.000
3) M1 - L4 Thickness [Å]           = 783.071 ±  9.631
4) M1 - L5 Thickness [Å]           = 788.861 ± 10.274
5) M2 - L1 Thickness [Å]           = 783.071 ±  0.000
6) M2 - L2 Thickness [Å]           = 788.861 ±  0.000
7) M1 - L2 % TiO2_Di52T2-1_mm16.dsp =  92.70 ±  0.00
8) M1 - L4 % TiO2_Di52T2-1_mm16.dsp =  92.70 ±  0.15
9) M2 - L1 % TiO2_Di52T2-1_mm16.dsp =  92.70 ±  0.00
10)TiO2_Di52T2-1_mm16  n∞          =   1.5105450 ±  0.0278058
11)TiO2_Di52T2-1_mm16  ωg          =   1.3667940 ±  0.1395556
12)TiO2_Di52T2-1_mm16  fj          =   0.0527662 ±  0.0133738
13)TiO2_Di52T2-1_mm16  ωj          =   6.6452490 ±  0.2127505
14)TiO2_Di52T2-1_mm16  Γj          =   0.6177589 ±  0.1276324
```

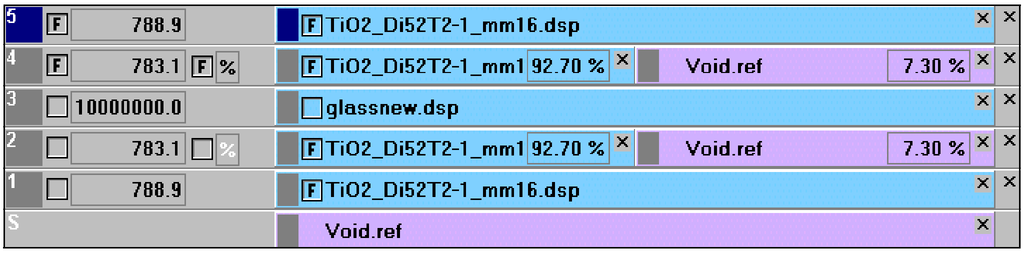
The next step is to update the models by clicking on ***update***. The models with the final parameters are then:

For reflection:



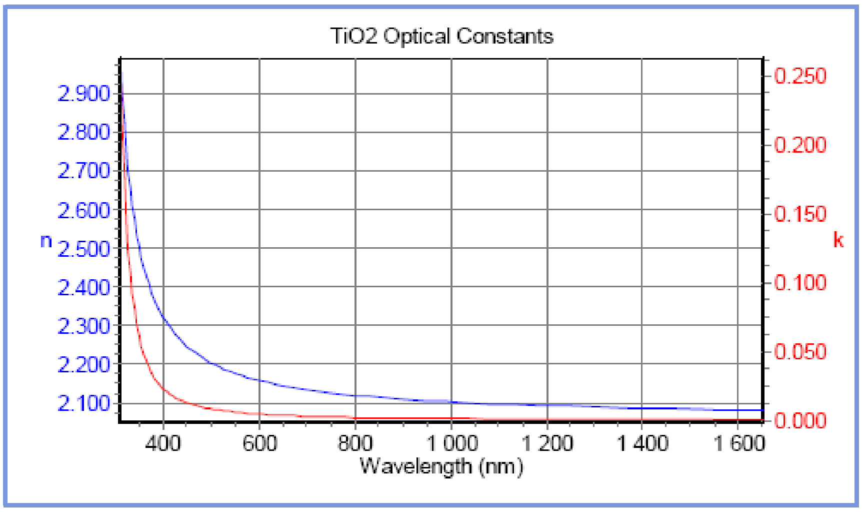
2	F	788.9			F TiO2_Di52T2-1_mm16.dsp			
1	F	783.1	F	%	F TiO2_Di52T2-1_mm1	92.70 %	Void.ref	7.30 %
S					☐ glassnew.dsp			

For transmission:



5	F	788.9			F TiO2_Di52T2-1_mm16.dsp			
4	F	783.1	F	%	F TiO2_Di52T2-1_mm1	92.70 %	Void.ref	7.30 %
3	☐	10000000.0			☐ glassnew.dsp			
2	☐	783.1	☐	%	F TiO2_Di52T2-1_mm1	92.70 %	Void.ref	7.30 %
1	☐	788.9			F TiO2_Di52T2-1_mm16.dsp			
S					Void.ref			

The thickness results are now written in the model. The dispersion of TiO_2 is shown below:



11.10Non-cubic Crystals

11.10.1 hexagonal Al_2O_3 / Al

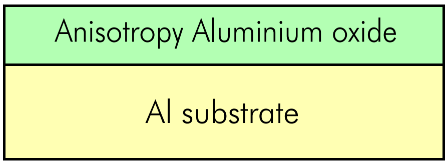
11.10.1.1 Key points

- uniaxial anisotropy

11.10.1.2 Typical settings of acquisition parameters:

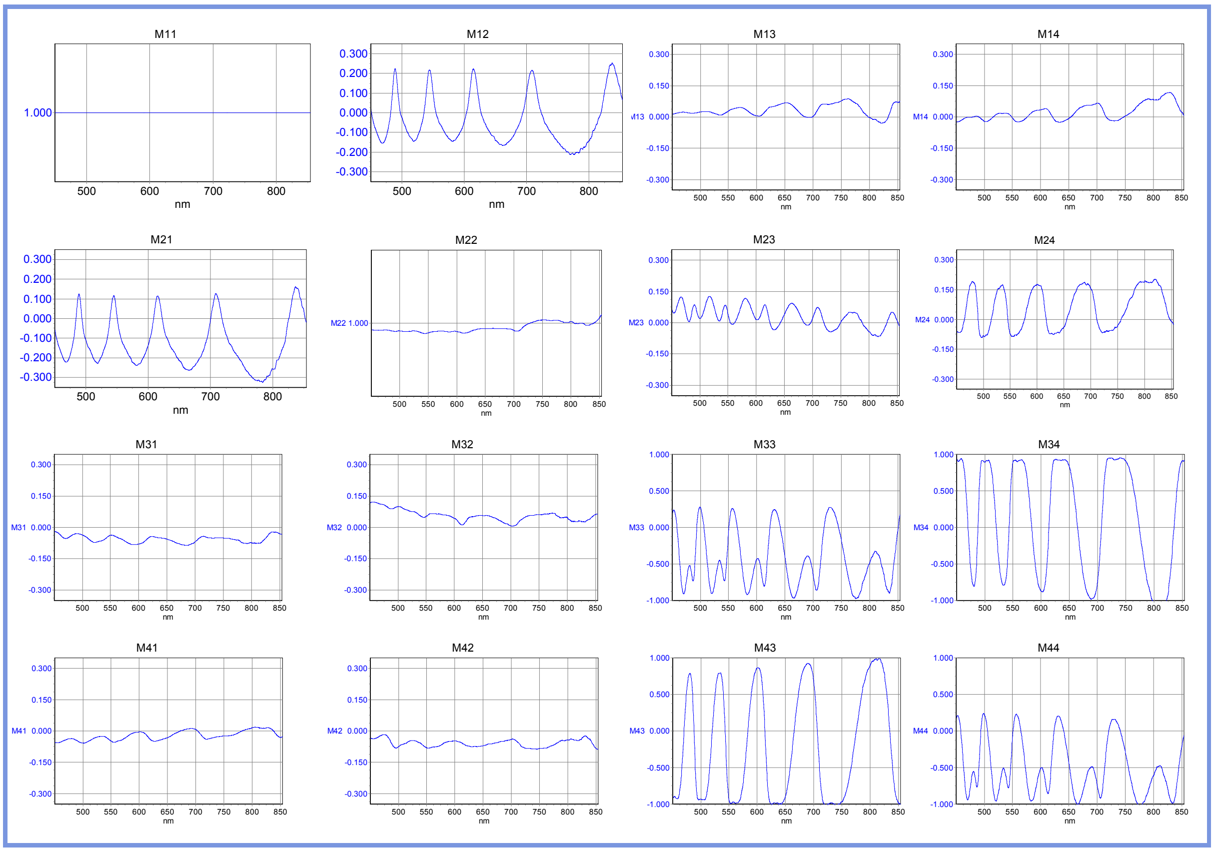
Sample	Al_2O_3 / Al
Spectral range	UVISEL: 1.5 – 6.5eV (825 – 190nm) (MM-16: 430 – 850nm)
Increment	UVISEL: 0.050eV
AOI	70°
Spot size	1mm x 3mm
Integration time	200ms
Configuration	II

Sample structure:



11.10.1.3 Experiment

Mueller Matrix measurements with the MM-16 show that the Al_2O_3 layer exhibits anisotropy because the off-diagonal elements are not 0 especially when the measurements are done in random positions that is away from the direction of the optical axis and at rotation of 90° from the optical axis and when the optical axis is not orthogonal to the sample plane.



Measurements with the UVISEL at the same spot but under different rotation around the sample normal are equal thus indicating uniaxial anisotropy of N-type. The corresponding layer model is therefore:


1 N LP S F 20000.0

E F Al2O3-E.dsp

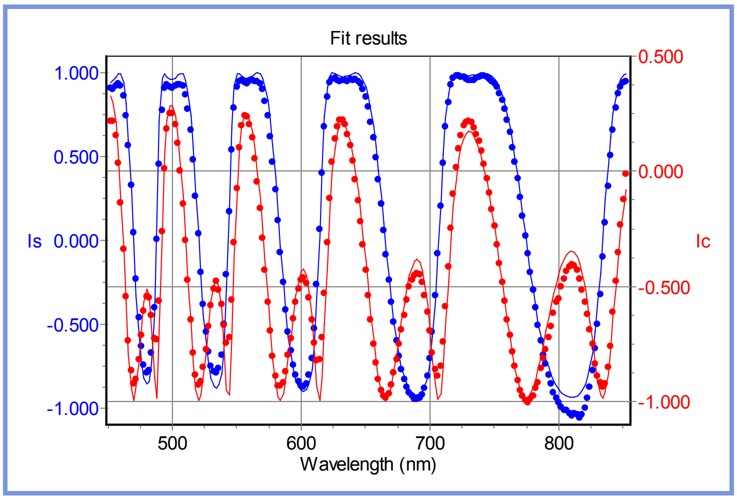
O F Al2O3-O.dsp

Al_asp.ref

It consists of one uniaxial anisotropic layer (N polarization) with two different dispersions for the ordinary (O) and the extra-ordinary direction (E). The dispersion model is the classical oscillator model:

$$\varepsilon = 1 + \frac{(\varepsilon_s - 1)\,\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\,\omega} \qquad \text{with } \Gamma_0 = 0$$

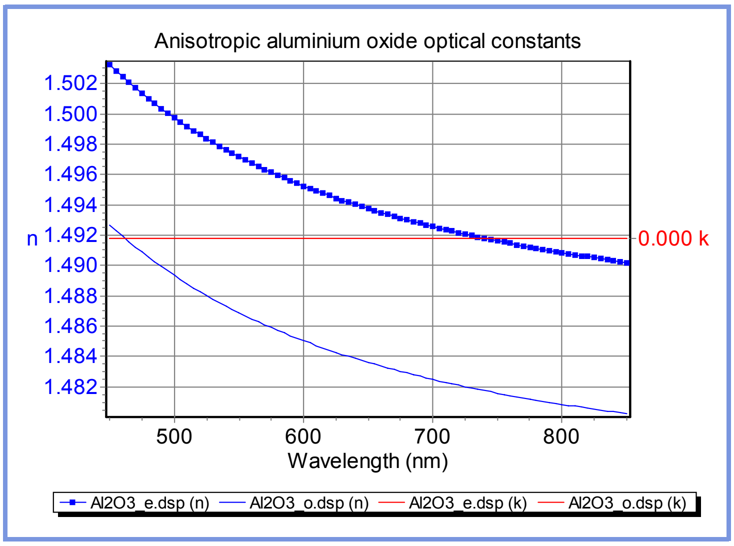
The experimental data and the fit are shown below:



As a result we get the thickness of the Al_2O_3 layer and the anisotropic optical constants:

Thickness Al_2O_3: 19940Å

Dispersions Al_2O_3:



One can observe a birefringence of n = 0.01 = n_o - n_E.

Note that the Al_2O_3 layer is porous and has therefore a rather low refractive index.

11.10.2 Strained materials

11.10.3 stretched polymer foil

11.10.3.1 Key points

- biaxial anisotropy

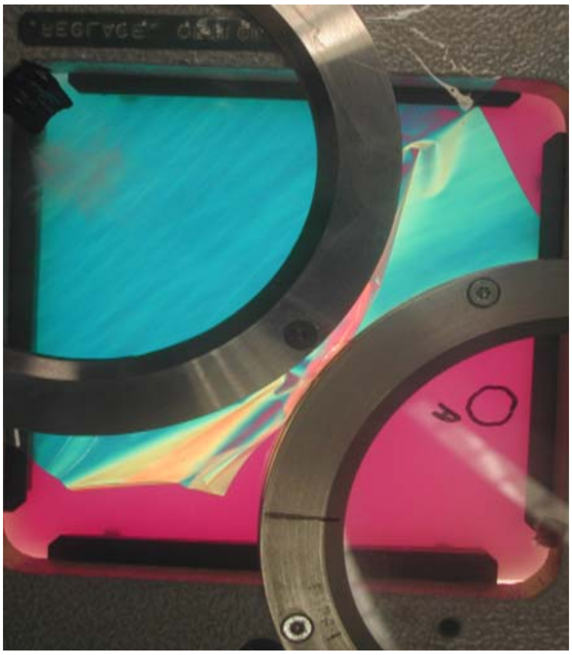
11.10.3.2 Typical settings of acquisition parameters:

Sample	PET foil
Spectral range	UVISEL: 1.5 – 6.5eV (825 – 190nm)
Increment	UVISEL: 0.050eV
AOI	70°
Spot size	1mm x 3mm
Integration time	200ms
Configuration	II

11.10.3.3 Experiment

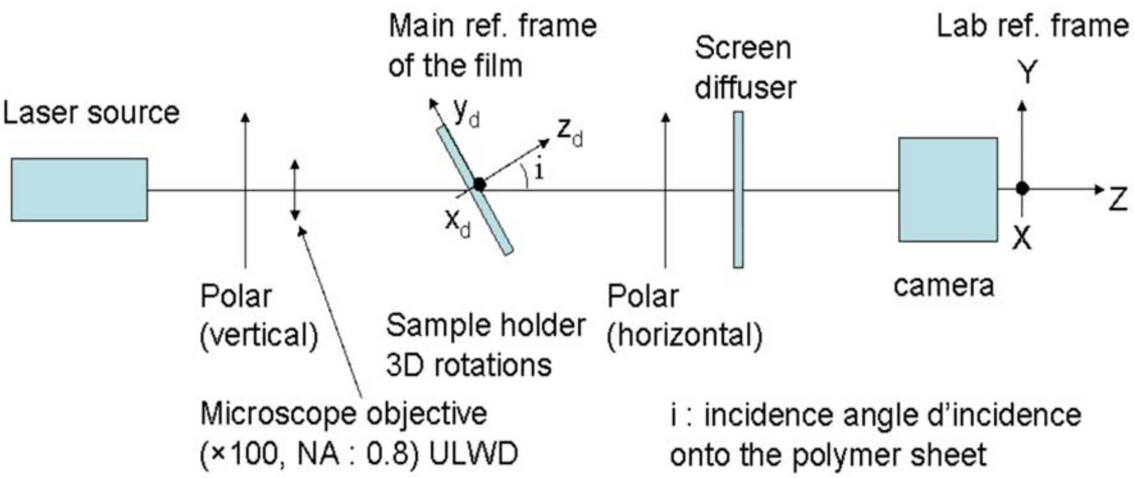
Mueller Matrix measurements with the MM-16 show that the PET foil exhibits anisotropy because the off-diagonal elements are not 0. Before the actual measurements were performed the optical axes of the sample have to be found. This is achieved by looking at the sample between crossed polarizers and by using a microscope in conoscopic mode.

With the crossed polarizers we can find the trace of the optical axes:

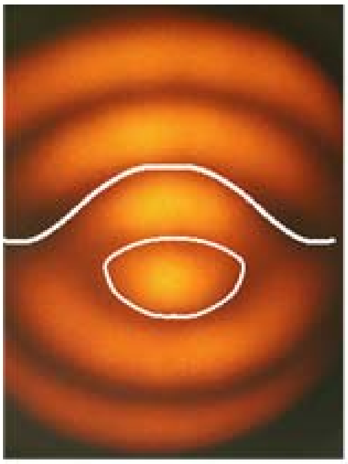


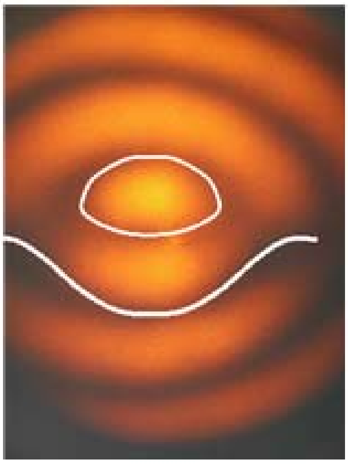
The microscope in conoscopic mode yields the type of anisotropy (uniaxial or biaxial) and the direction of the optical axes by comparing the images with references from literature.

The microscope in conoscopic configuration:



Below we see the image compared with theoretical shapes:





From there we get the information that the anisotropy is biaxial and the direction of the optical axes.

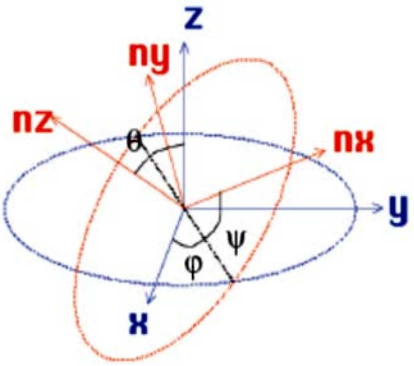
We now can align the sample for subsequent ellipsometer and transmission measurements.

The layer model is:

1
☐ 90.00000
Z 504 ellitrans vase z.dsp
X 504 ellitrans vase x.dsp
Y 504 ellitrans vase y.dsp
S void.dsp

containing a biaxial layer with Euler angles and taking into account backside reflections.

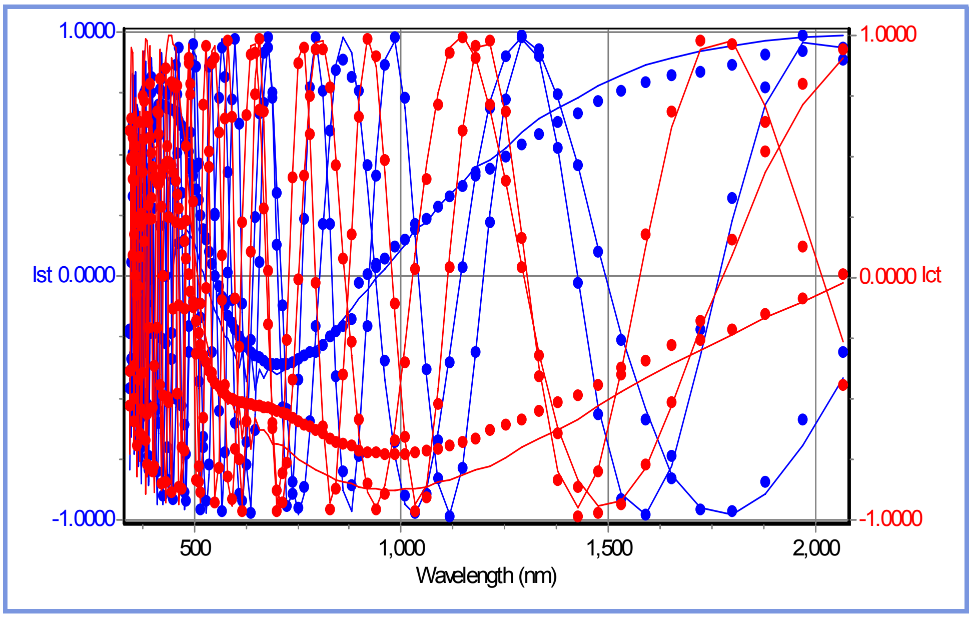
Euler angles:



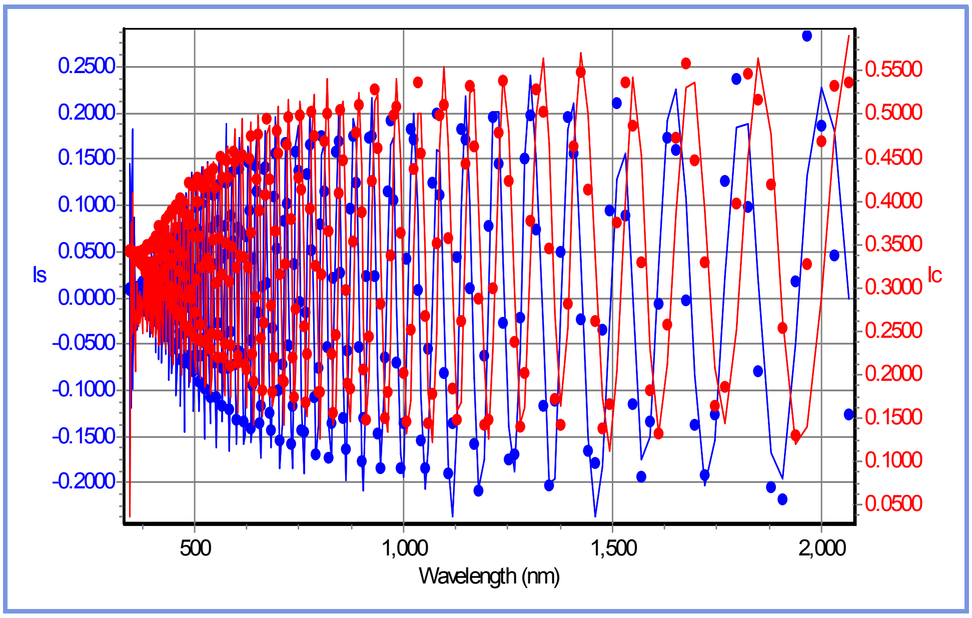
The dispersions for x, y, z are described with a classical oscillator model:

$$\varepsilon = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\Gamma_0\omega}$$

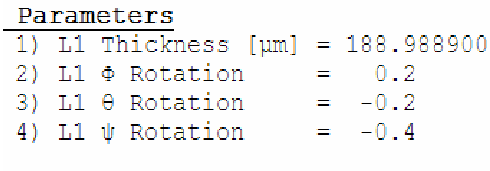
First we fitted measured ellipsometric transmission data (three AOI: 5°, 20°, 35°):



The results could be confirmed by fitting the ellipsometric data in reflection (AOI = 70°):

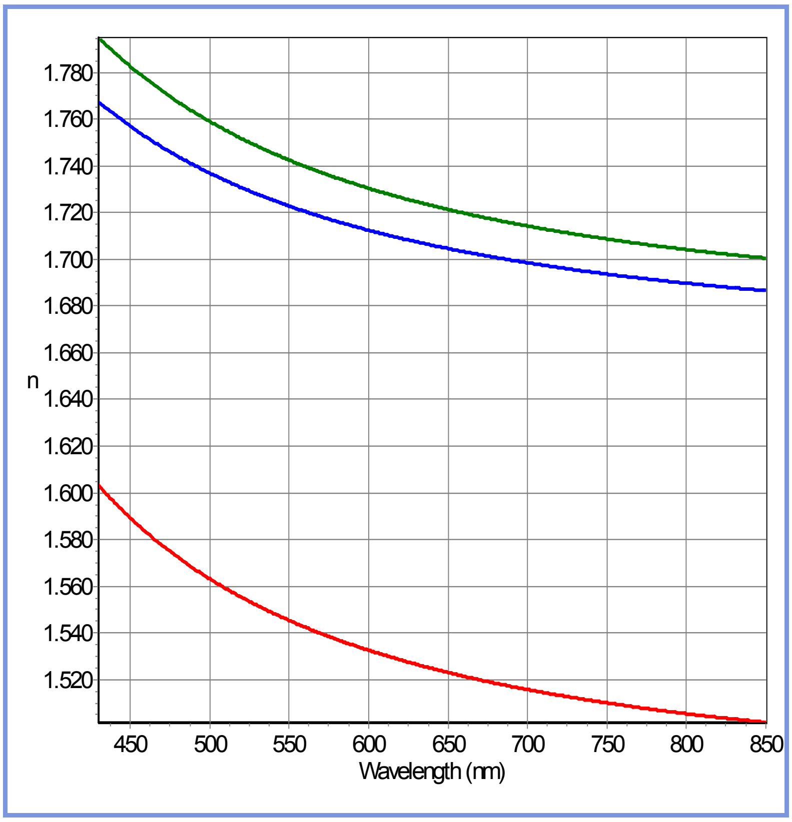


As a result we get the thickness of the foil:



```
Parameters
 1) L1 Thickness [µm] = 188.988900
 2) L1 Φ Rotation     =   0.2
 3) L1 θ Rotation     =  -0.2
 4) L1 ψ Rotation     =  -0.4
```

and the optical constants:



where:

n_x at 633nm = 1.684

$n_x - n_y = -0.021$

$n_x - n_z = 0.168$

12 Application Data Sheets

Next pages show some Application Models sum up on Data Sheets.

Spectroscopic Ellipsometry Data Sheets **1**

SiO_2 / c-Si Substrate

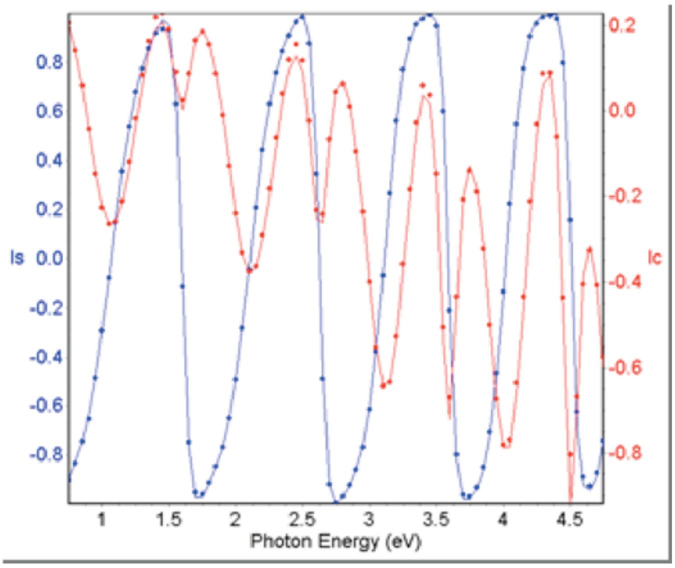
Model

2	F 73.3 ☐ %	Sio2_isa.ref 50.00 %	Void.ref 50.00 %	×
1	F 5227.5	Sio2_isa.ref		×
S		C-si_isa.ref		

Fit Conditions

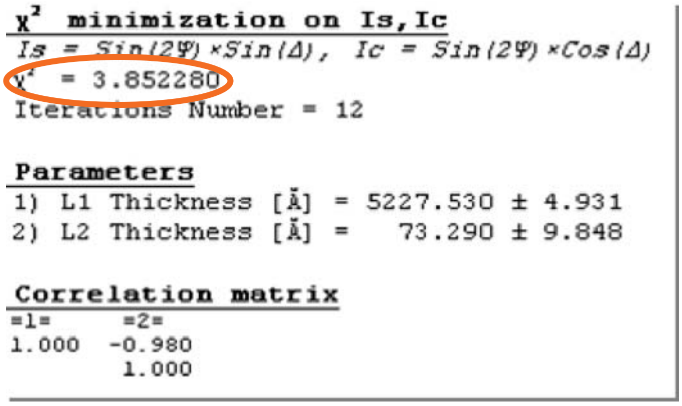
- Spectral range : 0.75-4.75 eV
- Step size: 0.05 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layers 1 and 2
- Materials
  - c-Si, SiO_2, void: Reference library

Fit Results



General Remarks

- Adding a surface roughness on top of the SiO_2 film provides an improvement of the χ^2 by a factor 2. Hence the final model takes into account the roughness.
- Using a dispersion formula for SiO_2 materials, eg adjusting the refractive index of SiO_2 doesn't provide an improvement of the χ^2.



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 3.852280
Iterations Number = 12

Parameters
1) L1 Thickness [Å] = 5227.530 ± 4.931
2) L2 Thickness [Å] =   73.290 ± 9.848

Correlation matrix
=1=      =2=
1.000   -0.980
         1.000
```

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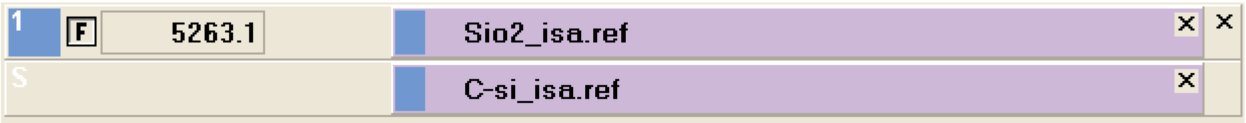
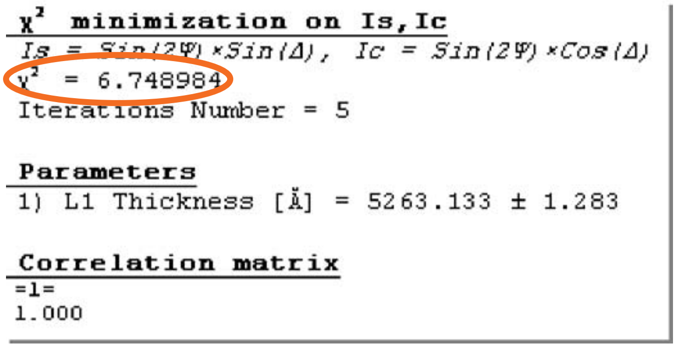
Model without roughness



1 F 5263.1 Sio2_isa.ref

S C-si_isa.ref

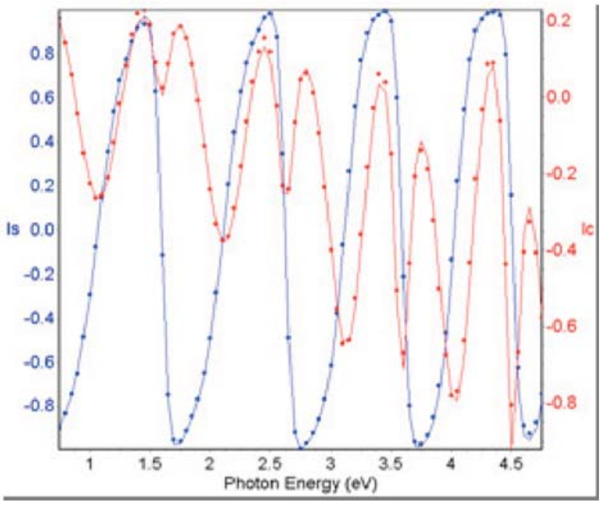
Fit Results



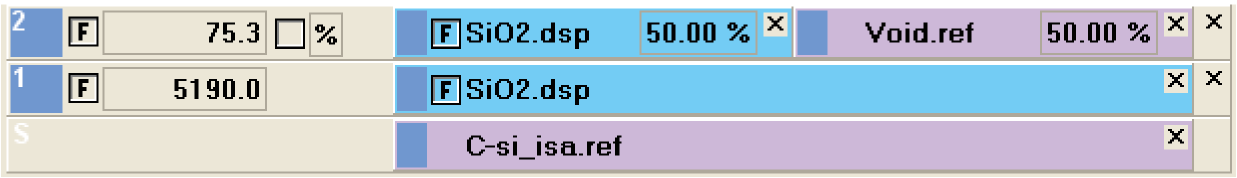
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 6.748984
Iterations Number = 5

Parameters
1) L1 Thickness [Å] = 5263.133 ± 1.283

Correlation matrix
=1=
1.000
```



Model with SiO_2 dispersion



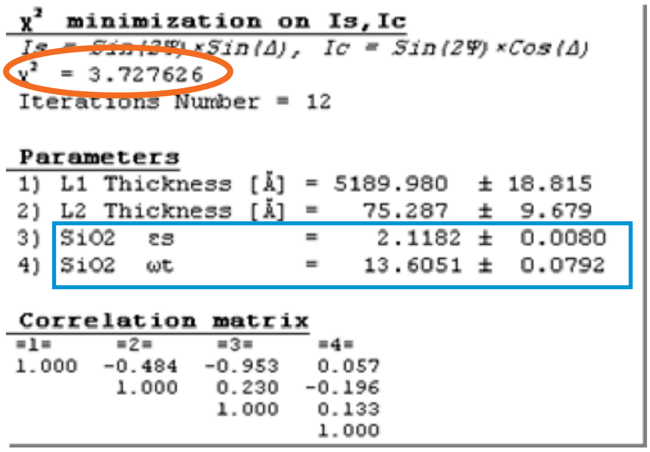
2 F 75.3 ☐ % F SiO2.dsp 50.00 % Void.ref 50.00 %

1 F 5190.0 F SiO2.dsp

S C-si_isa.ref

- Model Information:
  - SiO_2:Classical formula, transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

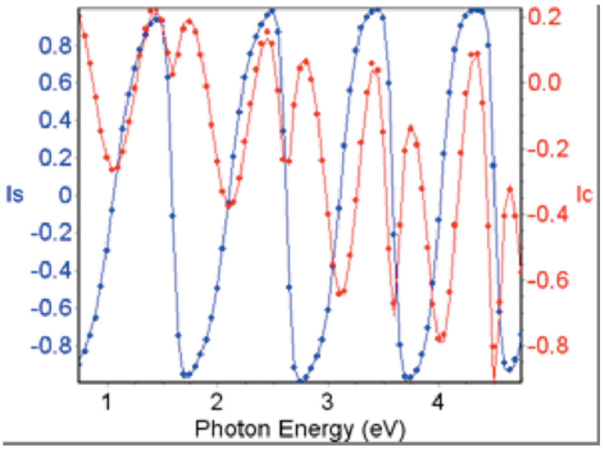
Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 3.727626
Iterations Number = 12

Parameters
1) L1 Thickness [Å] = 5189.980  ± 18.815
2) L2 Thickness [Å] =   75.287  ±  9.679
3) SiO2  εs         =    2.1182 ±  0.0080
4) SiO2  ωt         =   13.6051 ±  0.0792

Correlation matrix
=1=     =2=     =3=     =4=
1.000  -0.484  -0.953   0.057
        1.000   0.230  -0.196
                1.000   0.133
                        1.000
```



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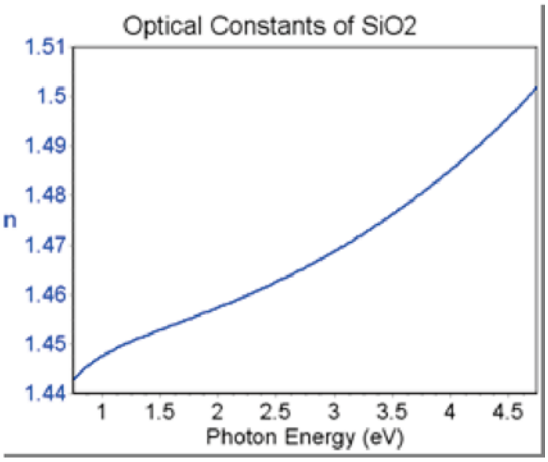
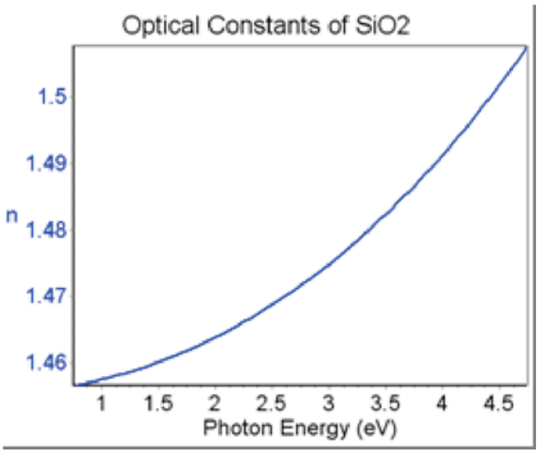
Optical Constants of SiO_2 Reference Library



Optical Constants of SiO_2 Dispersion Formula



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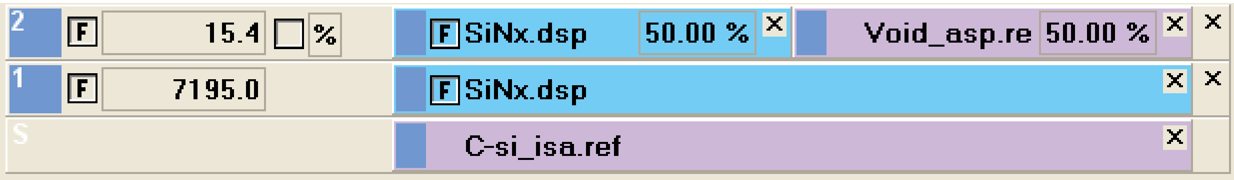
Spectroscopic Ellipsometry Data Sheets

2

SiN_x / c-Si Substrate

Model

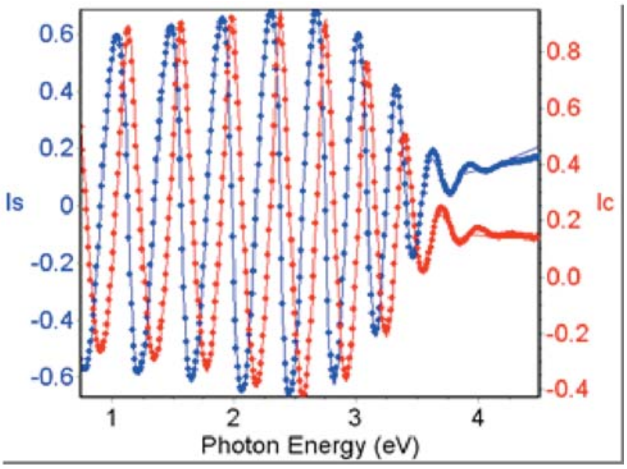


2	F	15.4 ☐ %	F SiNx.dsp 50.00 % ✕	Void_asp.re 50.00 % ✕	✕
1	F	7195.0	F SiNx.dsp ✕		✕
S			C-si_isa.ref ✕		

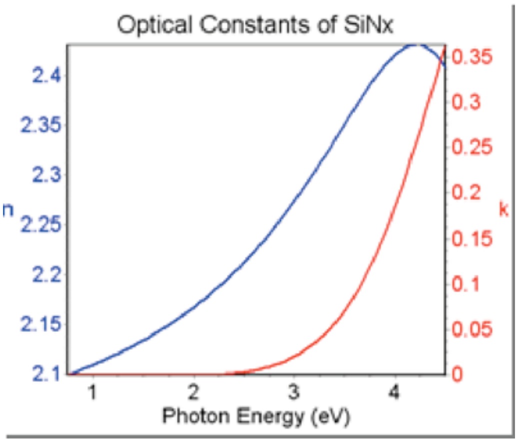
Fit Conditions

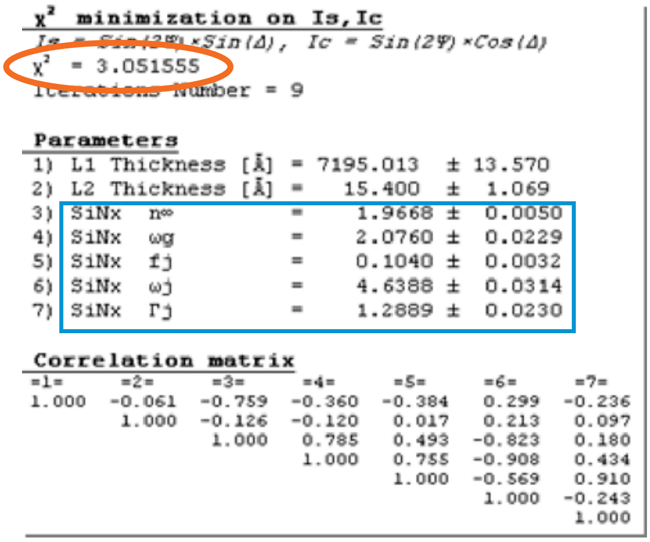
- Spectral range: 0.75 - 4.5 eV
- Step size: 0.01 eV
- Angle of incidence: 70°
- Fit parameters
  - Thickness: Layers 1 and 2
  - Optical constants: SiN_x
- Materials
  - c-Si: Reference materials
  - **SiN_x** : Double new amorphous formula

Fit Results



Optical constants of SiN_x





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 3.051555
Iterations Number = 9

Parameters
1) L1 Thickness [Å] = 7195.013  ± 13.570
2) L2 Thickness [Å] =   15.400  ±  1.069
3) SiNx  n∞         =    1.9668 ±  0.0050
4) SiNx  ωg         =    2.0760 ±  0.0229
5) SiNx  fj         =    0.1040 ±  0.0032
6) SiNx  ωj         =    4.6388 ±  0.0314
7) SiNx  Γj         =    1.2889 ±  0.0230

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.061  -0.759  -0.360  -0.384   0.299  -0.236
        1.000  -0.126  -0.120   0.017   0.213   0.097
                1.000   0.785   0.493  -0.823   0.180
                        1.000   0.755  -0.908   0.434
                                1.000  -0.569   0.910
                                        1.000  -0.243
                                                1.000
```

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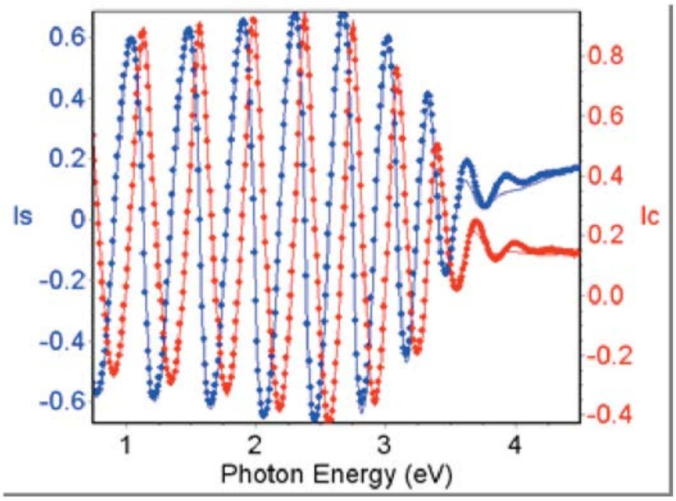
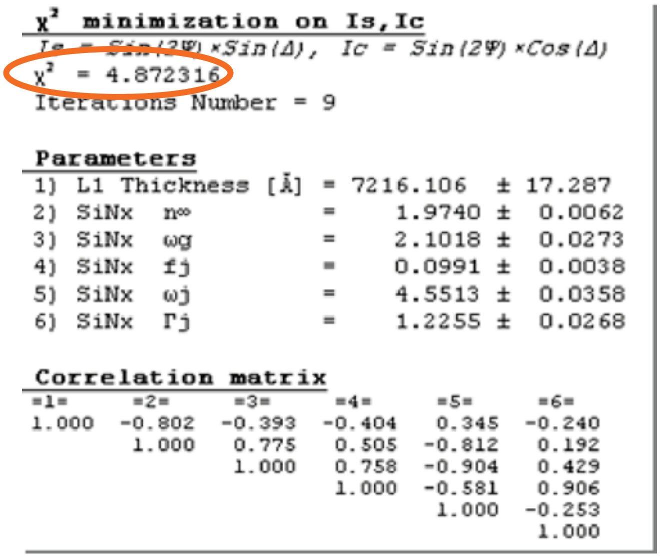
Model without roughness


1 F 7216.1 F SiNx.dsp

S C-si_isa.ref

Fit Results





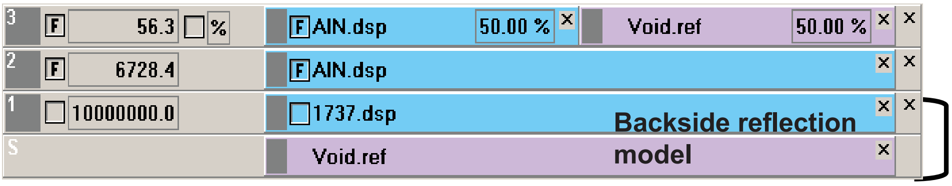
```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 4.872316
Iterations Number = 9

Parameters
1) L1 Thickness [Å]  = 7216.106  ± 17.287
2) SiNx  n∞          =    1.9740 ±  0.0062
3) SiNx  ωg          =    2.1018 ±  0.0273
4) SiNx  fj          =    0.0991 ±  0.0038
5) SiNx  ωj          =    4.5513 ±  0.0358
6) SiNx  Γj          =    1.2255 ±  0.0268

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000  -0.802  -0.393  -0.404   0.345  -0.240
        1.000   0.775   0.505  -0.812   0.192
                1.000   0.758  -0.904   0.429
                        1.000  -0.581   0.906
                                1.000  -0.253
                                        1.000
```

General Remarks

- Adding a roughness layer on top doesn't improve significantly the results. Others techniques may help to state on the final model.

AlN/ Glass Substrate BR

Model



3 F 56.3 ☐ % | F AlN.dsp 50.00 % | Void.ref 50.00 %

2 F 6728.4 | F AlN.dsp

1 ☐ 10000000.0 | ☐ 1737.dsp

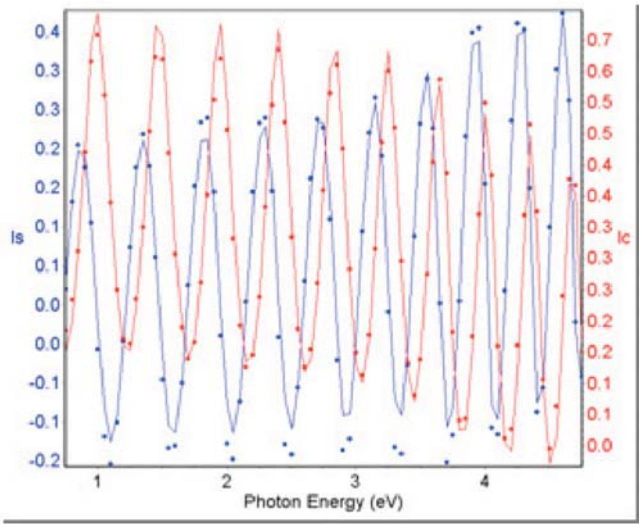
S | Void.ref

Backside reflection model

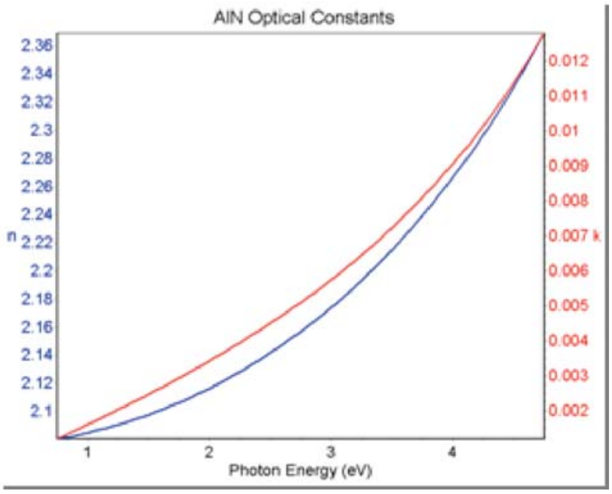
Fit Conditions

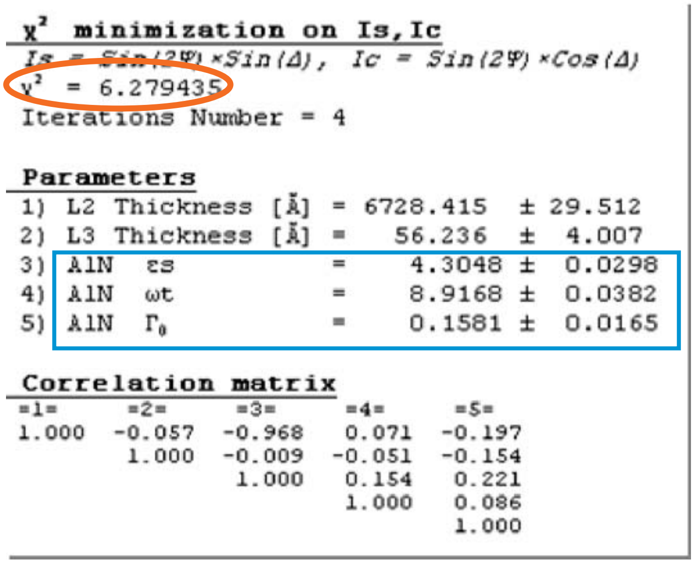
- Spectral range : 0.75 - 4.75 eV
- Step size: 0.05 eV
- Angle of incidence : 70°
- Model Information: Backside reflection model
- Fit parameters
  - Thickness : layers 2 and 3
  - Optical constants: AlN
- Materials
  - 1737, Void: Reference library
  - **AlN**: Classical formula, transparent Lorentz oscillator with $\varepsilon_{\infty} = 1.0$

Fit Results



Optical constants of AlN





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)*Sin(Δ),  Ic = Sin(2Ψ)*Cos(Δ)
χ² = 6.279435
Iterations Number = 4

Parameters
1) L2 Thickness [Å]  = 6728.415  ± 29.512
2) L3 Thickness [Å]  =   56.236  ±  4.007
3) AlN   εs          =    4.3048 ±  0.0298
4) AlN   ωt          =    8.9168 ±  0.0382
5) AlN   Γ0          =    0.1581 ±  0.0165

Correlation matrix
=1=     =2=     =3=     =4=     =5=
1.000  -0.057  -0.968   0.071  -0.197
        1.000  -0.009  -0.051  -0.154
                1.000   0.154   0.221
                        1.000   0.086
                                1.000
```

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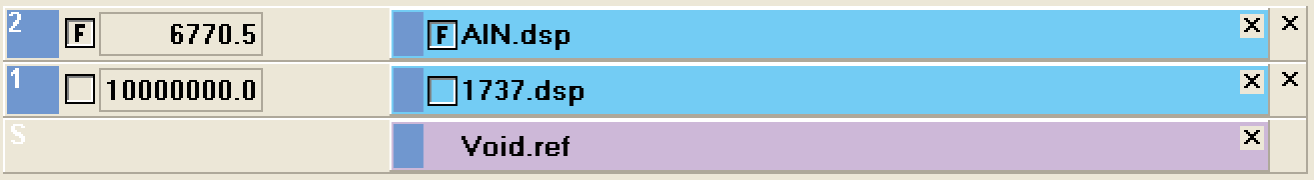
Model without roughness

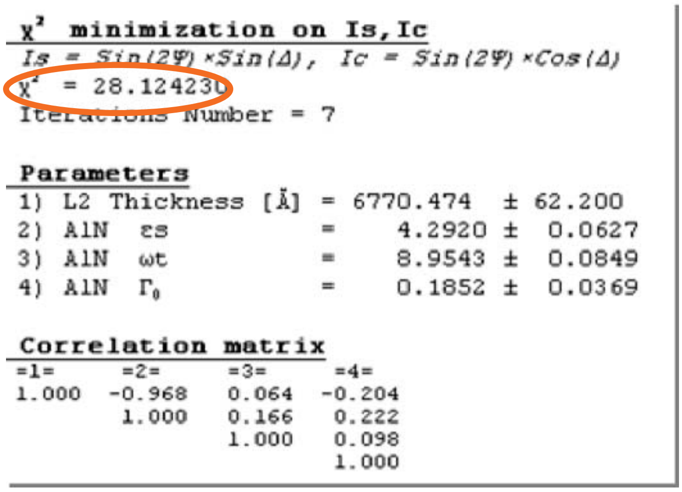


2 ☒ 6770.5 ☒ AlN.dsp

1 ☐ 10000000.0 ☐ 1737.dsp

S Void.ref

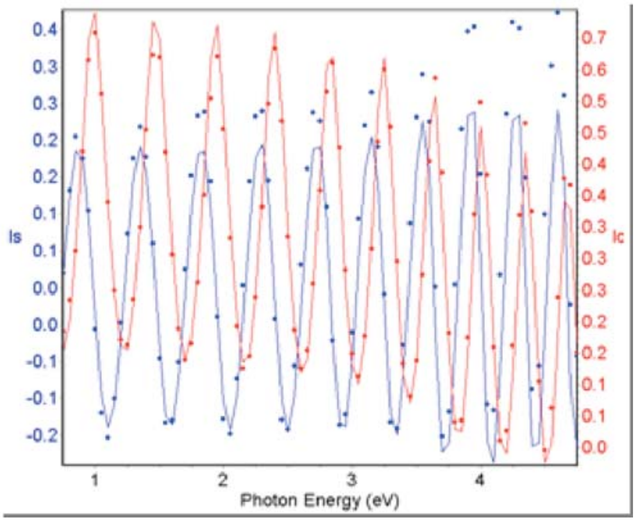
Fit Results



```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 28.124230
Iterations Number = 7

Parameters
1) L2 Thickness [Å] = 6770.474  ± 62.200
2) AlN  εs          =    4.2920 ±  0.0627
3) AlN  ωt          =    8.9543 ±  0.0849
4) AlN  Γ0          =    0.1852 ±  0.0369

Correlation matrix
=1=     =2=     =3=     =4=
1.000  -0.968   0.064  -0.204
        1.000   0.166   0.222
                1.000   0.098
                        1.000
```



General Remarks

- Adding a rough surface layer provides a decrease of the χ^2 from 28 to 6, hence the final model chosen includes the rough overlayer.

TiO_2 / c-Si Substrate

Model

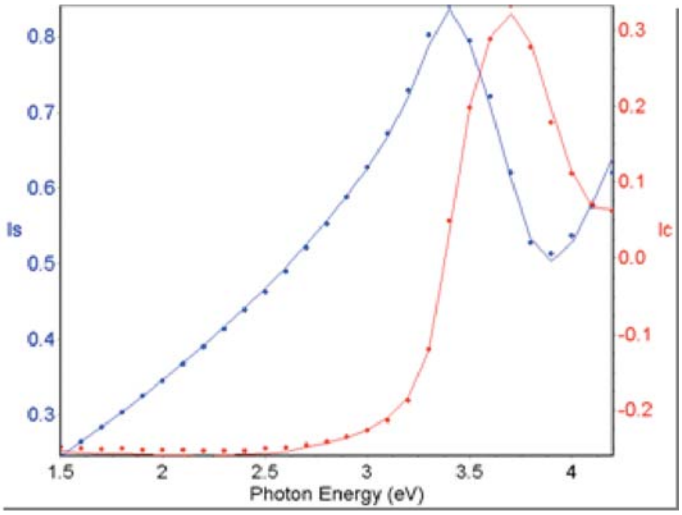
1 F 167.1 F tio2.dsp

S Csi_wor.ref

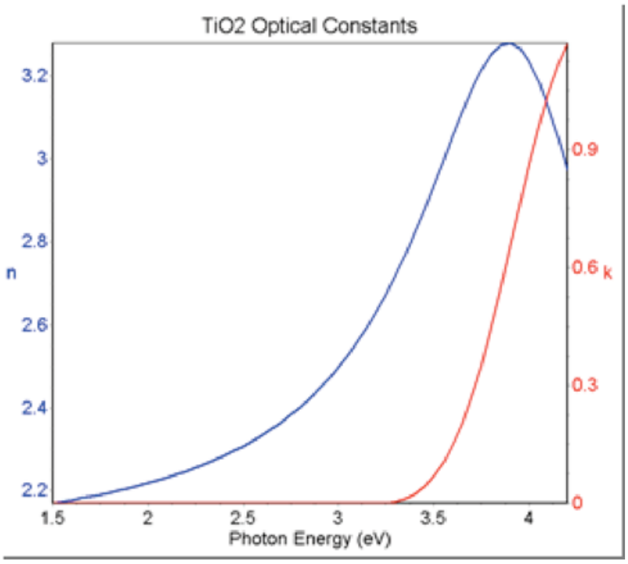
Fit Conditions

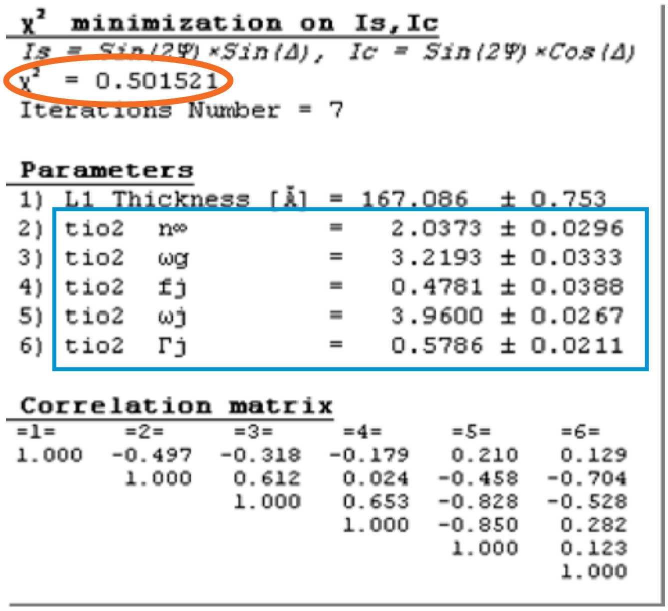
- Spectral range : 1.5-4.2 eV
- Step size: 0.1 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layer 1
  - Optical constants: TiO_2
- Materials
  - c-Si: Reference library
  - TiO_2: New amorphous formula

Fit Results



Optical constants of TiO_2





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.501521
Iterations Number = 7

Parameters
1)  L1 Thickness [Å]  = 167.086   ± 0.753
2)  tio2   n∞          =    2.0373 ± 0.0296
3)  tio2   ωg          =    3.2193 ± 0.0333
4)  tio2   fj          =    0.4781 ± 0.0388
5)  tio2   ωj          =    3.9600 ± 0.0267
6)  tio2   Γj          =    0.5786 ± 0.0211

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000  -0.497  -0.318  -0.179   0.210   0.129
        1.000   0.612   0.024  -0.458  -0.704
                1.000   0.653  -0.828  -0.528
                        1.000  -0.850   0.282
                                1.000   0.123
                                        1.000
```

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Al_2O_3 / c-Si Substrate

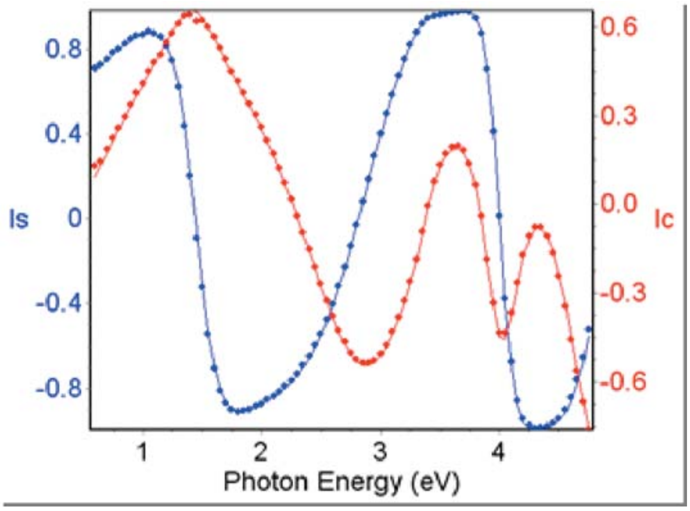
Model

1644.1
Al2O3.dsp
c-Si_Jy.clc

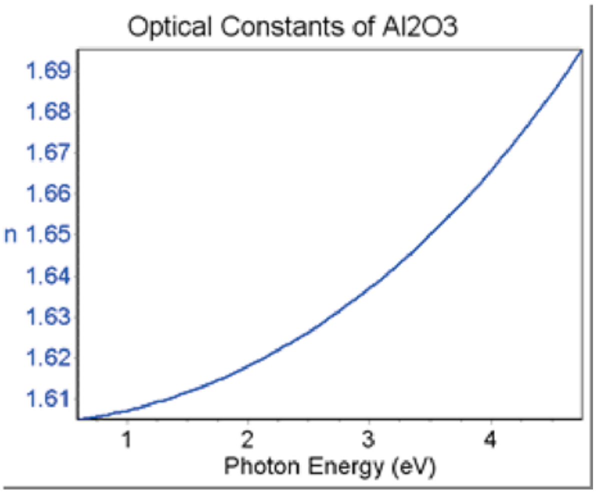
Fit Conditions

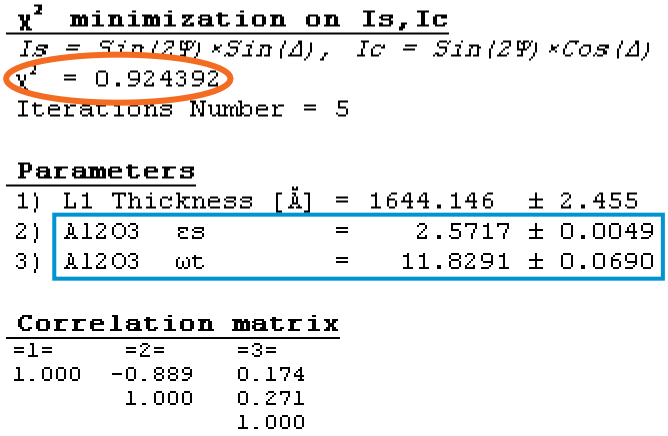
- Spectral range : 0.6 - 4.75 eV
- Step size: 0.05 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layer 1
  - Optical constants: Al_2O_3
- Materials
  - c-Si: Reference library
  - **Al_2O_3**:Classical formula, transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Fit Results



Optical constants of Al_2O_3





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)*Sin(Δ),  Ic = Sin(2Ψ)*Cos(Δ)
χ²  = 0.924392
Iterations Number = 5

Parameters
1) L1 Thickness [Å]  = 1644.146  ± 2.455
2) Al2O3  εs         =    2.5717 ± 0.0049
3) Al2O3  ωt         =   11.8291 ± 0.0690

Correlation matrix
=1=     =2=     =3=
1.000  -0.889   0.174
        1.000   0.271
                1.000
```

SiON / c-Si Substrate BR

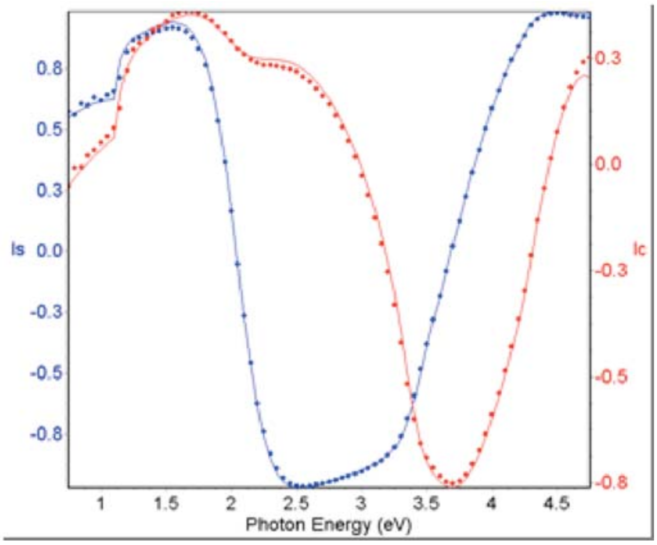
Model

2	F	1237.5	F SiON.dsp	
1	☐	3800000.0	C-si_isa.ref	Backside reflection model
S			Void.ref	

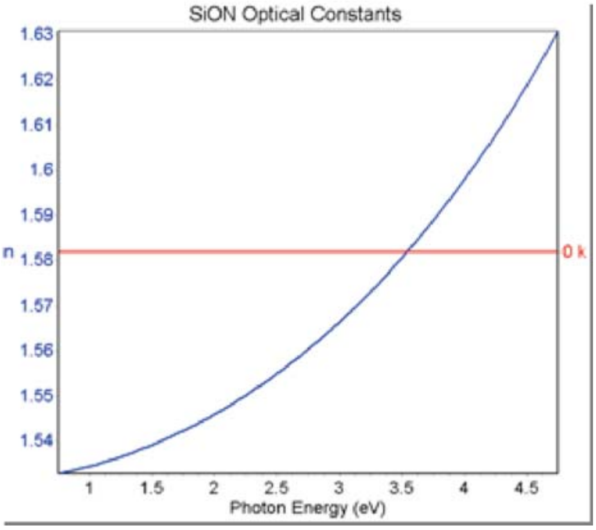
Fit Conditions

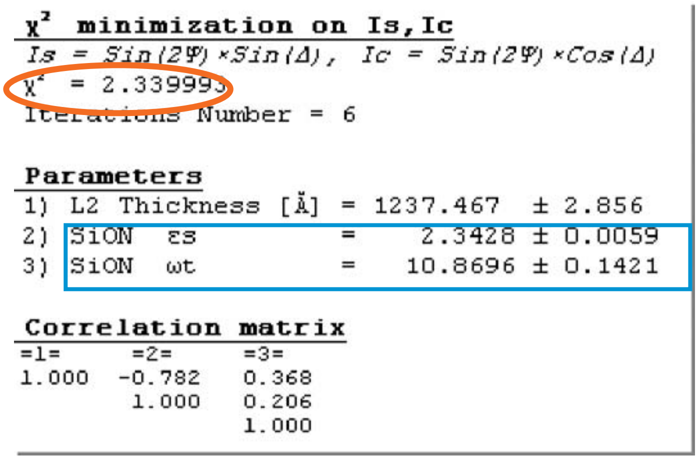
- Spectral range : 0.75-4.75 eV
- Angle of incidence : 70°
- Model Information:
  - Backside reflection model
  - Thin polished c-Si substrate
  - Measurement performed in NIR which is the transparent region of c-Si
- Fit parameters
  - Thickness : layer 2
  - Optical constants: SiON
- Materials
  - c-Si, Void: Reference library
  - **SiON**: Classical formula, transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Fit Results



Optical constants of SiON





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)*Sin(Δ), Ic = Sin(2Ψ)*Cos(Δ)
χ² = 2.339993
Iterations Number = 6

Parameters
1) L2 Thickness [Å]  = 1237.467  ± 2.856
2) SiON   εs         =    2.3428 ± 0.0059
3) SiON   ωt         =   10.8696 ± 0.1421

Correlation matrix
=1=      =2=      =3=
1.000   -0.782    0.368
         1.000    0.206
                  1.000
```

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Spectroscopic Ellipsometry Data Sheets 7

Si_3N_4/ SiO_2/ c-Si Substrate

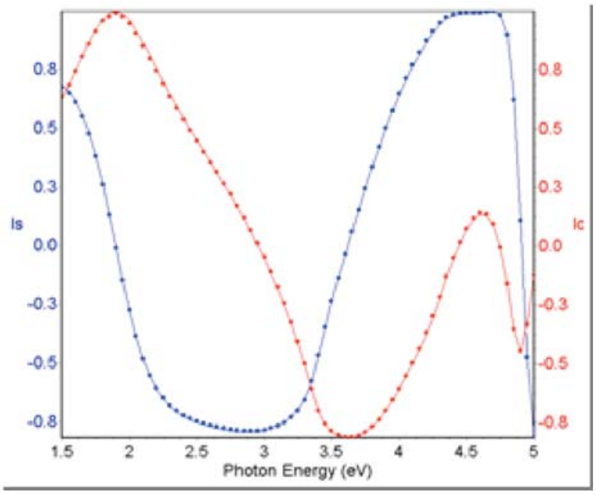
Model

2	F	695.0	F SI3N4.dsp	×
1	F	221.8	SiO2_wor.ref	×
S			Csi_wor.ref	

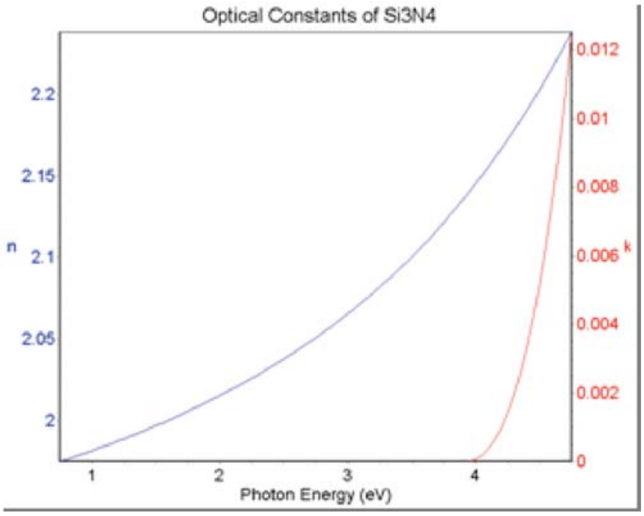
Fit Conditions

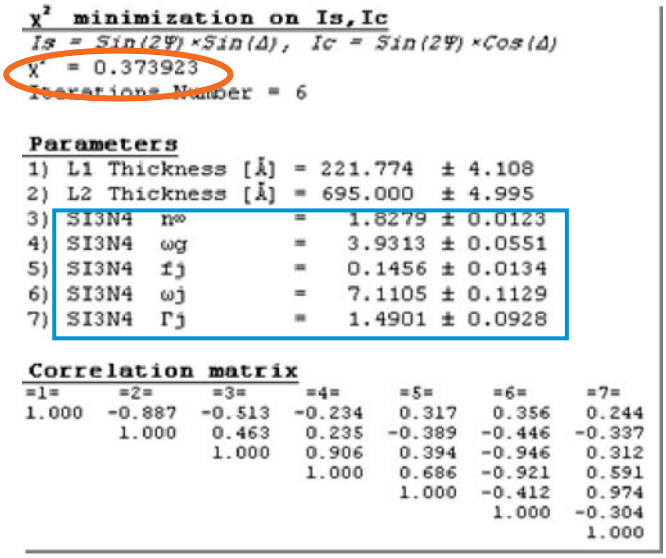
- Spectral range : 1.5-5 eV
- Step size: 0.05 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layers 1 and 2
  - Optical constants: Si_3N_4
- Materials
  - SiO_2, c-Si : Reference library
  - **Si_3N_4**: New amorphous formula

Fit Results



Optical constants of Si_3N_4





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.373923
Iterations Number = 6

Parameters
1) L1 Thickness [Å] = 221.774  ± 4.108
2) L2 Thickness [Å] = 695.000  ± 4.995
3) SI3N4  n∞        =   1.8279 ± 0.0123
4) SI3N4  ωg        =   3.9313 ± 0.0551
5) SI3N4  fj        =   0.1456 ± 0.0134
6) SI3N4  ωj        =   7.1105 ± 0.1129
7) SI3N4  Γj        =   1.4901 ± 0.0928

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.887  -0.513  -0.234   0.317   0.356   0.244
        1.000   0.463   0.235  -0.389  -0.446  -0.337
                1.000   0.906   0.394  -0.946   0.312
                        1.000   0.686  -0.921   0.591
                                1.000  -0.412   0.974
                                        1.000  -0.304
                                                1.000
```

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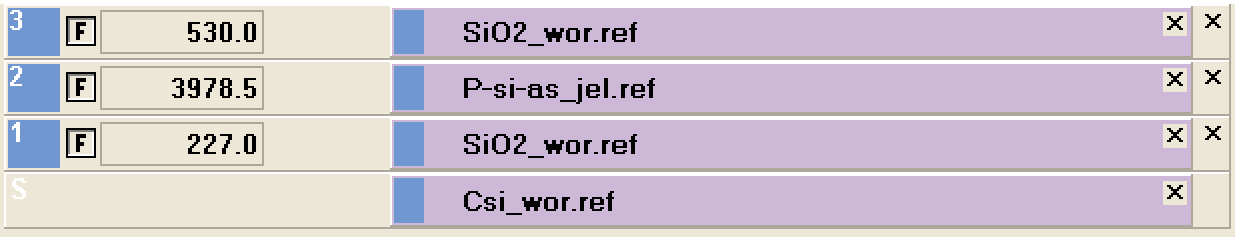
SiO_2 /p-Si / SiO_2 / c-Si Substrate

Model

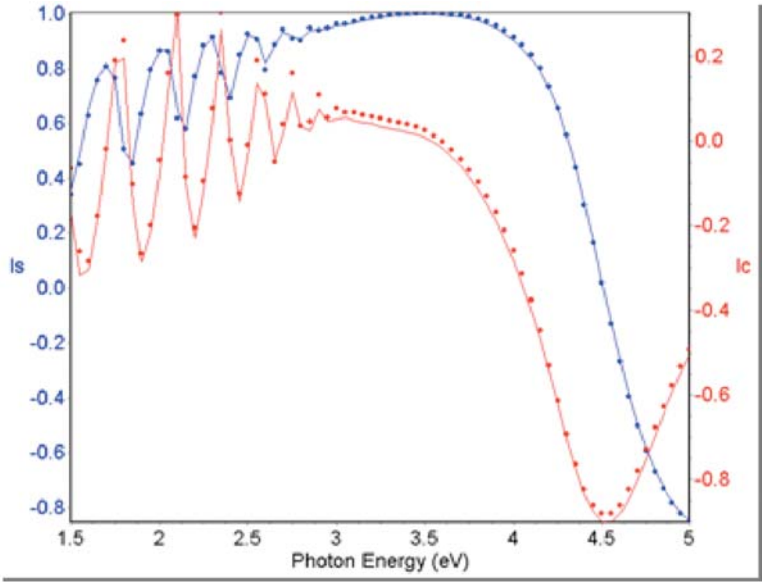


3	F	530.0	SiO2_wor.ref	×
2	F	3978.5	P-si-as_jel.ref	×
1	F	227.0	SiO2_wor.ref	×
S			Csi_wor.ref	

Fit Conditions

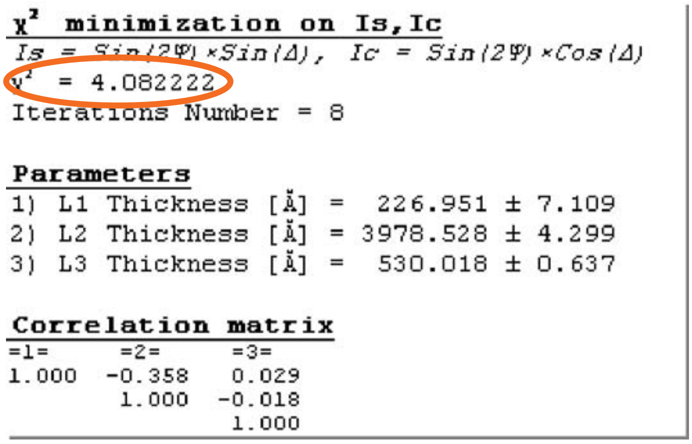
- Spectral range : 1.5-5.0 eV
- Step size: 0.05 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layers 1, 2 and 3
- Materials
  - SiO_2, p-Si (as doped), c-Si: Reference library

Fit Results



General Remarks

- The fit results is quite good by using the reference materials of the library.
- It may be improved by improving the p-Si optical constants.



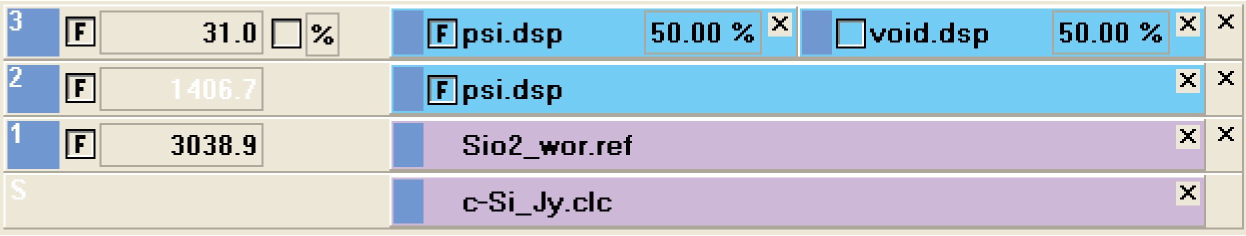
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 4.082222
Iterations Number = 8

Parameters
1) L1 Thickness [Å] =  226.951 ± 7.109
2) L2 Thickness [Å] = 3978.528 ± 4.299
3) L3 Thickness [Å] =  530.018 ± 0.637

Correlation matrix
=1=      =2=      =3=
1.000  -0.358    0.029
         1.000  -0.018
                 1.000
```

p-Si / SiO_2 / c-Si Substrate

Model

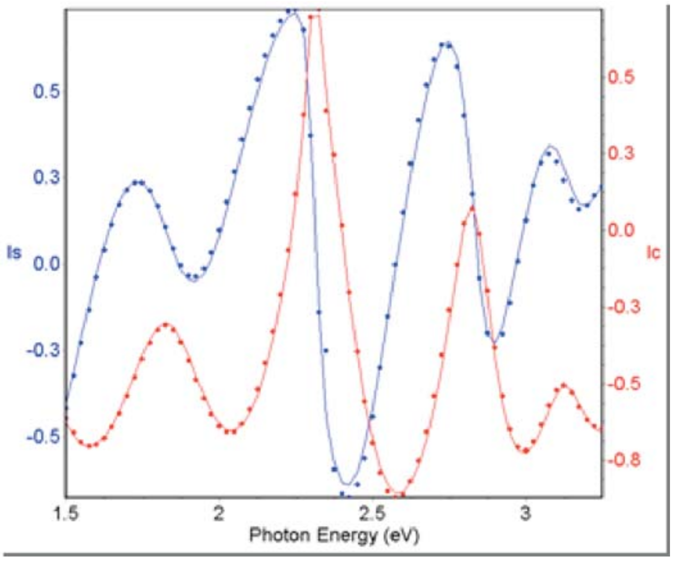


3	F	31.0	☐ %	F psi.dsp	50.00 %	☐ void.dsp	50.00 %
2	F	1406.7		F psi.dsp			
1	F	3038.9		Sio2_wor.ref			
S				c-Si_Jy.clc			

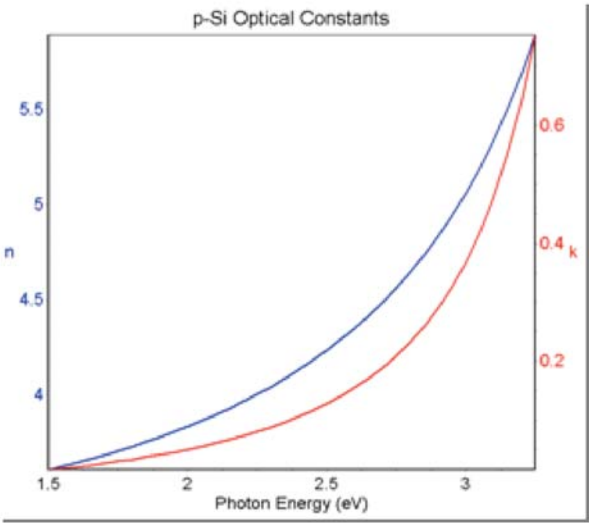
Fit Conditions

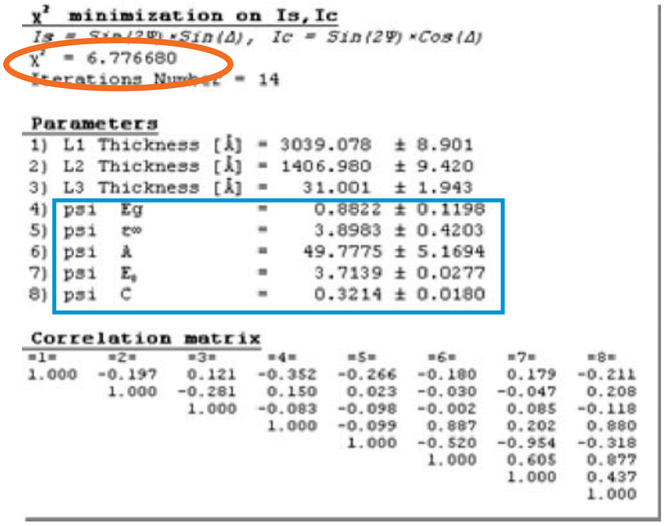
- Spectral range : 1.5-3.25 eV
- Step size: 0.025 eV
- Angle of incidence : 70.1°
- Fit parameters
  - Thickness : layers 1 (with multiguess), 2 and 3
  - Optical constants: p-Si
- Materials
  - SiO_2, c-Si: Reference library
  - **p-Si**: Tauc Lorentz formula

Fit Results



Optical constants of p-Si





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 6.776680
Iterations Number = 14

Parameters
1) L1 Thickness [Å] = 3039.078  ± 8.901
2) L2 Thickness [Å] = 1406.980  ± 9.420
3) L3 Thickness [Å] =   31.001  ± 1.943
4) psi  Eg          =    0.8822 ± 0.1198
5) psi  ε∞          =    3.8983 ± 0.4203
6) psi  A           =   49.7775 ± 5.1694
7) psi  E0          =    3.7139 ± 0.0277
8) psi  C           =    0.3214 ± 0.0180

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=     =8=
1.000  -0.197   0.121  -0.352  -0.266  -0.180   0.179  -0.211
        1.000  -0.281   0.150   0.023  -0.030  -0.047   0.208
                1.000  -0.083  -0.098  -0.002   0.085  -0.118
                        1.000  -0.099   0.887   0.202   0.880
                                1.000  -0.520  -0.954  -0.318
                                        1.000   0.605   0.877
                                                1.000   0.437
                                                        1.000
```

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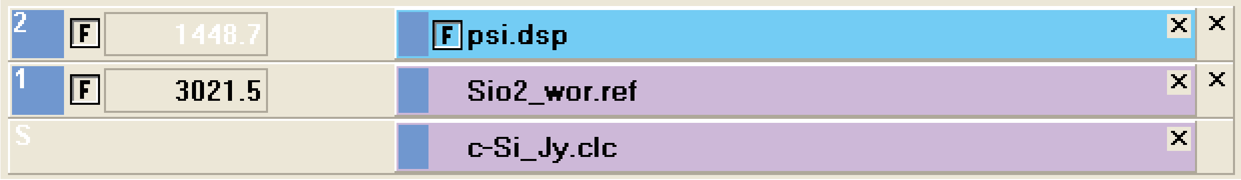
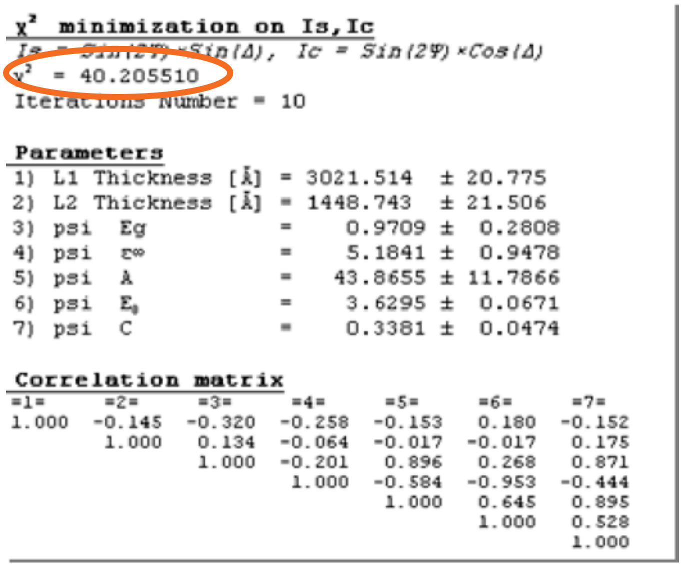
Model without roughness



2	F	1448.7	F psi.dsp	☒
1	F	3021.5	Sio2_wor.ref	☒
S			c-Si_Jy.clc	☒

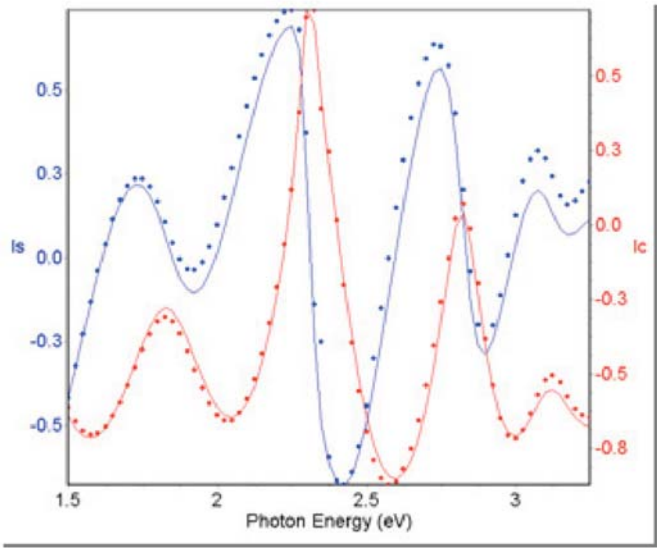
Fit Results



```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 40.205510
Iterations Number = 10

Parameters
1) L1 Thickness [Å] = 3021.514  ± 20.775
2) L2 Thickness [Å] = 1448.743  ± 21.506
3) psi  Eg          =     0.9709 ±  0.2808
4) psi  ε∞          =     5.1841 ±  0.9478
5) psi  A           =    43.8655 ± 11.7866
6) psi  E₀          =     3.6295 ±  0.0671
7) psi  C           =     0.3381 ±  0.0474

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.145  -0.320  -0.258  -0.153   0.180  -0.152
        1.000   0.134  -0.064  -0.017  -0.017   0.175
                1.000  -0.201   0.896   0.268   0.871
                        1.000  -0.584  -0.953  -0.444
                                1.000   0.645   0.895
                                        1.000   0.528
                                                1.000
```



General Remarks

- Adding a rough overlayer strongly decreases the χ^2 value.

Amorphous Silicon/ Glass Substrate

Model

2 F 64.9 ☐ % F aSi_TL.dsp 50.00 % Void.ref 50.00 %

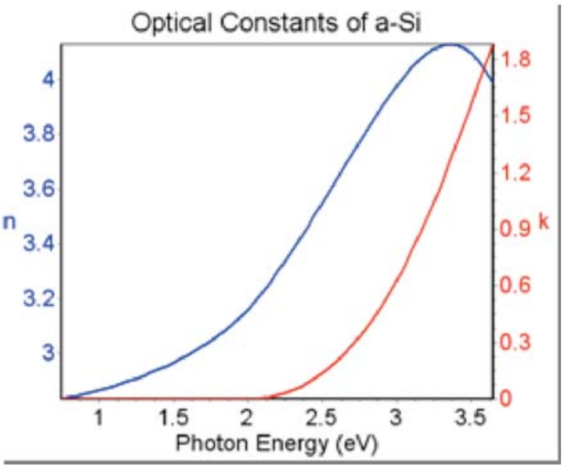
1 F 8268.3 F aSi_TL.dsp

S ☐ glass new.dsp

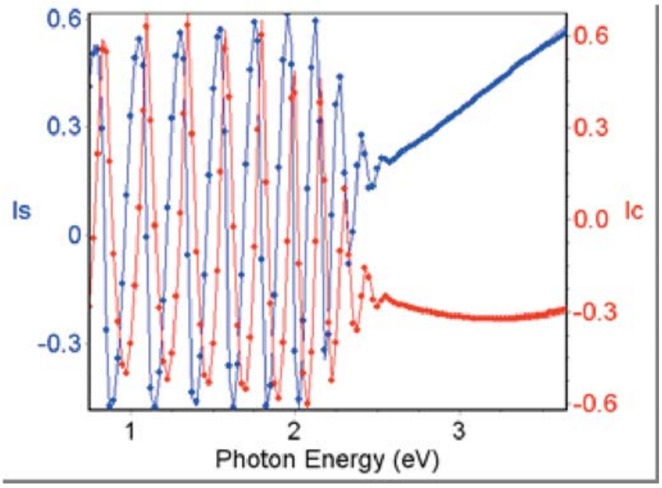
Fit Conditions

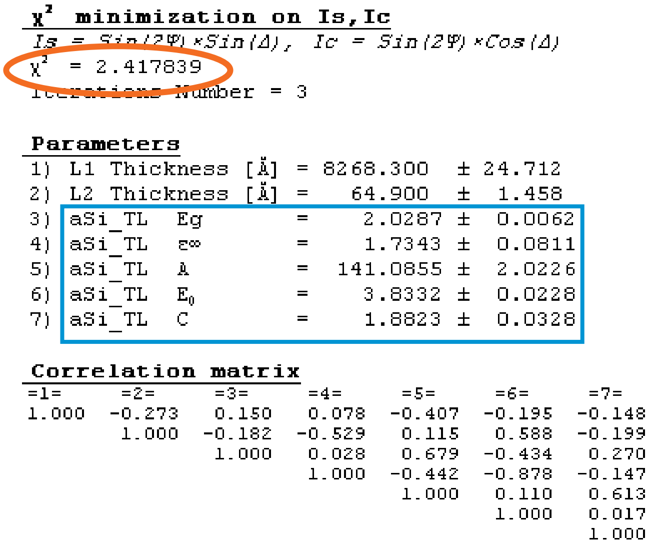
- Spectral range : 0.75 - 3.65 eV
- Step size: 0.025 eV
- Angle of incidence : 70°
- Fit parameters
    - Thickness : layers 1 & 2
    - Optical constants: a-Si
- Materials
    - Void, Glass new: Reference library
    - **a-Si**: Tauc Lorentz

Optical constants of a-Silicon



Fit Results





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 2.417839
Iterations Number = 3

Parameters
1) L1 Thickness [Å] = 8268.300  ± 24.712
2) L2 Thickness [Å] =   64.900  ±  1.458
3) aSi_TL  Eg       =    2.0287 ±  0.0062
4) aSi_TL  ε∞       =    1.7343 ±  0.0811
5) aSi_TL  A        =  141.0855 ±  2.0226
6) aSi_TL  E0       =    3.8332 ±  0.0228
7) aSi_TL  C        =    1.8823 ±  0.0328

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.273   0.150   0.078  -0.407  -0.195  -0.148
        1.000  -0.182  -0.529   0.115   0.588  -0.199
                1.000   0.028   0.679  -0.434   0.270
                        1.000  -0.442  -0.878  -0.147
                                1.000   0.110   0.613
                                        1.000   0.017
                                                1.000
```

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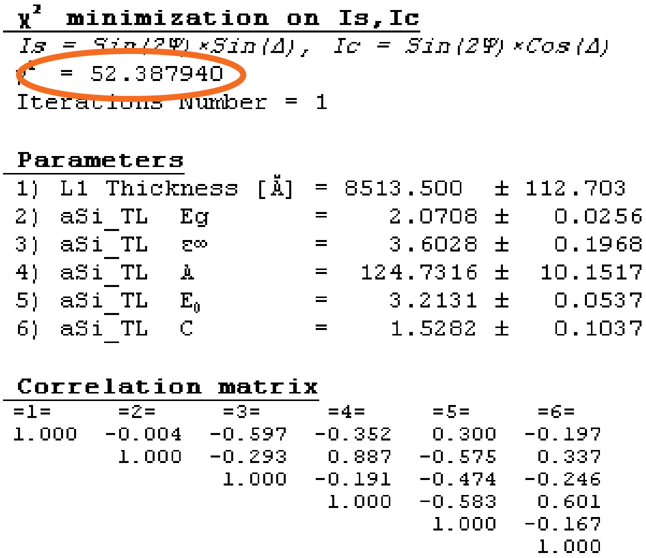
Model without roughness

```
1  F  8513.5   F aSi_TL.dsp
S              ☐ glass new.dsp
```

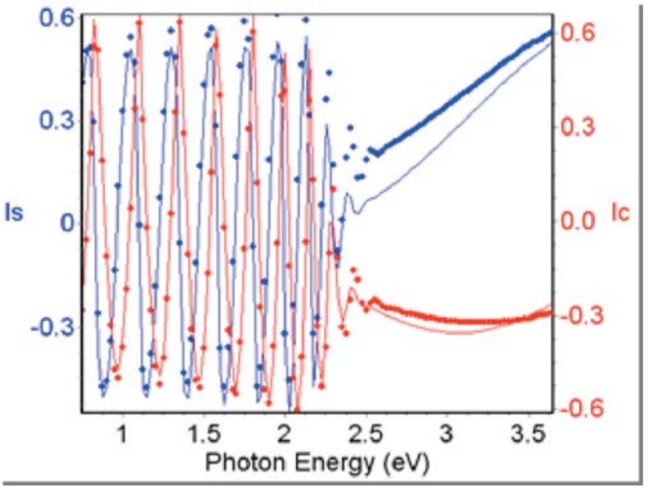
Fit Results



```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 52.387940
Iterations Number = 1

Parameters
1) L1 Thickness [Å]  = 8513.500  ± 112.703
2) aSi_TL  Eg        =     2.0708 ±   0.0256
3) aSi_TL  ε∞        =     3.6028 ±   0.1968
4) aSi_TL  A         =   124.7316 ±  10.1517
5) aSi_TL  E0        =     3.2131 ±   0.0537
6) aSi_TL  C         =     1.5282 ±   0.1037

Correlation matrix
 =1=     =2=     =3=     =4=     =5=     =6=
1.000  -0.004  -0.597  -0.352   0.300  -0.197
        1.000  -0.293   0.887  -0.575   0.337
                1.000  -0.191  -0.474  -0.246
                        1.000  -0.583   0.601
                                1.000  -0.167
                                        1.000
```



General Remarks

- Amorphous silicon is very often a rough material, and adding a rough overlayer is of major importance to increase the fit results.

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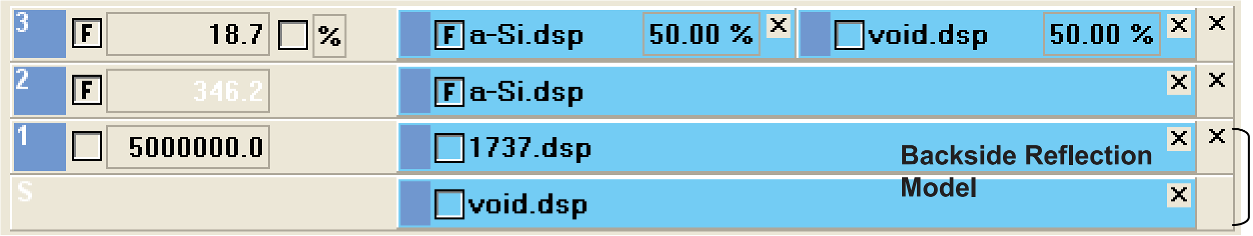
Amorphous Silicon/ Glass Substrate BR

Model



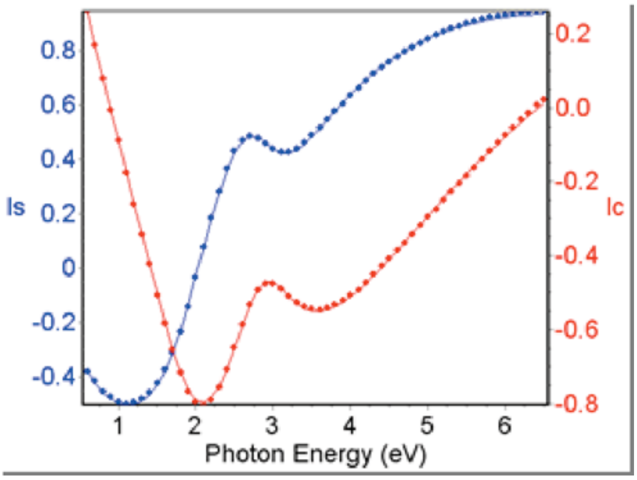
3	☐F 18.7 ☐ %	☐F a-Si.dsp 50.00 %	☐ void.dsp 50.00 %	✕
2	☐F 346.2	☐F a-Si.dsp		✕
1	☐ 5000000.0	☐ 1737.dsp		✕
S		☐ void.dsp		✕

Backside Reflection Model

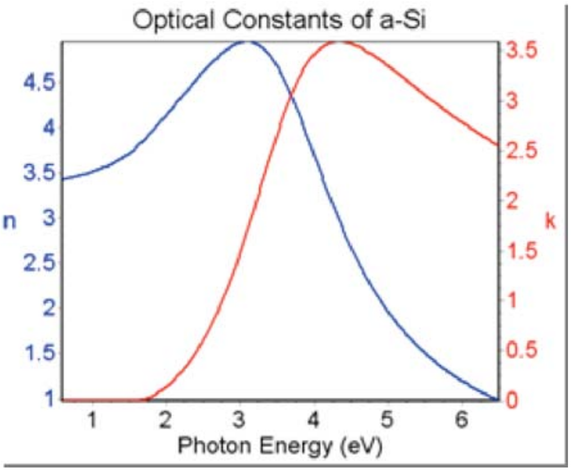
Fit Conditions

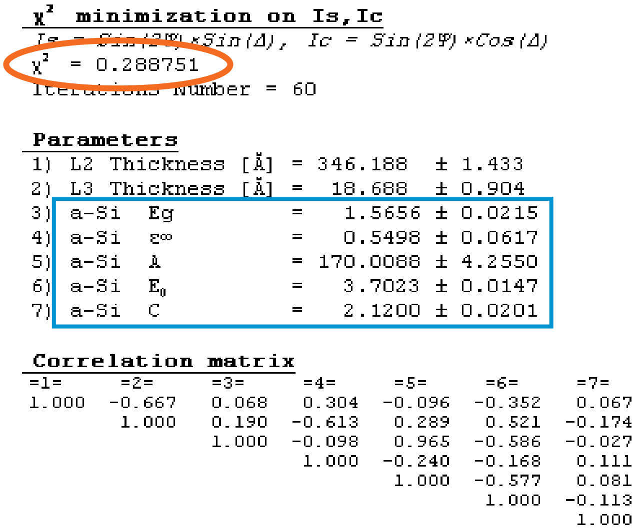
- Spectral range : 0.6 - 6.5 eV
- Step size: 0.1 eV
- Angle of incidence : 70°
- Model information:
    - Multiguess on layer 2 varying the thickness between 0 to 1000 Å by step of 250 Å.
    - Backside reflection model
- Fit parameters
    - Thickness : layers 2 & 3
    - Optical constants: a-Si
- Materials
    - Void, 1737: Reference library
    - a-Si: Tauc Lorentz

Fit Results



Optical constants of a-Silicon



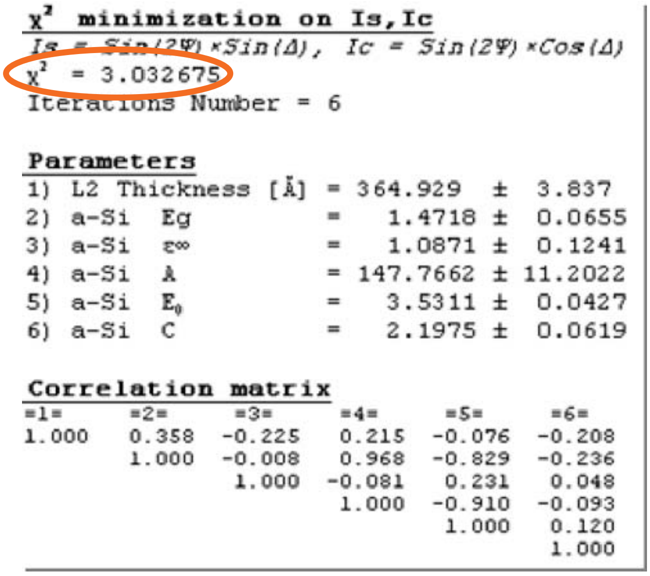


```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.288751
Iterations Number = 60

Parameters
1)  L2 Thickness [Å] = 346.188  ± 1.433
2)  L3 Thickness [Å] =  18.688  ± 0.904
3)  a-Si  Eg         =   1.5656 ± 0.0215
4)  a-Si  ε∞         =   0.5498 ± 0.0617
5)  a-Si  A          = 170.0088 ± 4.2550
6)  a-Si  E0         =   3.7023 ± 0.0147
7)  a-Si  C          =   2.1200 ± 0.0201

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.667   0.068   0.304  -0.096  -0.352   0.067
        1.000   0.190  -0.613   0.289   0.521  -0.174
                1.000  -0.098   0.965  -0.586  -0.027
                        1.000  -0.240  -0.168   0.111
                                1.000  -0.577   0.081
                                        1.000  -0.113
                                                1.000
```

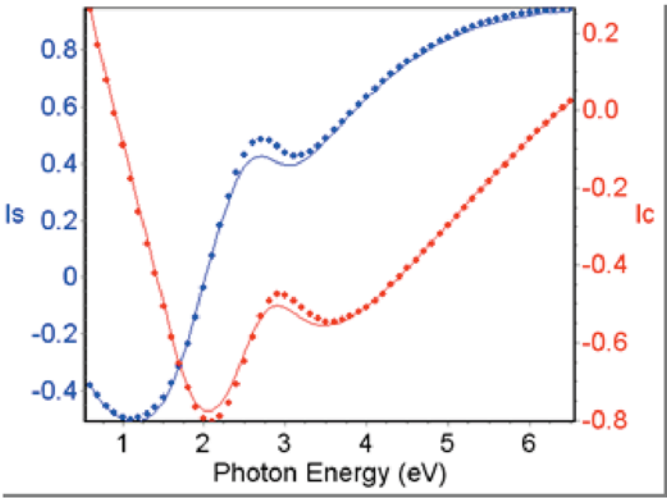
Model without roughness

2	F	364.9	F a-Si.dsp
1	☐	5000000.0	☐ 1737.dsp
S			☐ void.dsp

Fit Results



```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)*Sin(Δ),  Ic = Sin(2Ψ)*Cos(Δ)
χ²  = 3.032675
Iterations Number = 6

Parameters
1)  L2 Thickness [Å]  = 364.929  ±  3.837
2)  a-Si   Eg         =    1.4718 ±  0.0655
3)  a-Si   ε∞         =    1.0871 ±  0.1241
4)  a-Si   A          = 147.7662 ± 11.2022
5)  a-Si   E₀         =    3.5311 ±  0.0427
6)  a-Si   C          =    2.1975 ±  0.0619

Correlation matrix
=1=      =2=      =3=      =4=      =5=      =6=
1.000    0.358   -0.225    0.215   -0.076   -0.208
         1.000   -0.008    0.968   -0.829   -0.236
                  1.000   -0.081    0.231    0.048
                           1.000   -0.910   -0.093
                                    1.000    0.120
                                             1.000
```

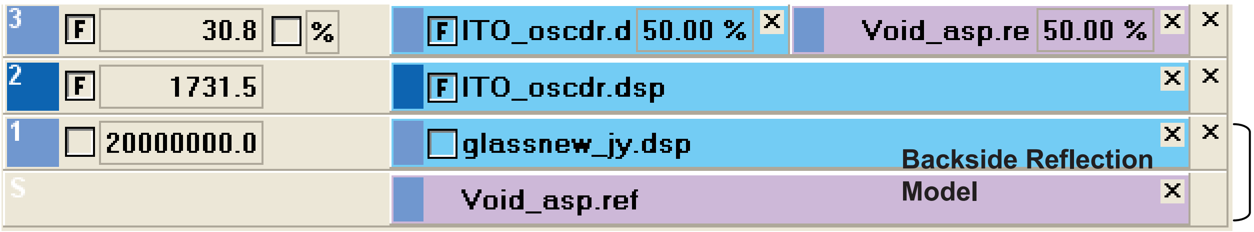


General Remarks

- The rough overlayer on top of amorphous silicon has a strong impact on the decrease of the χ^2. Hence the final model includes the rough overlayer on top.

ITO / Glass Substrate BR

Model



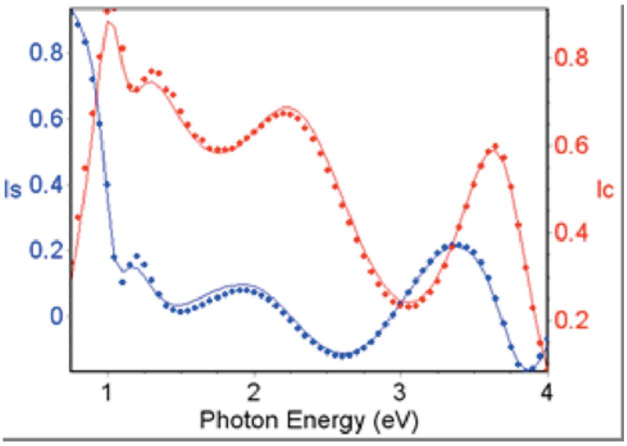
```
3  F  30.8  ☐ %   F ITO_oscdr.d 50.00 %  ✕   Void_asp.re 50.00 %  ✕  ✕
2  F  1731.5      F ITO_oscdr.dsp                                    ✕  ✕
1  ☐  20000000.0  ☐ glassnew_jy.dsp                                  ✕  ✕
S                 Void_asp.ref                                       ✕
```

Backside Reflection Model

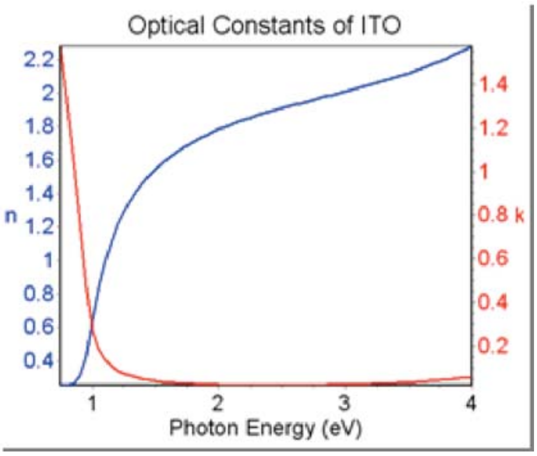
Fit Conditions

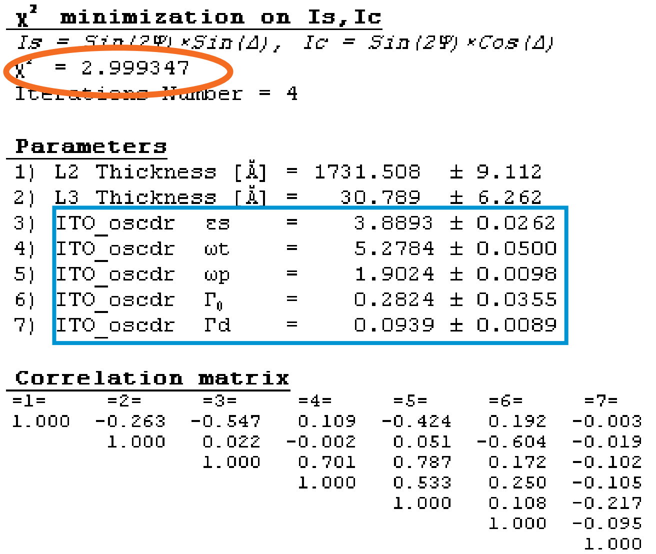
- Spectral range : 0.75 - 4.0 eV
- Step size: 0.05 eV
- Angle of incidence : 70.1°
- Model information:
    - Backside reflection model
- Fit parameters
    - Thickness : layers 2 & 3
    - Optical constants: ITO
- Materials
    - Void, glassnew_jy: Reference library
    - **ITO**: Classical formula mixing absorbing Lorentz oscillator + Drude

Fit Results



Optical constants of ITO





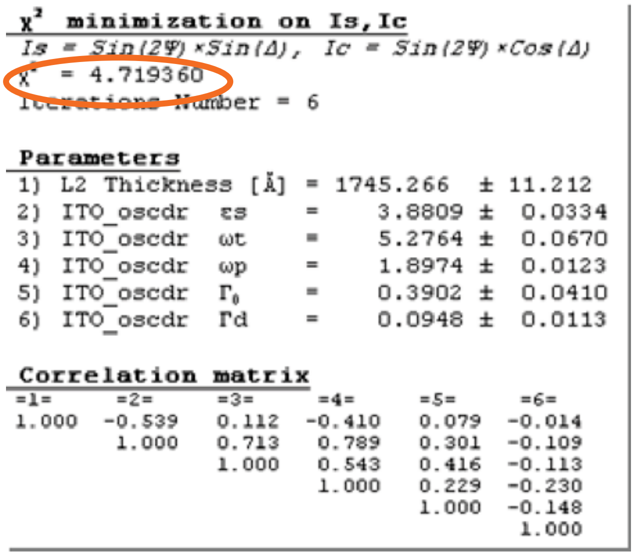
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 2.999347
Iterations Number = 4

Parameters
1) L2 Thickness [Å] = 1731.508  ± 9.112
2) L3 Thickness [Å] =   30.789  ± 6.262
3) ITO_oscdr  εs    =   3.8893 ± 0.0262
4) ITO_oscdr  ωt    =   5.2784 ± 0.0500
5) ITO_oscdr  ωp    =   1.9024 ± 0.0098
6) ITO_oscdr  Γ0    =   0.2824 ± 0.0355
7) ITO_oscdr  Γd    =   0.0939 ± 0.0089

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.263  -0.547   0.109  -0.424   0.192  -0.003
        1.000   0.022  -0.002   0.051  -0.604  -0.019
                1.000   0.701   0.787   0.172  -0.102
                        1.000   0.533   0.250  -0.105
                                1.000   0.108  -0.217
                                        1.000  -0.095
                                                1.000
```

9/2/08

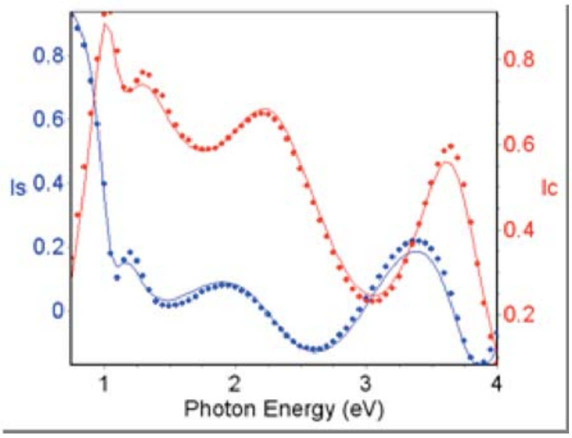
Model without roughness

2	F	1745.3	F ITO_oscdr.dsp
1	☐	20000000.0	☐ glassnew_jy.dsp
S			Void_asp.ref

Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 4.719360
Iterations Number = 6

Parameters
1) L2 Thickness [Å] = 1745.266  ± 11.212
2) ITO_oscdr  εs    =    3.8809 ±  0.0334
3) ITO_oscdr  ωt    =    5.2764 ±  0.0670
4) ITO_oscdr  ωp    =    1.8974 ±  0.0123
5) ITO_oscdr  Γ0    =    0.3902 ±  0.0410
6) ITO_oscdr  Γd    =    0.0948 ±  0.0113

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000  -0.539   0.112  -0.410   0.079  -0.014
        1.000   0.713   0.789   0.301  -0.109
                1.000   0.543   0.416  -0.113
                        1.000   0.229  -0.230
                                1.000  -0.148
                                        1.000
```

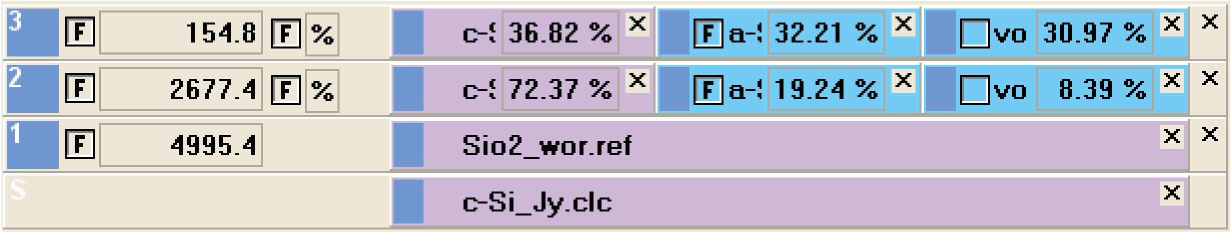


General Remarks

- The presence of the rough overlayer improves the goodness of fit.
- ITO films are often known as inhomogeneous, and / or rough. We advise to test different models including single layer + roughness, single graded layer, 2 layers with 2 different ITO optical constants. To choose between those different models, weight the benefit gained on the χ^2 against the added complication (more regression parameters, more complicated model, etc).

PolySilicon / SiO_2 / c-Si Substrate

Model



3 F 154.8 F % | c-S 36.82 % × | F a-S 32.21 % × | ☐ vo 30.97 % × ×

2 F 2677.4 F % | c-S 72.37 % × | F a-S 19.24 % × | ☐ vo 8.39 % × ×

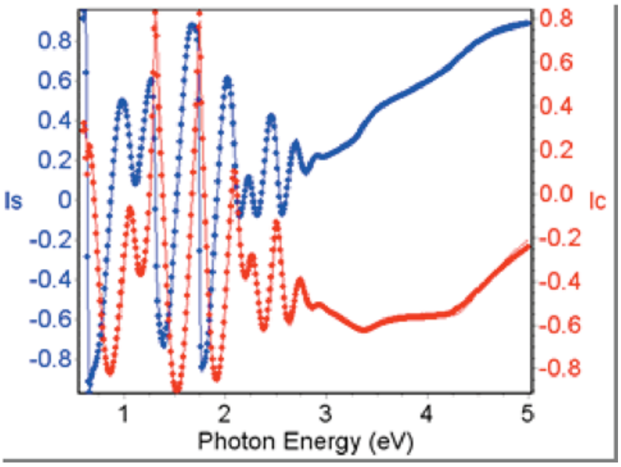
1 F 4995.4 | Sio2_wor.ref × ×

S | c-Si_Jy.clc ×

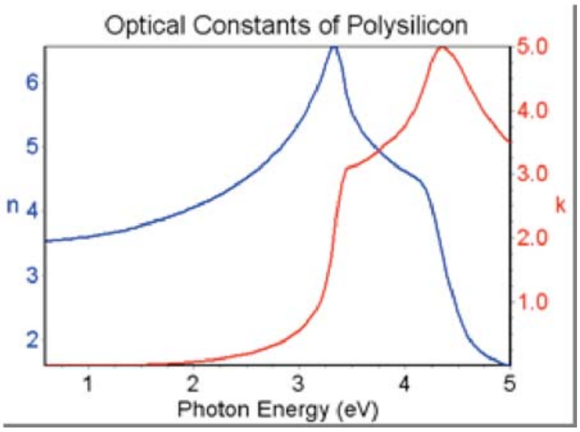
Fit Conditions

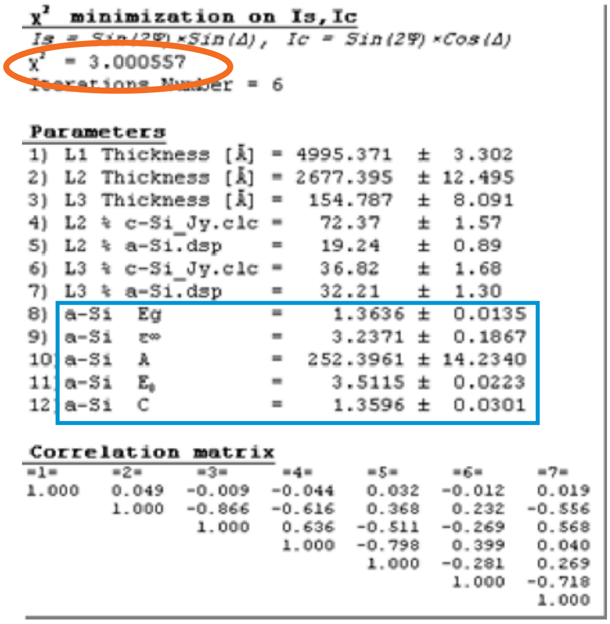
- Spectral range : 0.6 – 5.0 eV
- Step size: 0.01 eV
- Angle of incidence : 70°
- Model information:
  - Polysilicon material is represented by a mixture of c-Si + a-Si + Void.
  - The layer 3 represents the surface layer which can be considered as the surface roughness.
- Fit parameters
  - Thickness : layers 1, 2 and 3
  - Optical constants: a-Si
  - Material composition: layers 2 and 3
- Materials
  - Void, c-Si, SiO_2: Reference library
  - a-Si: Tauc Lorentz

Fit Results



Optical constants of p-Silicon of layer 2*





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 3.000557
Iterations Number = 6

Parameters
1)  L1 Thickness [Å] = 4995.371  ±  3.302
2)  L2 Thickness [Å] = 2677.395  ± 12.495
3)  L3 Thickness [Å] =  154.787  ±  8.091
4)  L2 % c-Si_Jy.clc =   72.37   ±  1.57
5)  L2 % a-Si.dsp    =   19.24   ±  0.89
6)  L3 % c-Si_Jy.clc =   36.82   ±  1.68
7)  L3 % a-Si.dsp    =   32.21   ±  1.30
8)  a-Si  Eg         =     1.3636 ±  0.0135
9)  a-Si  ε∞         =     3.2371 ±  0.1867
10) a-Si  A          =   252.3961 ± 14.2340
11) a-Si  E0         =     3.5115 ±  0.0223
12) a-Si  C          =     1.3596 ±  0.0301

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000   0.049  -0.009  -0.044   0.032  -0.012   0.019
        1.000  -0.866  -0.616   0.368   0.232  -0.556
                1.000   0.636  -0.511  -0.269   0.568
                        1.000  -0.798   0.399   0.040
                                1.000  -0.281   0.269
                                        1.000  -0.718
                                                1.000
```

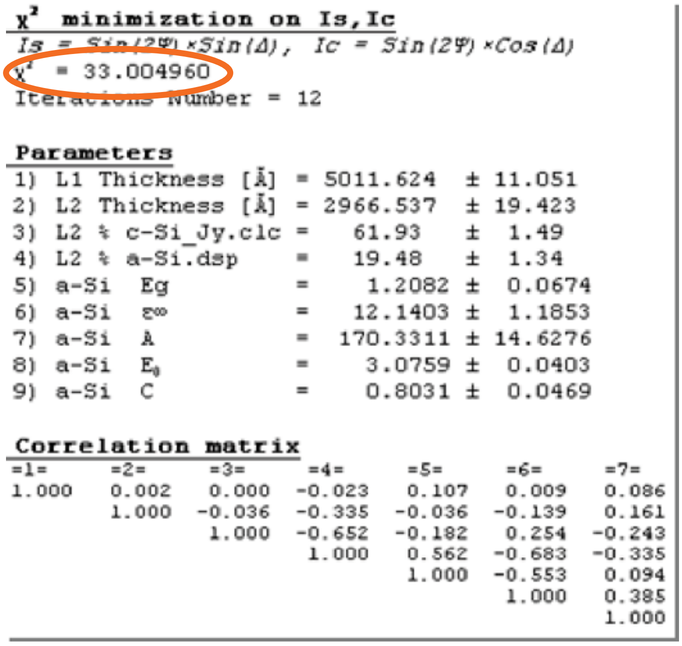
*In deltapsi2, build a new spectroscopic model, and put in the substrate the results found for layer 2, eg 72.37% c-Si + 19.24% a-Si + 8.39% void. Then under modeling description, click on edit, and in the modeling conditions tab, choose “User defined spectral range” and put 0.6-5 eV. Then, click on simulation, and in the results display area, select the (n,k) axis.

9/27/08

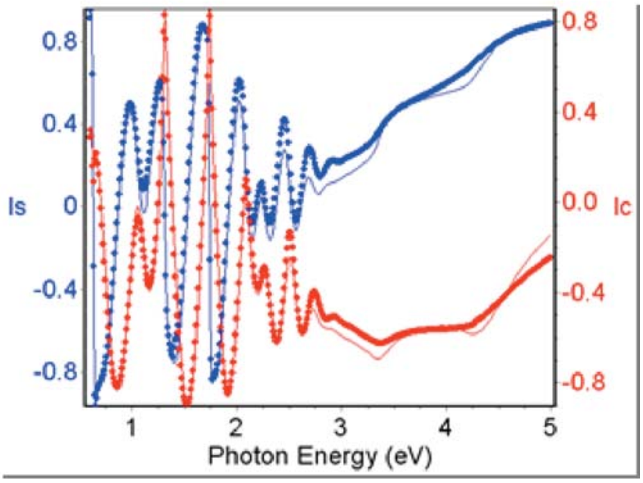
Model without roughness

```
2  F  2966.5  F  %  |  c-!  61.93 %  ×  |  F  a-!  19.48 %  ×  |  ☐  vo  18.59 %  ×  ×
1  F  5011.6        |  Sio2_wor.ref                                               ×  ×
S                   |  c-Si_Jy.clc                                                ×
```

Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 33.004960
Iterations Number = 12

Parameters
1) L1 Thickness [Å] = 5011.624  ± 11.051
2) L2 Thickness [Å] = 2966.537  ± 19.423
3) L2 % c-Si_Jy.clc =   61.93   ±  1.49
4) L2 % a-Si.dsp    =   19.48   ±  1.34
5) a-Si  Eg         =    1.2082 ±  0.0674
6) a-Si  ε∞         =   12.1403 ±  1.1853
7) a-Si  A          =  170.3311 ± 14.6276
8) a-Si  E0         =    3.0759 ±  0.0403
9) a-Si  C          =    0.8031 ±  0.0469

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000   0.002   0.000  -0.023   0.107   0.009   0.086
        1.000  -0.036  -0.335  -0.036  -0.139   0.161
                1.000  -0.652  -0.182   0.254  -0.243
                        1.000   0.562  -0.683  -0.335
                                1.000  -0.553   0.094
                                        1.000   0.385
                                                1.000
```

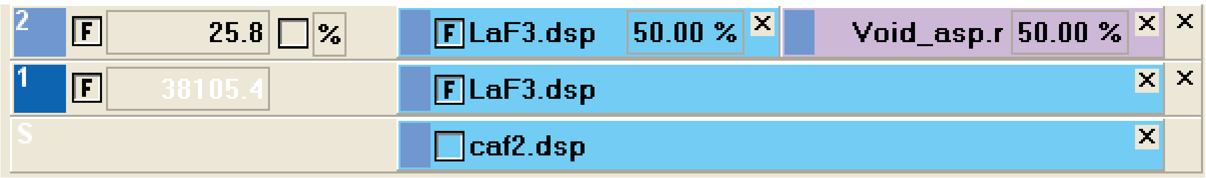


General Remarks

- The rough overlayer on top of layer 2 decreases the χ^2 by a factor 10 !. Hence the final model includes the rough overlayer on top.

LaF_3 / CaF_2 Substrate

Model

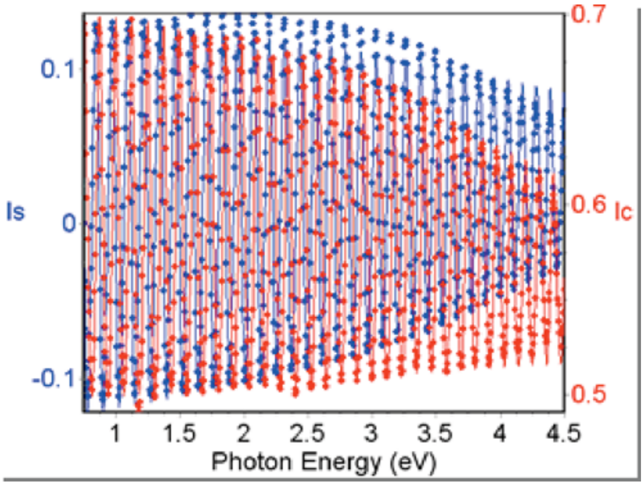


2	F	25.8	☐ %	F LaF3.dsp	50.00 %	Void_asp.r 50.00 %
1	F	38105.4		F LaF3.dsp		
S				☐ caf2.dsp		

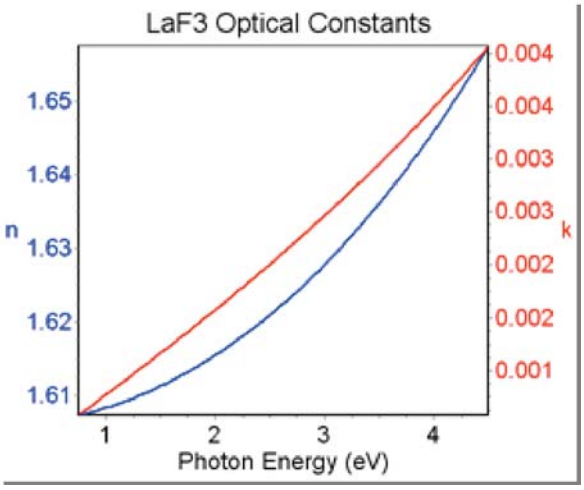
Fit Conditions

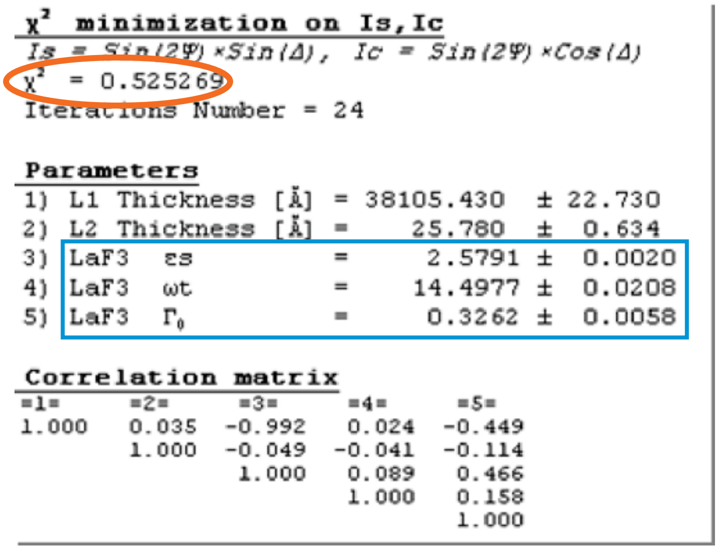
- Spectral range: 0.75 - 4.5 eV
- Step size: 0.005 eV
- Angle of incidence: 70°
- Model Information: Multiguess used for the 1st layer because the thickness is very thick.
- Fit parameters
  - Thickness: Layers 1 and 2
  - Optical constants: LaF_3
- Materials
  - Glassnew: Reference material
  - LaF_3: Classical formula, transparent lorentz oscillator with $\varepsilon_\infty = 1.0$

Fit Results



Optical constants of LaF_3

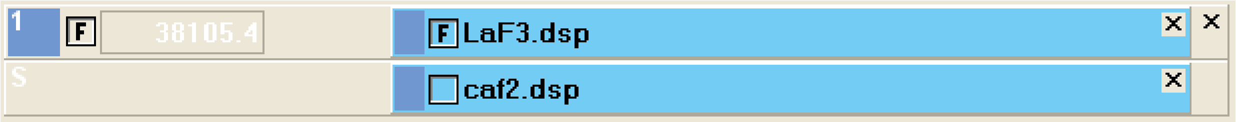




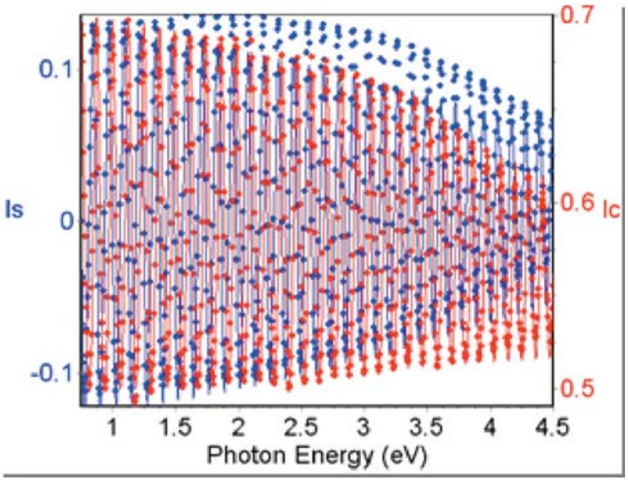
```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.525269
Iterations Number = 24

Parameters
1) L1 Thickness [Å] = 38105.430  ± 22.730
2) L2 Thickness [Å] =    25.780  ±  0.634
3) LaF3  εs         =    2.5791 ±  0.0020
4) LaF3  ωt         =   14.4977 ±  0.0208
5) LaF3  Γ0         =    0.3262 ±  0.0058

Correlation matrix
=1=     =2=     =3=     =4=     =5=
1.000   0.035  -0.992   0.024  -0.449
        1.000  -0.049  -0.041  -0.114
                1.000   0.089   0.466
                        1.000   0.158
                                1.000
```

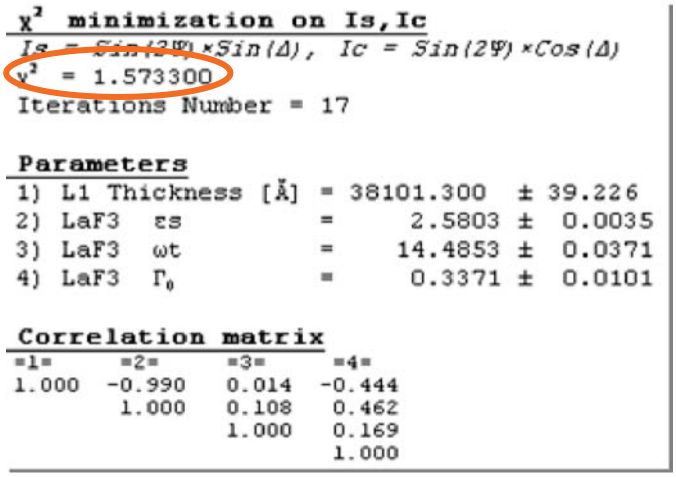
9/2/08

Model without roughness



Fit Results





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 1.573300
Iterations Number = 17

Parameters
1) L1 Thickness [Å] = 38101.300 ± 39.226
2) LaF3  εs         =     2.5803 ±  0.0035
3) LaF3  ωt         =    14.4853 ±  0.0371
4) LaF3  Γ0         =     0.3371 ±  0.0101

Correlation matrix
=1=     =2=     =3=     =4=
1.000  -0.990   0.014  -0.444
        1.000   0.108   0.462
                1.000   0.169
                        1.000
```

General Remarks

- Adding a rough overlayer on top of the film stack decreases the χ^2 by a factor 3. Hence the final model takes into account the roughness.

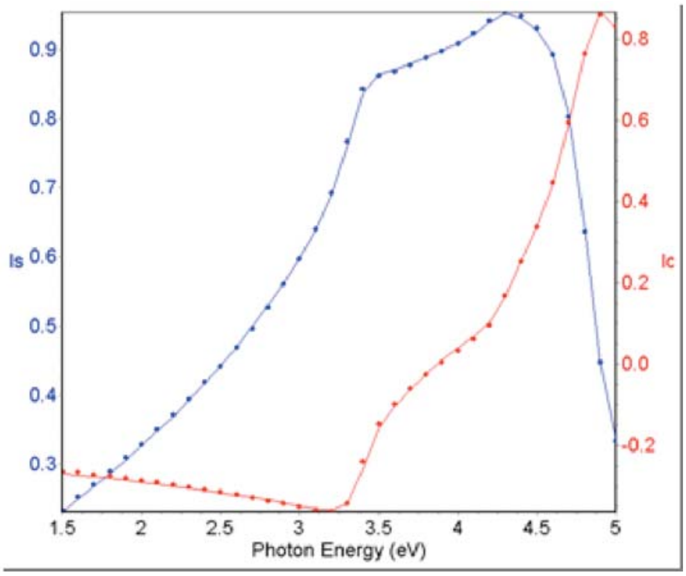
Ta_2O_5 / c-Si Substrate

Model

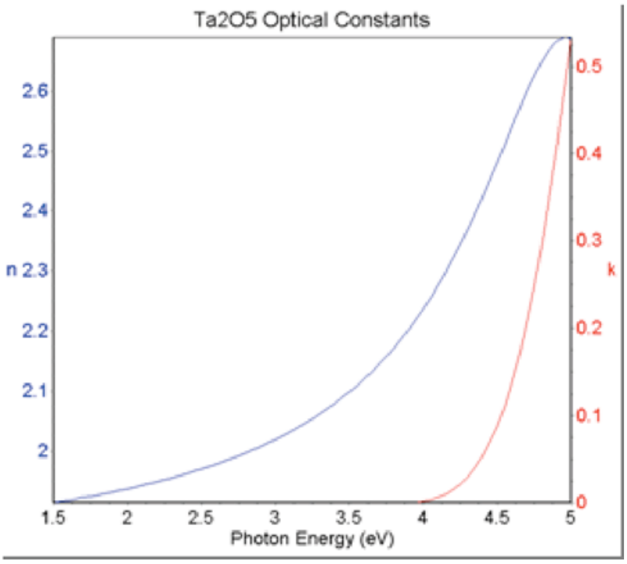
Fit Conditions

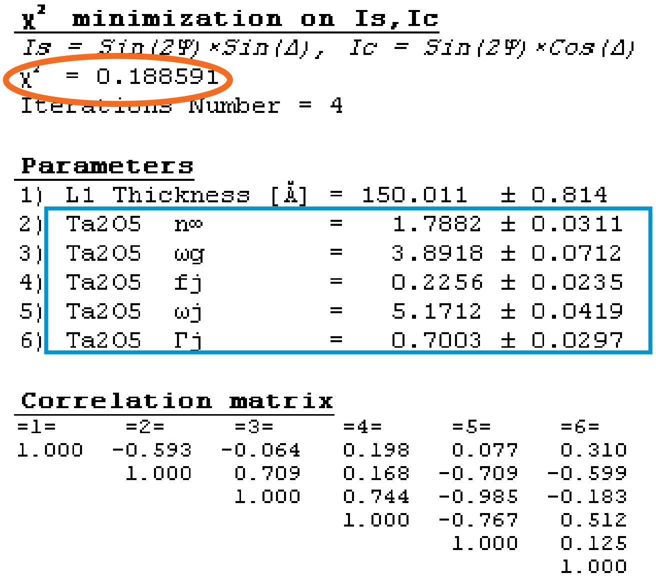
- Spectral range : 1.5-5.0 eV
- Step size: 0.1 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layer 1
  - Optical constants: Ta_2O_5
- Materials
  - c-Si: Reference library
  - **Ta_2O_5**: New amorphous formula

Fit Results



Optical constants of Ta_2O_5

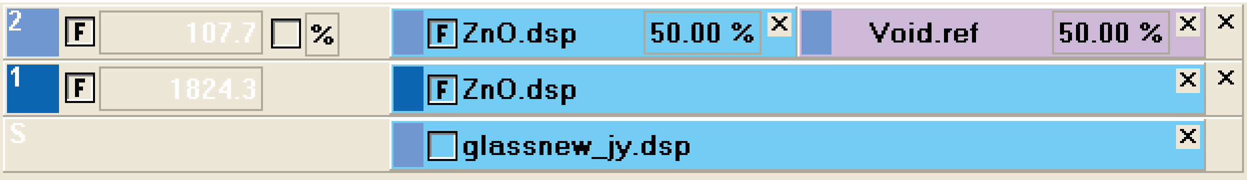




```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.188591
Iterations Number = 4

Parameters
1)  L1 Thickness [Å]  = 150.011   ± 0.814
2)  Ta2O5   n∞         =    1.7882 ± 0.0311
3)  Ta2O5   ωg         =    3.8918 ± 0.0712
4)  Ta2O5   fj         =    0.2256 ± 0.0235
5)  Ta2O5   ωj         =    5.1712 ± 0.0419
6)  Ta2O5   Γj         =    0.7003 ± 0.0297

Correlation matrix
=1=      =2=      =3=      =4=      =5=      =6=
1.000   -0.593   -0.064    0.198    0.077    0.310
         1.000    0.709    0.168   -0.709   -0.599
                  1.000    0.744   -0.985   -0.183
                           1.000   -0.767    0.512
                                    1.000    0.125
                                             1.000
```

ZnO / Glass substrate

Model



2 F 107.7 ☐ % ☑ ZnO.dsp 50.00 % ✕ Void.ref 50.00 % ✕ ✕

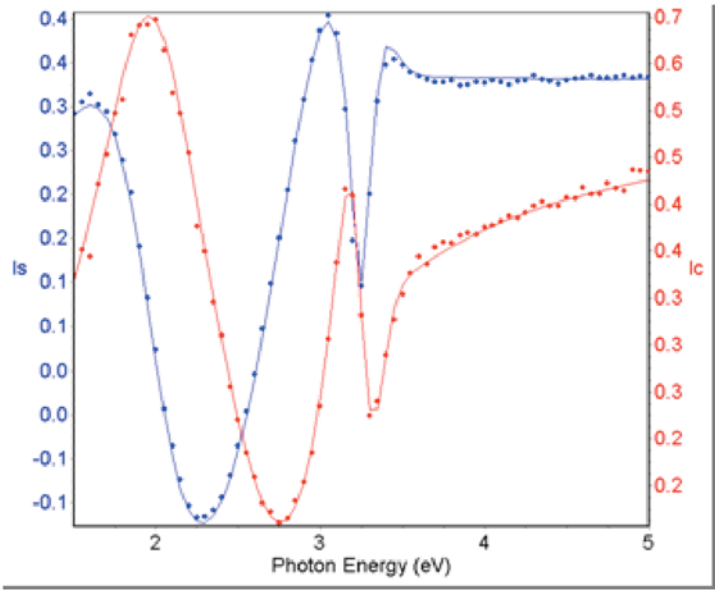
1 F 1824.3 ☑ ZnO.dsp ✕ ✕

S ☐ glassnew_jy.dsp ✕

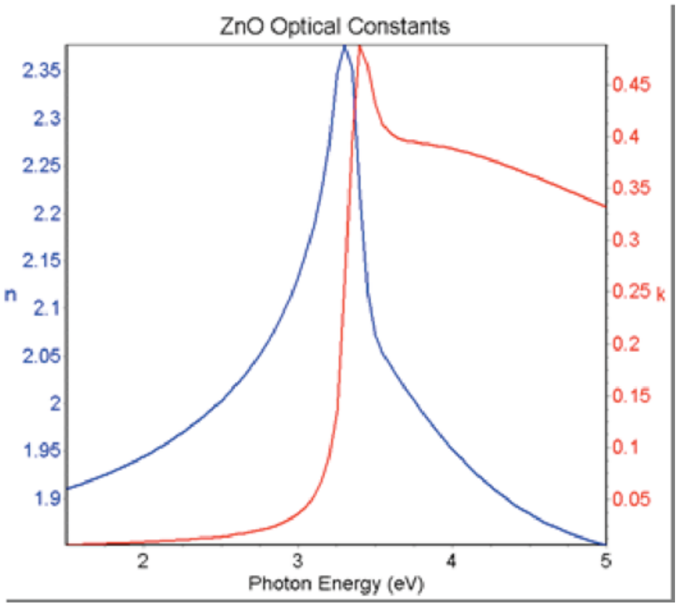
Fit Conditions

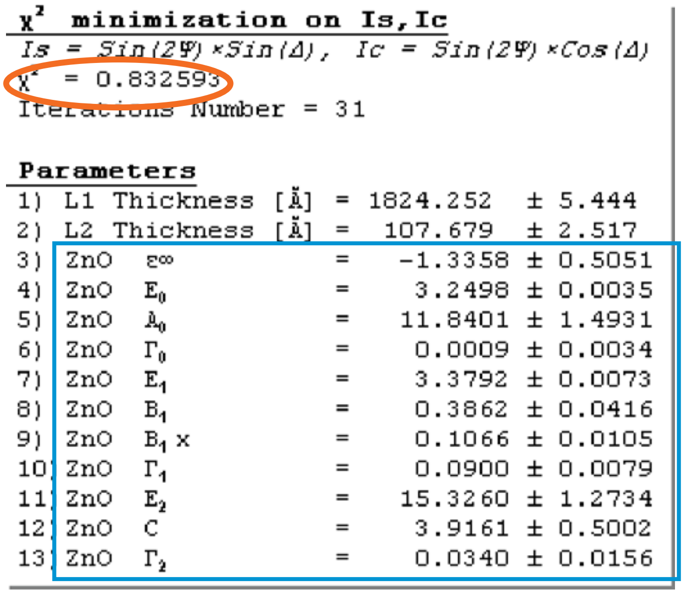
- Spectral range : 1.5-5.0 eV
- Step size: 0.05 eV
- Angle of incidence : 69.9°
- Model: Backside reflections coming from the transparent glass substrate have been masked.
- Fit parameters
  - Thickness : layers 1 and 2 with multiguess
  - Optical constants: ZnO
- Materials
  - Glass new_jy, void : Reference library
  - **AIN**: Kato Adachi formula

Fit Results



Optical constants of ZnO





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 0.832593
Iterations Number = 31

Parameters
1) L1 Thickness [Å] = 1824.252  ± 5.444
2) L2 Thickness [Å] =  107.679  ± 2.517
3) ZnO  ε∞          =   -1.3358 ± 0.5051
4) ZnO  E0          =    3.2498 ± 0.0035
5) ZnO  A0          =   11.8401 ± 1.4931
6) ZnO  Γ0          =    0.0009 ± 0.0034
7) ZnO  E1          =    3.3792 ± 0.0073
8) ZnO  B1          =    0.3862 ± 0.0416
9) ZnO  B1 x        =    0.1066 ± 0.0105
10) ZnO Γ1          =    0.0900 ± 0.0079
11) ZnO E2          =   15.3260 ± 1.2734
12) ZnO C           =    3.9161 ± 0.5002
13) ZnO Γ2          =    0.0340 ± 0.0156
```

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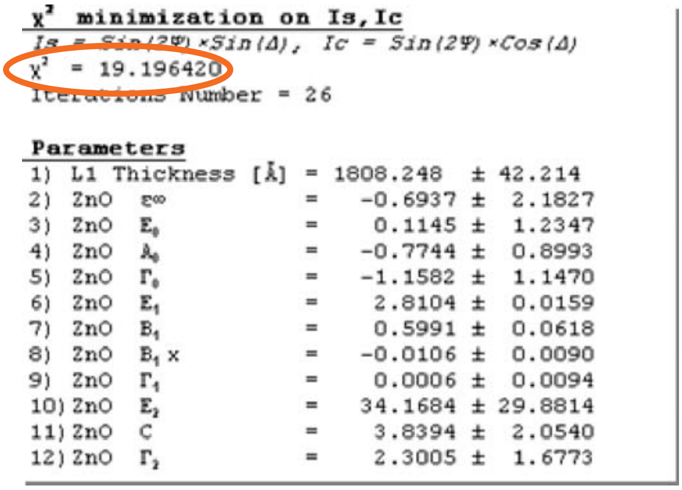
Model without roughness

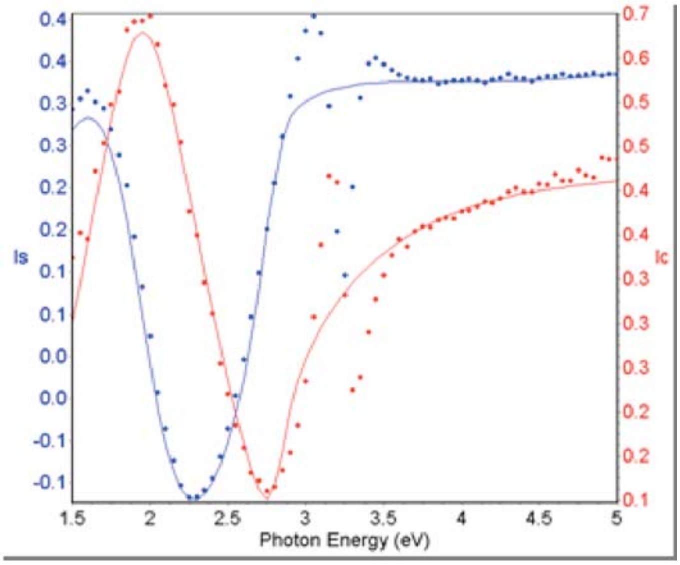
1 F 1808.2 F ZnO.dsp

S glassnew_jy.dsp

Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 19.196420
Iterations Number = 26

Parameters
1) L1 Thickness [Å] = 1808.248  ± 42.214
2) ZnO  ε∞          =  -0.6937 ±  2.1827
3) ZnO  E0          =   0.1145 ±  1.2347
4) ZnO  A0          =  -0.7744 ±  0.8993
5) ZnO  Γ0          =  -1.1582 ±  1.1470
6) ZnO  E1          =   2.8104 ±  0.0159
7) ZnO  B1          =   0.5991 ±  0.0618
8) ZnO  B1 x        =  -0.0106 ±  0.0090
9) ZnO  Γ1          =   0.0006 ±  0.0094
10) ZnO E2          =  34.1684 ± 29.8814
11) ZnO C           =   3.8394 ±  2.0540
12) ZnO Γ2          =   2.3005 ±  1.6773
```



General Remarks

- The final model includes a rough overlayer on top that provides an excellent fit results.

9/2/08

GaAs Oxide/ GaAs Substrate

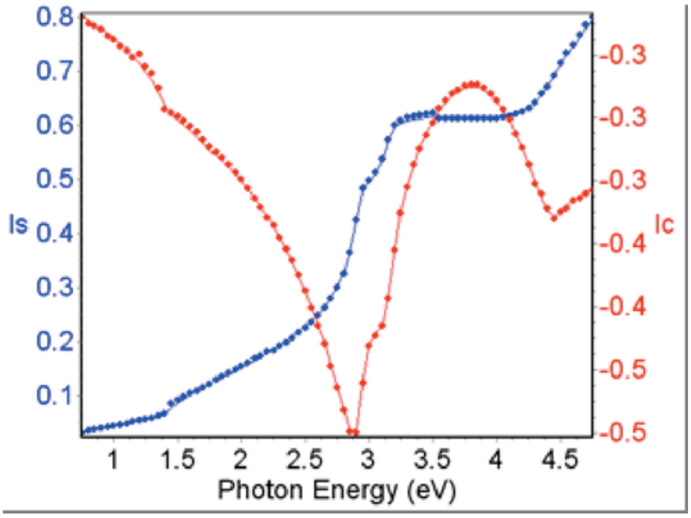
Model

1 F 49.7 F gaas-oxide.dsp
S Gaas_isa.ref

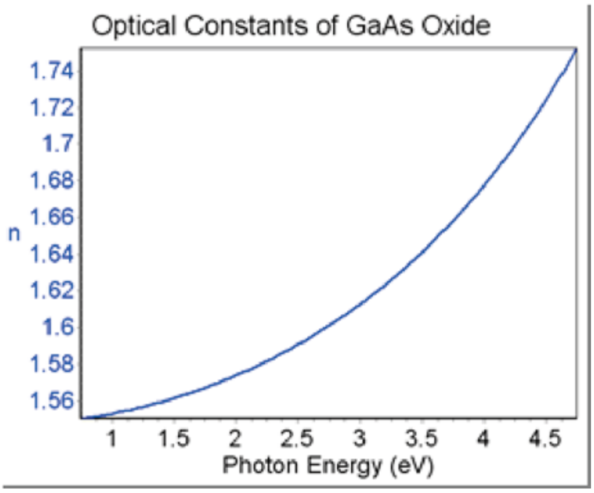
Fit Conditions

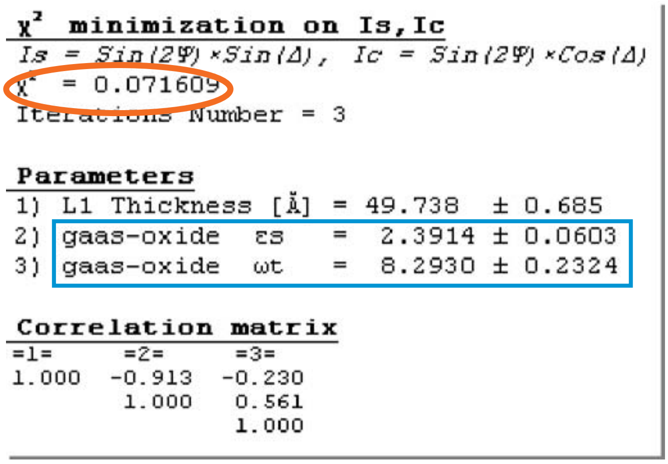
- Spectral range : 0.75 - 4.75 eV
- Step size: 0.05 eV
- Angle of incidence : 70°
- Model: Backside reflection model
- Fit parameters
  - Thickness : layer 1
  - Optical constants: GaAs oxide
- Materials
  - GaAs_isa: Reference library
  - **GaAs oxide**: Classical formula, transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Fit Results



Optical constants of GaAs oxide





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.071609
Iterations Number = 3

Parameters
1) L1 Thickness [Å]  = 49.738  ± 0.685
2) gaas-oxide  εs    =  2.3914 ± 0.0603
3) gaas-oxide  ωt    =  8.2930 ± 0.2324

Correlation matrix
=1=     =2=     =3=
1.000  -0.913  -0.230
        1.000   0.561
                1.000
```

PVK / SiO_2 Substrate

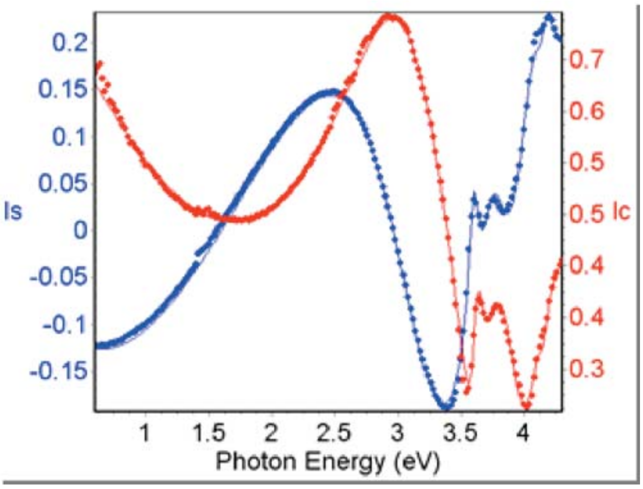
Model

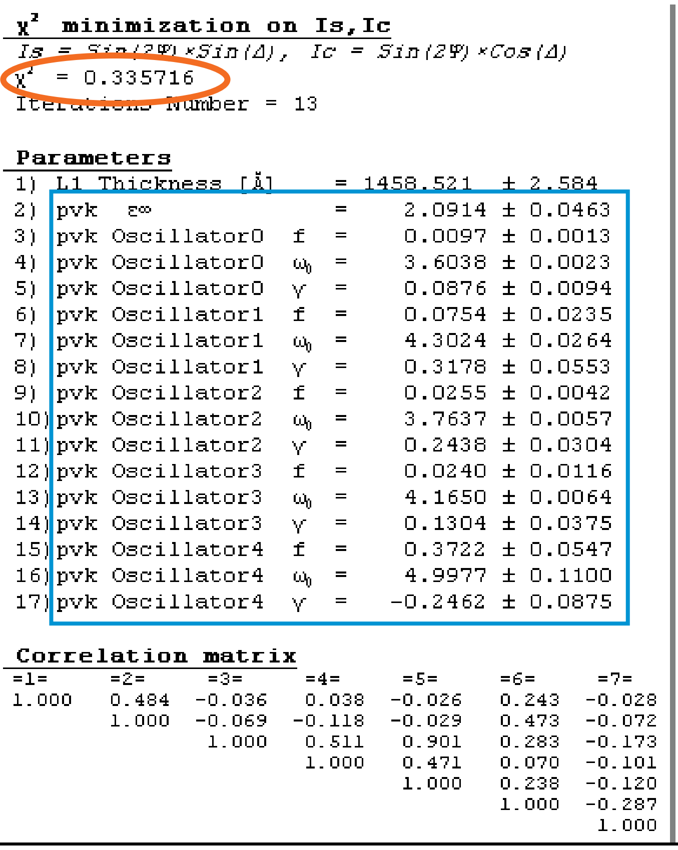

1 F 1458.5
F pvk.udf
S
Sio2_wor.ref

Fit Conditions

- Spectral range : 0.6 - 4.3 eV
- Step size: 0.05 eV
- Angle of incidence : 70.3°
- Fit parameters
  - Thickness : layer 1
  - Optical constants: PVK
- Materials
  - SiO_2: Reference library
  - **PVK**: Absorbing Lorentz 5 oscillators

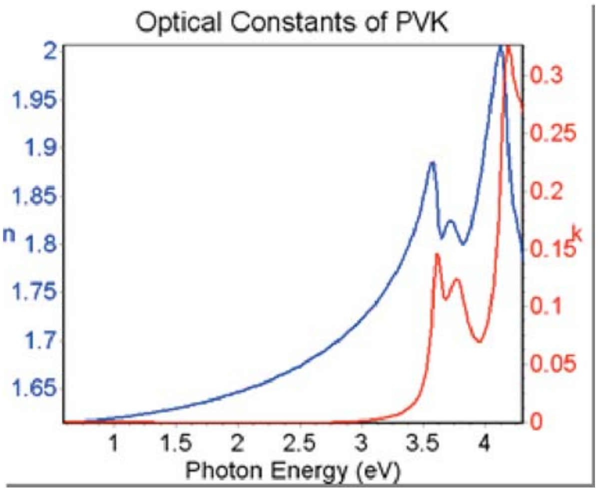
Fit Results





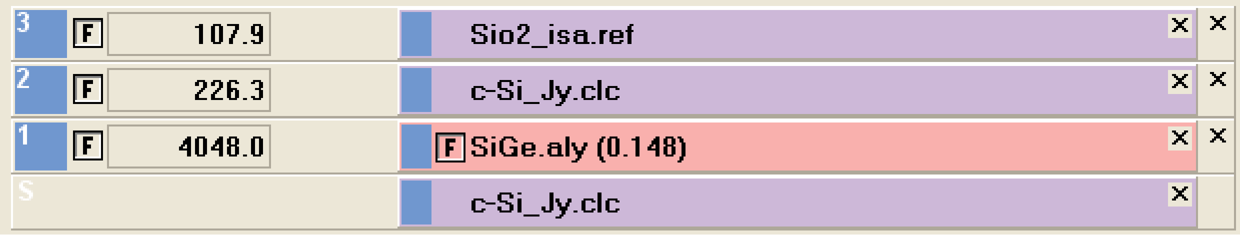
```
χ²  minimization on Is,Ic
 Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
 χ²  = 0.335716
 Iterations Number = 13

 Parameters
 1) L1 Thickness [Å]      = 1458.521  ± 2.584
 2) pvk   ε∞              =    2.0914 ± 0.0463
 3) pvk Oscillator0  f    =    0.0097 ± 0.0013
 4) pvk Oscillator0  ω0   =    3.6038 ± 0.0023
 5) pvk Oscillator0  γ    =    0.0876 ± 0.0094
 6) pvk Oscillator1  f    =    0.0754 ± 0.0235
 7) pvk Oscillator1  ω0   =    4.3024 ± 0.0264
 8) pvk Oscillator1  γ    =    0.3178 ± 0.0553
 9) pvk Oscillator2  f    =    0.0255 ± 0.0042
10) pvk Oscillator2  ω0   =    3.7637 ± 0.0057
11) pvk Oscillator2  γ    =    0.2438 ± 0.0304
12) pvk Oscillator3  f    =    0.0240 ± 0.0116
13) pvk Oscillator3  ω0   =    4.1650 ± 0.0064
14) pvk Oscillator3  γ    =    0.1304 ± 0.0375
15) pvk Oscillator4  f    =    0.3722 ± 0.0547
16) pvk Oscillator4  ω0   =    4.9977 ± 0.1100
17) pvk Oscillator4  γ    =   -0.2462 ± 0.0875

 Correlation matrix
 =1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000   0.484  -0.036   0.038  -0.026   0.243  -0.028
        1.000  -0.069  -0.118  -0.029   0.473  -0.072
                1.000   0.511   0.901   0.283  -0.173
                        1.000   0.471   0.070  -0.101
                                1.000   0.238  -0.120
                                        1.000  -0.287
                                                1.000
```

Optical constants of PVK



SiO_2 / c-Si / SiGe / c-Si Substrate

Model



3 F 107.9 Sio2_isa.ref

2 F 226.3 c-Si_Jy.clc

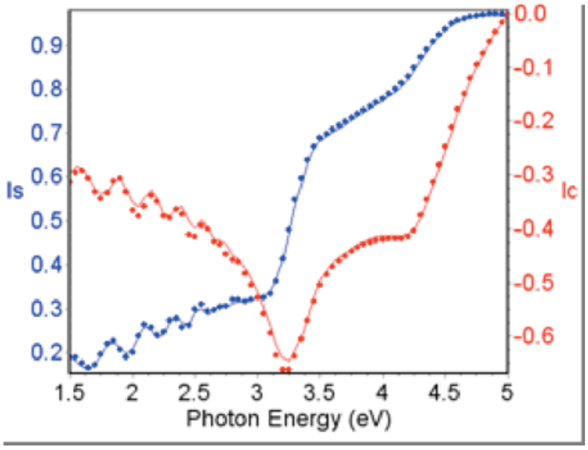
1 F 4048.0 F SiGe.aly (0.148)

S c-Si_Jy.clc

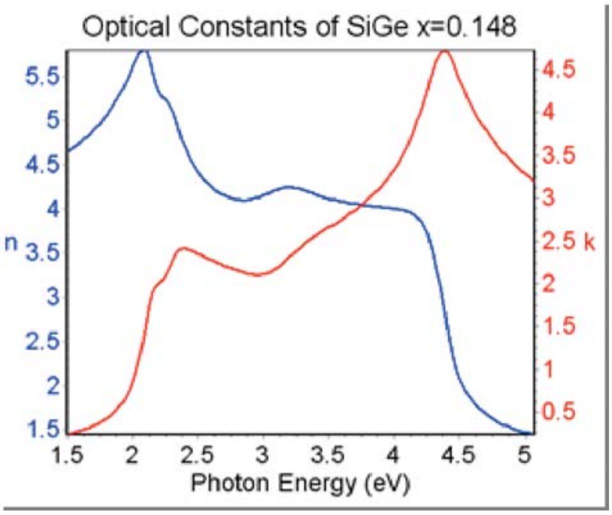
Fit Conditions

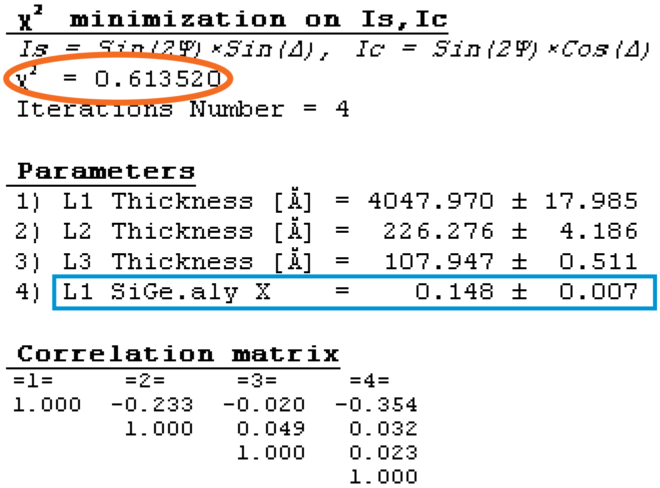
- Spectral range : 1.5 - 5.0 eV
- Step size : 0.05 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layers 1, 2, 3
  - Composition: SiGe alloy
- Materials
  - c-Si, SiO_2: Reference library
  - **SiGe**: Alloy

Fit Results



Optical constants of SiGe x=0.148





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)*Sin(Δ),  Ic = Sin(2Ψ)*Cos(Δ)
χ²  = 0.613520
Iterations Number = 4

Parameters
1)  L1 Thickness [Å]  = 4047.970 ± 17.985
2)  L2 Thickness [Å]  =  226.276 ±  4.186
3)  L3 Thickness [Å]  =  107.947 ±  0.511
4)  L1 SiGe.aly X     =    0.148 ±  0.007

Correlation matrix
=1=     =2=     =3=     =4=
1.000  -0.233  -0.020  -0.354
        1.000   0.049   0.032
                1.000   0.023
                        1.000
```

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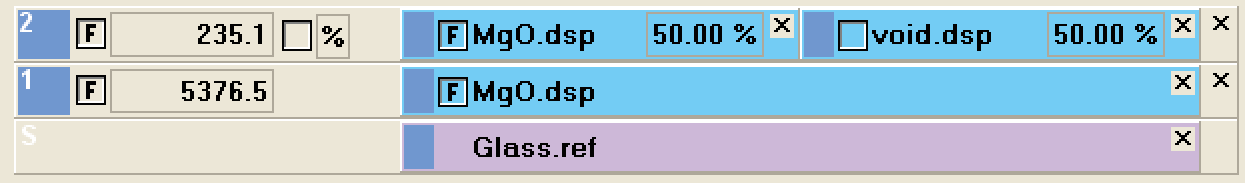
MgO / Glass Substrate

Model



2 F 235.1 ☐ % | F MgO.dsp 50.00 % | ☐ void.dsp 50.00 %

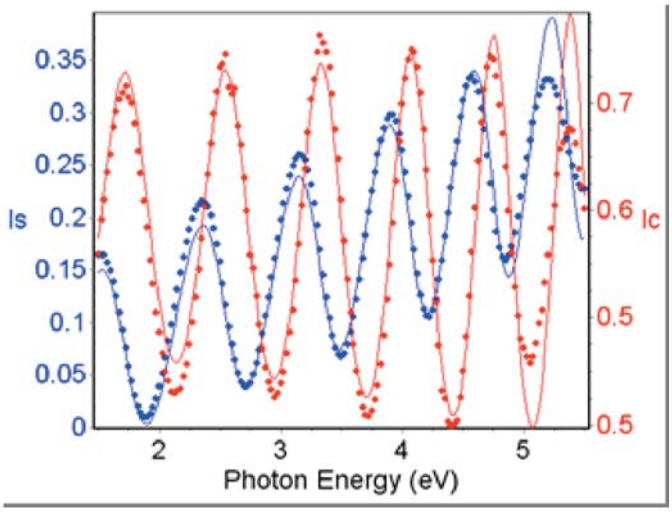
1 F 5376.5 | F MgO.dsp

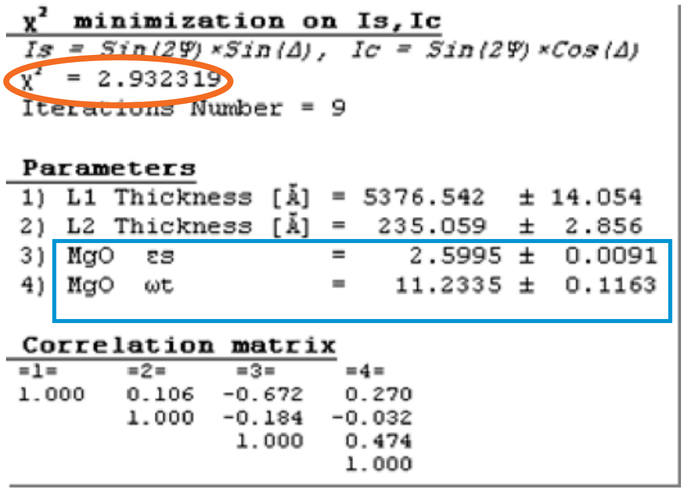
S | Glass.ref

Fit Conditions

- Spectral range : 1.5 - 5.5 eV
- Step size: 0.025
- Angle of incidence : 70.2°
- Fit parameters
  - Thickness : layers 1 and 2
  - Optical constants: MgO
- Materials
  - Glass: Reference library
  - **MgO**: Classical formula, transparent Lorentz oscillator, with $\varepsilon_\infty = 1.0$

Fit Results



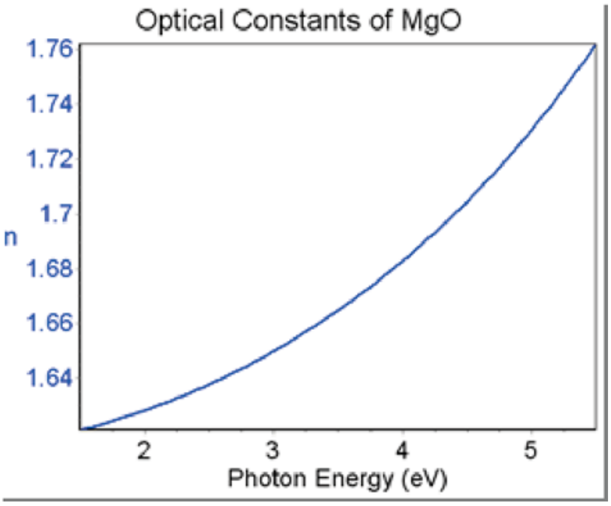


```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 2.932319
Iterations Number = 9

Parameters
1) L1 Thickness [Å] = 5376.542  ± 14.054
2) L2 Thickness [Å] =  235.059  ±  2.856
3) MgO  εs          =     2.5995 ±  0.0091
4) MgO  ωt          =    11.2335 ±  0.1163

Correlation matrix
=1=      =2=      =3=      =4=
1.000    0.106   -0.672    0.270
         1.000   -0.184   -0.032
                  1.000    0.474
                           1.000
```

Optical constants of MgO



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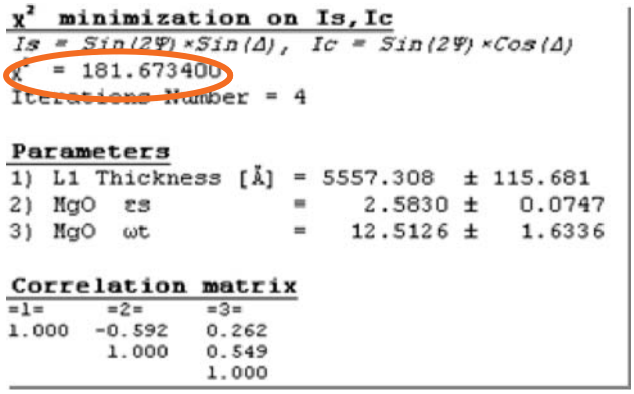
Model without Roughness

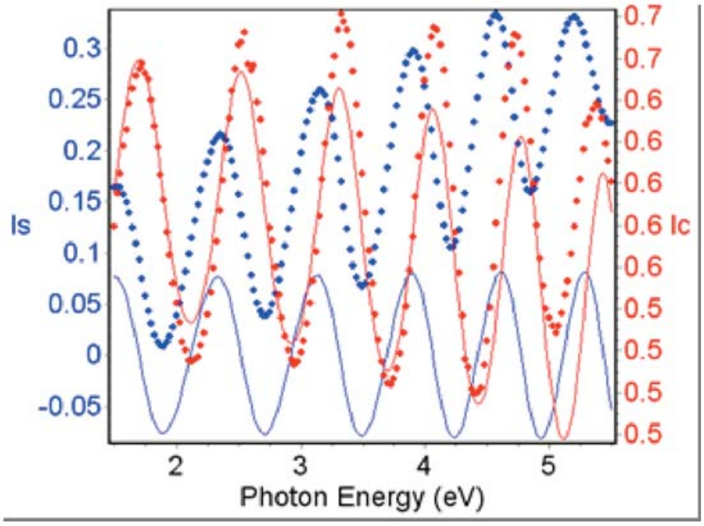
Fit Results



```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 181.673400
Iterations Number = 4

Parameters
1) L1 Thickness [Å]  = 5557.308  ± 115.681
2) MgO  εs           =     2.5830 ±    0.0747
3) MgO  ωt           =    12.5126 ±    1.6336

Correlation matrix
=1=      =2=      =3=
1.000   -0.592    0.262
         1.000    0.549
                  1.000
```



General Remarks

- The MgO exhibits a strong rough overlayer that must be taken into account in the final model.

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BaSrTiO$_3$ / Sapphire Substrate BR

Model

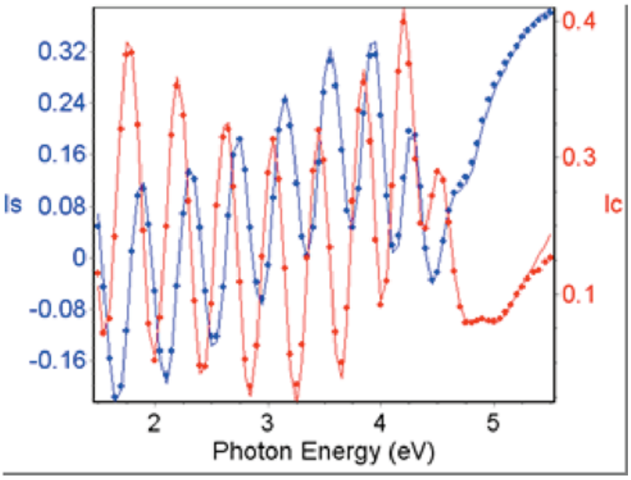
3	F 35.6 ☐ %	F BST.dsp 50.00 %	Void.ref 50.00 %
2	F 645.8	F BST.dsp	
1	☐ 5200000.0 E	☐ AL2O3_E.dsp	
	O	☐ AL2O3_O.dsp	
S		Void.ref	

Backside reflection model

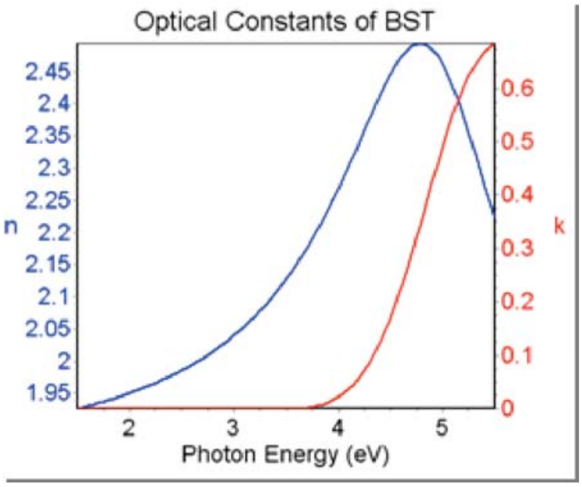
Fit Conditions

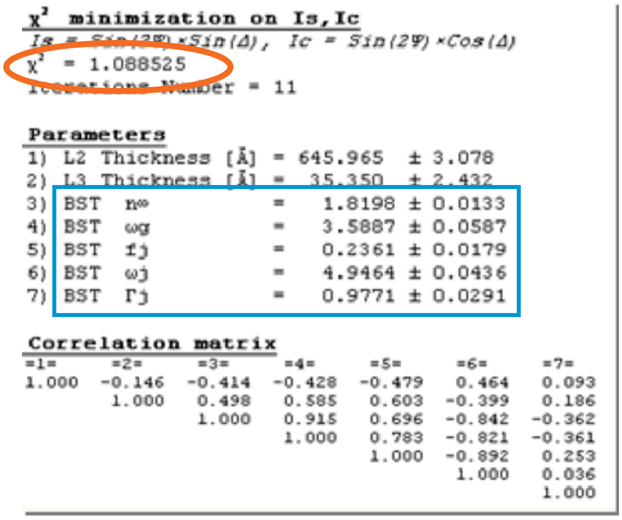
- Spectral range: 1.5-5.5 eV
- Step size: 0.05 eV
- Angle of incidence: 70°
- Model: Backside reflections
- Fit parameters
    - Thickness: Layers 1 and 2
    - Optical constants: BST
- Materials
    - Al$_2$O$_3$ void : Reference library
    - BST: New amorphous formula

Fit Results



Optical constants of BST



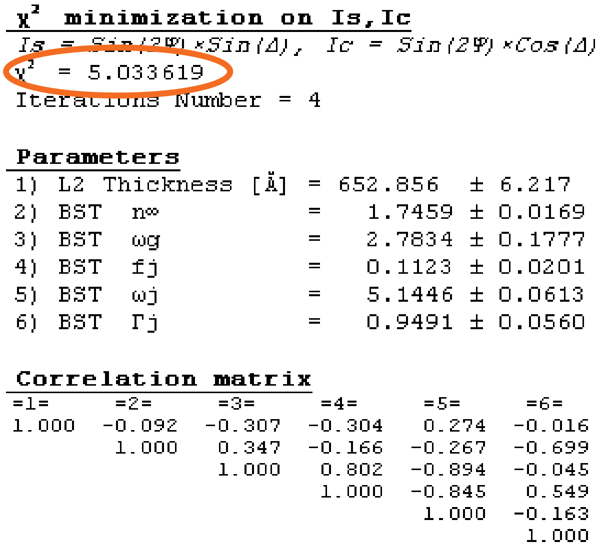


```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 1.088525
Iterations Number = 11

Parameters
1)  L2 Thickness [Å]  = 645.965  ± 3.078
2)  L3 Thickness [Å]  =  35.350  ± 2.432
3)  BST  n∞           =   1.8198 ± 0.0133
4)  BST  ωg           =   3.5887 ± 0.0587
5)  BST  fj           =   0.2361 ± 0.0179
6)  BST  ωj           =   4.9464 ± 0.0436
7)  BST  Γj           =   0.9771 ± 0.0291

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.146  -0.414  -0.428  -0.479   0.464   0.093
        1.000   0.498   0.585   0.603  -0.399   0.186
                1.000   0.915   0.696  -0.842  -0.362
                        1.000   0.783  -0.821  -0.361
                                1.000  -0.892   0.253
                                        1.000   0.036
                                                1.000
```

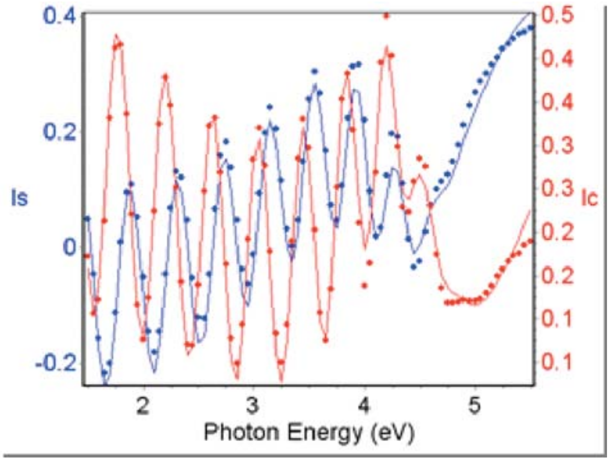
Model without roughness

```
2  F  652.8              F BST.dsp
1  ☐  5200000.0   E      ☐ AL2O3_E.dsp
                  O      ☐ AL2O3_O.dsp
S                        Void.ref
```

Fit Results



```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 5.033619
Iterations Number = 4

Parameters
1) L2 Thickness [Å] = 652.856  ± 6.217
2) BST  n∞          =   1.7459 ± 0.0169
3) BST  ωg          =   2.7834 ± 0.1777
4) BST  fj          =   0.1123 ± 0.0201
5) BST  ωj          =   5.1446 ± 0.0613
6) BST  Γj          =   0.9491 ± 0.0560

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000  -0.092  -0.307  -0.304   0.274  -0.016
        1.000   0.347  -0.166  -0.267  -0.699
                1.000   0.802  -0.894  -0.045
                        1.000  -0.845   0.549
                                1.000  -0.163
                                        1.000
```



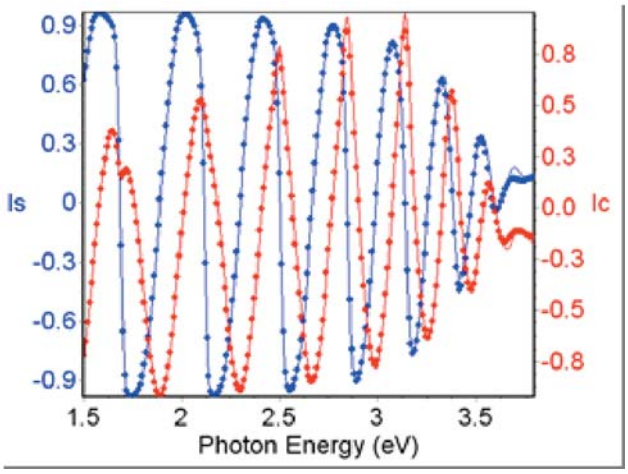
PZT / Pt Substrate

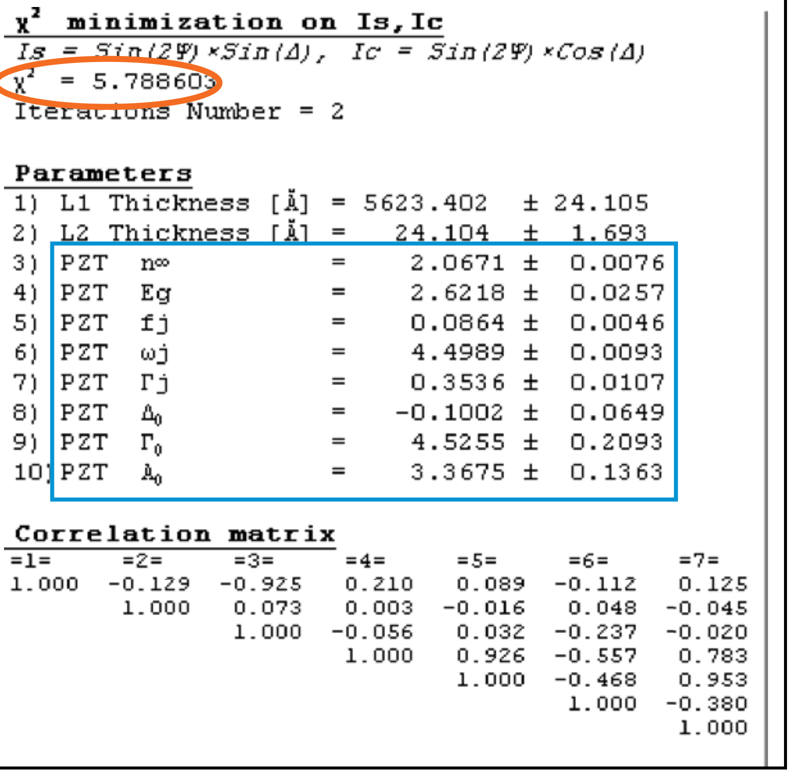
Model

Fit Conditions

- Spectral range: 1.5 - 3.8 eV
- Step size: 0.01 eV
- Angle of incidence: 70°
- Model Information: Pt substrate was measured in a 1st step to be able to use the « spe » file directly in the substrate.
- Fit parameters
  - Thickness: Layers 1 and 2
  - Optical constants: PZT
- Materials
  - Pt: Spe file – raw data
  - **PZT**: Adachi New Forouhi formula

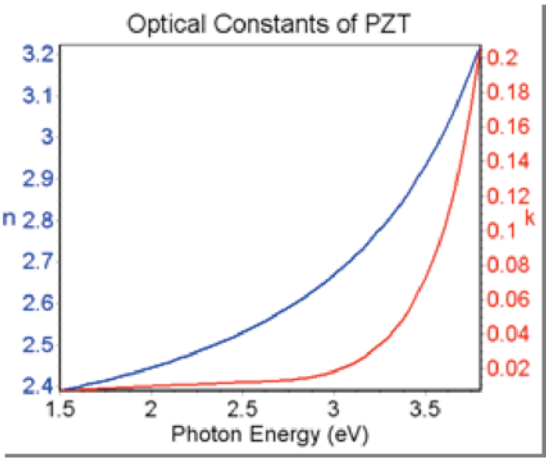
Fit Results





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 5.788603
Iterations Number = 2

Parameters
1) L1 Thickness [Å] = 5623.402   ± 24.105
2) L2 Thickness [Å] =   24.104   ±  1.693
3) PZT  n∞            =    2.0671 ±  0.0076
4) PZT  Eg            =    2.6218 ±  0.0257
5) PZT  fj            =    0.0864 ±  0.0046
6) PZT  ωj            =    4.4989 ±  0.0093
7) PZT  Γj            =    0.3536 ±  0.0107
8) PZT  Δ0            =   -0.1002 ±  0.0649
9) PZT  Γ0            =    4.5255 ±  0.2093
10)PZT  A0            =    3.3675 ±  0.1363

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.129  -0.925   0.210   0.089  -0.112   0.125
        1.000   0.073   0.003  -0.016   0.048  -0.045
                1.000  -0.056   0.032  -0.237  -0.020
                        1.000   0.926  -0.557   0.783
                                1.000  -0.468   0.953
                                        1.000  -0.380
                                                1.000
```

Optical constants of PZT

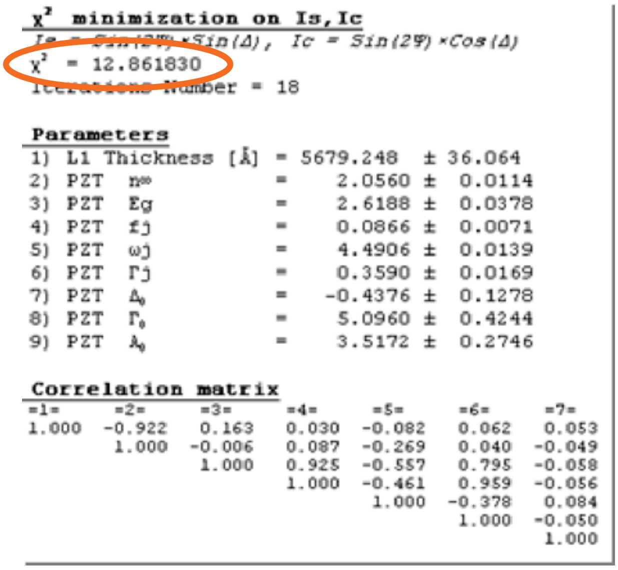


Model without roughness

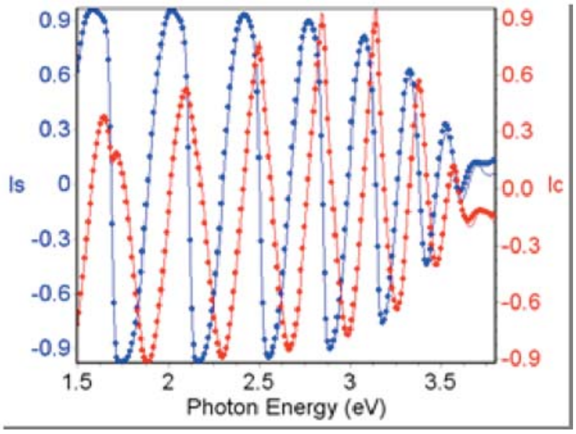
1 F 5679.2 F PZT.dsp

S Pt.spe

Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 12.861830
Iterations Number = 18

Parameters
1) L1 Thickness [Å] = 5679.248  ± 36.064
2) PZT  n∞          =    2.0560 ±  0.0114
3) PZT  Eg          =    2.6188 ±  0.0378
4) PZT  fj          =    0.0866 ±  0.0071
5) PZT  ωj          =    4.4906 ±  0.0139
6) PZT  Γj          =    0.3590 ±  0.0169
7) PZT  Δ0          =   -0.4376 ±  0.1278
8) PZT  Γ0          =    5.0960 ±  0.4244
9) PZT  A0          =    3.5172 ±  0.2746

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.922   0.163   0.030  -0.082   0.062   0.053
        1.000  -0.006   0.087  -0.269   0.040  -0.049
                1.000   0.925  -0.557   0.795  -0.058
                        1.000  -0.461   0.959  -0.056
                                1.000  -0.378   0.084
                                        1.000  -0.050
                                                1.000
```



General Remarks

- Adding a rough overlayer on top of the film stack provides a significant decrease of the χ^2. So the final model takes into account the roughness.
- The sample substrate was platinum. The material is listed in the application library of the software. Nevertheless, the optical properties (n,k) of metals vary strongly vs their composition. Thus as metals are strongly absorbing materials, the solution is to measure them and use the “spe” experimental file directly in the substrate.

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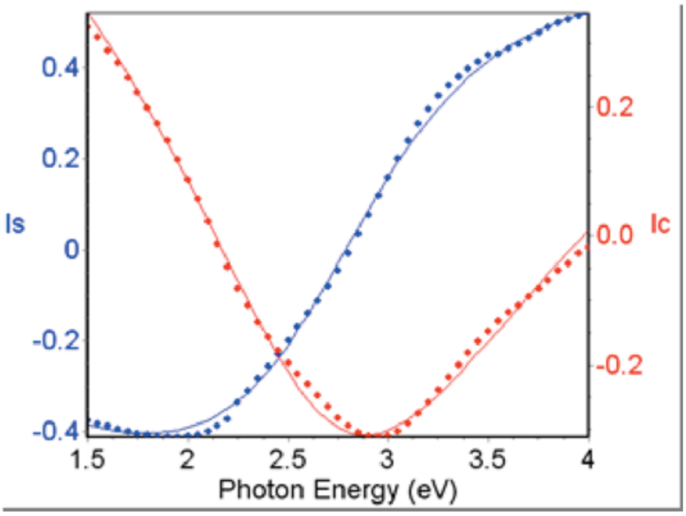
FeO / Glass Substrate

Model

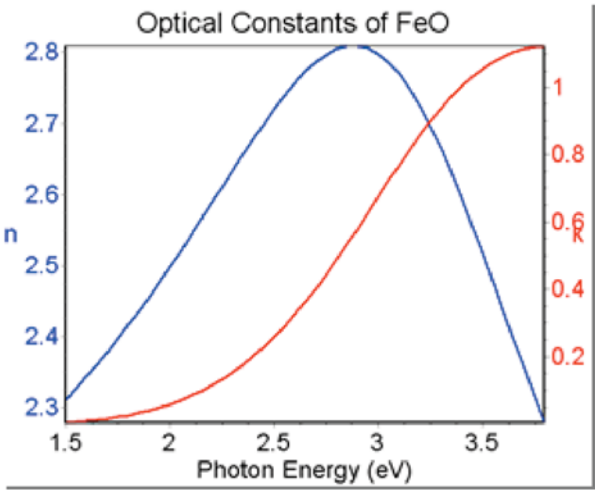
Fit Conditions

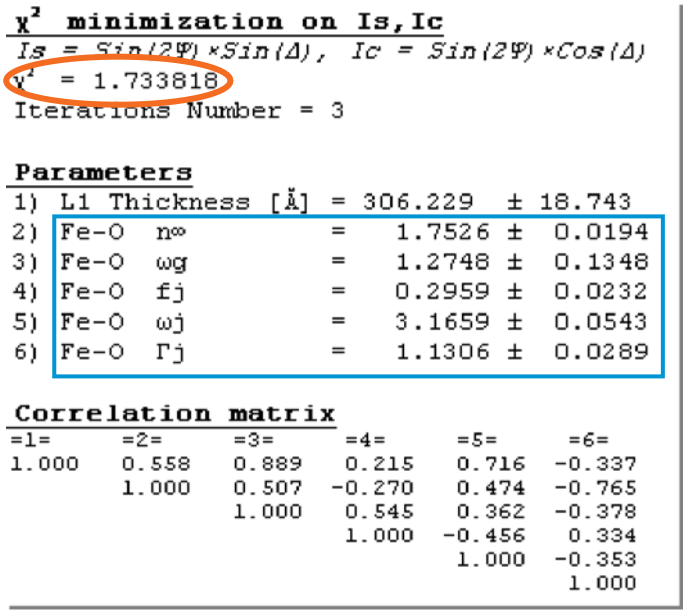
- Spectral range: 1.5 - 4.0 eV
- Step size: 0.05 eV
- Angle of incidence: 70.3°
- Model Information: The backside of the glass substrate was roughened (hence the backside reflection model is not used here).
- Fit parameters
  - Thickness: Layer 1
  - Optical constants: Fe-O
- Materials
  - Glassnew: Reference material
  - **FeO**: New amorphous formula

Fit Results



Optical constants of FeO





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 1.733818
Iterations Number = 3

Parameters
1) L1 Thickness [Å]  = 306.229  ± 18.743
2) Fe-O  n∞          =   1.7526 ±  0.0194
3) Fe-O  ωg          =   1.2748 ±  0.1348
4) Fe-O  fj          =   0.2959 ±  0.0232
5) Fe-O  ωj          =   3.1659 ±  0.0543
6) Fe-O  Γj          =   1.1306 ±  0.0289

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000   0.558   0.889   0.215   0.716  -0.337
        1.000   0.507  -0.270   0.474  -0.765
                1.000   0.545   0.362  -0.378
                        1.000  -0.456   0.334
                                1.000  -0.353
                                        1.000
```

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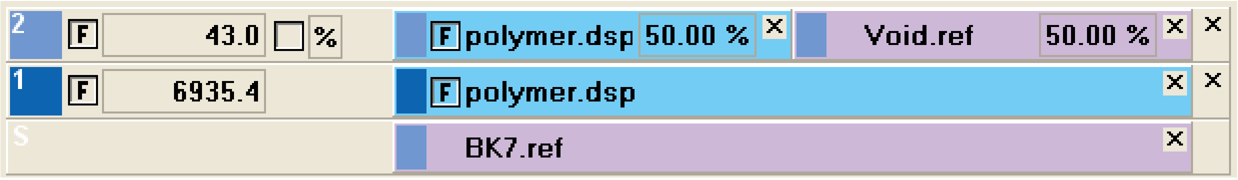
Polymer / BK7 Substrate

Model

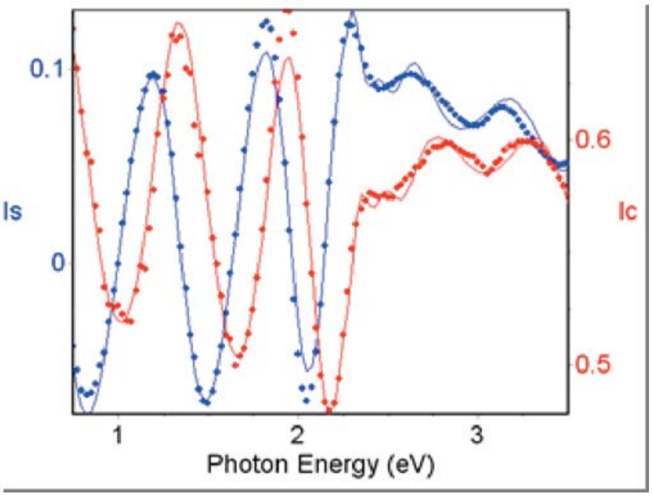


2 F 43.0 ☐ % F polymer.dsp 50.00 % × Void.ref 50.00 % × ×
1 F 6935.4 F polymer.dsp × ×
S BK7.ref ×

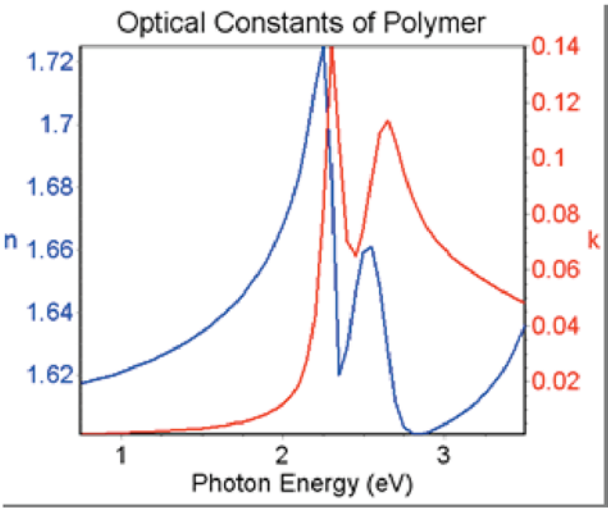
Fit Conditions

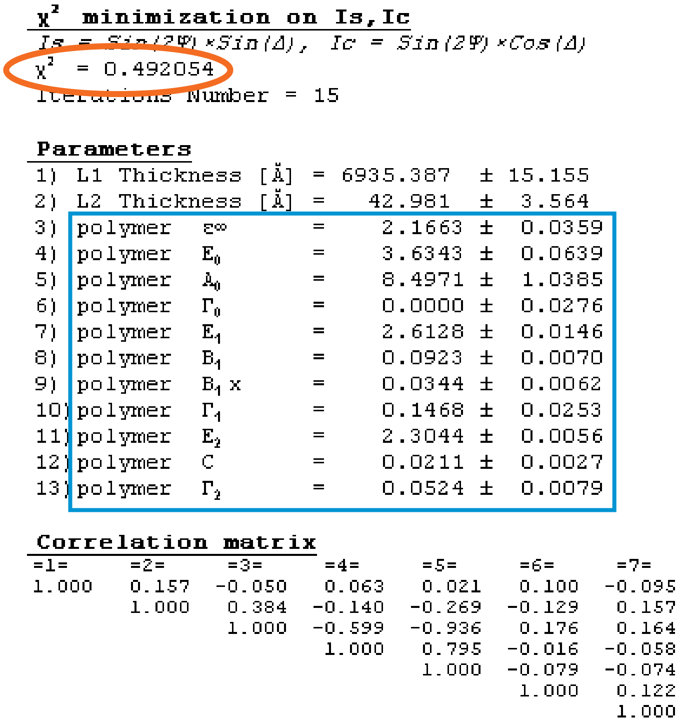
- Spectral range: 0.75 - 3.5 eV
- Step size: 0.025 eV
- Angle of incidence: 70°
- Model Information: The backside of the glass substrate was roughened (hence the backside reflection model is not used here).
- Fit parameters
    - Thickness: Layers 1 and 2
    - Optical constants: Polymer
- Materials
    - BK7: Reference material
    - **Polymer**: Kato-Adachi

Fit Results



Optical constants of Polymer

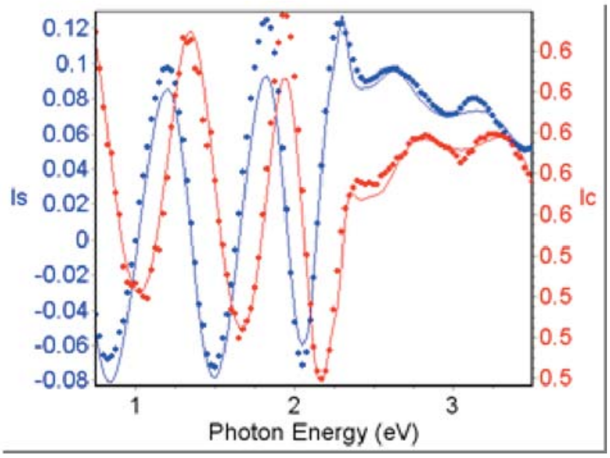


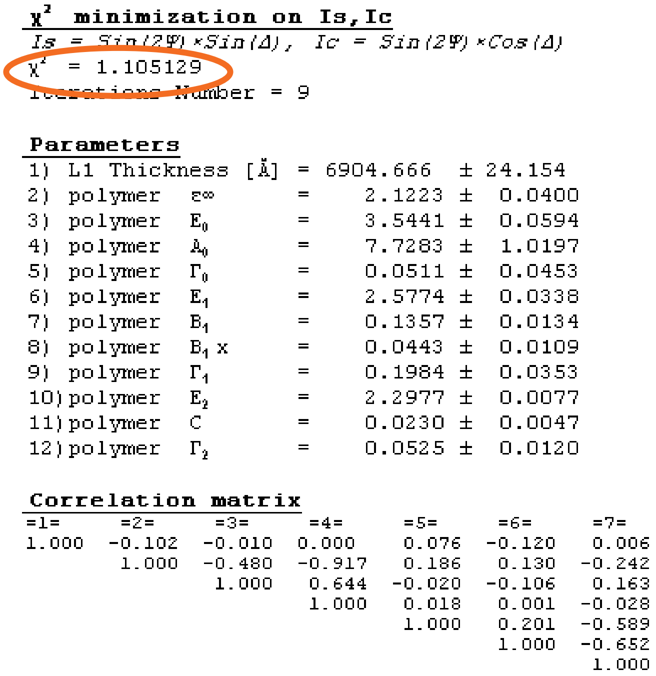


```
χ2  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ2  = 0.492054
Iterations Number = 15

Parameters
1) L1 Thickness [Å] = 6935.387  ± 15.155
2) L2 Thickness [Å] =   42.981  ±  3.564
3) polymer  ε∞        =   2.1663 ±  0.0359
4) polymer  E0        =   3.6343 ±  0.0639
5) polymer  A0        =   8.4971 ±  1.0385
6) polymer  Γ0        =   0.0000 ±  0.0276
7) polymer  E1        =   2.6128 ±  0.0146
8) polymer  B1        =   0.0923 ±  0.0070
9) polymer  B1 x      =   0.0344 ±  0.0062
10) polymer Γ1        =   0.1468 ±  0.0253
11) polymer E2        =   2.3044 ±  0.0056
12) polymer C         =   0.0211 ±  0.0027
13) polymer Γ2        =   0.0524 ±  0.0079

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000   0.157  -0.050   0.063   0.021   0.100  -0.095
        1.000   0.384  -0.140  -0.269  -0.129   0.157
                1.000  -0.599  -0.936   0.176   0.164
                        1.000   0.795  -0.016  -0.058
                                1.000  -0.079  -0.074
                                        1.000   0.122
                                                1.000
```

Model without roughness

Fit Results





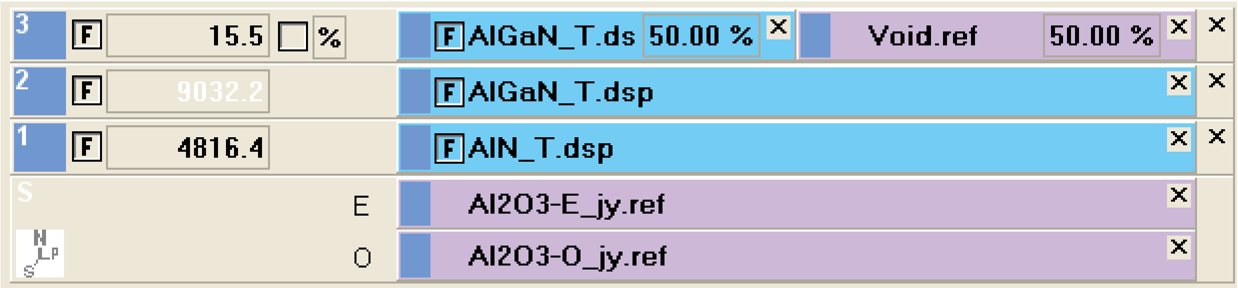
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 1.105129
Iterations Number = 9

Parameters
1) L1 Thickness [Å]  = 6904.666  ± 24.154
2) polymer  ε∞        =    2.1223 ±  0.0400
3) polymer  E0        =    3.5441 ±  0.0594
4) polymer  A0        =    7.7283 ±  1.0197
5) polymer  Γ0        =    0.0511 ±  0.0453
6) polymer  E1        =    2.5774 ±  0.0338
7) polymer  B1        =    0.1357 ±  0.0134
8) polymer  B1 x      =    0.0443 ±  0.0109
9) polymer  Γ1        =    0.1984 ±  0.0353
10)polymer  E2        =    2.2977 ±  0.0077
11)polymer  C         =    0.0230 ±  0.0047
12)polymer  Γ2        =    0.0525 ±  0.0120

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.102  -0.010  0.000    0.076  -0.120   0.006
        1.000  -0.480  -0.917    0.186   0.130  -0.242
                1.000   0.644   -0.020  -0.106   0.163
                        1.000    0.018   0.001  -0.028
                                 1.000   0.201  -0.589
                                         1.000  -0.652
                                                 1.000
```

General Remarks

- Adding a rough overlayer on top of the film stack decreases the χ^2 by a factor 2. Hence the final model takes into account the roughness.
- It is important noticing that the E_0, E_1, and E_2 values correspond to the energy at which the 3 extinction peaks (k) displayed on the graph “Optical constants of polymer” are maximum.
- We guess the presence of these absorption peaks directly on the raw (Is,Ic) data.

AlGaN / AlN / Sapphire Substrate

Model



3 F 15.5 ☐ % F AlGaN_T.ds 50.00 % ☒ Void.ref 50.00 % ☒ ☒

2 F 9032.2 F AlGaN_T.dsp ☒ ☒

1 F 4816.4 F AlN_T.dsp ☒ ☒

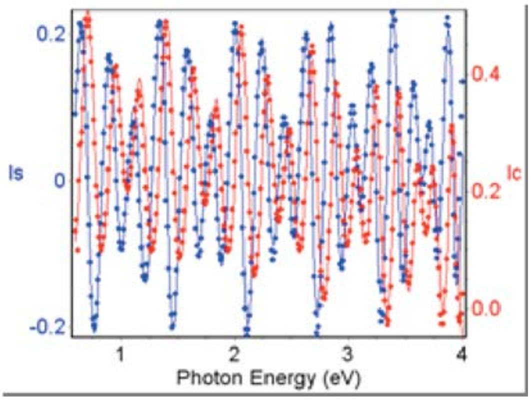
S E Al2O3-E_jy.ref ☒

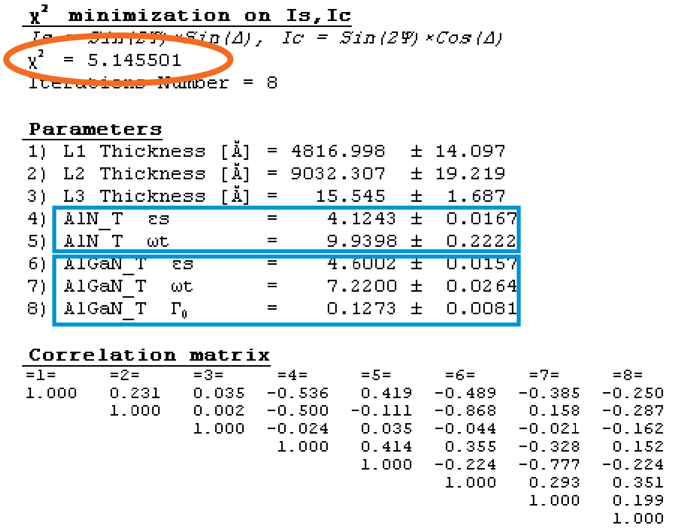
O Al2O3-O_jy.ref ☒

Fit Conditions

- Spectral range: 0.6 - 4.0 eV
- Step size: 0.01 eV
- Angle of incidence: 70.07°
- Model Information:
  - Sapphire is an anisotropic material (in this example N oriented).
  - Multiguess on AlGaN thickness varying from 7000 to 13 000 Å by step of 1000 Å.
- Fit parameters
  - Thickness: Layers 1, 2 and 3
  - Optical constants: AlN, AlGaN
- Materials
  - Al_2O_3-O, Al_2O_3-E, Void: Reference materials
  - **AlN, AlGaN** : Classical formula, respectively transparent and absorbing lorentz oscillator with $\varepsilon_\infty = 1.0$

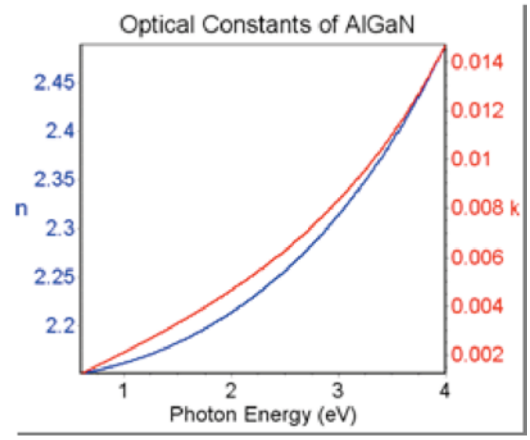
Fit Results





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 5.145501
Iterations Number = 8

Parameters
1) L1 Thickness [Å] = 4816.998  ± 14.097
2) L2 Thickness [Å] = 9032.307  ± 19.219
3) L3 Thickness [Å] =   15.545  ±  1.687
4) AlN_T   εs        =    4.1243 ±  0.0167
5) AlN_T   ωt        =    9.9398 ±  0.2222
6) AlGaN_T  εs       =    4.6002 ±  0.0157
7) AlGaN_T  ωt       =    7.2200 ±  0.0264
8) AlGaN_T  Γ0       =    0.1273 ±  0.0081

Correlation matrix
=1=    =2=    =3=    =4=     =5=    =6=     =7=     =8=
1.000  0.231  0.035  -0.536  0.419  -0.489  -0.385  -0.250
       1.000  0.002  -0.500 -0.111  -0.868   0.158  -0.287
              1.000  -0.024  0.035  -0.044  -0.021  -0.162
                      1.000  0.414   0.355  -0.328   0.152
                             1.000  -0.224  -0.777  -0.224
                                     1.000   0.293   0.351
                                             1.000   0.199
                                                     1.000
```

Optical constants of AlGaN



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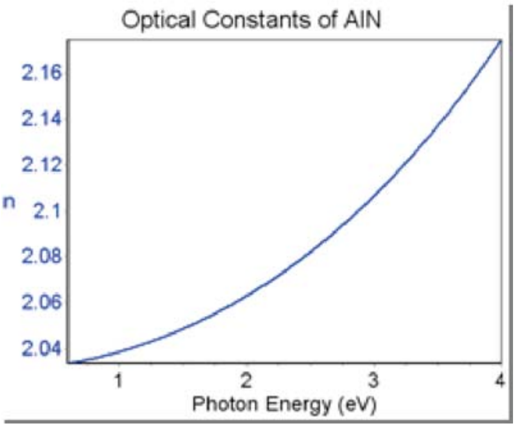
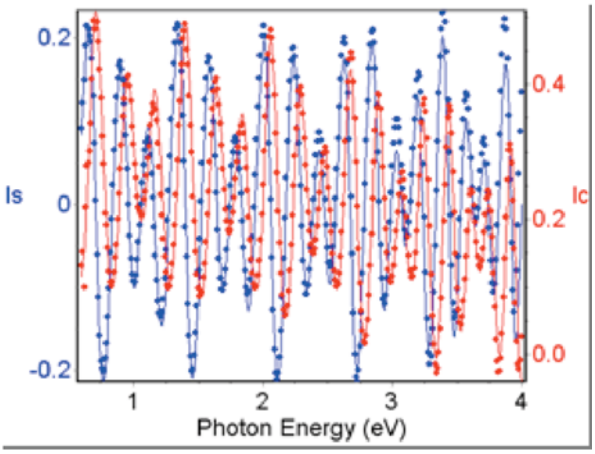
Optical constants of AlN

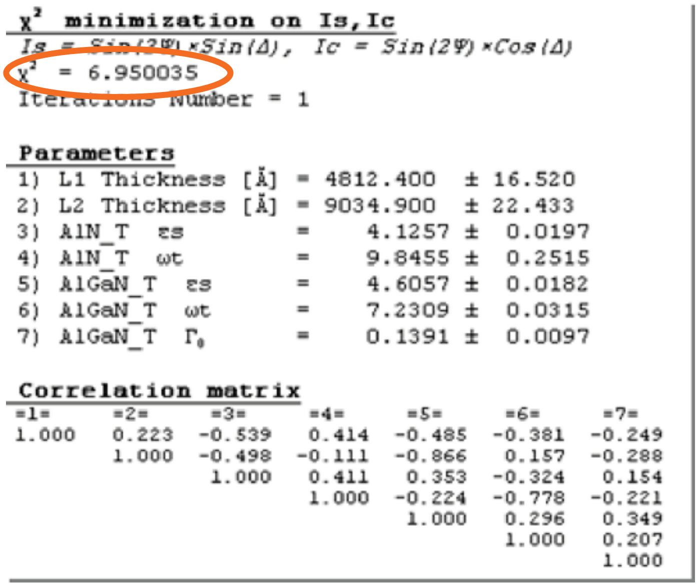


Model without roughness

2	F	9034.9	F AlGaN_T.dsp
1	F	4812.4	F AlN_T.dsp
S		E	Al2O3-E_jy.ref
		O	Al2O3-O_jy.ref

Fit Results





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 6.950035
Iterations Number = 1

Parameters
1)  L1 Thickness [Å] = 4812.400  ± 16.520
2)  L2 Thickness [Å] = 9034.900  ± 22.433
3)  AlN_T   εs       =    4.1257 ±  0.0197
4)  AlN_T   ωt       =    9.8455 ±  0.2515
5)  AlGaN_T   εs     =    4.6057 ±  0.0182
6)  AlGaN_T   ωt     =    7.2309 ±  0.0315
7)  AlGaN_T   Γ0     =    0.1391 ±  0.0097

Correlation matrix
=1=      =2=      =3=      =4=      =5=      =6=      =7=
1.000    0.223   -0.539    0.414   -0.485   -0.381   -0.249
         1.000   -0.498   -0.111   -0.866    0.157   -0.288
                  1.000    0.411    0.353   -0.324    0.154
                           1.000   -0.224   -0.778   -0.221
                                    1.000    0.296    0.349
                                             1.000    0.207
                                                      1.000
```

General Remarks

- Adding a rough overlayer on top of the film stack decreases the χ^2 from approximatively 7 to 5. Hence the final model takes into account the roughness.

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GaAs / InGaP / Germanium Substrate

Model

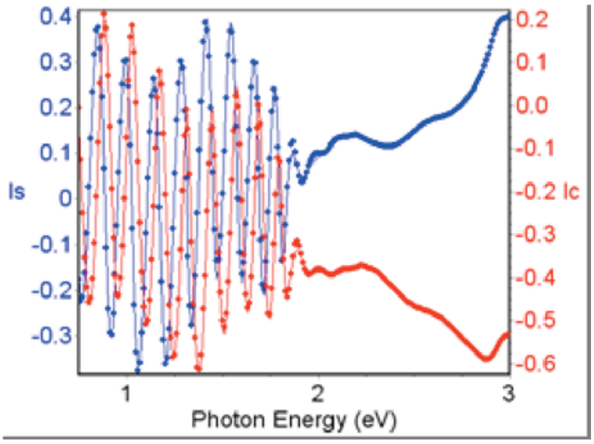
Layer		Thickness	Material
4	F	19.4 ☐ %	Gaas_isa.re 50.00 % Void.ref 50.00 %
3	F	2025.4	Gaas_isa.ref
2	F	10619.7	F InGaP.dsp
1	☐	1500000.0	Ge_palik 1102.ref
S			Void.ref

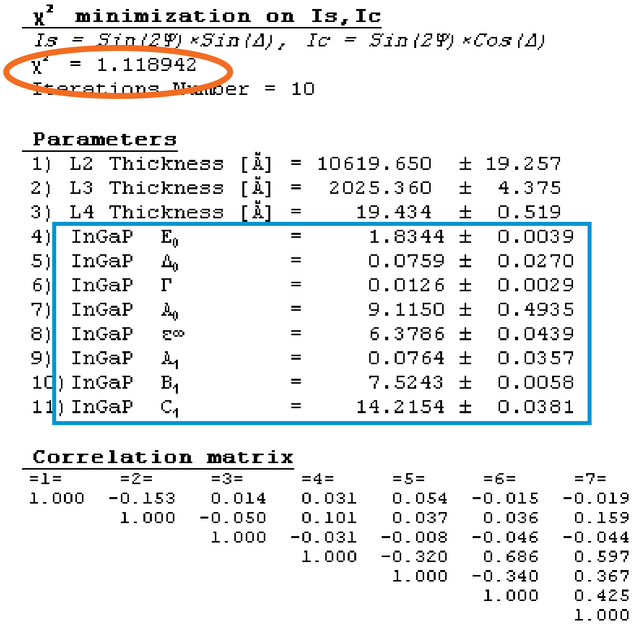
Backside reflection model

Fit Conditions

- Spectral range: 0.75 - 3.0 eV
- Step size: 0.01 eV
- Angle of incidence: 70.0°
- Model Information: Backside reflections model is used as Germanium substrate is transparent in the NIR wavelength range.
- Fit parameters
  - Thickness: Layers 1, 2 and 3
  - Optical constants: InGaP
- Materials
  - GaAs, Ge, Void: Reference materials
  - **InGaP** : Adachi-Forouhi

Fit Results



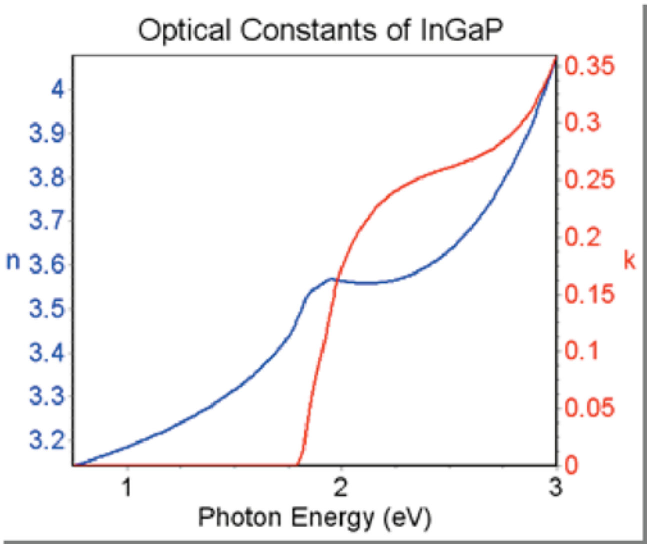


```
χ²  minimization on Is,Ic
 Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
 χ²  = 1.118942
 Iterations Number = 10

 Parameters
 1)  L2 Thickness [Å]  =  10619.650  ± 19.257
 2)  L3 Thickness [Å]  =   2025.360  ±  4.375
 3)  L4 Thickness [Å]  =     19.434  ±  0.519
 4)  InGaP  E0         =      1.8344 ±  0.0039
 5)  InGaP  Δ0         =      0.0759 ±  0.0270
 6)  InGaP  Γ          =      0.0126 ±  0.0029
 7)  InGaP  A0         =      9.1150 ±  0.4935
 8)  InGaP  ε∞         =      6.3786 ±  0.0439
 9)  InGaP  A1         =      0.0764 ±  0.0357
 10) InGaP  B1         =      7.5243 ±  0.0058
 11) InGaP  C1         =     14.2154 ±  0.0381

 Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.153   0.014   0.031   0.054  -0.015  -0.019
        1.000  -0.050   0.101   0.037   0.036   0.159
                1.000  -0.031  -0.008  -0.046  -0.044
                        1.000  -0.320   0.686   0.597
                                1.000  -0.340   0.367
                                        1.000   0.425
                                                1.000
```

Optical constants of InGaP



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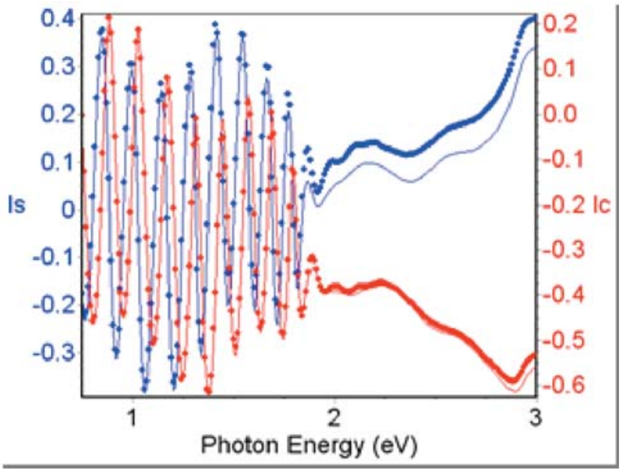
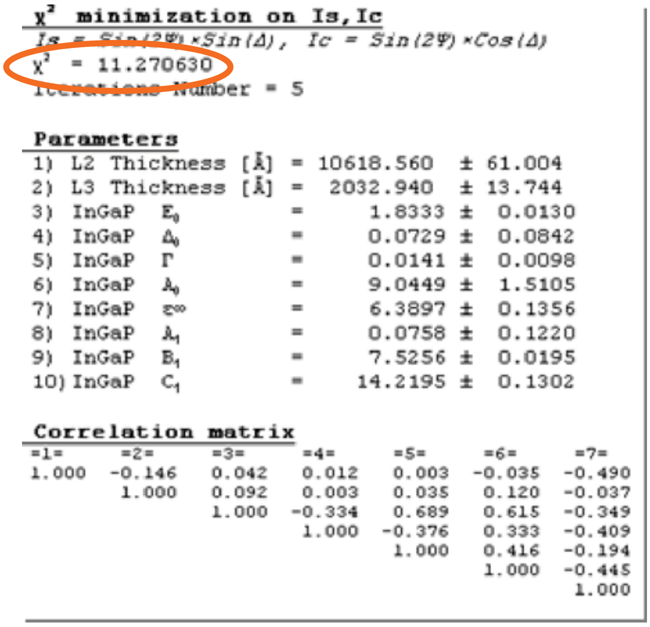
Model without roughness

3	☒ F	2032.9	Gaas_isa.ref	✕ ✕
2	☒ F	10618.6	F InGaP.dsp	✕ ✕
1	☐	1500000.0	Ge_palik 1102.ref	✕ ✕
S			Void.ref	✕

Fit Results





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 11.270630
Iterations Number = 5

Parameters
1)  L2 Thickness [Å] = 10618.560  ± 61.004
2)  L3 Thickness [Å] =  2032.940  ± 13.744
3)  InGaP  E0           =     1.8333 ±  0.0130
4)  InGaP  Δ0           =     0.0729 ±  0.0842
5)  InGaP  Γ            =     0.0141 ±  0.0098
6)  InGaP  A0           =     9.0449 ±  1.5105
7)  InGaP  ε∞           =     6.3897 ±  0.1356
8)  InGaP  A1           =     0.0758 ±  0.1220
9)  InGaP  B1           =     7.5256 ±  0.0195
10) InGaP  C1           =    14.2195 ±  0.1302

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.146   0.042   0.012   0.003  -0.035  -0.490
        1.000   0.092   0.003   0.035   0.120  -0.037
                1.000  -0.334   0.689   0.615  -0.349
                        1.000  -0.376   0.333  -0.409
                                1.000   0.416  -0.194
                                        1.000  -0.445
                                                1.000
```

General Remarks

- Adding a rough overlayer on top of the film stack decreases strongly the χ^2. Hence the final model takes into account the roughness.

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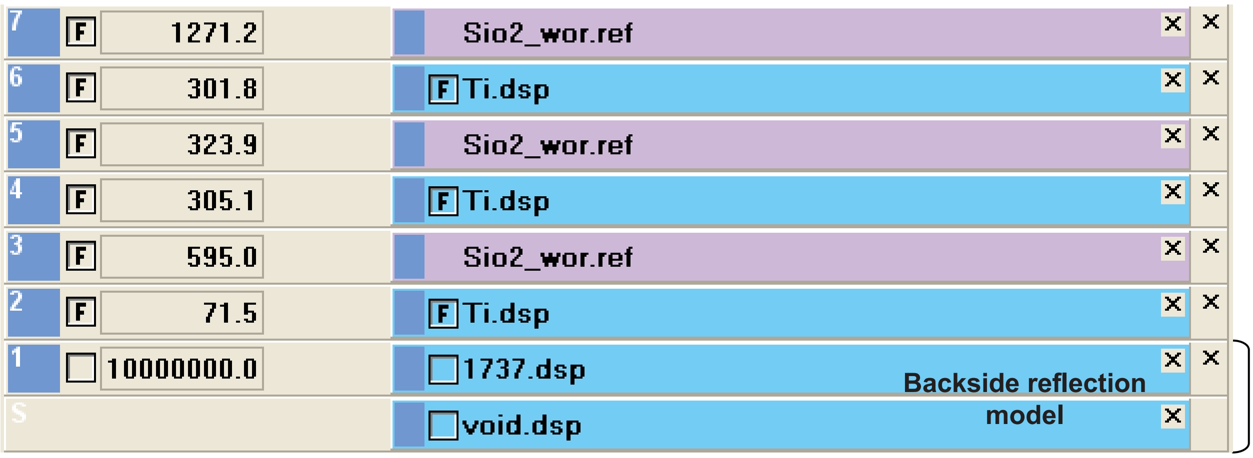
3x(SiO_2 / Ti) / Glass Substrate

Model

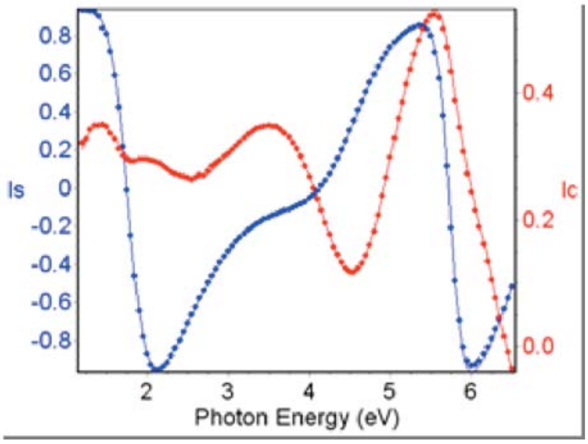


7	F	1271.2	Sio2_wor.ref
6	F	301.8	F Ti.dsp
5	F	323.9	Sio2_wor.ref
4	F	305.1	F Ti.dsp
3	F	595.0	Sio2_wor.ref
2	F	71.5	F Ti.dsp
1	☐	10000000.0	☐ 1737.dsp
S			☐ void.dsp

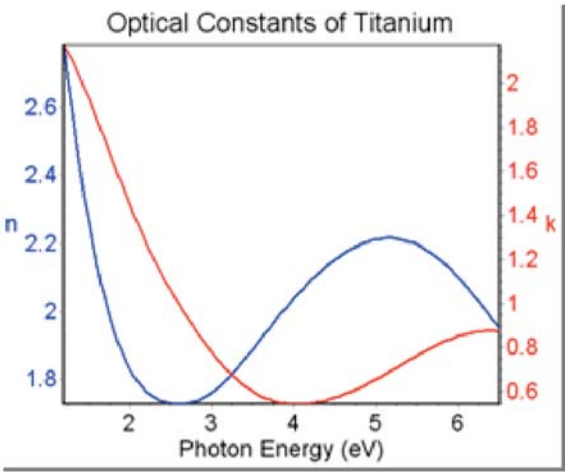
Backside reflection model

Fit Conditions

- Spectral range: 1.2 - 6.5 eV
- Step size: 0.05 eV
- Angle of incidence: 70.0°
- Model Information: Backside reflections model is used as Glass is a transparent material.
- Fit parameters
  - Thickness: Layers 1, 2, 3, 4, 5, 6 and 7
  - Optical constants: Ti
- Materials
  - 1737, Void, SiO_2: Reference materials
  - Ti : Full classical formula including 3 absorbing lorentz oscillator + drude oscillator



Optical constants of Titanium



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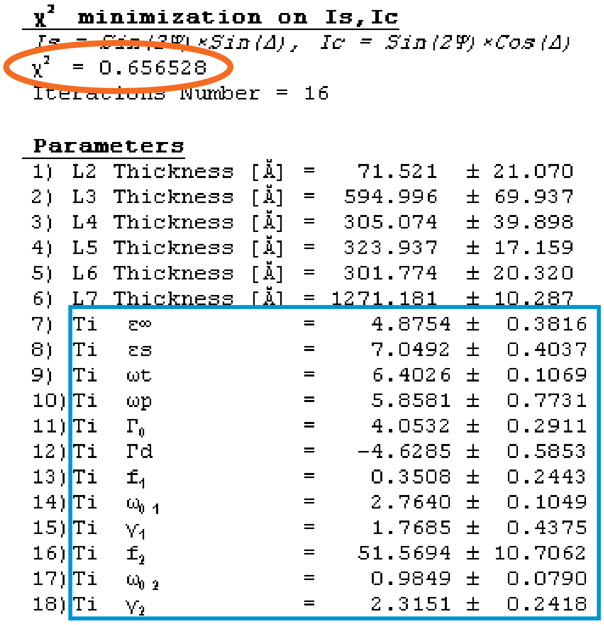


```
χ2 minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ2  = 0.656528
Iterations Number = 16

Parameters
1)  L2 Thickness [Å] =   71.521  ± 21.070
2)  L3 Thickness [Å] =  594.996  ± 69.937
3)  L4 Thickness [Å] =  305.074  ± 39.898
4)  L5 Thickness [Å] =  323.937  ± 17.159
5)  L6 Thickness [Å] =  301.774  ± 20.320
6)  L7 Thickness [Å] = 1271.181  ± 10.287
7)  Ti   ε∞              =     4.8754 ±  0.3816
8)  Ti   εs              =     7.0492 ±  0.4037
9)  Ti   ωt              =     6.4026 ±  0.1069
10) Ti   ωp              =     5.8581 ±  0.7731
11) Ti   Γ0              =     4.0532 ±  0.2911
12) Ti   Γd              =    -4.6285 ±  0.5853
13) Ti   f1              =     0.3508 ±  0.2443
14) Ti   ω0 1            =     2.7640 ±  0.1049
15) Ti   γ1              =     1.7685 ±  0.4375
16) Ti   f2              =    51.5694 ± 10.7062
17) Ti   ω0 2            =     0.9849 ±  0.0790
18) Ti   γ2              =     2.3151 ±  0.2418
```

General Remarks

- Negative parameters have been found in the Titanium dispersion parameters. Nevertheless the optical constants found are physical.

YBaCuO / $SrTiO_3$ Substrate

Model

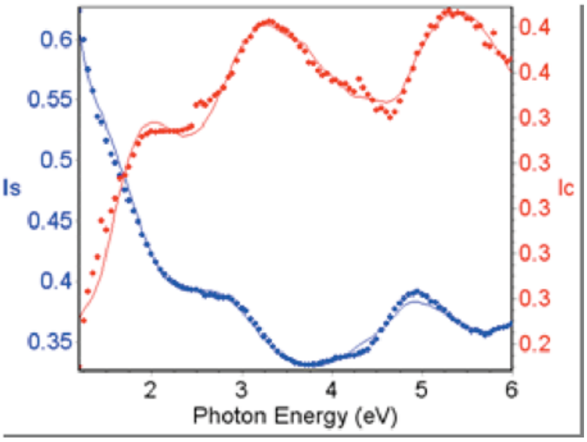
1 F 997.8 F YBaCuO.dsp

S SrTiO3 substrate.spe

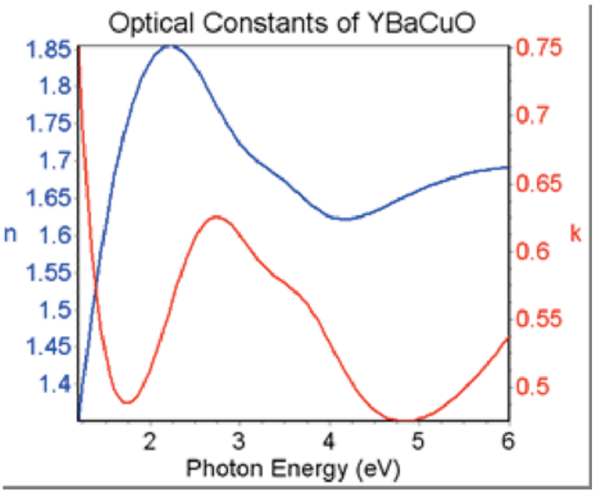
Fit Conditions

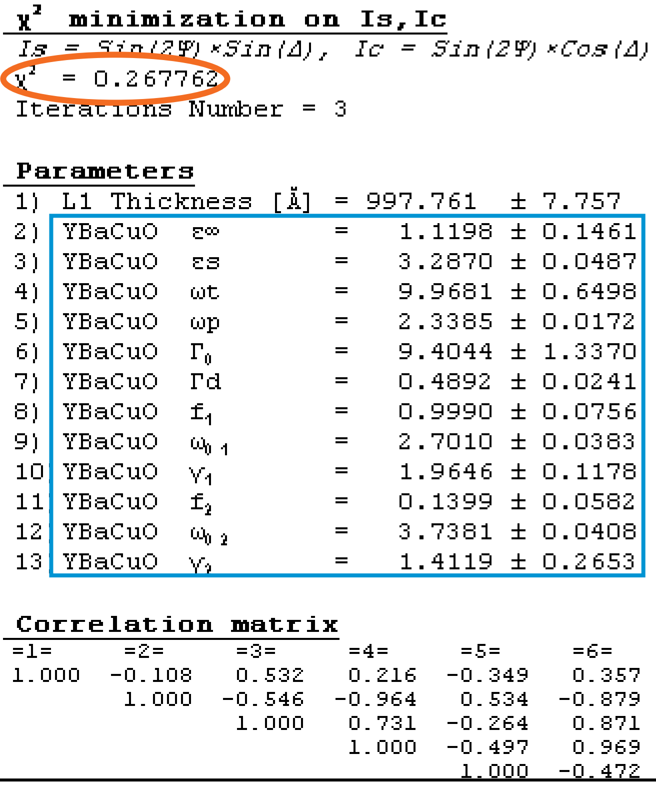
- Spectral range: 1.2 - 6.0 eV
- Step size: 0.05 eV
- Angle of incidence: 67.9°
- Model Information: $SrTiO_3$ substrate was measured in a 1st step to be able to use the « spe » file directly in the substrate.
- Fit parameters
  - Thickness: Layer 1
  - Optical constants: YBaCuO
- Materials
  - 1737, Void, SiO_2: Reference materials
  - **YBaCuO** : Full classical formula including 3 absorbing lorentz oscillator + drude oscillator

Fit Results



Optical constants of YBaCuO





```
χ^2  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ^2  = 0.267762
Iterations Number = 3

Parameters
1)  L1 Thickness [Å] = 997.761  ± 7.757
2)  YBaCuO  ε∞        =   1.1198 ± 0.1461
3)  YBaCuO  εs        =   3.2870 ± 0.0487
4)  YBaCuO  ωt        =   9.9681 ± 0.6498
5)  YBaCuO  ωp        =   2.3385 ± 0.0172
6)  YBaCuO  Γ0        =   9.4044 ± 1.3370
7)  YBaCuO  Γd        =   0.4892 ± 0.0241
8)  YBaCuO  f1        =   0.9990 ± 0.0756
9)  YBaCuO  ω0 1      =   2.7010 ± 0.0383
10  YBaCuO  γ1        =   1.9646 ± 0.1178
11  YBaCuO  f2        =   0.1399 ± 0.0582
12  YBaCuO  ω0 2      =   3.7381 ± 0.0408
13  YBaCuO  γ2        =   1.4119 ± 0.2653

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000  -0.108   0.532   0.216  -0.349   0.357
        1.000  -0.546  -0.964   0.534  -0.879
                1.000   0.731  -0.264   0.871
                        1.000  -0.497   0.969
                                1.000  -0.472
```

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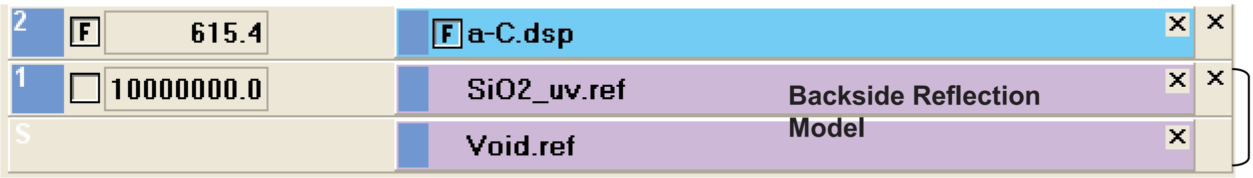
Amorphous Carbon / Glass Substrate BR

Model



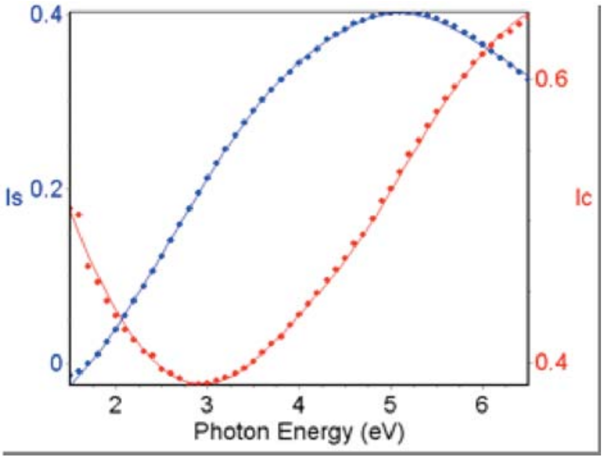
2	☒ F	615.4	F a-C.dsp
1	☐	10000000.0	SiO2_uv.ref
S			Void.ref

Backside Reflection Model

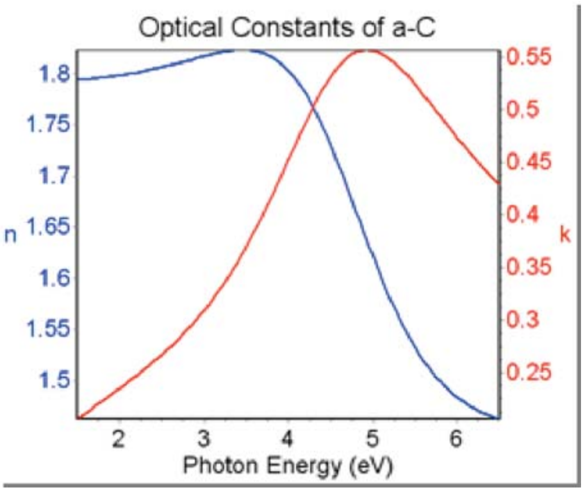
Fit Conditions

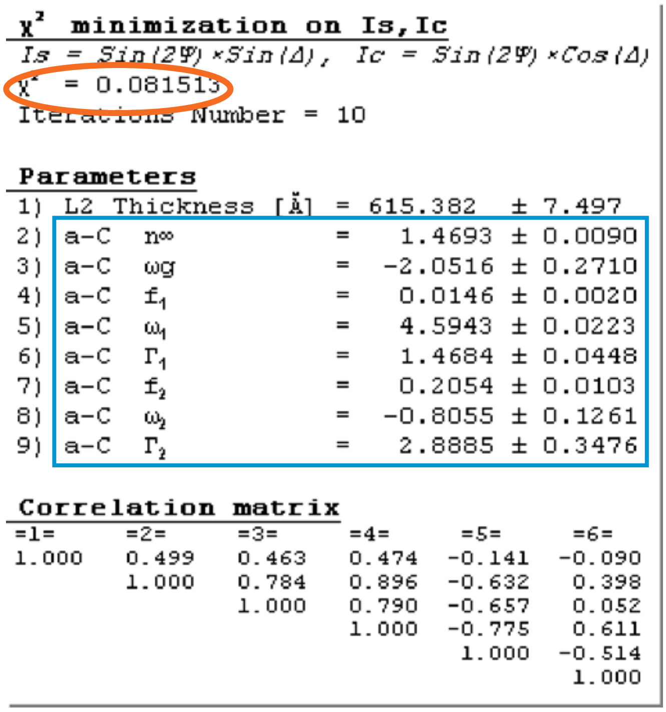
- Spectral range: 1.2 - 6.5 eV
- Step size: 0.1 eV
- Angle of incidence: 70.5°
- Model Information: Backside reflection model was used as Glass is a transparent material.
- Fit parameters
  - Thickness: Layer 2
  - Optical constants: a-C
- Materials
  - Void, SiO_2: Reference materials
  - **a-C** : Double new amorphous formula

Fit Results



Optical constants of a-Carbon





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 0.081513
Iterations Number = 10

Parameters
1)  L2 Thickness [Å]  = 615.382   ± 7.497
2)  a-C   n∞            =    1.4693 ± 0.0090
3)  a-C   ωg            =   -2.0516 ± 0.2710
4)  a-C   f1            =    0.0146 ± 0.0020
5)  a-C   ω1            =    4.5943 ± 0.0223
6)  a-C   Γ1            =    1.4684 ± 0.0448
7)  a-C   f2            =    0.2054 ± 0.0103
8)  a-C   ω2            =   -0.8055 ± 0.1261
9)  a-C   Γ2            =    2.8885 ± 0.3476

Correlation matrix
=1=      =2=      =3=      =4=      =5=      =6=
1.000    0.499    0.463    0.474   -0.141   -0.090
         1.000    0.784    0.896   -0.632    0.398
                  1.000    0.790   -0.657    0.052
                           1.000   -0.775    0.611
                                    1.000   -0.514
                                             1.000
```

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MgF_2/ TiO_2/ c-Si Substrate

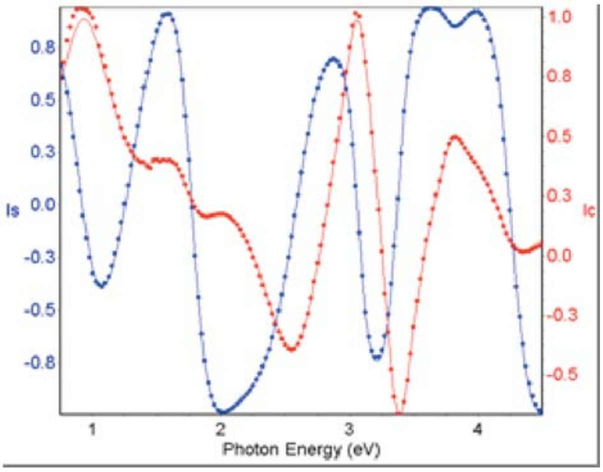
Model

Linear graded layer

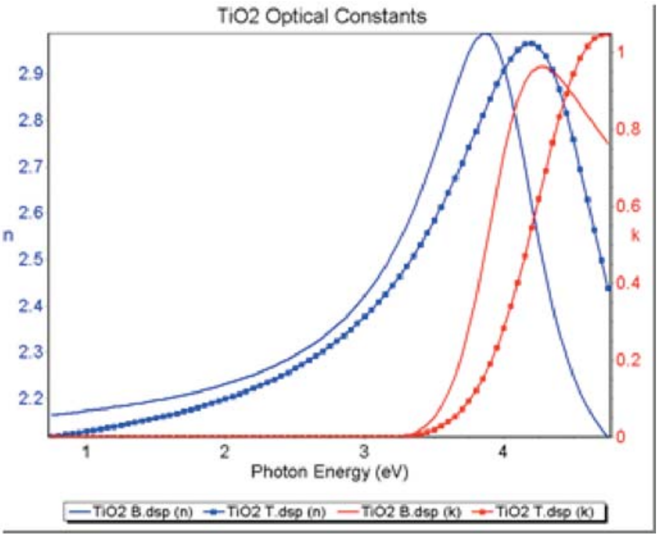
Fit Conditions

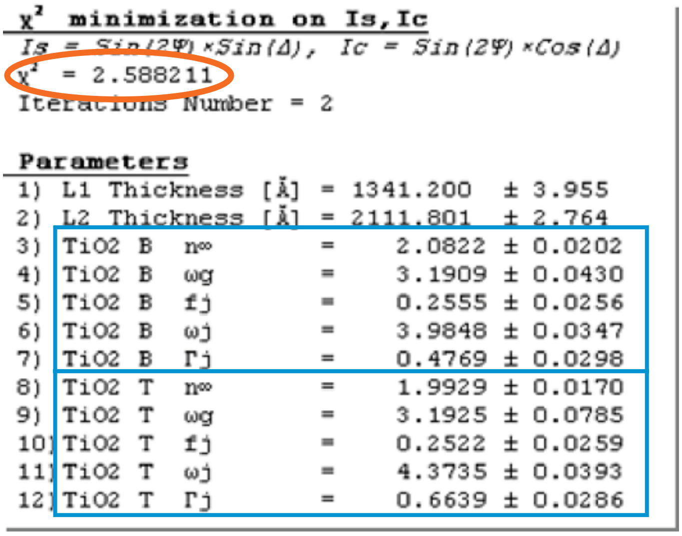
- Spectral range : 0.75-4.5 eV
- Step size: 0.025 eV
- Angle of incidence : 70°
- Fit parameters
  - Thickness : layers 1 and 2
  - Optical constants: TiO_2 linear gradient
- Materials
  - c-Si : reference library
  - TiO_2 : New amorphous formula
  - MgF_2: Classical formula, transparent Lorentz oscillator

Fit Results



Optical constants of TiO_2 – B Bottom, T Top of the graded layer





```
χ²  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 2.588211
Iterations Number = 2

Parameters
1) L1 Thickness [Å] = 1341.200  ± 3.955
2) L2 Thickness [Å] = 2111.801  ± 2.764
3) TiO2 B  n∞       =    2.0822 ± 0.0202
4) TiO2 B  ωg       =    3.1909 ± 0.0430
5) TiO2 B  fj       =    0.2555 ± 0.0256
6) TiO2 B  ωj       =    3.9848 ± 0.0347
7) TiO2 B  Γj       =    0.4769 ± 0.0298
8) TiO2 T  n∞       =    1.9929 ± 0.0170
9) TiO2 T  ωg       =    3.1925 ± 0.0785
10)TiO2 T  fj       =    0.2522 ± 0.0259
11)TiO2 T  ωj       =    4.3735 ± 0.0393
12)TiO2 T  Γj       =    0.6639 ± 0.0286
```

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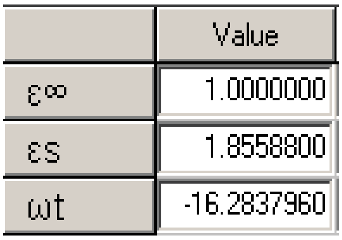
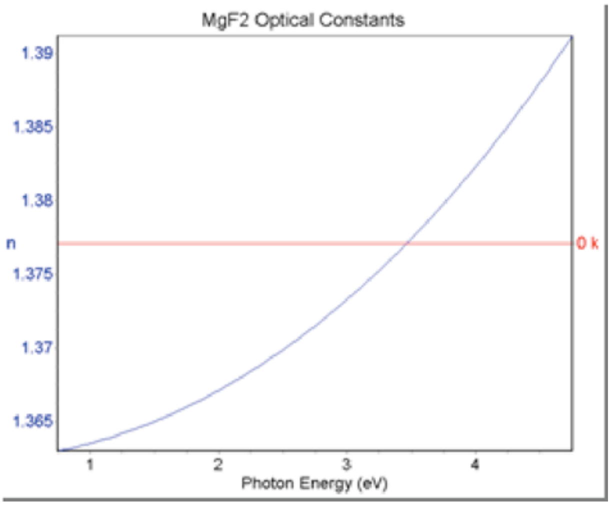
Optical constants of MgF_2



	Value
ε∞	1.0000000
εs	1.8558800
ωt	-16.2837960

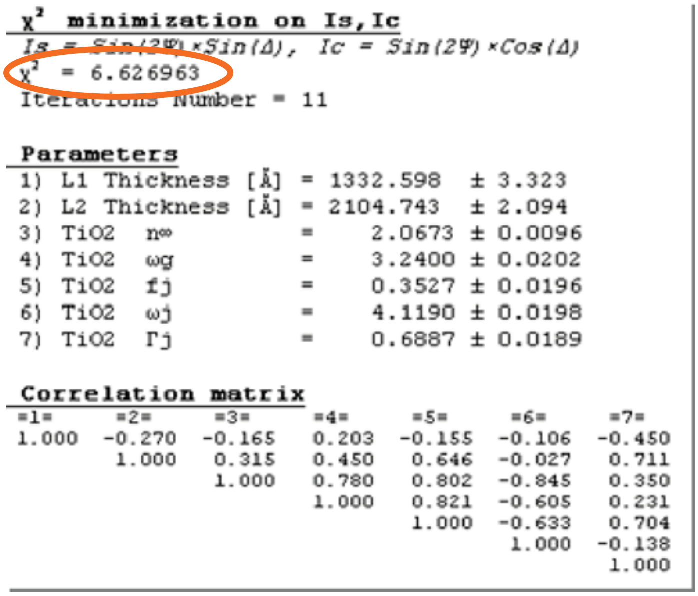


- In the physical formula of the Lorentz oscillator, the ωt parameter is squared so that the negative parameter found for ωt is good and provides physical optical constants (as shown on the right).

Model without gradient

2	F 2104.7	MgF2.dsp
1	F 1332.6	F TiO2.dsp
S		Csi_wor.ref

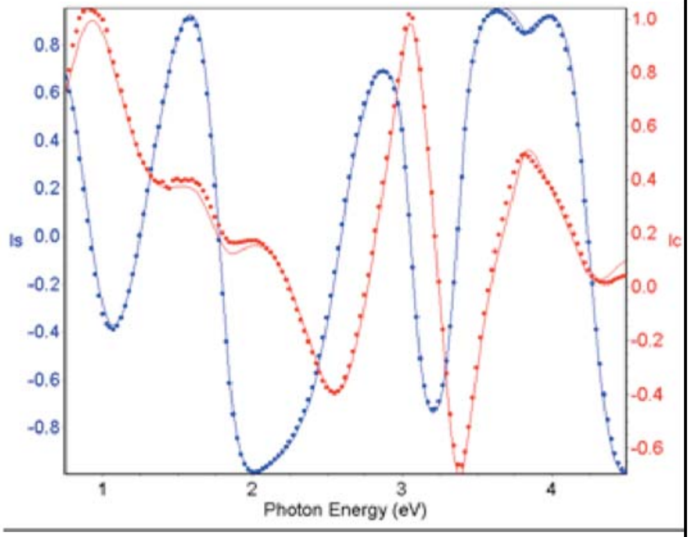
Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 6.626963
Iterations Number = 11

Parameters
1) L1 Thickness [Å] = 1332.598  ± 3.323
2) L2 Thickness [Å] = 2104.743  ± 2.094
3) TiO2   n∞        =    2.0673 ± 0.0096
4) TiO2   ωg        =    3.2400 ± 0.0202
5) TiO2   fj        =    0.3527 ± 0.0196
6) TiO2   ωj        =    4.1190 ± 0.0198
7) TiO2   Γj        =    0.6887 ± 0.0189

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.270  -0.165   0.203  -0.155  -0.106  -0.450
        1.000   0.315   0.450   0.646  -0.027   0.711
                1.000   0.780   0.802  -0.845   0.350
                        1.000   0.821  -0.605   0.231
                                1.000  -0.633   0.704
                                        1.000  -0.138
                                                1.000
```



General Remarks

- The TiO_2 gradient improves strongly the fit results, hence the final model contains it.
- MgF_2 optical properties are not fitted as they were previously analyzed.

GeSbTe / c-Si Substrate

Model

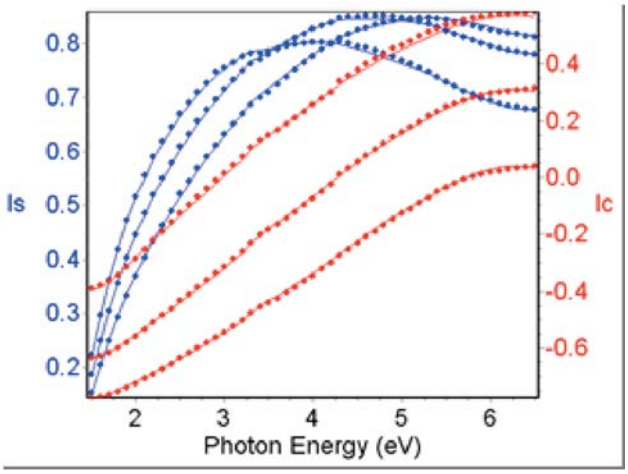
1 F 332.7 F GeSbTe.dsp

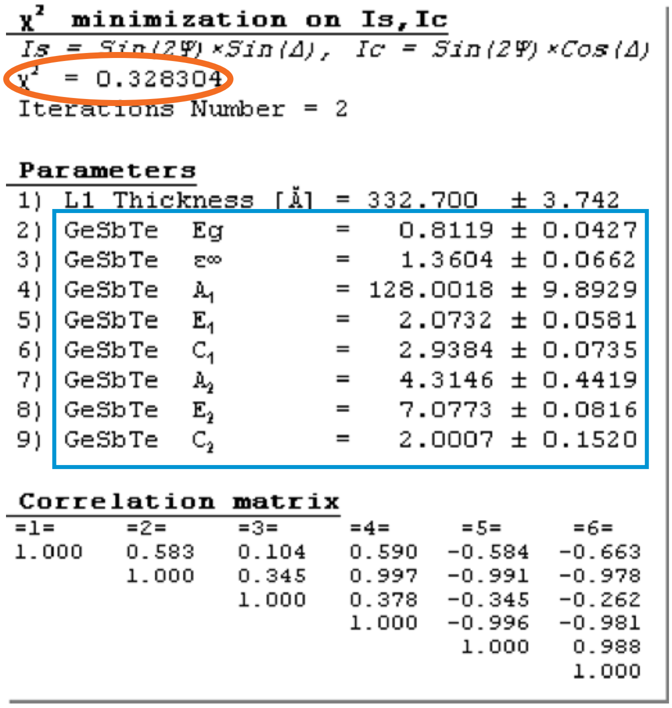
S c-Si_Jy.clc

Fit Conditions

- Spectral range: 1.5 - 6.5 eV
- Step size: 0.1 eV
- Angle of incidence: VASE 65-70-75°
- Model information: VASE was used in the model, in order to increase the results stability. Nevertheless, it is not mandatory.
- Fit parameters
  - Thickness: Layer 1
  - Optical constants: GeSbTe
- Materials
  - c-Si: Reference materials
  - **GeSbTe** : Double tauc-lorentz formula

Fit Results



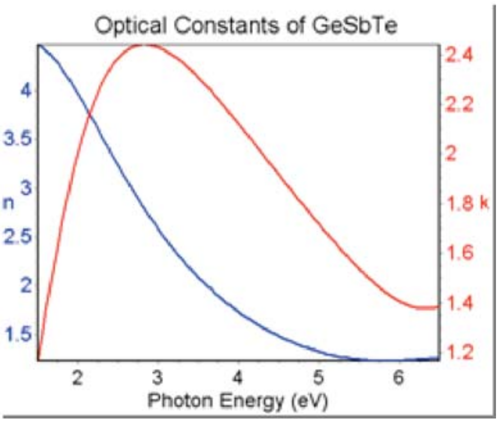


```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 0.328304
Iterations Number = 2

Parameters
1) L1 Thickness [Å] = 332.700 ± 3.742
2) GeSbTe   Eg      =   0.8119 ± 0.0427
3) GeSbTe   ε∞      =   1.3604 ± 0.0662
4) GeSbTe   A1      = 128.0018 ± 9.8929
5) GeSbTe   E1      =   2.0732 ± 0.0581
6) GeSbTe   C1      =   2.9384 ± 0.0735
7) GeSbTe   A2      =   4.3146 ± 0.4419
8) GeSbTe   E2      =   7.0773 ± 0.0816
9) GeSbTe   C2      =   2.0007 ± 0.1520

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=
1.000   0.583   0.104   0.590  -0.584  -0.663
        1.000   0.345   0.997  -0.991  -0.978
                1.000   0.378  -0.345  -0.262
                        1.000  -0.996  -0.981
                                1.000   0.988
                                        1.000
```

Optical constants of GeSbTe



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Spectroscopic Ellipsometry Data Sheets **32**

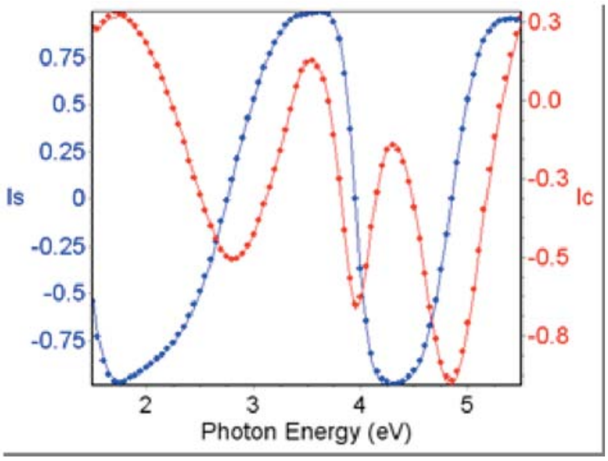
PMMA / c-Si Substrate

Model

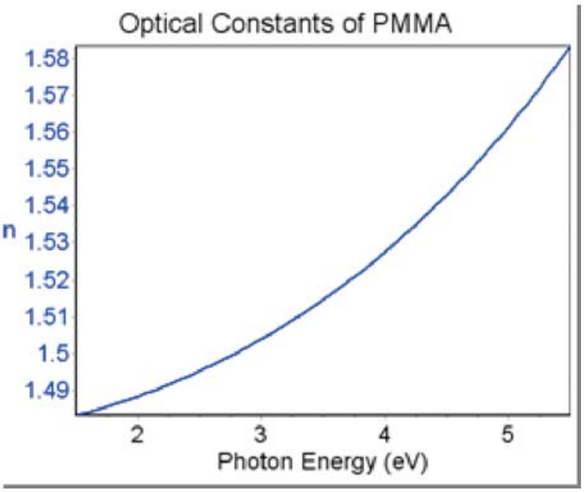
Fit Conditions

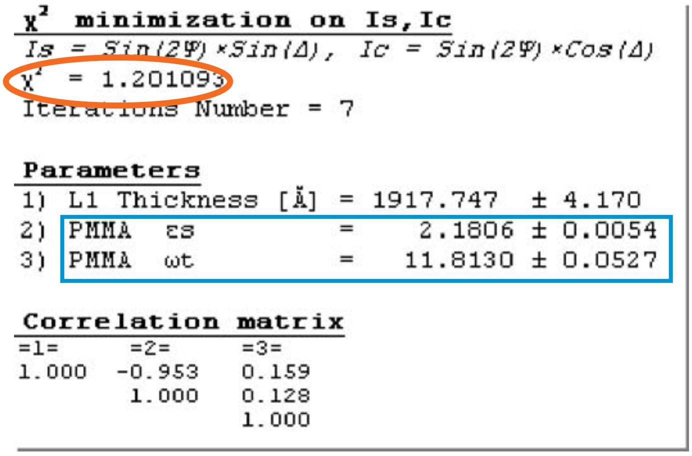
- Spectral range: 1.5 - 5.5 eV
- Step size: 0.05 eV
- Angle of incidence: 70.5°
- Fit parameters
  - Thickness: Layer 1
  - Optical constants: PMMA
- Materials
  - c-Si: Reference materials
  - **PMMA** : Classical formula, Transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Fit Results



Optical constants of PMMA





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 1.201093
Iterations Number = 7

Parameters
1) L1 Thickness [Å] = 1917.747  ± 4.170
2) PMMA  εs         =    2.1806 ± 0.0054
3) PMMA  ωt         =   11.8130 ± 0.0527

Correlation matrix
=1=      =2=      =3=
1.000   -0.953    0.159
         1.000    0.128
                  1.000
```

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4(SiO_2-TiO_2) / Glass Substrate

Model

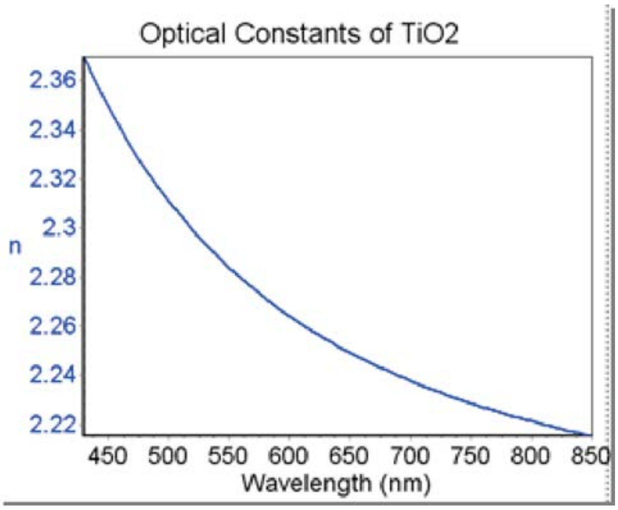
4	3	F 1118.1	Sio2_isa.ref
	2	F 673.4	F TiO2.dsp
	1	☐ 10000000.0	☐ Glass.dsp
	S		Void.ref

Backside reflection model

Fit Conditions

- Spectral range: 430 - 850 nm
- Angle of incidence: 70°
- Model Information:
  - Backside reflection model
  - The repeated layer function was used to repeat 4 times the TiO_2/SiO_2 layers. The results provide an average thickness of these 4 times repeated layers.
  - It is worth noticing that the wavelength range is limited from 430 to 850 nm. Hence the TiO_2 dispersion used is a transparent Lorentz oscillator providing an extinction coefficient (k) equal to 0.
- Fit parameters
  - Thickness: Repeated layers 1 and 2
  - Optical constants: TiO_2
- Materials
  - Glass, Void: Reference materials
  - TiO_2 : Classical formula, Transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Optical constants of TiO_2



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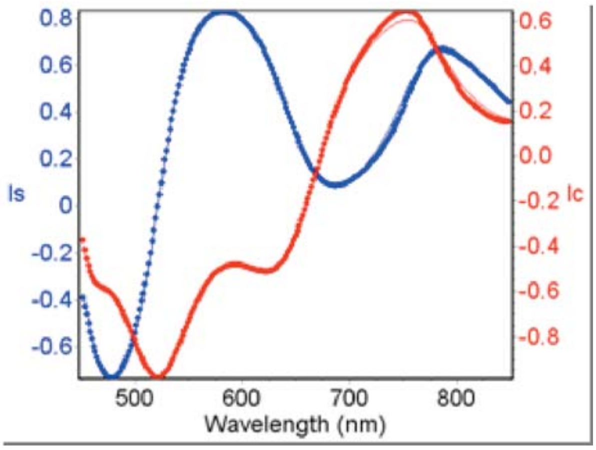
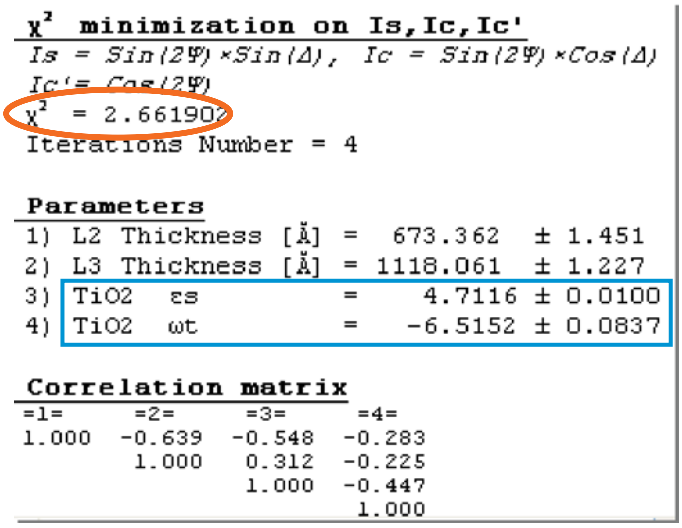
Fit Results





```
χ² minimization on Is,Ic,Ic'
Is = Sin(2Ψ)*Sin(Δ), Ic = Sin(2Ψ)*Cos(Δ)
Ic'= Cos(2Ψ)
χ² = 2.661902
Iterations Number = 4

Parameters
1) L2 Thickness [Å] =  673.362  ± 1.451
2) L3 Thickness [Å] = 1118.061  ± 1.227
3) TiO2  εs         =     4.7116 ± 0.0100
4) TiO2  ωt         =    -6.5152 ± 0.0837

Correlation matrix
=1=     =2=     =3=     =4=
1.000  -0.639  -0.548  -0.283
        1.000   0.312  -0.225
                1.000  -0.447
                        1.000
```

- Negative ωt parameter is possible as in Lorentz oscillator formula ωt is squared.

$Y_3Fe_5O_{12}$ / SiO_2 / c-Si Substrate

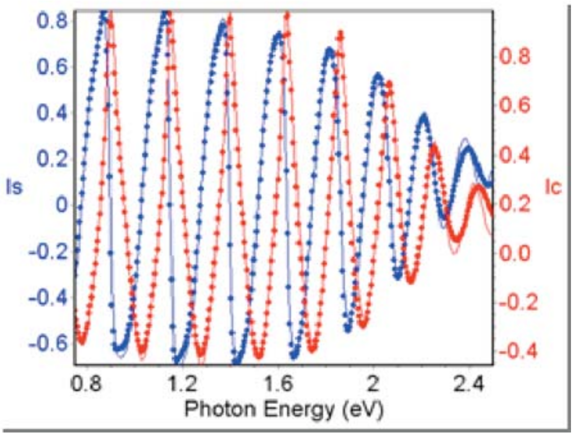
Model

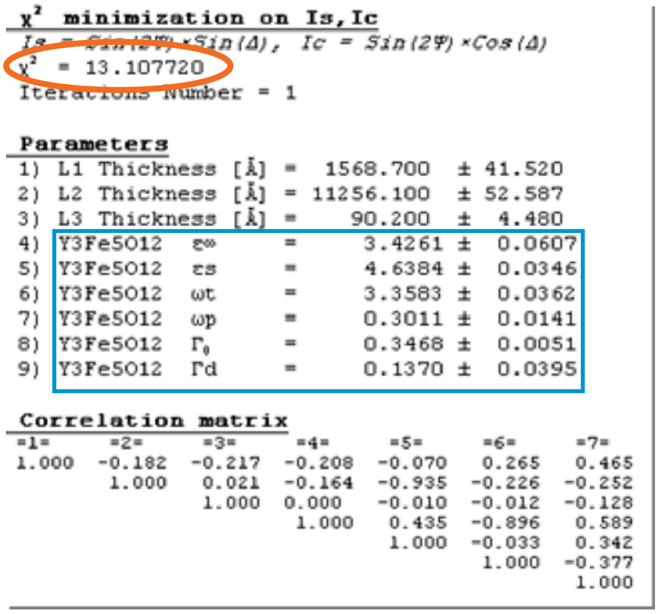
3 F 90.2 ☐ % | F Y3Fe5O12.d 50.00 % | Void_asp.re 50.00 %
2 F 11256.1 | F Y3Fe5O12.dsp
1 F 1568.7 | Sio2_isa.ref
S | C-si_isa.ref

Fit Conditions

- Spectral range: 0.75 – 2.50 eV
- Step size: 0.005 eV
- Angle of incidence: 70°
- Model Information:
  - The fit was performed on a restricted spectral range due to the strong absorption of $Y_3Fe_5O_{12}$ material above 2.5 eV. More investigation is necessary to extend the spectral range of fitting, eg. Testing others dispersion formulae.
- Fit parameters
  - Thickness: Layers 1, 2 and 3
  - Optical constants: $Y_3Fe_5O_{12}$
- Materials
  - c-Si, SiO_2: Reference materials
  - **$Y_3Fe_5O_{12}$** : Classical formula, Absorbing Lorentz + Drude oscillators

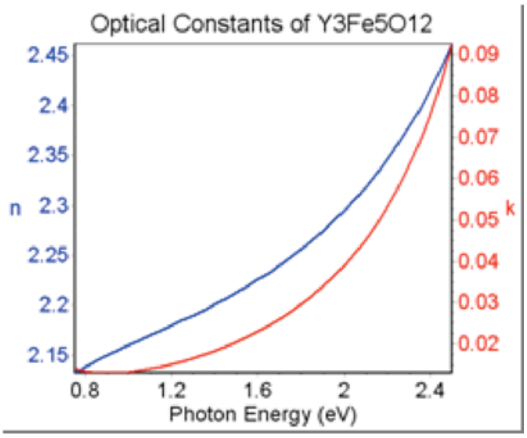
Fit Results





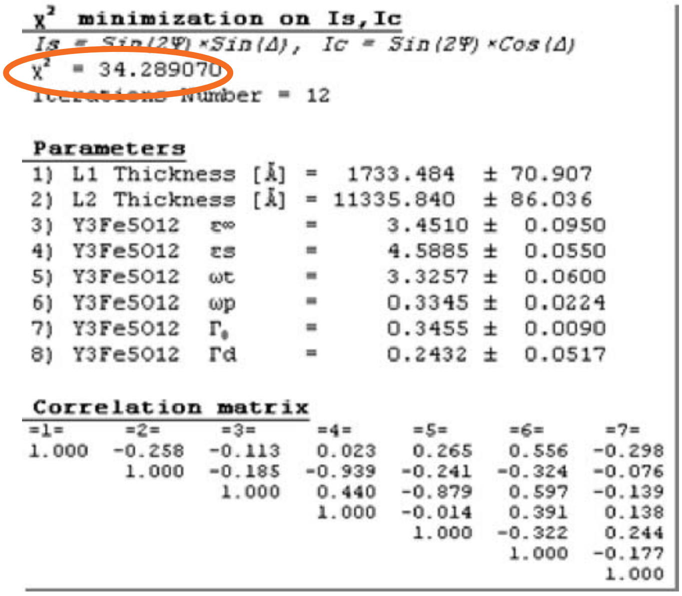
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ²  = 13.107720
Iterations Number = 1

Parameters
1)  L1 Thickness [Å] =   1568.700  ± 41.520
2)  L2 Thickness [Å] =  11256.100  ± 52.587
3)  L3 Thickness [Å] =     90.200  ±  4.480
4)  Y3Fe5O12   ε∞    =       3.4261 ±  0.0607
5)  Y3Fe5O12   εs    =       4.6384 ±  0.0346
6)  Y3Fe5O12   ωt    =       3.3583 ±  0.0362
7)  Y3Fe5O12   ωp    =       0.3011 ±  0.0141
8)  Y3Fe5O12   Γ0    =       0.3468 ±  0.0051
9)  Y3Fe5O12   Γd    =       0.1370 ±  0.0395

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.182  -0.217  -0.208  -0.070   0.265   0.465
        1.000   0.021  -0.164  -0.935  -0.226  -0.252
                1.000   0.000  -0.010  -0.012  -0.128
                        1.000   0.435  -0.896   0.589
                                1.000  -0.033   0.342
                                        1.000  -0.377
                                                1.000
```

Optical constants of $Y_3Fe_5O_{12}$

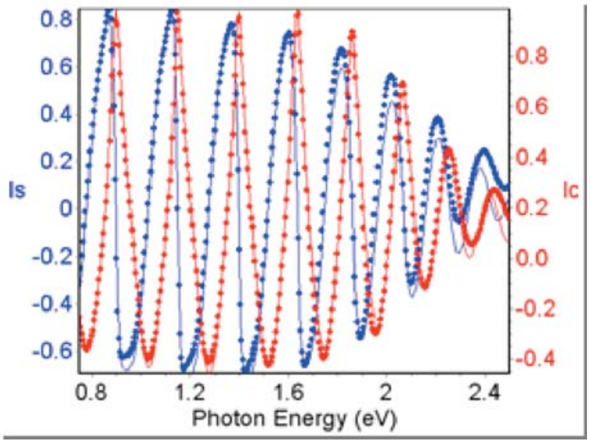


Model without roughness

Fit Results



```
χ2  minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ2  = 34.289070
Iterations Number = 12

Parameters
1)  L1 Thickness [Å]  =  1733.484  ± 70.907
2)  L2 Thickness [Å]  = 11335.840  ± 86.036
3)  Y3Fe5O12  ε∞      =      3.4510 ±  0.0950
4)  Y3Fe5O12  εs      =      4.5885 ±  0.0550
5)  Y3Fe5O12  ωt      =      3.3257 ±  0.0600
6)  Y3Fe5O12  ωp      =      0.3345 ±  0.0224
7)  Y3Fe5O12  Γ0      =      0.3455 ±  0.0090
8)  Y3Fe5O12  Γd      =      0.2432 ±  0.0517

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.258  -0.113   0.023   0.265   0.556  -0.298
        1.000  -0.185  -0.939  -0.241  -0.324  -0.076
                1.000   0.440  -0.879   0.597  -0.139
                        1.000  -0.014   0.391   0.138
                                1.000  -0.322   0.244
                                        1.000  -0.177
                                                1.000
```



General Remarks

- Adding a surface roughness improves the χ^2 by a factor 3.

9/2/08

Anodised Al / Al_2O_3 / Al Substrate

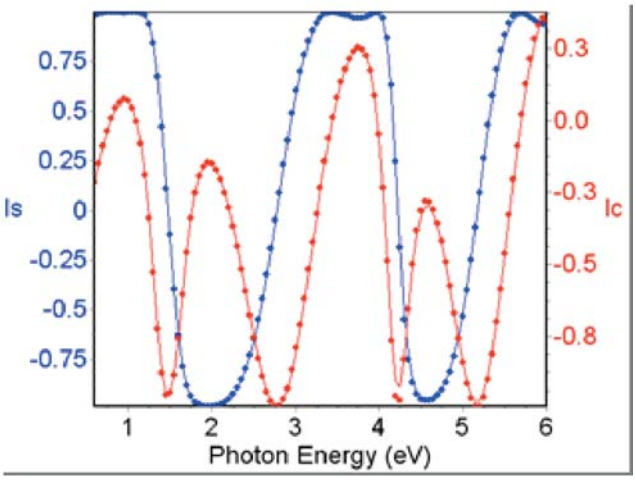
Model

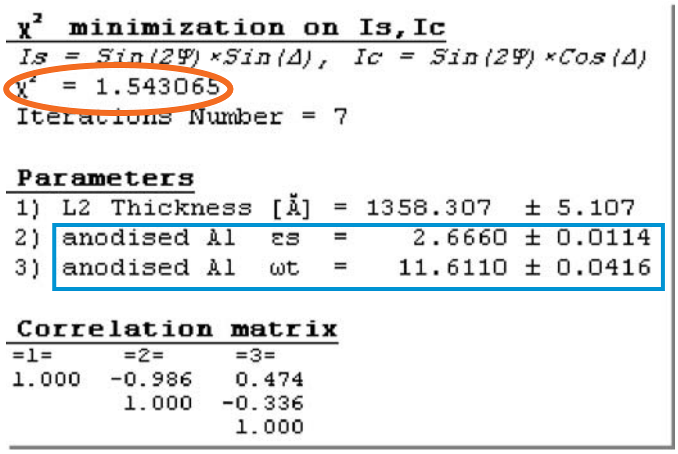
2	F	1358.3	F anodised Al.dsp
1	☐	70.9	Al2O3_pal.ref
S			nk Al.clc

Fit Conditions

- Spectral range: 0.6 – 6.0 eV
- Step size: 0.05 eV
- Angle of incidence: 70°
- Model Information:
  - The substrate is the measurement file of the Aluminium substrate itself. Cleaning the substrate is required as Aluminium surface always exhibits a native Al_2O_3 film.
  - A remaining Al_2O_3 interface film was found (from previous results explaining the non-fitting of this film).
  - A merge acquisition is necessary for metals.
- Fit parameters
  - Thickness: Layer 2
  - Optical constants: Anodised Al
- Materials
  - Al_2O_3: Reference materials
  - **Anodised Al**: Classical formula, Transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

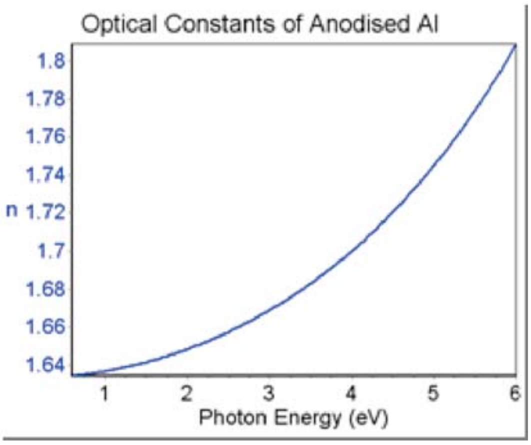
Fit Results





```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 1.543065
Iterations Number = 7

Parameters
1) L2 Thickness [Å] = 1358.307 ± 5.107
2) anodised Al  εs =     2.6660 ± 0.0114
3) anodised Al  ωt =    11.6110 ± 0.0416

Correlation matrix
=1=     =2=     =3=
1.000  -0.986   0.474
        1.000  -0.336
                1.000
```

Optical constants of Anodised Al



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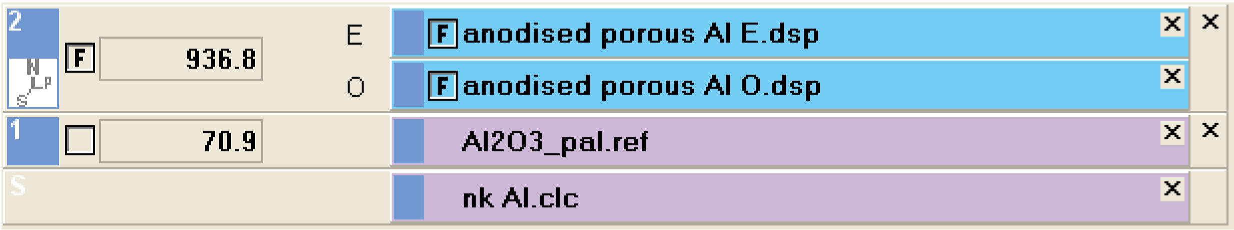
Anodised Porous Al / Al_2O_3 / Al Substrate

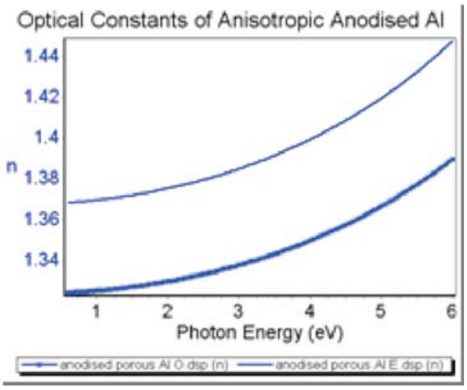
Model



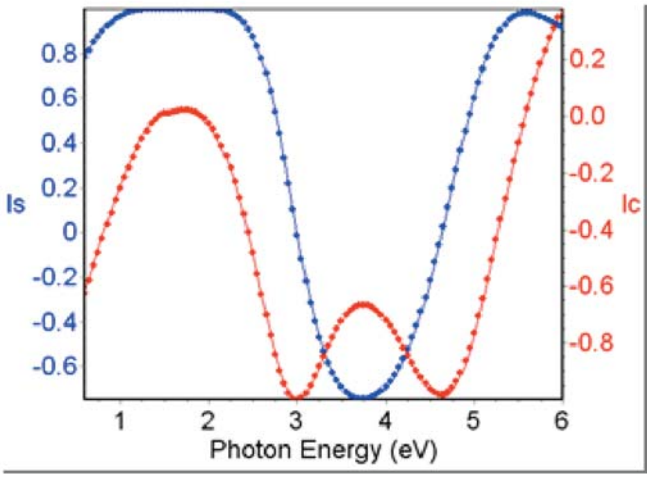
Fit Conditions

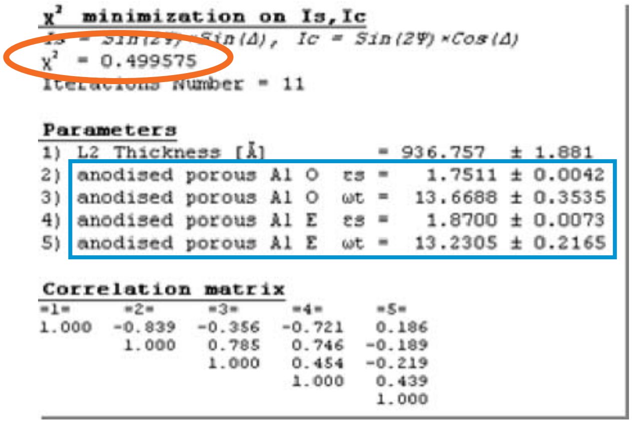
- Spectral range: 0.6 – 6.0 eV
- Step size: 0.05 eV
- Angle of incidence: 70°
- Model Information:
  - The substrate is the measurement file of the Aluminium substrate itself. Cleaning the substrate is required as Aluminium surface always exhibits a native Al_2O_3 film.
  - A remaining Al_2O_3 interface film was found (from previous results explaining the non-fitting of this film).
  - A merge acquisition is necessary for metals.
  - The conditions of elaboration of anodised Aluminium film introduces uniformly distributed pores on the surface. This is modeling by using an anisotropic film (N oriented as pores are perpendicular to the surface).
- Fit parameters
  - Thickness: Layer 2
  - Optical constants: Anodised Al
- Materials
  - Al_2O_3: Reference materials
  - **Anodised Al**: Classical formula, Transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Optical constants of anisotropic anodised Al



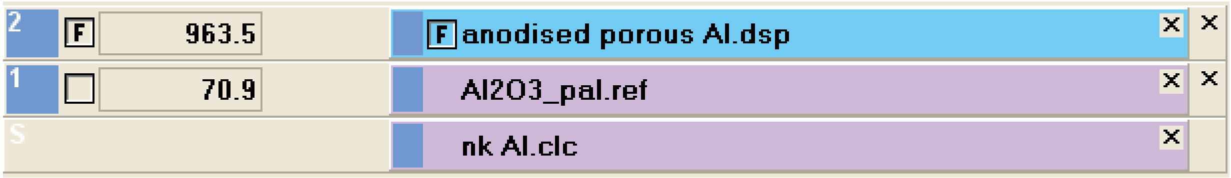
Fit Results





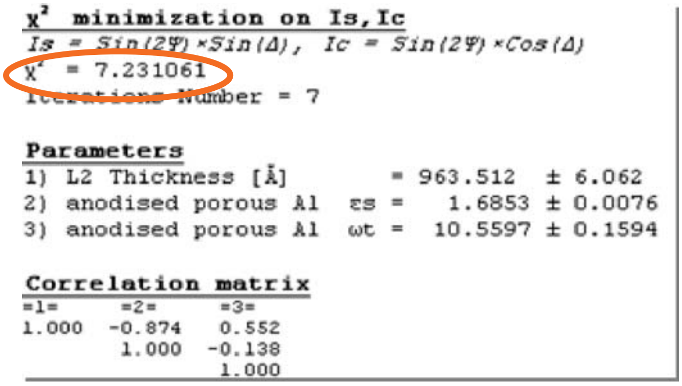
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 0.499575
Iterations Number = 11

Parameters
1) L2 Thickness [Å]              = 936.757  ± 1.881
2) anodised porous Al O  εs =    1.7511 ± 0.0042
3) anodised porous Al O  ωt =   13.6688 ± 0.3535
4) anodised porous Al E  εs =    1.8700 ± 0.0073
5) anodised porous Al E  ωt =   13.2305 ± 0.2165

Correlation matrix
=1=     =2=     =3=     =4=     =5=
1.000  -0.839  -0.356  -0.721   0.186
        1.000   0.785   0.746  -0.189
                1.000   0.454  -0.219
                        1.000   0.439
                                1.000
```

Model without anisotropy

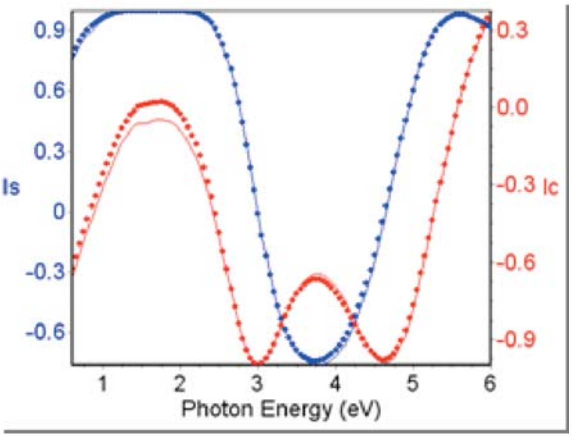


```
2  [F]  963.5   [F] anodised porous Al.dsp
1  [ ]   70.9       Al2O3_pal.ref
S                   nk Al.clc
```

Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 7.231061
Iterations Number = 7

Parameters
1) L2 Thickness [Å]          = 963.512  ± 6.062
2) anodised porous Al  εs =    1.6853 ± 0.0076
3) anodised porous Al  ωt =   10.5597 ± 0.1594

Correlation matrix
=1=      =2=      =3=
1.000  -0.874    0.552
        1.000   -0.138
                 1.000
```

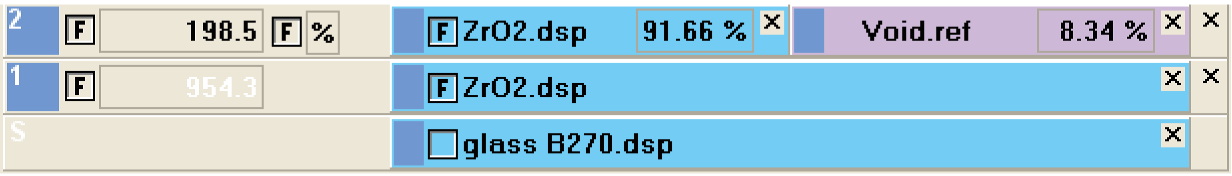


General Remarks

- The anisotropic layer contained in the final model results a χ^2=0.5 compared to 7.2 for a simple layer.

ZrO_2 / Glass Substrate

Model



2 F 198.5 F % | F ZrO2.dsp 91.66 % | Void.ref 8.34 %

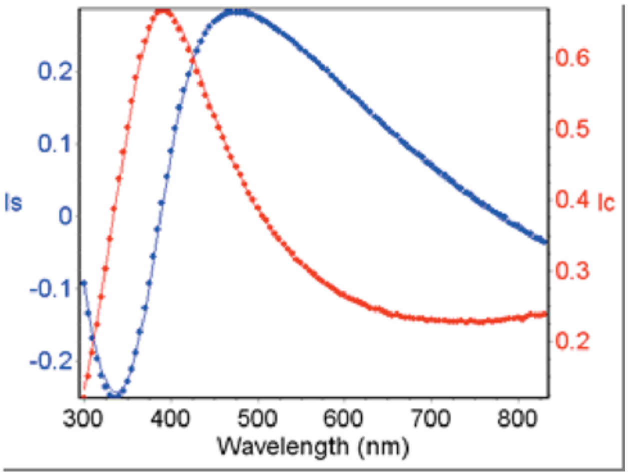
1 F 954.3 | F ZrO2.dsp

S | glass B270.dsp

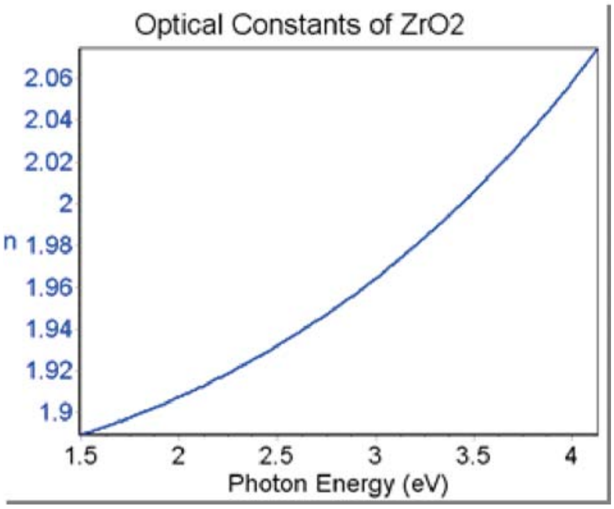
Fit Conditions

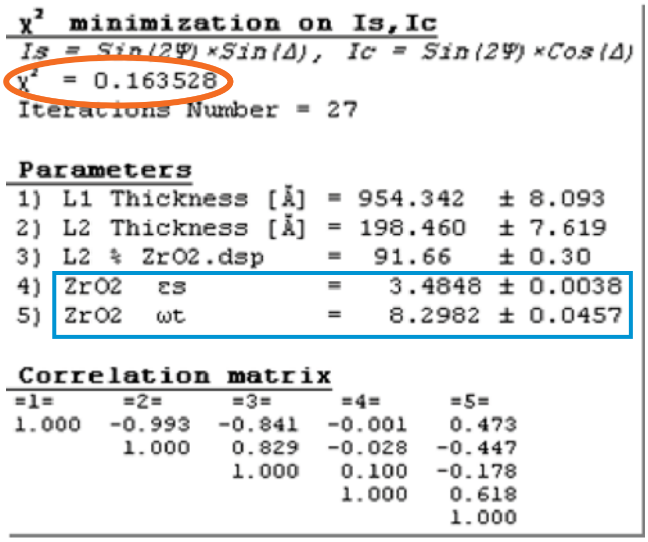
- Spectral range: 300 – 830 nm
- Step size: 5 nm
- Angle of incidence: 70°
- Model Information:
  - Multiguess on thickness varying from 800 to 1500 nm by step of 100 nm for layer 1.
  - The model includes a top surface layer which is very porous (percentage of void ~ 8%).
  - The glass substrate is a dispersion file. It means that it has been separately measured and modeled.
- Fit parameters
  - Thickness: Layers 1 and 2
  - Optical constants: ZrO_2
  - Composition of layer 2: % void + % ZrO_2
- Materials
  - Void: Reference materials
  - **ZrO_2**: Classical formula, Transparent Lorentz oscillator with $\varepsilon_\infty = 1.0$

Fit Results



Optical constants of ZrO_2





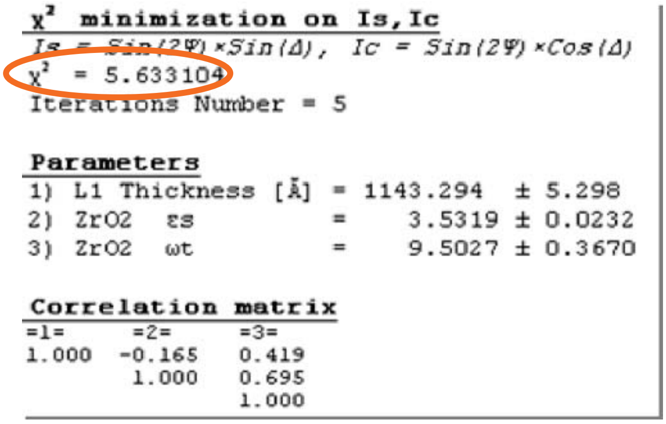
```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 0.163528
Iterations Number = 27

Parameters
1) L1 Thickness [Å]  = 954.342  ± 8.093
2) L2 Thickness [Å]  = 198.460  ± 7.619
3) L2 % ZrO2.dsp     =  91.66   ± 0.30
4) ZrO2   εs         =    3.4848 ± 0.0038
5) ZrO2   ωt         =    8.2982 ± 0.0457

Correlation matrix
=1=     =2=     =3=     =4=     =5=
1.000  -0.993  -0.841  -0.001   0.473
        1.000   0.829  -0.028  -0.447
                1.000   0.100  -0.178
                        1.000   0.618
                                1.000
```

Model without porous surface layer

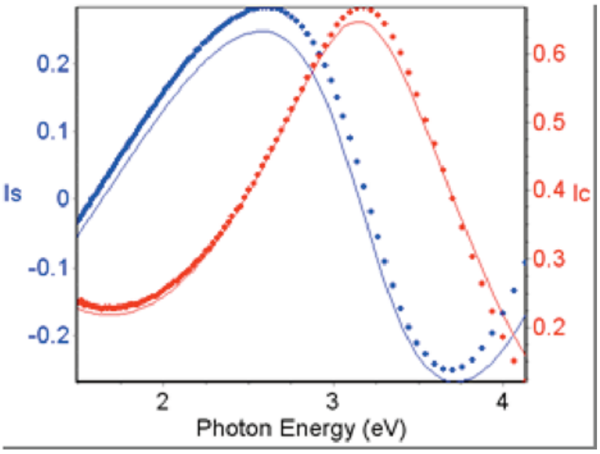
1 F 1143.3 F ZrO2.dsp

S glass B270.dsp

Fit Results



```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ), Ic = Sin(2Ψ)×Cos(Δ)
χ² = 5.633104
Iterations Number = 5

Parameters
1) L1 Thickness [Å] = 1143.294  ± 5.298
2) ZrO2  εs         =    3.5319 ± 0.0232
3) ZrO2  ωt         =    9.5027 ± 0.3670

Correlation matrix
=1=    =2=     =3=
1.000  -0.165  0.419
        1.000  0.695
               1.000
```



General Remarks

- The anisotropic layer contained in the final model results a χ^2=0.5 compared to 7.2 for a simple layer.

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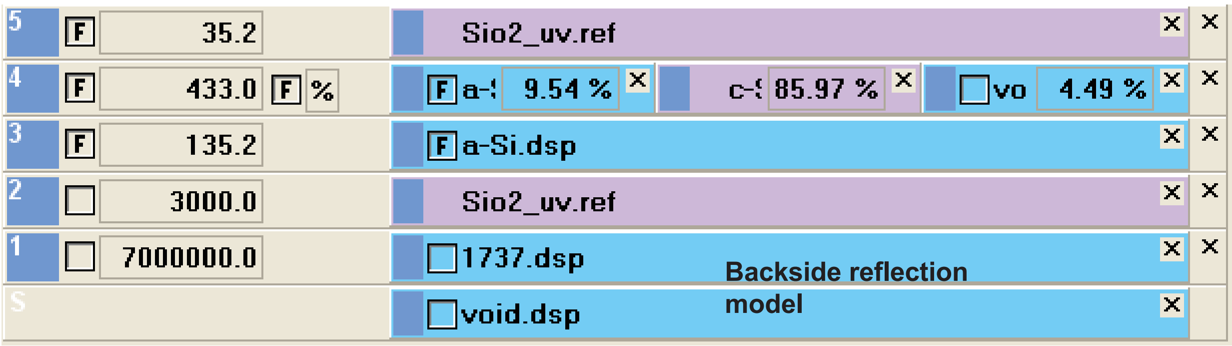
PolySilicon / a-Si / SiO_2 / Glass Substrate

Model



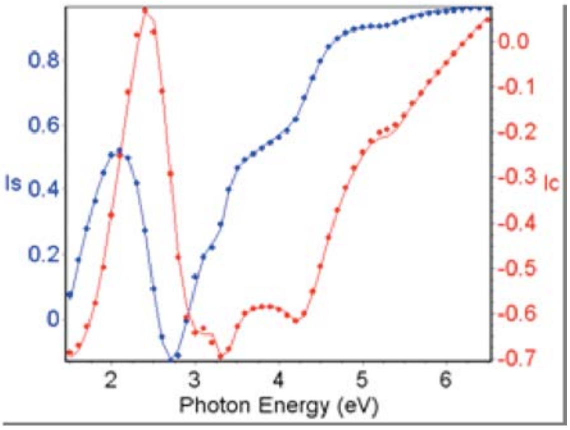
5	F	35.2	Sio2_uv.ref
4	F	433.0 F %	F a- 9.54 % ☒ c- 85.97 % ☒ ☐ vo 4.49 % ☒
3	F	135.2	F a-Si.dsp
2	☐	3000.0	Sio2_uv.ref
1	☐	7000000.0	☐ 1737.dsp
S			☐ void.dsp

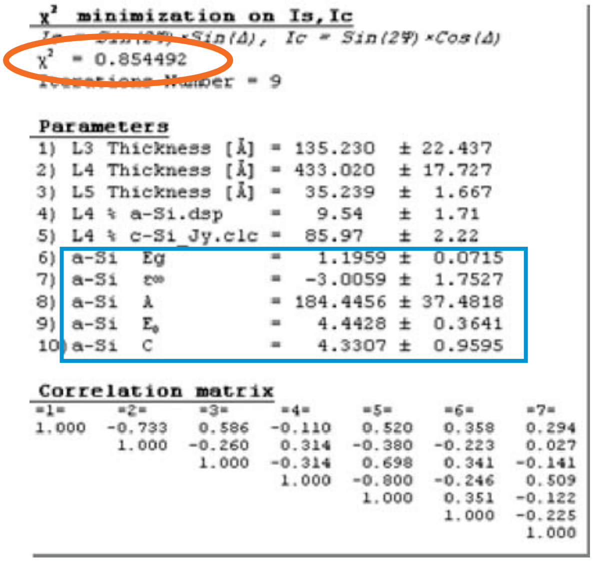
Backside reflection model

Fit Conditions

- Spectral range: 1.5 – 6.5 eV
- Step size: 0.1 eV
- Angle of incidence: 70°
- Model Information:
  - Backside reflection model
  - Polysilicon material is represented by a mixture of a-Si + c-Si + void
  - Native oxide on top surface of the sample
  - SiO_2 layer is not fitted as it comes from previous results.
- Fit parameters
  - Thickness: Layers 1, 2, 3, 4 and 5
  - Optical constants: a-Si
  - Composition of layer 4: % a-Si + % c-Si + % void
- Materials
  - Void, Glass, SiO_2: Reference materials
  - a-Si: Tauc Lorentz formula

Fit Results



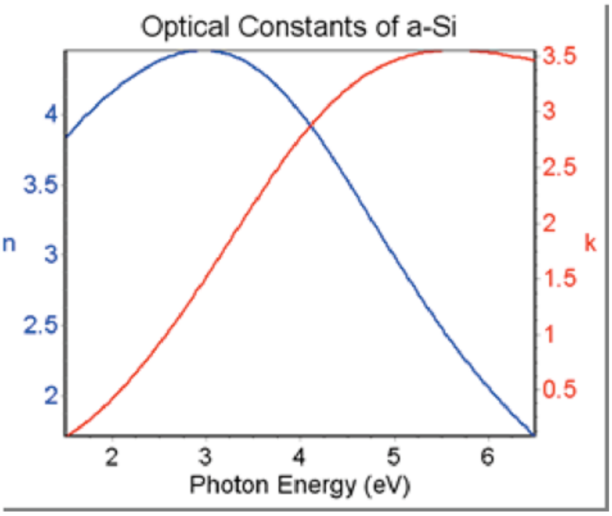


```
χ² minimization on Is,Ic
Is = Sin(2Ψ)×Sin(Δ),  Ic = Sin(2Ψ)×Cos(Δ)
χ² = 0.854492
Iterations Number = 9

Parameters
1) L3 Thickness [Å] = 135.230  ± 22.437
2) L4 Thickness [Å] = 433.020  ± 17.727
3) L5 Thickness [Å] =  35.239  ±  1.667
4) L4 % a-Si.dsp    =   9.54   ±  1.71
5) L4 % c-Si_Jy.clc =  85.97   ±  2.22
6) a-Si  Eg         =   1.1959 ±  0.0715
7) a-Si  ε∞         =  -3.0059 ±  1.7527
8) a-Si  A          = 184.4456 ± 37.4818
9) a-Si  E0         =   4.4428 ±  0.3641
10)a-Si  C          =   4.3307 ±  0.9595

Correlation matrix
=1=     =2=     =3=     =4=     =5=     =6=     =7=
1.000  -0.733   0.586  -0.110   0.520   0.358   0.294
        1.000  -0.260   0.314  -0.380  -0.223   0.027
                1.000  -0.314   0.698   0.341  -0.141
                        1.000  -0.800  -0.246   0.509
                                1.000   0.351  -0.122
                                        1.000  -0.225
                                                1.000
```

Optical constants of a-Si



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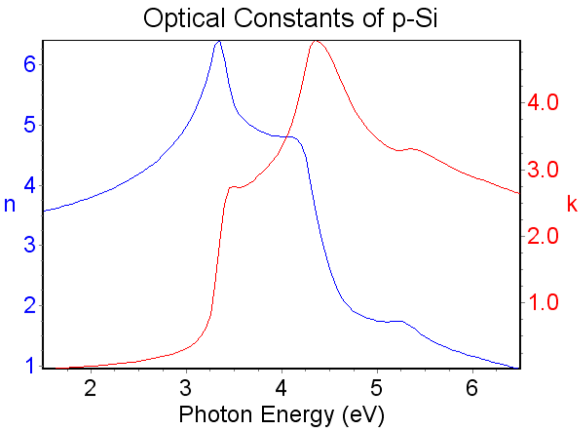
Optical constants of p-Si of layer 4*



*In deltapsi2, build a new spectroscopic model, and put in the substrate the results found for layer 2, eg 9.54% c-Si + 85.97% a-Si + 4.49% void. Then under modeling description, click on edit, and in the modeling conditions tab, choose “User defined spectral range” and put 1.5-6.5 eV. Then, click on simulation, and in the results display area, select the (n,k) axis.

Appendix A Detailed Description of Dispersion Formulae and Settings

Next pages detail each Dispersion Model available from DeltaPsi2 Software.

Appendix A1: Lorentz Dispersion Model

Spectroscopic Ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected polarized light in order to characterize thin film optical functions and other properties. The measured SE data is described by a model where layers refer to a given material. The model uses mathematical relations called dispersion formulas that help to evaluate the material's optical properties by adjusting specific fit parameters.
This technical note deals with the Drude dispersion formula.

Note that the technical notes «Classical dispersion model» and «Lorentz dispersion model» are complementary to

Theoretical model

Drude's model (1900) is based on the kinetic theory of electrons in a metal which assumes that the material has motionless positive ions and a non-interacting electron gas. This simple model uses classical mechanical theory of free electron. It was constructed in order to explain the transport properties of conduction electrons in metals (due to intra-band transitions in a quantum-mechanical interpretation), conductive oxides and heavily doped semiconductors.

Since the conduction electrons are considered to be free, Drude oscillator is an extension of the single Lorentz oscillator to a case where the restoring force and the resonance frequency are null ($\Gamma_0=0$, $\omega_t = 0$) - see «Lorentz dispersion model» technical note.

The equation of motion is:

$$\boxed{m\cdot\frac{d\vec{v}}{dt}+m\cdot\Gamma_d\cdot\vec{v}=-e\cdot\vec{E}\ \ (1)}$$

where:

- m (dv/dt) is the acceleration force; m is the mass of the oscillator (here the electron) and v is the speed of the gas of electron;
- m Γ_d v is the friction force;
- the term -e.E is the electric force; it contains the term $E=E_0\, e^{i\omega t}$ which is the electric field of pulsation ω and -e which is the electric charge.

The solution of the previous equation is given by the following expression for oscillation amplitude:

$$\vec{v}(\omega)=\vec{v}_0\cdot e^{i\omega t}=\frac{-e}{m}\cdot\frac{\vec{E}_0}{i\omega+\Gamma_d}\ \ (2)$$

The conduction density of current J_c corresponding to the movement of the N electrons per unit volume is:

$$\vec{J}_c(\omega)=-Ne\vec{v}=\frac{Ne^2}{m\cdot(\Gamma_d+i\omega)}\vec{E}\ \ (3)$$

The displacement density of current of vacuum is expressed by:

$$\vec{J}_d=\frac{\partial\vec{D}}{\partial t}=i\omega\varepsilon_0\vec{E}\ \ (4)$$

where D is the electric displacement of vacuum: $D = \varepsilon_0 E$.

The total density of current J is given by:

$$\vec{J}(\omega)=\vec{J}_c+\vec{J}_d=\left[\frac{N\cdot e^2}{m\cdot(\Gamma_d+i\omega)}+i\omega\varepsilon_0\right]\vec{E}\ \ (5)$$

Assuming that the plasma can also be characterized by identifying the total density of current to a global displacement current Dtot $= \varepsilon_0\varepsilon_r E$. A new expression for the total density of current is then given by:

$$\vec{J}(\omega)=\frac{\partial\vec{D}_{tot}}{\partial t}=i\omega\varepsilon_0\,\tilde{\varepsilon}\,\vec{E}\ \ (6)$$

The identification of the two last formulations of the total density of current J yields:

$$\vec{J}(\omega)=\left[\frac{N\cdot e^2}{m\cdot(\Gamma_d+i\omega)}+i\omega\varepsilon_0\right]\cdot\vec{E}=i\omega\varepsilon_0\tilde{\varepsilon}(\omega)\cdot\vec{E}\ \ (7)$$

By simplifying that last expression, it is possible to deduce Drude's dielectric function $\varepsilon(\omega)$ given by the following equation:

$$\boxed{\tilde{\varepsilon}(\omega)=1-\frac{Ne^2}{m\varepsilon_0}\cdot\frac{1}{(\omega^2-i\Gamma_d\omega)}=1-\frac{\omega_p^2}{-\omega^2+i\cdot\Gamma_d\cdot\omega}\ \ (8)}$$

Note that for $\omega \rightarrow \infty$, $\varepsilon(\infty) \rightarrow 1$ then it is possible to rewrite the dielectric function as:

$$\boxed{\tilde{\varepsilon}(\omega)=\varepsilon(\infty)-\frac{\omega_p^2}{-\omega^2+i\cdot\Gamma_d\cdot\omega}\ \ (9)}$$

like in DP2 software, where $\varepsilon(\infty)$ is the high-frequency contribution that is usually superior or equal to one.

The real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of the dielectric function are given by:

$$\varepsilon_1(\omega)=1(\varepsilon(\infty))-\frac{\omega_p^2}{\omega^2+\Gamma^2} \quad (10.1)$$

and

$$\varepsilon_2(\omega)=\frac{\omega_p^2\cdot\Gamma}{\omega\cdot\left(\omega^2+\Gamma^2\right)} \quad (10.2)$$

Behaviour of Drude dielectric function

- If $\omega<\omega_p$ then the real part of ε is negative: any electrical field cannot penetrate the metal that is totally reflective. **The optical constants of the material are complex.**
- If $\omega=\omega_p$ then the real part of the dielectric function is zero. This means that all electrons oscillate in phase throughout the material propagation length.
- If $\omega>\omega_p$ the reflectivity decreases and the metal becomes transparent. **The refractive index of the material is almost real.**
- When $\omega^2>>\Gamma_d^2$ then $\varepsilon_r(\omega)=1-(\omega_p^2/\omega^2)$. The imaginary part of the dielectric function can be approximated by $\varepsilon_i(\omega) = (\omega_p^2\,\Gamma/\omega^2)$ and there is no absorption at the high frequency limit.

The parameters of the dispersion formula

2 parameters are used in the Drude's model. Both ω_p and Γ_d influence the real and imaginary parts of the dielectric function.

$$\omega_p=\sqrt{\frac{N\cdot e^2}{m\cdot\varepsilon_0}}$$

- ω_p is the plasma frequency. It corresponds to the photon energy position where $\varepsilon_r(\omega)$ is approximately zero. As ω_p increases the amplitude of $\varepsilon_r(\omega)$ and $\varepsilon_i(\omega)$ increases too.
- Γ_d (in eV) is the collision frequency. Generally, for metals $0 < \Gamma_d < 4$. As Γ_d increases the broadening of the absorption tail increases too.

Limitation of the model

The Drude oscillator describes well the optical properties of metals but does not take into account the notion of optical energy band gap E_g semiconductors and the quantum effects.

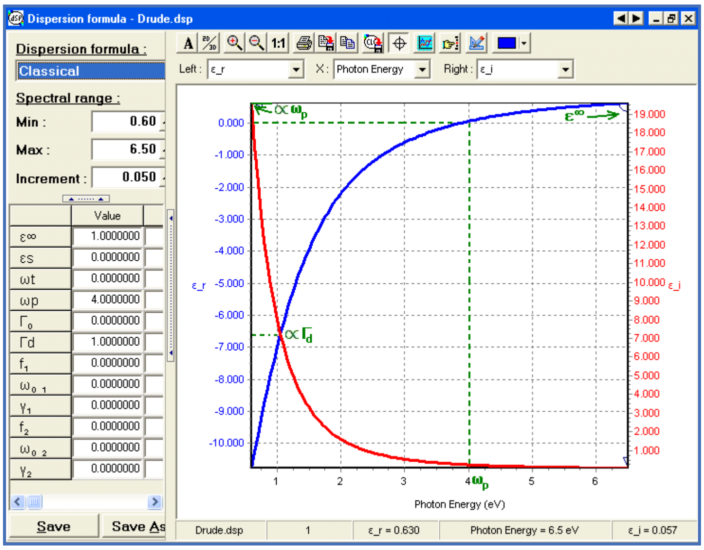
Parameter setup

Note that:

1 - The Drude's dielectric function is available in the Classical dispersion formula in the DeltaPsi2 software.

2 - The sign $\propto$ before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

Drude's model predicts monotonous decrease of $\varepsilon_r(\omega)$ for decreasing photon energy. It is also characterized by monotonous increase of $\varepsilon_i(\omega)$ (absorption tail) with decreasing photon energy towards the NIR region.



Dispersion formula - Drude.dsp

Dispersion formula : Classical

Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.050

	Value
$\varepsilon\infty$	1.0000000
εs	0.0000000
ωt	0.0000000
ωp	4.0000000
Γ_0	0.0000000
Γd	1.0000000
f_1	0.0000000
$\omega_{0\,1}$	0.0000000
γ_1	0.0000000
f_2	0.0000000
$\omega_{0\,2}$	0.0000000
γ_2	0.0000000

Left : ε_r
X : Photon Energy
Right : ε_i

Drude.dsp | 1 | ε_r = 0.630 | Photon Energy = 6.5 eV | ε_i = 0.057

Starting values of a classical Drude function

Application to materials

This model fits well the optical properties of metallic samples and heavily doped semiconductors. The spectral range used for fitting depends on the material as shown in the array below.

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

S.R. means Spectral Range.

Materials	$\varepsilon\wp$	ω_p	Γ_d	S. R. (eV)
Al	1.0	15.702	0.696	1.5 - 6.5
Co	3.694	12.175	5.799	0.75 - 4.75
Mo	-1.366*	19.972	8.357	1.5 - 5
NiCr	1.0	14.270	4.020	1.5 - 5
NiFe	1.0	14.790	4.780	1.5 - 5
Ti	1.0	10.9	2.53	1.0 - 6.0

References

1) J. M. Cazaux, *Introduction a la physique du Solide*, Masson (1996)
2) H. M. Rosenberg, *The Solid State*, Oxford University Press (1988)
3) F. Wooten, *Optical Properties of Solids*, Academic Press (1972)
4) E. Hecht, *Optics*, Chap. 3, Hardcover (2001)
5) www.ece.tamu.edu/People/bios/hemmer_files/15-dispersion.ppt

Appendix A2: Drude Dispersion Model

Spectroscopic Ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected polarized light in order to characterize thin film optical functions and other properties. The measured SE data is described by a model where layers refer to a given material. The model uses mathematical relations called dispersion formulas that help to evaluate the material's optical properties by adjusting specific fit parameters.
This technical note deals with the Drude dispersion formula.

Note that the technical notes «Classical dispersion model» and «Lorentz dispersion model» are complementary to this one.

Theoretical model

Drude's model (1900) is based on the kinetic theory of electrons in a metal which assumes that the material has motionless positive ions and a non-interacting electron gas. This simple model uses classical mechanical theory of free electron. It was constructed in order to explain the transport properties of conduction electrons in metals (due to intra-band transitions in a quantum-mechanical interpretation), conductive oxides and heavily doped semiconductors.

Since the conduction electrons are considered to be free, Drude oscillator is an extension of the single Lorentz oscillator to a case where the restoring force and the resonance frequency are null ($\Gamma_0=0$, $\omega_t = 0$) - see «Lorentz dispersion model» technical note.

The equation of motion is:

$$\boxed{m\cdot\frac{d\vec{v}}{dt}+m\cdot\Gamma_d\cdot\vec{v}=-e\cdot\vec{E}\ \ (1)}$$

where:

- m (d**v**/dt) is the acceleration force; m is the mass of the oscillator (here the electron) and v is the speed of the gas of electron;
- m Γ_d **v** is the friction force;
- the term -e.**E** is the electric force; it contains the term $E=E_0\, e^{i\omega t}$ which is the electric field of pulsation ω and -e which is the electric charge.

The solution of the previous equation is given by the following expression for oscillation amplitude:

$$\vec{v}(\omega)=\vec{v}_0\cdot e^{i\omega t}=\frac{-e}{m}\cdot\frac{\vec{E}_0}{i\omega+\Gamma_d}\ \ (2)$$

The conduction density of current J_c corresponding to the movement of the N electrons per unit volume is:

$$\vec{J}_c(\omega)=-N\,e\,\vec{v}=\frac{N\,e^2}{m\cdot(\Gamma_d+i\,\omega)}\vec{E}\ \ (3)$$

The displacement density of current of vacuum is expressed by:

$$\vec{J}_d=\frac{\partial\vec{D}}{\partial t}=i\,\omega\,\varepsilon_0\,\vec{E}\ \ (4)$$

where D is the electric displacement of vacuum: $D = \varepsilon_0 E$.

The total density of current J is given by:

$$\vec{J}(\omega)=\vec{J}_c+\vec{J}_d=\left[\frac{N\cdot e^2}{m\cdot(\Gamma_d+i\,\omega)}+i\,\omega\,\varepsilon_0\right]\vec{E}\ \ (5)$$

Assuming that the plasma can also be characterized by identifying the total density of current to a global displacement current Dtot $= \varepsilon_0\varepsilon_r E$. A new expression for the total density of current is then given by:

$$\vec{J}(\omega)=\frac{\partial\vec{D}_{tot}}{\partial t}=i\,\omega\,\varepsilon_0\,\tilde{\varepsilon}\,\vec{E}\ \ (6)$$

The identification of the two last formulations of the total density of current J yields:

$$\vec{J}(\omega)=\left[\frac{N\cdot e^2}{m\cdot(\Gamma_d+i\,\omega)}+i\,\omega\,\varepsilon_0\right]\cdot\vec{E}=i\,\omega\,\varepsilon_0\,\tilde{\varepsilon}(\omega)\cdot\vec{E}\ \ (7)$$

By simplifying that last expression, it is possible to deduce Drude's dielectric function ε(ω) given by the following equation:

$$\boxed{\tilde{\varepsilon}(\omega)=1-\frac{N\,e^2}{m\,\varepsilon_0}\cdot\frac{1}{(\omega^2-i\,\Gamma_d\,\omega)}=1-\frac{\omega_p^2}{-\omega^2+i\cdot\Gamma_d\cdot\omega}\ \ (8)}$$

Note that for ω → ∞, ε(∞) → 1 then it is possible to rewrite the dielectric function as:

$$\boxed{\tilde{\varepsilon}(\omega)=\varepsilon(\infty)-\frac{\omega_p^2}{-\omega^2+i\cdot\Gamma_d\cdot\omega}\ \ (9)}$$

like in DP2 software, where ε(∞) is the high-frequency contribution that is usually superior or equal to one.

The real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of the dielectric function are given by:

$$\varepsilon_1(\omega) = 1(\varepsilon(\infty)) - \frac{\omega_p^2}{\omega^2 + \Gamma^2} \quad (10.1)$$

and

$$\varepsilon_2(\omega) = \frac{\omega_p^2 \cdot \Gamma}{\omega \cdot \left(\omega^2 + \Gamma^2\right)} \quad (10.2)$$

Behaviour of Drude dielectric function

- If $\omega < \omega_p$ then the real part of ε is negative: any electrical field cannot penetrate the metal that is totally reflective. **The optical constants of the material are complex**.
- If $\omega = \omega_p$ then the real part of the dielectric function is zero. This means that all electrons oscillate in phase throughout the material propagation length.
- If $\omega > \omega_p$ the reflectivity decreases and the metal becomes transparent. **The refractive index of the material is almost real**.
- When $\omega^2 >> \Gamma_d^2$ then $\varepsilon_r(\omega) = 1 - (\omega_p^2/\omega^2)$. The imaginary part of the dielectric function can be approximated by $\varepsilon_i(\omega) = (\omega_p^2\ \Gamma/\omega^2)$ and there is no absorption at the high frequency limit.

The parameters of the dispersion formula

2 parameters are used in the Drude's model. Both ω_p and Γ_d influence the real and imaginary parts of the dielectric function.

$$\omega_p = \sqrt{\frac{N \cdot e^2}{m \cdot \varepsilon_0}}$$

- ω_p is the plasma frequency. It corresponds to the photon energy position where $\varepsilon_r(\omega)$ is approximately zero. As ω_p increases the amplitude of $\varepsilon_r(\omega)$ and $\varepsilon_i(\omega)$ increases too.
- Γ_d (in eV) is the collision frequency. Generally, for metals $0 < \Gamma_d < 4$. As Γ_d increases the broadening of the absorption tail increases too.

Limitation of the model

The Drude oscillator describes well the optical properties of metals but does not take into account the notion of optical energy band gap E_g semiconductors and the quantum effects.

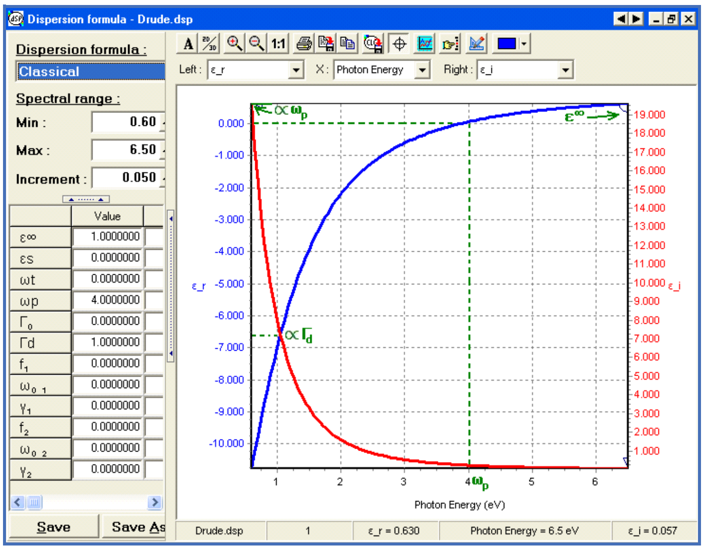
Parameter setup

Note that:

1 - The Drude's dielectric function is available in the Classical dispersion formula in the DeltaPsi2 software.

2 - The sign ∝ before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

Drude's model predicts monotonous decrease of $\varepsilon_r(\omega)$ for decreasing photon energy. It is also characterized by monotonous increase of $\varepsilon_i(\omega)$ (absorption tail) with decreasing photon energy towards the NIR region.



Dispersion formula - Drude.dsp

Dispersion formula : Classical

Spectral range :

Min : 0.60

Max : 6.50

Increment : 0.050

	Value
ε∞	1.0000000
εs	0.0000000
ωt	0.0000000
ωp	4.0000000
Γ_0	0.0000000
Γd	1.0000000
f_1	0.0000000
$\omega_{0\ 1}$	0.0000000
γ_1	0.0000000
f_2	0.0000000
$\omega_{0\ 2}$	0.0000000
γ_2	0.0000000

Left : ε_r X : Photon Energy Right : ε_i

Drude.dsp | 1 | ε_r = 0.630 | Photon Energy = 6.5 eV | ε_i = 0.057

Starting values of a classical Drude function

Application to materials

This model fits well the optical properties of metallic samples and heavily doped semiconductors. The spectral range used for fitting depends on the material as shown in the array below.

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

S.R. means Spectral Range.

Materials	ε ℘	ω_p	Γ_d	S. R. (eV)
Al	1.0	15.702	0.696	1.5 - 6.5
Co	3.694	12.175	5.799	0.75 - 4.75
Mo	-1.366*	19.972	8.357	1.5 - 5
NiCr	1.0	14.270	4.020	1.5 - 5
NiFe	1.0	14.790	4.780	1.5 - 5
Ti	1.0	10.9	2.53	1.0 - 6.0

References

1) J. M. Cazaux, *Introduction a la physique du Solide*, Masson (1996)
2) H. M. Rosenberg, *The Solid State*, Oxford University Press (1988)
3) F. Wooten, *Optical Properties of Solids*, Academic Press (1972)
4) E. Hecht, *Optics*, Chap. 3, Hardcover (2001)
5) www.ece.tamu.edu/People/bios/hemmer_files/15-dispersion.ppt

Appendix A3: Classical Dispersion Model

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured data are used to describe a model where each layer refers to a given material. The model uses mathematical relations called dispersion formulae that help to evaluate the thickness and optical properties of the material by adjusting specific fit parameters.

This application note deals with the classical dispersion formula. Note that more detailed explanation are given in the technical notes: Drude's and Lorentz dispersion model.

Theoretical model

The classical dispersion model is based on the sum of the single and double Lorentz, and Drude oscillators.

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\cdot\omega_t^2}{\omega_t^2 - \omega^2 + i\cdot\Gamma_0\cdot\omega} + \frac{\omega_p^2}{-\omega^2 + i\cdot\Gamma_d\cdot\omega} + \sum_{j=1}^{2}\frac{f_j\cdot\omega_{0j}^2}{\omega_{0j}^2 - \omega^2 + i\cdot\gamma_j\cdot\omega}$$

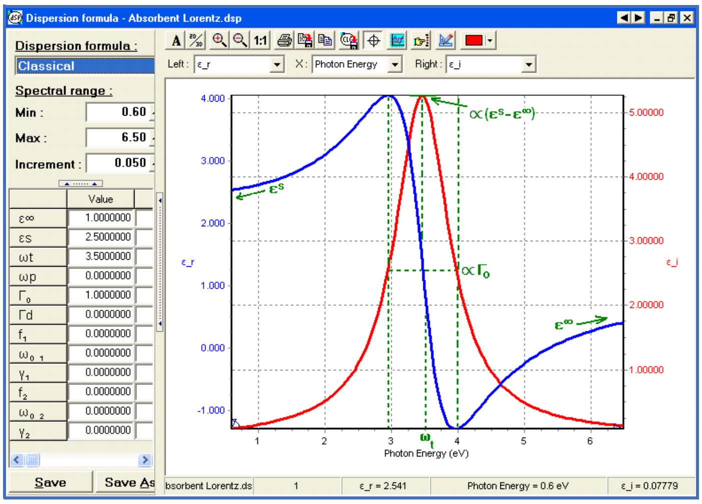
- Lorentz dispersion model

The Lorentz classical theory (1878) is based on the classical theory of interaction between light and matter and is used to describe frequency dependent polarization due to bound charge.

The Lorentzian dispersion formula comes from the solution of the equation of an electron bound to a nucleus driven by an oscillating electric field E. The response is equivalent to the classical mass on a spring which has damping and an external driving force. It generates damped harmonic oscillations.

In the DeltaPsi2 software the classical dispersion formula contains three oscillators.

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\cdot\omega_t^2}{\omega_t^2 - \omega^2 + i\cdot\Gamma_0\cdot\omega} + \sum_{j=1}^{2}\frac{f_j\cdot\omega_{0j}^2}{\omega_{oj}^2 - \omega^2 + i\cdot\gamma_j\cdot\omega}$$



Dispersion formula - Absorbent Lorentz.dsp

Dispersion formula : Classical

Spectral range :

Min : 0.60

Max : 6.50

Increment : 0.050

	Value
ε∞	1.0000000
εs	2.5000000
ωt	3.5000000
ωp	0.0000000
Γ_0	1.0000000
Γd	0.0000000
f_1	0.0000000
$\omega_{0\,1}$	0.0000000
γ_1	0.0000000
f_2	0.0000000
$\omega_{0\,2}$	0.0000000
γ_2	0.0000000

Left : ε_r X : Photon Energy Right : ε_i

bsorbent Lorentz.ds 1 ε_r = 2.541 Photon Energy = 0.6 eV ε_i = 0.07779

Single Lorentz oscillator

Parameters describing the real part of the dielectric function

- The constant ε_∞ is the high frequency dielectric constant. Generally, $\varepsilon_\infty = 1$ but can be greater than 1 if oscillators in higher enegies exist and are not taken into account.
- The constant ε_s ($\varepsilon_s > \varepsilon_\infty$) gives the value of the static dielectric function at a zero frequency. The difference $\varepsilon_s - \varepsilon_\infty$ represents the strength of the single Lorentz oscillator. The larger it is then the smaller the width Γ_0 of the peak of the single Lorentz oscillator.

Parameters describing the imaginary part of the single Lorentz oscillator dielectric function

- ω_t (in eV) is the resonant frequency of the oscillator whose energy corresponds to the absorption peak. When ω_t increases then the peak is shifted to higher photon energies. Generally, $1 \le \omega_t \le 20$.
- Γ_0 (in eV) is the broadening of each oscillator also known as the damping factor. The damping effect is due to the absorption process involving transitions between two states. On a graphic representing $\varepsilon_i(\omega)$, Γ_0 is generally equal to the Full Width At Half Maximum (FWHM) of the peak. As Γ_0 increases the width of the peak increases, but the amplitude of that decreases. Generally, $0 \le \Gamma_0 \le 10$.

Parameters describing the imaginary part of the multiple Lorentz oscillators dielectric function

- f_j (j = 1, 2 … N) term is the oscillator strength present in the expression of the multiple Lorentz oscillator. As fj increases then the peak amplitude increases, but the width of the peak γ_j decreases. Generally, $0 \le f_j \le 10$.
- ω_{0j} (in eV) (j = 1, 2 … N) is the resonant (peak) energy of an oscillator for a collection of several Lorentzian oscillators. It is similar to ω_t . Generally, $1 \le \omega_{0j} \le 8$.
- γ_j (in eV) (j = 1, 2 … N) parameter is the broadening parameter corresponding to the peak energy of each oscillator. It behaves like Γ_0 . Generally, $0 \le \gamma_j \le 10$.

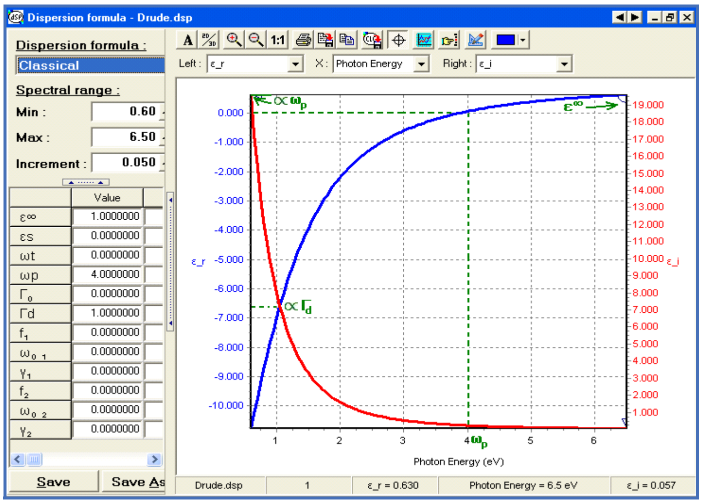
- Drude dispersion model

Drude's model (1900) is based on the kinetic theory of electrons in a metal which assumes that the material has motionless positive ions and a non-interacting electron gas. This simple model uses classical mechanical theory of free electron. It was constructed in order to explain the transport properties of conduction electrons in metals (due to intra-band transitions in a quantum-mechanical interpretation), conductive oxides and heavily doped semiconductors.

Since the conduction electrons are considered to be free, Drude oscillator is an extension of the single Lorentz oscillator to a case where the restoring force and the resonance frequency are null ($\Gamma_0=0$, $\omega_t = 0$).

In the DeltaPsi2 software the classical dispersion formula contains the Drude model expressed as below:

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{-\omega^2 + i \cdot \Gamma_d \cdot \omega}$$



Dispersion formula : Classical

Left : ε_r X : Photon Energy Right : ε_i

Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.050

	Value
ε∞	1.0000000
εs	0.0000000
ωt	0.0000000
ωp	4.0000000
Γ_o	0.0000000
Γd	1.0000000
f_1	0.0000000
$\omega_{o\ 1}$	0.0000000
γ_1	0.0000000
f_2	0.0000000
$\omega_{o\ 2}$	0.0000000
γ_2	0.0000000

Drude.dsp | 1 | ε_r = 0.630 | Photon Energy = 6.5 eV | ε_i = 0.057

Classical Drude function

- ω_p is the plasma frequency corresponding to the photon energy position where $\varepsilon_r(\omega)$ is approximately zero. When ω_p increases then the amplitude of the $\varepsilon_r(\omega)$ and $\varepsilon_i(\omega)$ increases too.

$$\boxed{\omega_p = \sqrt{\frac{N \cdot e^2}{m \cdot \varepsilon_0}}}$$

- Γ_d (in eV) is the collision frequency. As Γ_d increases the broadening of the absorption tail increases too. Generally, for metals $0.4 < \Gamma_d < 4$.

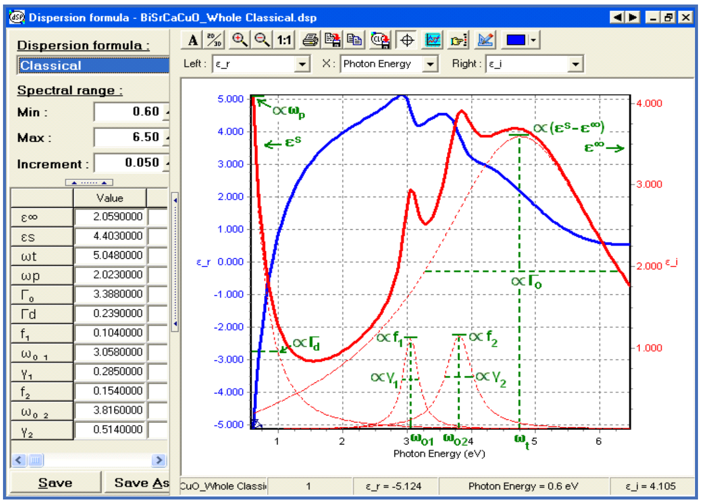
Application to Materials

The Lorentz oscillator model works well for insulators and semiconductors above the band gap.

The Drude model describes well the optical properties of metals but does not take into account the notion of optical band gap energy E_g .

The combination of both is often adequate when the material is a little conductive and has a metallic character (like conducting oxides ITO, RuO_2).

The graph above typically shows the influence of Drude's function characterized by an increasing absorption (imaginary part of the dielectric function) toward the IR region.



Dispersion formula : Classical

Left : ε_r X : Photon Energy Right : ε_i

Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.050

	Value
ε∞	2.0590000
εs	4.4030000
ωt	5.0480000
ωp	2.0230000
Γ_o	3.3880000
Γd	0.2390000
f_1	0.1040000
$\omega_{o\ 1}$	3.0580000
γ_1	0.2850000
f_2	0.1540000
$\omega_{o\ 2}$	3.8160000
γ_2	0.5140000

CuO_Whole Classi | 1 | ε_r = -5.124 | Photon Energy = 0.6 eV | ε_i = 4.105

Dielectric function of BiSrCaCuO

List of materials following Drude and Lorentzian dispersion models

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

Materials	ε_∞	ε_s	ω_t	ω_p	Γ_0	Γ_d
Ag	-2.875*	3.401	9.6310	8.707	1.783	0.073
Al	0.959	16.787	1.637	13.320	0.705	0.119
Cr	3.9	4	0	20.000	0	100.000
Cu	1	1.65	1.80	4.00	3.00	0.85
IrO_2	1.0	6.209	6.650	3.989	9.002	0.819
ITO/PET	1.0	4.077	6.841	1.244	2.365	0.107
ITO/glass	3.201	4.039	4.935	1.850	0.302	0.0854
MoSi	1	7.948	6.628	2.714	9.081	7.870
NiCr	1	0.890	0	14.270	0	4.020
NiFe	1	0.880	0	14.790	0	4.780
Si_3N_4	1.0	5.377	3.186	0	0	0
SnO_2	0.714	0.792	4.933	7.814	1.141	15.546
Ta	1	1.790	0	21.530	0	19.799
TiN	1.348	3.610	5.067	4.769	6.339	4.343
YAG:Tb(10%)	1.0	2.545	10.342	0.793	0	0
$Y_3Fe_5O_{12}$	3.410	4.636	3.369	0.305	0.346	0.165
ZnO	1	2.900	7.250	5.450	2.700	17.150

List of materials following Drude and double Lorentz oscillator models

Materials	$\varepsilon_{\wp}$	ε_s	ω_t	ω_p	Γ_0	Γ_d
Al	0.884	0	0	13.346	0	0.119
Au	-4.230*	6.956	8.481	7.971	7.449	0.078
BiSrCuO	2.059	4.403	5.048	2.023	3.388	0.239
C60	2.306	3.362	4.556	0.000	1.046	0.000
Cr	1.769	56.676	1.311	4.179	5.715	0.609
Cu	3.070	8.173	2.234	8.896	0.880	-0.047*
CuPC	2.551	0	0	0	0	0
Mo - Pal	2.216	10.869	4.190	8.306	2.048	0.347
p-Si	7.000	0	0	0	0	0
SiC - pal	2.922	6.401	6.843	0.000	0.974	0.000
Ta	1.129	2.617	3.140	7.683	1.527	0.045
Ti	-0.551*	0	0	5.415	0	1.942
TiN	3.050	0	0	12.071	0	11.321

Materials	f_1	$\omega_{0,1}$	γ_1	f_2	$\omega_{0,2}$	γ_2
Al	9.255	1.990	1.667	7.766	1.572	0.391
Au	-1.476*	0.182	4.243	-3.011*	6.619	2.692
BiSrCuO	0.104	3.058	0.285	0.154	3.816	0.514
C60	0.223	2.704	0.439	0.364	3.523	0.420
Cu	-6.330*	-2.137*	0.909	9.926	4.597	10.564
Cr	1.648	6.769	3.606	0	0	0
CuPC	0.425	2.022	0.210	0.149	3.574	0.334
Mo - Pal	3.093	1.712	0.557	11.119	2.426	1.475
p-Si	6.000	3.400	1.000	5.500	4.400	1.250
SiC - pal	0.154	2.403	2.188	0.080	4.042	1.203
Ta	-1.935*	-1.971*	0.926	18.717	7.896	26.969
Ti	0.300	-5.789*	-0.404*	2.102	-3.328*	2.203
TiN	-1.089*	2.006	1.026	0.929	4.743	1.011

References

1) H.M. Rosenberg, The Solid State, Oxford University Press.
2) F. Wooten, Optical Properties of Solids, Academic Press (1972).
3) Eugene Hecht, Optics, Addison-Wesley, NY (1997)
4) http://www.ifm.liu.se/~boser/surfacemodes/L3.pdf
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6) F. Wooten, Optical Properties of Solids, Academic Press (1972)
7) H. M. Rosenberg, The Solid State, Oxford University Press (1988)
8) J. M. Cazaux, Introduction a la physique du Solide, Masson (199)
9) E. Hecht, Optics, Chap. 3, Hardcover (2001)
10) www.ece.tamu.edu/People/bios/hemmer_files/15-dispersion.ppt

Appendix A4: New Amorphous Dispersion Formula

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured data are used to describe a model where each layer refers to a given material. The model uses mathematical relations called dispersion formulae that help to evaluate the material's optical properties by adjusting specific fit parameters.

This application note deals with the new amorphous dispersion formula. For further information about the original theory derived from Forouhi-Bloomer, please refer to the technical note «Forouhi Bloomer alias Amorphous dispersion formula».

New Amorphous theoretical model

The «New Amorphous» dispersion formula was derived by Horiba Jobin Yvon on the basis of Forouhi-Bloomer formulation. This new formulation was established in order to give a Lorentzian shape to the expressions of the extinction coefficient and refractive index. The absorption coefficient is given by :

$$k(\omega)=\begin{cases}\dfrac{f_j\cdot(\omega-\omega_g)^2}{(\omega-\omega_j)^2+\Gamma_j^2} & ;\text{for } \omega>\omega_g\\ 0 & ;\text{for } \omega\le\omega_g\end{cases}\qquad(1)$$

The refractive index is written through this formula :

$$n(\omega)=n_\infty+\frac{B\cdot(\omega-\omega_j)+C}{(\omega-\omega_j)^2+\Gamma_j^2}\qquad(2)$$

where :

$$\begin{cases}B_j=\dfrac{f_j}{\Gamma_j}\cdot\left(\Gamma_j^2-(\omega_j-\omega_g)^2\right)\\ C_j=2\cdot f_j\cdot\Gamma_j\cdot(\omega_j-\omega_g)\end{cases}\qquad(3)$$

Extension to multiple oscillators: «N - New Amorphous»

The New Amorphous formulation can be extended to the case where many oscillators are present in the material. Such dispersions are called « N – New Amorphous » and are given in the array below.

Formula	Number of oscillators	Number of parameters
New Amorphous	N=1	5
Double New Amorphous	N=2	8
Triple New Amorphous	N=3	11

The equations for k(ω) and n(ω) for N oscillators are given below :

- for the extinction coefficient :

$$k(\omega)=\begin{cases}\displaystyle\sum_{j=1}^{N}\frac{f_j\cdot(\omega-\omega_g)^2}{(\omega-\omega_j)^2+\Gamma_j^2} & ;\text{for } \omega>\omega_g\\ 0 & ;\text{for } \omega\le\omega_g\end{cases}\qquad(4)$$

- for the refractive index :

$$n(\omega)=n_\infty+\sum_{j=1}^{N}\frac{B_j\cdot(\omega-\omega_j)+C_j}{(\omega-\omega_j)^2+\Gamma_j^2}\qquad(5)$$

Increasing the number of oscillators leads to a shift of the peaks of absorption toward the ultraviolet region.

The parameters of the equation

Parameter describing the refractive index

The term n(∞) is an additional parameter, at least greater than one and equal to the value of the refractive index when $\omega\rightarrow\infty$.

4 parameters describe the extinction coefficient.

- f_j (j=1, 2, 3) (in eV) is related to the strength (amplitude) of the extinction coefficient peak. As the value of f_j increases both values of the refractive index and extinction coefficient increases. Generally, $0<f_j<1$.
- Γ_j (j=1, 2, 3) (in eV) is the broadening term of the peak of absorption. The larger Γ_j is the larger the absorption peak but the smaller its amplitude. Generally, $0.2<\Gamma_j<8$.
- ω_j (in eV) is approximately the energy at which the extinction coefficient is maximum (peak of absorption). As the value of ω_j increases the absorption peak is shifted towards the UV region. Generally, $1.5<\omega_j<10$.
- ω_g (in eV) is the energy band gap. It is equal to the minimum of energy required for a transition from the valence band to the conduction band. It is the energy from which the absorption starts to be non-zero: $k(E \geq Eg) \geq 0$. Always, $\omega_g < \omega_j$.

Relations between «Amorphous» and «New Amorphous» parameters

The array below gives the relations between the parameters of Forouhi-Bloomer and New Amorphous dispersion formulae.

Forouhi-Bloomer	New Amorphous
A	f_j
B	$2.\omega_j$
C	$\omega^2_j+\Gamma^2_j$
$\sqrt{\varepsilon_\infty}$	n_∞
E_g	ω_g

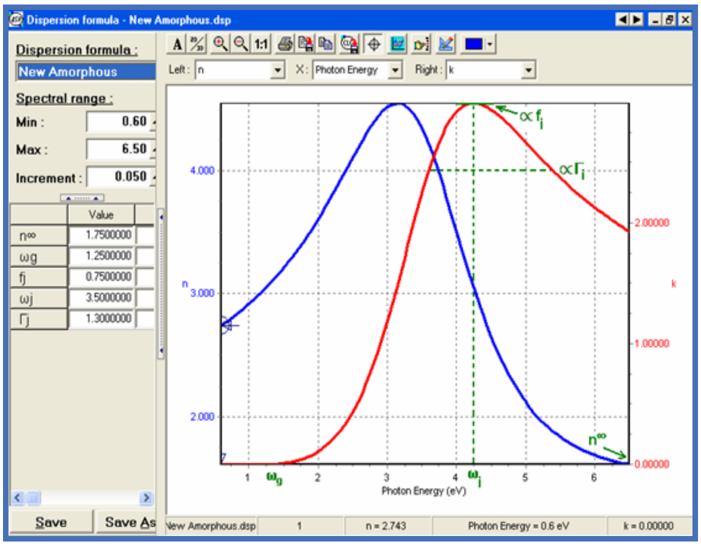
N.B: In DeltaPsi2 software, the user is advised to perform fitting using the «New Amorphous» formula (and its extensions) instead of the «Amorphous» one because *B* and *C* parameters are often correlated.

Parameter setup

Note that :

- The graphs below show the different contributions (in red dashed lines) to the imaginary part of the Double New Amorphous dielectric function (in red bold line).
- The sign « ∝ » before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

New Amorphous function



Dispersion formula - New Amorphous.dsp

Dispersion formula : New Amorphous

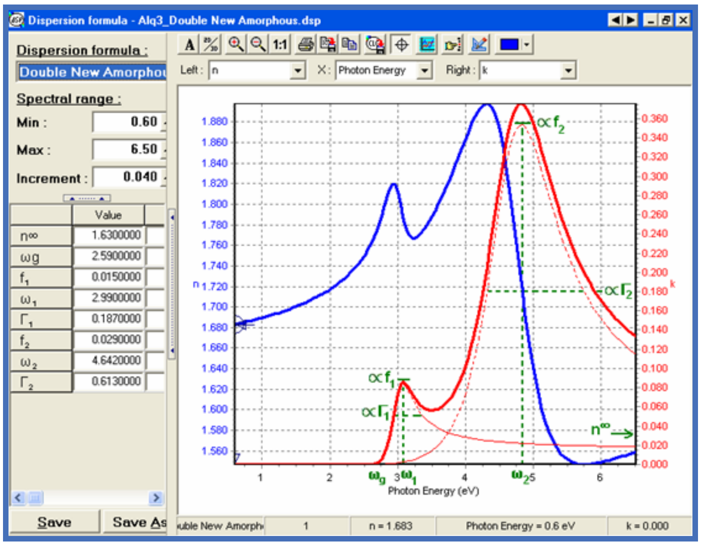
Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.050

	Value
n∞	1.7500000
ωg	1.2500000
fj	0.7500000
ωj	3.5000000
Γj	1.3000000

Left : n X : Photon Energy Right : k

New Amorphous.dsp | 1 | n = 2.743 | Photon Energy = 0.6 eV | k = 0.00000

Double New Amorphous function



Dispersion formula - Alq3_Double New Amorphous.dsp

Dispersion formula : Double New Amorphou

Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.040

	Value
n∞	1.6300000
ωg	2.5900000
f_1	0.0150000
ω_1	2.9900000
Γ_1	0.1870000
f_2	0.0290000
ω_2	4.6420000
Γ_2	0.6130000

Left : n X : Photon Energy Right : k

uble New Amorph | 1 | n = 1.683 | Photon Energy = 0.6 eV | k = 0.000

Optical properties of Alq3 given by the Double New Amorphous function

Applications to materials

The new amorphous model works particularly well for amorphous materials exhibiting an absorption in the visible and/or FUV range (absorbing dielectrics, semiconductors, polymers).

We advise the user to compare the results obtained between the new amorphous and Tauc-Lorentz dispersion formula. The Tauc-Lorentz model may fit better the absorption part of the experimental spectrum.

Materials following the New Amorphous model

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

Materials	n ℘	ω_g	f_j	ω_j	Γ_j	S. R. (eV)
a-C	1.564	0.542	0.123	3.620	2.645	1.5 - 3.5
AlGaAs	1.123	4.170	2.192	5.569	0.510	0.6 - 3
Al_2O_3	1.56	9.85	2.46	10.4	0.44	0.73 - 4.73
AlN	1.574	0.490	0.558	5.604	7.897	1.5 - 5
Alq3	1.526	0.422	0.061	8.465	2.278	0.75 - 4
Amino-Silane	1.298	1.342	0.181	4.659	3.166	1.5 - 6
a-Si	1.750	1.250	0.750	3.5	1.3	1.5 - 5
p-Si	2.626	0.599	0.123	3.908	0.510	1.5 - 5
AsSe	2.499	1.686	0.242	2.471	0.562	0.75 - 4.5
AZO	1.923	2.828	0.134	3.575	0.516	0.6 - 2
$Ba_{0.5}Sr_{0.5}TiO_3$	1.843	3.702	0.256	4.892	0.940	1.5 - 5.5
$BaTiO_3$	1.500	3.000	0.100	5.000	0.500	1.5 - 5.5
BaFeO	2.538	0.936	0.022	2.374	0.213	0.75 - 4.7
BK7	1.456	5.500	0.073	8.127	1.347	1.5 - 5.5
Ge doped CH	3.270	-3.336*	0.010	2.550	0.245	1.5 - 6
CH	1.650	0.488	0.084	3.443	1.839	0.7 - 3
CFx	1.361	2.108	0.023	4.299	1.186	0.7 - 4.75
DLC	1.501	0.420	0.093	2.783	2.237	0.75 - 4.75
Organic EL/HTL	0.580	-1.104*	0.222	11.552	4.026	0.75 - 4
Fe oxide	1.787	0.510	0.179	3.282	1.149	0.75 - 4.75
GaN	2.145	2.620	0.048	4.298	0.290	0.65 - 3
GeO_2	1.576	1.172	0.199	1.262	6.064	0.75 - 2
Glass	1.130	3.428	0.009	16.953	0.282	0.65 - 5
Glass 1737	0.626	3.238	0.0549	41.765	2.309	1.5 - 6.5
HfO_2	1.436	4.831	0.259	12.138	2.718	0.75 - 4.5
InN	2.200	1.900	0.200	2.250	0.250	
$In_xGa_{1-x}N$	1.857	-6.448*	0.006	4.915	0.762	0.75 - 3
In_2O_3	1.526	3.429	0.111	3.631	0.484	1.5 - 5
$LiAlO_3$	2.139	-12.354*	0.003	2.533	0.518	
$LiNbO_3$	2.149	4.183	0.478	4.902	0.556	1.5 - 5
MoSi	2.089	-5.109*	0.172	2.928	4.385	0.75 - 4.5
LPCVD Nitride	1.834	2.192	0.164	5.412	2.170	1.5 - 4.7
NPD	1.781	2.763	0.054	3.374	0.318	0.75 - 4

Materials	n ℘	ω_g	f_1	ω_1	Γ_1	S. R. (eV)
e-PEDOT-PSS	1.563	4.149	0.0027	5.163	0.152	0.8 - 5.4
o-PEDOT-PSS	1.471	3.374	0.025	6.542	0.773	
PI	1.485	3.604	0.092	5.375	1.322	1.5 - 6.5
Photoresist	1.557	1.301	0.011	5.352	0.490	1.5 - 6.5
Polymer	1.660	0.875	0.0434	2.435	0.442	0.6 - 4
PMMA	1.456	3.667	0.130	4.212	7.144	0.6 - 6
e - PPV	1.516	2.878	0.0832	3.144	0.126	0.8 - 5.3
o-PPV	1.538	1.766	0.0763	2.383	0.241	
PZT	2.345	3.000	0.183	4.350	0.424	0.6 - 4.7
Resist	1.537	2.629	0.00364	5.312	0.079	1.5 - 3
SiGeC	3.023	0.500	0.100	4.000	0.900	0.8 - 3
SiN_x	2.071	4.388	0.657	5.288	2.848	1.5 - 6.5
SiN_x	1.750	3.420	0.160	7.310	1.700	0.75 - 4.5
Si_3N_4	1.794	2.221	0.031	7.340	0.623	0.75 - 4.75
SiO	1.500	2.362	0.0841	5.878	1.561	0.6 - 6
TAC	1.448	2.947	0.0507	5.244	1.966	1.5 - 4
Ta_2O_5	1.788	3.892	0.225	5.170	0.700	1.4 - 5
TeO_2	2.096	2.952	0.278	4.282	0.652	0.75 - 4
TiO_2	2.096	2.952	0.278	4.282	0.652	0.75 - 4
$TiVO_x$	1.879	1.479	0.124	3.848	0.849	0.75 - 4
WO_3	1.818	2.199	0.025	4.734	0.325	1.5 - 4.5
WO_x	2.646	2.952	0.802	3.105	1.011	1.5 - 4.5
ZnO_x	1.405	2.737	0.102	3.385	0.305	1.5 - 4
ZnO_2	1.852	3.062	0.127	3.372	0.218	1.5 - 4

Materials following the Double New Amorphous model

Materials	n ℘	ω_g	f_1	ω_1
Alq3	1.630	2.590	0.029	4.642
AZO	1.605	1.825	0.001	3.520
EIL	1.329	0.376	0.0203	5.420
EML	1.329	0.376	0.0203	5.420
ETL	1.702	2.881	0.0979	2.976
FeCo oxide	1.266	0.524	0.142	2.230
Blue Filter	1.616	1.463	0.0333	1.620
Ge	2.389	-0.918*	0.366	4.436
HIL	1.695	2.695	0.135	3.275
HTL	1.702	2.658	0.097	3.201
In_2O_3	1.427	3.047	0.020	4.922
ITO	1.555	2.866	0.777	3.385
LaTeMnO	1.650	0.227	0.049	4.307
NPD	1.717	2.893	0.066	3.167
p-Si	1.800	2.250	0.550	3.250
TPD	1.571	2.515	0.00723	3.933
Varnish	1.604	-0.519*	0.053	-1.662*

Materials	Γ_1	f_2	ω_2	Γ_2	S. R. (eV)
Alq3	0.613	0.015	2.990	0.187	0.75 - 4
AZO	0.176	0.022	4.126	0.761	
EIL	0.385	0.003	3.031	0.169	0.8 - 4
EML	0.385	0.003	3.031	0.169	0.8 - 4
ETL	0.100	-0.060*	3.398	-0.538*	0.8 - 4
FeCo oxide	0.976	0.905	0.346	-0.016*	0.75 - 4
Blue Filter	0.0634	0.00588	1.928	0.117	0.7 - 2
Ge	1.862	0.003	2.248	0.119	0.8 - 2
HIL	0.369	0.0109	3.688	0.229	0.8 - 4
HTL	0.298	0.0071	3.604	0.167	0.8 - 4
In_2O_3	0.740	0.049	4.049	0.662	1.5 - 5
ITO	0.230	0.003	5.025	0.075	0.8 - 4
LaTeMnO	0.771	0.059	1.815	0.459	
NPD	0.185	0.031	3.493	0.232	0.75 - 4
p-Si	0.450	0.250	4.250	0.500	
TPD	0.232	0.0206	3.440	0.202	
Varnish	0.201	0.001	6.367	0.654	1.5 - 6.5

Materials following the Triple New Amorphous model

Materials	n℘	ω_g	f_1	ω_1	Γ_1	f_2
CuPc	1.300	1.000	0.003	1.700	0.050	0.002
PET	1.653	2.216	0.00036	4.174	0.133	0.0095
Poly-carbonate	1.000	3.500	0.010	4.500	0.200	0.100
ARC coating Polymer	1.565	4.373	0.00289	5.451	0.189	0.0316
Photoresist	1.480	3.980	0.00048	5.426	0.0536	0.0046

Materials	ω_2	Γ_2	f_3	ω_3	Γ_3	S. R. (eV)
CuPc	2.000	0.050	0.020	3.750	0.479	0.6 - 4
PET	5.018	0.303	0.00704	6.421	0.339	1.5 - 6.5
Poly-carbonate	5.500	1.000	0.050	6.300	1.000	1.5 - 6.5
ARC coating Polymer	4.385	0.0204	0.0248	6.363	0.455	1.5 - 6.5
Photoresist	4.397	0.115	0.0242	6.453	0.366	1.5 - 6.5

References

1. E. D. Palik, Handbook of Optical Constants of Solids II, Chap. 7.
2. A. R. Forouhi, I. Bloomer, Phys. Rev. B 34, 7018-7026 (1986).
3. A. R. Forouhi, I. Bloomer, Phys. Rev. B 38, 1865 (1988).
4. G.E Jellison, F. A. Modine, Phys. Rev. , 69(3), 371-374 (1996).

Appendix A5: Tauc-Lorentz Dispersion Formula

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured SE data are used to describe a model where layers refer to given materials. The model uses mathematical relations called dispersion formulae that help to evaluate the material's optical properties by adjusting specific fit parameters.

This technical note deals with Tauc-Lorentz dispersion formula.

Theoretical model

Jellison and Modine developed this model (1996) using the Tauc joint density of states and the Lorentz oscillator. The complex dielectric function is :

$$\tilde{\varepsilon}_{TL} = \varepsilon_{r,TL} + i \cdot \varepsilon_{i,TL} = \varepsilon_{r,TL} + i \cdot \left(\varepsilon_{i,T} \times \varepsilon_{i,L}\right) \quad (1)$$

Here the imaginary part $\varepsilon_{i,TL}$ of the dielectric function is given by the product of imaginary part of Tauc's (1966) dielectric $\varepsilon_{i,T}$ function with Lorentz one $\varepsilon_{i,L}$. In the approximation of parabolic bands, Tauc's dielectric function describes inter-band transitions above the band edge as :

$$\varepsilon_{i,T}\left(E > E_g\right) = A_T \cdot \left(\frac{E - E_g}{E}\right)^2 \quad (2)$$

where :

- A_T is the Tauc coefficient
- E is the photon energy
- E_g is the optical band gap

The imaginary part of Tauc's dielectric function gives the response of the material caused by inter-band mechanisms only : thus $\varepsilon_{i,T}$ $(E \leq E_g) = 0$.

The imaginary part of the Lorentzian oscillator model is given by :

$$\varepsilon_{i,L}(E) = \frac{A_L \cdot E_0 \cdot C \cdot E}{\left(E^2 - E_0^2\right)^2 + C^2 \cdot E^2} \quad (3)$$

where :

- A_L is the strength of the $\varepsilon_{2,TL}(E)$ peak
- C is the broadening term of the peak
- E_0 is the peak central energy

By multiplying equation (2) by equation (3), Jellison sets up a new expression for $\varepsilon_{i,L}(E)$:

$$\varepsilon_{i,TL}(E) = \varepsilon_{i,L} \times \varepsilon_{i,T} = \begin{cases} \dfrac{1}{E} \dfrac{A E_0 C \left(E - E_g\right)^2}{\left(E^2 - E_0^2\right)^2 + C^2 E^2} & \text{for } E > E_g \\ 0 & \text{for } E \leq E_g \end{cases} \quad (4)$$

where $A = A_T \times A_L$.

The real part $\varepsilon_{r,TL}$ of the dielectric function is derived from the expression of ε_i using the Kramers-Kronig integration. Then, it comes the following expression for ε_i:

$$\varepsilon_r(E) = \varepsilon_r(\infty) + \frac{2}{\pi} \cdot P \cdot \int_{E_g}^{\infty} \frac{\xi \cdot \varepsilon_i(\xi)}{\xi^2 - E^2} d\xi \quad (5)$$

where P is the Cauchy principal value containing the residues of the integral at poles located on lower half of the complex plane and along the real axis.

According to Jellison and Modine (*Ref. 1*), the derivation of the previous integral yields :

$$\begin{aligned} \varepsilon_{r,TL}(E) = \varepsilon_\infty &+ \frac{A \cdot C \cdot a_{\ln}}{2 \cdot \pi \cdot \zeta^4 \cdot \alpha \cdot E_0} \cdot \ln\left[\frac{E_0^2 + E_g^2 + \alpha \cdot E_g}{E_0^2 + E_g^2 - \alpha \cdot E_g}\right] \\ &- \frac{A}{\pi} \cdot \frac{a_{a\tan}}{\zeta^4 \cdot E_0} \cdot \left[\pi - \arctan\left(\frac{2 \cdot E_g + \alpha}{C}\right) + \ldots \right. \\ &\qquad \left. + \arctan\left(\frac{\alpha - 2 \cdot E_g}{C}\right)\right] \\ &+ \frac{4 \cdot A \cdot E_0 \cdot E_g \cdot \left(E^2 - \gamma^2\right)}{\pi \cdot \zeta^4 \cdot \alpha} \times \ldots \\ &\times \left[\arctan\left(\frac{\alpha + 2 \cdot E_g}{C}\right) + \arctan\left(\frac{\alpha - 2 \cdot E_g}{C}\right)\right] \\ &- \frac{A \cdot E_0 \cdot C \cdot \left(E^2 + E_g^2\right)}{\pi \cdot \zeta^4 \cdot E} \cdot \ln\left(\frac{\left|E - E_g\right|}{E + E_g}\right) + \ldots \\ &+ \frac{2 \cdot A \cdot E_0 \cdot C}{\pi \cdot \zeta^4} \times E_g \cdot \ln\left[\frac{\left|E - E_g\right| \cdot \left(E + E_g\right)}{\sqrt{\left(E_0^2 - E_g^2\right)^2 + E_g^2 \cdot C^2}}\right] \end{aligned} \quad (6)$$

where:

$$\begin{cases} a_{\ln} = \left(E_g^2 - E_0^2\right)\cdot E^2 + E_g^2 \cdot C^2 - E_0^2 \cdot \left(E_0^2 + 3 \cdot E_g^2\right) \\ a_{a\tan} = \left(E^2 - E_0^2\right)\cdot\left(E_0^2 + E_g^2\right) + E_g^2 \cdot C^2 \\ \alpha = \sqrt{4 \cdot E_0^2 - C^2} \\ \gamma = \sqrt{E_0^2 - C^2/2} \\ \zeta^4 = \left(E^2 - \gamma^2\right)^2 + \alpha^2 \cdot C^2/4 \end{cases} \qquad (7)$$

Extension to multiple oscillators

In the case of multiple oscillators (N>1) the expression of ε_i contains now a series over all the oscillators.

$$\varepsilon_i = \begin{cases} \sum_{i=1}^{N} \frac{1}{E} \times \frac{A_i \cdot E_i \cdot C_i \cdot \left(E - E_g\right)^2}{\left(E^2 - E_i^2\right)^2 + C_i^2 \cdot E^2} & \text{for } \mathrm{E} > \mathrm{E_g} \\ 0 & \text{for } \mathrm{E} \le \mathrm{E_g} \end{cases} \qquad (8)$$

and ε_r is re-written as the following sum :

$$\varepsilon_r(E) = \varepsilon_r(\infty) + \sum_{i=1}^{N} \frac{2}{\pi} \cdot P \cdot \int_{E_g}^{\infty} \frac{\xi \cdot \varepsilon_i(\xi)}{\xi^2 - E^2}\, \mathrm{d}\xi \quad (9)$$

Deriving this integral yields the analytical expression of the real part of the dielectric function :

$$\begin{aligned} \varepsilon_r(E) = \varepsilon_r(\infty) + \sum_{i=1}^{N} \Bigg\{ & \frac{A_i \cdot C_i \cdot a_{\ln}}{2 \cdot \pi \cdot \zeta^4 \cdot \alpha \cdot E_i} \cdot \ln\left[\frac{E_i^2 + E_g^2 + \alpha \cdot E_g}{E_i^2 + E_g^2 - \alpha \cdot E_g}\right] \\ & - \frac{A_i}{\pi} \cdot \frac{a_{a\tan}}{\zeta^4 \cdot E_i} \cdot \left[\pi - \arctan\left(\frac{2 \cdot E_g + \alpha}{C_i}\right) + \ldots \right. \\ & \left. + \arctan\left(\frac{\alpha - 2 \cdot E_g}{C_i}\right)\right] \\ & + \frac{4 \cdot A_i \cdot E_i \cdot E_g \cdot \left(E^2 - \gamma^2\right)}{\pi \cdot \zeta^4 \cdot \alpha} \cdot \left[\arctan\left(\frac{\alpha + 2 \cdot E_g}{C_i}\right) \right. \\ & \left. + \arctan\left(\frac{\alpha - 2 \cdot E_g}{C_i}\right)\right] \\ & - \frac{A_i \cdot E_i \cdot C_i \cdot \left(E^2 + E_g^2\right)}{\pi \cdot \zeta^4 \cdot E} \cdot \ln\left(\frac{\left|E - E_g\right|}{E + E_g}\right) \\ & + \frac{2\, A_i\, E_i\, C_i}{\pi \cdot \zeta^4} E_g \ln\left[\frac{\left|E - E_g\right|\left(E + E_g\right)}{\sqrt{\left(E_0^2 - E_g^2\right)^2 + E_g^2\, C_i^2}}\right] \Bigg\} \end{aligned} \quad (10)$$

The parameters of the equations

The name of the different Tauc-Lorentz formulae present in the DeltaPsi2 software depending on the number of oscillators are given below. It indicates the number of parameters too.

Formula	Number of oscillators	Number of parameters
Tauc-Lorentz	N=1	5
Tauc-Lorentz 2	N=2	8
Tauc-Lorentz 3	N=3	11

Increasing the number of oscillators leads to a shift of the peaks of absorption toward the ultraviolet region.

1 parameter is linked to the real part of the dielectric function

- ε_r (∞) = ε_∞ is the high frequency dielectric constant. This is an additional fitting parameter that prevents ε_1 from converging to zero for energies below the band gap. Generally, $\varepsilon_\infty > 1$.

At least 4 parameters describe the imaginary part of the dielectric function

- A_i (in eV) is related to the strength of the i$^{\text{th}}$ absorption peak. The subscript «i» refers to the number (i=1, 2 or 3) of oscillators. As A_i increases, the amplitude of the peak increases and the Full Width At Half Maximum (FWHM) of that peak gets slightly larger. Generally, $10 < A_i < 200$.
- C_i (in eV) is the broadening term ; it is a damping coefficient linked to FWHM of the i$^{\text{th}}$ peak of absorption. The higher it is the larger that peak becomes and at the same time the smaller its amplitude is. Generally $0 < C_i < 10$.
- E_g (in eV) is the optical band gap energy.
- E_i (in eV) is the energy of maximum transition probability or the energy position of the peak of absorption. The subscript «i» refers to the number (i=1, 2 or 3) of oscillators. Always, $Eg < Ei$.

Limitation of the model

The Tauc-Lorentz model requires ε_i to be zero for energies less than the band gap. Consequently, Tauc-Lorentz model does not take into account intra-band absorption: any defect or intra-band absorption increases ε_i below the band gap and generates bad fits in that region.

Valid spectral range

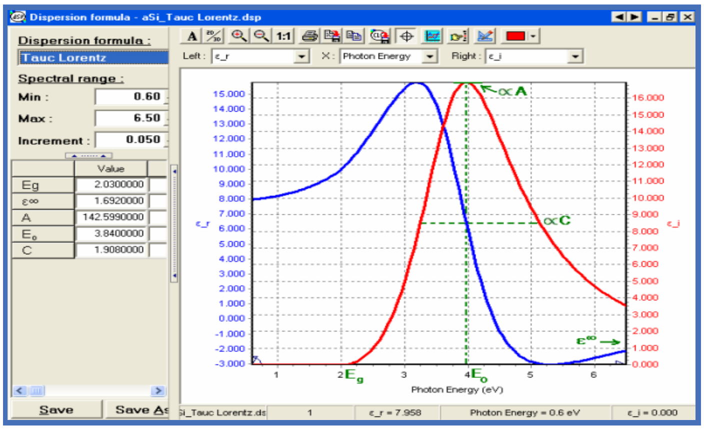
The Tauc-Lorentz model well describes the behaviour of materials for energies $E \le E_i$ where E_i is the transition energy of the oscillator of highest order.

Parameter setup

The Tauc-Lorentz model works particularly well for amorphous materials exhibiting an absorption in the visible and/or FUV range (absorbing dielectrics, semiconductors, polymers).
Note that :

- The graph below shows the different contributions (in red dashed lines) to the imaginary part of the Tauc Lorentz dielectric function (in red bold line).
- The sign « ∝ » before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

Tauc-Lorentz function


Dispersion formula - aSi_Tauc Lorentz.dsp

Dispersion formula : Tauc Lorentz

Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.050

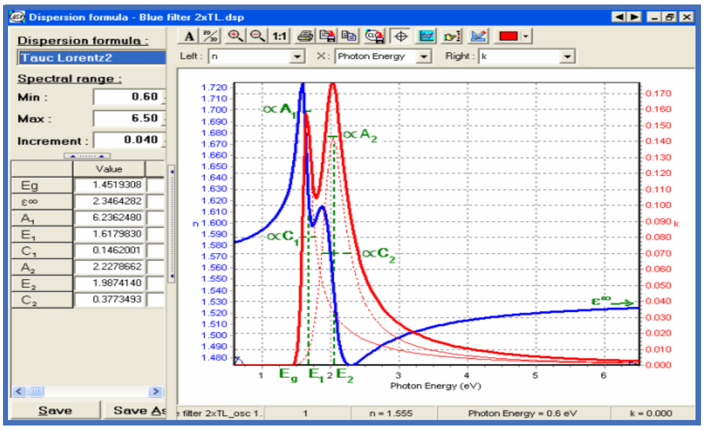
	Value
Eg	2.0300000
ε∞	1.6920000
A	142.5990000
E₀	3.8400000
C	1.9080000

Left : ε_r X : Photon Energy Right : ε_i

Si_Tauc Lorentz.ds 1 ε_r = 7.958 Photon Energy = 0.6 eV ε_i = 0.000

Dielectric function of a-Si represented by a single Tauc-Lorentz oscillator

Double Tauc-Lorentz function


Dispersion formula - Blue filter 2xTL.dsp

Dispersion formula : Tauc Lorentz2

Spectral range :
Min : 0.60
Max : 6.50
Increment : 0.040

	Value
Eg	1.4519308
ε∞	2.3464282
A₁	6.2362480
E₁	1.6179830
C₁	0.1462001
A₂	2.2278662
E₂	1.9874140
C₂	0.3773493

Left : n X : Photon Energy Right : k

filter 2xTL_osc 1. 1 n = 1.555 Photon Energy = 0.6 eV k = 0.000

Dielectric function of a blue filter represented by a double Tauc-Lorentz oscillator

Applications to materials

Materials following the Tauc-Lorentz model

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

Materials	Eg	ε℘	A	E_0	C	S. R. (eV)
a-C	1.305	3.774	38.835	6.335	6.227	1.5 - 5
AlGaN	3.300	3.000	100.000	4.500	1.000	1.5 - 2.5
As_2S_3	2.349	1.240	133.819	4.574	5.935	0.75 - 4.75
AsSSe	1.000	1.600	50.000	3.500	2.000	0.75 - 4.5
DLC	0.374	2.960	11.558	3.533	3.346	0.7 - 2
GaN	3.200	3.500	100.000	4.500	1.000	1,5 - 3
GeSbSe	1.851	2.062	54.703	3.412	2.045	0.65 - 3
InGaN	3.000	3.500	100.000	4.500	1.000	1,5 - 3
Polymer	3.027	1.701	32.921	5.759	2.416	0.7 - 4
poly-Si	0.882	3.937	49.597	3.711	0.321	1.5 - 3.25
a-Si	2.030	1.692	142.599	3.840	1.908	0.75 - 3.65
a-Si:B	1.267	2.148	143.380	3.617	1.994	0.75 - 4.75
a-Si:H	1.393	0.626	171.105	3.582	2.201	0.75 - 4.75
$Si_xO_yN_z$	3.864	1.760	77.340	8.363	3.550	1.5 - 6.5
Ta-C	1.395	2.558	67.312	8.713	9.760	1.5 - 5
ZnS	2.976	4.500	57.167	3.954	1.200	1.5 - 6.5
GeSbTe	0,450	2,024	158,795	1,688	2,397	0,65 - 3

Materials following the Double Tauc-Lorentz model

Materials	Eg	ε℘	A_1	E_1
Blue Filter	1.451	2.346	6.236	1.617
Oxide coating	1.168	0.894	41.060	6.464
Polymer	3.420	2.771	113.260	4.234
SiC	1.521	-1.657*	4.026	5.678
Ta_2O_5	4.261	1.827	188.580	4.188

Materials	C_1	A_2	E_2	C_2	S. R. (eV)
Blue Filter	0.146	2.227	1.987	0.377	0.6 - 2.2
Oxide coating	4.140	-6.269*	3.763	2.390	1.5 - 5
Polymer	1.455	6.870	4.806	8.345	0.7 - 5
SiC	-5.129*	51.264	9.561	3.869	1.5 - 6.5
Ta_2O_5	5.278	58.367	5.354	1.246	1.5 - 6.5

Materials following the Triple Tauc-Lorentz model

Materials	Eg	ε℘	A_1	E_1	C_1	A_2
a - Si	1.405	1.029	-16.227*	6.800	5.454	1.310
HfO_2	4.972	2.764	80.221	7.451	0.876	4.604

Materials	E_2	C_2	A_3	E_3	C_3	S. R. (eV)
a - Si	0.807	2.215	185.343	3.707	2.379	0.6 - 6
HfO_2	4.192	6.834	4.469	6.368	0.599	1.5 - 6.5

References

1) *G.E. Jellison and F.A. Modine, Appl. Phys. Lett. 69 (3), 371-374 (1996).*
2) *Erratum, G. E. Jellison & F. A. Modine, Appl. Phys. Lett. 69 (14), 2137 (1996).*
3) *H. Chen, W. Z. Shen, Eur. Phys. J. B. 43, 503-507 (2005).*

Appendix A6: Cauchy and related Empirical Dispersion Formulae for Transparent Materials

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured data are used to describe a model where each layer refers to a given material. The model uses mathematical relations called dispersion formulae that help to evaluate the thickness and optical properties of the material by adjusting specific fit parameters.

This technical note deals with the Cauchy and related empirical transparent dispersion formulae to calculate the real (n) and imaginary (k) parts of the complex refractive index for a material.

Theoretical Model

Equation of Cauchy Transparent

The earliest dispersion formula was established by Cauchy (1836) who set up simple empirical dispersion law. The "Cauchy Transparent" dispersion works best when the material has no optical absorption in the visible spectral range and consequently generally has a normal dispersion which means a monotonous decreasing refractive index with increasing wavelength in this way:

$$1 < n(\lambda_{red}) < n(\lambda_{blue})$$

The following equation connects the refractive index to the wavelength (in nm):

$$\boxed{\begin{cases} n(\lambda) = A + \dfrac{10^4 \cdot B}{\lambda^2} + \dfrac{10^9 \cdot C}{\lambda^4} \\ k(\lambda) = 0 \end{cases} \quad (1)}$$

Equation of Cauchy Absorbent

A second formulation of the Cauchy model is the «Cauchy Absorbing» dispersion and it is more suitable to describe the optical properties of weakly absorbing materials. Here a non-zero extinction coefficient is given in an expression similar to the previous used for the refractive index:

$$\boxed{\begin{cases} n(\lambda) = A + \dfrac{10^4 \cdot B}{\lambda^2} + \dfrac{10^9 \cdot C}{\lambda^4} \\ k(\lambda) = 10^{-5} \cdot D + \dfrac{10^4 \cdot E}{\lambda^2} + \dfrac{10^9 \cdot F}{\lambda^4} \end{cases} \quad (2)}$$

The parameters of the equations

3 parameters are used in the equation of the Cauchy transparent model and 6 parameters in the Cauchy absorbing model.

Parameters describing the refractive index

- A is a dimensionless parameter: when $\lambda \to \infty$ then $n(\lambda) \to A$.
- B (nm^2) affects the curvature and the amplitude of the refractive index for medium wavelengths in the visible.
- C (nm^4) affects the curvature and amplitude for smaller wavelengths in the UV. Generally,

$$\boxed{0 < |C| < |B| < 1 < A \quad (3).}$$

3 parameters describe the extinction coefficient.

- D is a dimensionless parameter similar to A,
- E (nm^2) is analogous to B,
- F (nm^4) behaves like C.

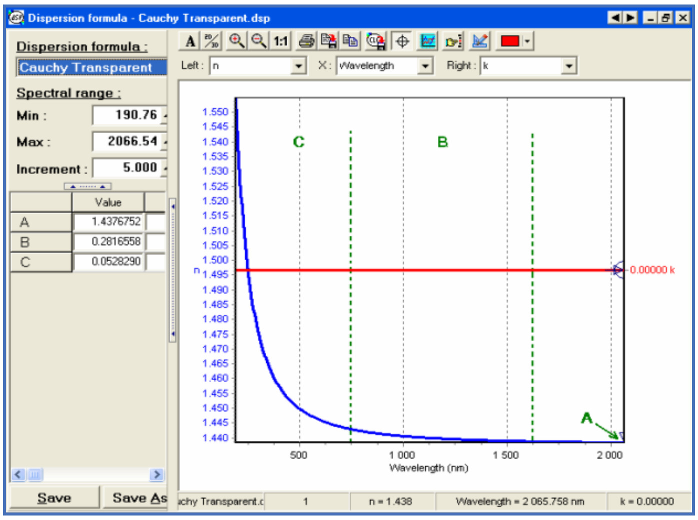
Limitation of the model

Cauchy's formulation cannot be easily applied to metals and semiconductors.

The parameters used do not have any physical meaning and therefore, these empirical relations are not Kramers-Kronig consistent. From first principles, the Kramers-Kronig relation relates the index of refraction and extinction coefficient parts; it means they are not independent quantities. In other words, if the value of the extinction coefficient is known over the entire spectral range, the index of refraction coefficient can be calculated.

Parameter setup

Cauchy Transparent function



Dispersion formula - Cauchy Transparent.dsp

Dispersion formula : Cauchy Transparent

Spectral range :

Min : 190.76

Max : 2066.54

Increment : 5.000

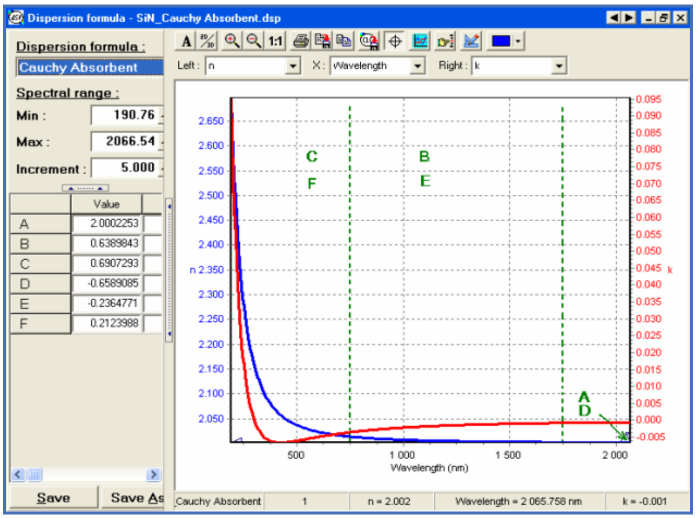
	Value
A	1.4376752
B	0.2816558
C	0.0528290

Left : n X : Wavelength Right : k

chy Transparent.c | 1 | n = 1.438 | Wavelength = 2 065.758 nm | k = 0.00000

Optical properties of SiO_2 given by the Cauchy transparent function

Cauchy Absorbent function



Dispersion formula - SiN_Cauchy Absorbent.dsp

Dispersion formula : Cauchy Absorbent

Spectral range :

Min : 190.76

Max : 2066.54

Increment : 5.000

	Value
A	2.0002253
B	0.6389843
C	0.6907293
D	-0.6589085
E	-0.2364771
F	0.2123988

Left : n X : Wavelength Right : k

Cauchy Absorbent | 1 | n = 2.002 | Wavelength = 2 065.758 nm | k = -0.001

Optical properties of SiN given by the Cauchy absorbent function

Application to materials

The Cauchy model is used for transparent materials like insulators, glasses exhibiting no or very low optical absorption in the Far Ultra Violet.

Materials	A	B	C	D	E	F	S.R (eV)
ChG Glass	6.5	0.7	0	0	0	0	
HfO	1.993	1.303	0.158	0	0	0	1.5 - 5.5
MgF	1.386	0.117	0.109	0	0	0	1.5 - 5.5
PI	1.631	0.497	1.337	771.776	- 0.587	1.117	
SiN	2.000	0.638	0.690	-0.658	-0.236	0.212	1 - 6.0
SiO_2	1.447	3660	0	0	0	0	1 - 6.0
TiO_2	2.374	1.932	6.855	0	0	0	1.5 - 6.0

References

1. L. Cauchy, Bull. des sc. Math., 14, 9 (1830).
2. http://en.wikipedia.org/wiki/Cauchy_equation.
3. G. Ghosh, Handbook of Thermo-Optic Coefficients of optical Materials with Applications, Academic Press.

Appendix A6a: Briot Dispersion Formula

Theoretical model

This dispersion model is based on a Laurent series (1864) expressing the equation for the refractive index of transparent materials:

$$\boxed{n^2(\lambda) = A_0 + 10^{-2}\cdot A_1\cdot\lambda^2 + \frac{10^{-2}\cdot A_2}{\lambda^2} + \frac{10^{-4}\cdot A_3}{\lambda^4} + \frac{10^{-6}\cdot A_4}{\lambda^6} + \frac{10^{-7}\cdot A_5}{\lambda^8} \quad (1)}$$

with:

$$\boxed{k(E) = 0 \ (2).}$$

The previous equation of the refractive index is also known as the *Schott* equation because it was used by the Schott company until 1992 when it was abandoned and replaced by the *Sellmeier* formula. However, Briot's equation remains widespread use elsewhere.

The parameters of the equations

Parameters describing the refractive index

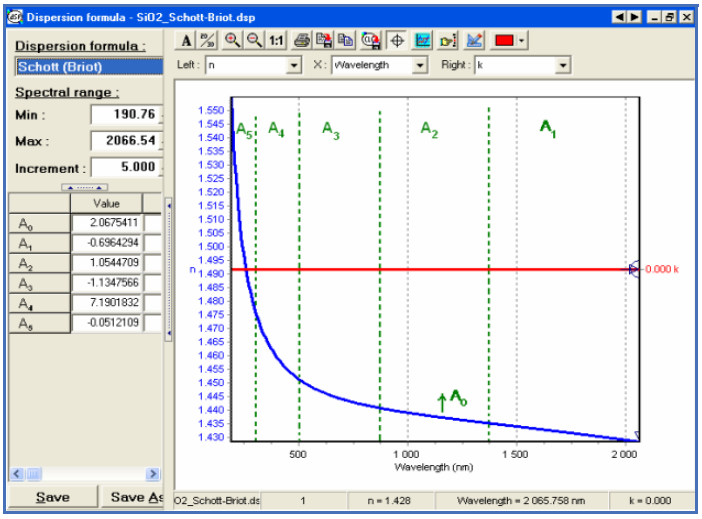
- A_0 (dimensionless), A_1 (in nm^{-2}), A_2 (in nm^2), A_3 (in nm^4), A_4 (in nm^6) and A_5 (in nm^8) are the different coefficients of the development in Laurent series.
- A_0 is a positive parameter that prevents $n^2(\lambda)$ from being negative.
- The low order terms of the development ($A_1 < 0$ and A_2) contribute to the intensity of the refractive index curve for long wavelengths in the visible and IR regions.
- The high order terms of the development (A_3, A_4 and A_5) contribute to the intensity of the refractive index curve for small wavelengths in the UV region.

Limitation of the model

Briot's formulation cannot be easily applied to metals and semiconductors.
This empirical relation is not Kramers-Kronig consistent and therefore does not have any physical meaning.

Parameter setup

Schott-Briot function



Dispersion formula - SiO2_Schott-Briot.dsp

Dispersion formula : Schott (Briot)

Spectral range :
Min : 190.76
Max : 2066.54
Increment : 5.000

	Value
A_0	2.0675411
A_1	-0.6964294
A_2	1.0544709
A_3	-1.1347566
A_4	7.1901832
A_5	-0.0512109

Left : n
X : Wavelength
Right : k

O2_Schott-Briot.ds | 1 | n = 1.428 | Wavelength = 2 065.758 nm | k = 0.000

Optical properties of SiO$_2$ given by the Schott-Briot function

Application to materials

The Briot model is used for transparent materials such as crystalline quartz across the range 300nm~1600nm.

References

1. C. Briot, Essais sur la théorie mathématique de la lumière. Paris, Mallet-Bachelier, (1864).
2. www.optics.arizona.edu/Palmer/cgi-bin/index/dispeqns.pdf

Appendix A6b: Hartmann Dispersion Formula

Theoretical model

The Hartmann's (1926) model, has the following general form:

$$\boxed{n(E) = A + \frac{C}{\lambda(E) - B} \quad (1)}$$

This equation works for transparent films that do not have absorption:

$$\boxed{k(E) = 0 \quad (2).}$$

The parameters of the equations

3 parameters are used in the equation of the Hartmann model and allow to define the refractive index.

- A ($A > 1$) is a dimensionless parameter; when $\lambda \to \infty$ then $n(\lambda) \to A$.
- B and C have the dimension of wavelengths (nm).
- B is the resonance wavelength for which the refractive
- index diverges. The fit must be performed for wavelengths $\lambda \neq B$ otherwise $n(\lambda) \to \infty$.
- C determines the amplitude (strength) of the refractive index for wavelengths $\lambda \to B$.

Limitation of the model

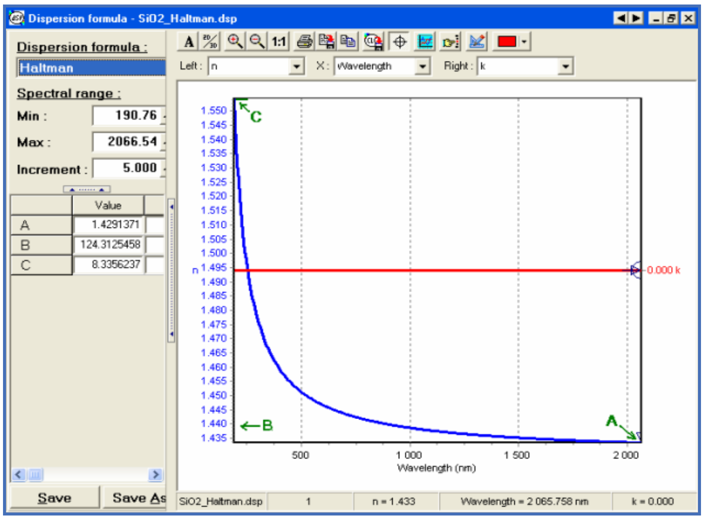
The Hartmann formula cannot be easily applied to metals and semiconductors.

This empirical formula is not Kramers-Kronig consistent and therefore does not have any physical meaning.

Parameter setup

The Hartmann function has similar application to the Cauchy Transparent dispersion. It is useful for transparent materials with normal dispersion.

Hartmann function



Dispersion formula - SiO2_Haltman.dsp

Dispersion formula : Haltman

Spectral range :
Min : 190.76
Max : 2066.54
Increment : 5.000

	Value
A	1.4291371
B	124.3125458
C	8.3356237

Left : n
X : Wavelength
Right : k

SiO2_Haltman.dsp | 1 | n = 1.433 | Wavelength = 2 065.758 nm | k = 0.000

Optical properties of SiO_2 given by the Hartmann function

Application to materials

The Hartmann model is used for transparent materials like insulators, glasses.

Materials	A	B	C	S.R (eV)
SiO_2	1.429	124.312	8.335	0.7 - 6
TiO_2	1.890	178.621	203.804	1.5 - 4

References

1. http://scienceworld.wolfram.com/physics/HartmannDispersion-Formula.html
2. H. W. Lee, Trans. Opt. Soc., Volume 28, Issue 3, 161-167 (1926).
3. www.optics.arizona.edu/Palmer/cgi-bin/index/dispeqns.pdf

Appendix A6c: Conrady Dispersion Formula

Theoretical model

Conrady's equation (1960) allows the refractive index to be derived using the following equation for n(λ):

$$\boxed{n(\lambda) = A + \frac{10^2 \cdot B}{\lambda} + \frac{10^9 \cdot C}{\lambda^{3.5}} \quad (1)}$$

for a transparent film for which:

$$\boxed{k(E) = 0 \quad (2).}$$

The parameters of the equations

3 parameters are used in the expression of the *Conrady model*.

Parameters describing the refractive index

- A is a dimensionless parameter: when $\lambda \to \infty$ then $n(\lambda) \to A$.
- B (nm) has the same dimension as a wavelength.

This parameter affects the curvature and amplitude of the refractive index for visible wavelengths.

- C ($\mathrm{nm}^{3.5}$) influences the behaviour (strength) of the refractive index at small wavelengths in the UV.

Generally,

$$\boxed{0 < |C| < |B| < 1 < A \quad (3)}$$

Limitation of the model

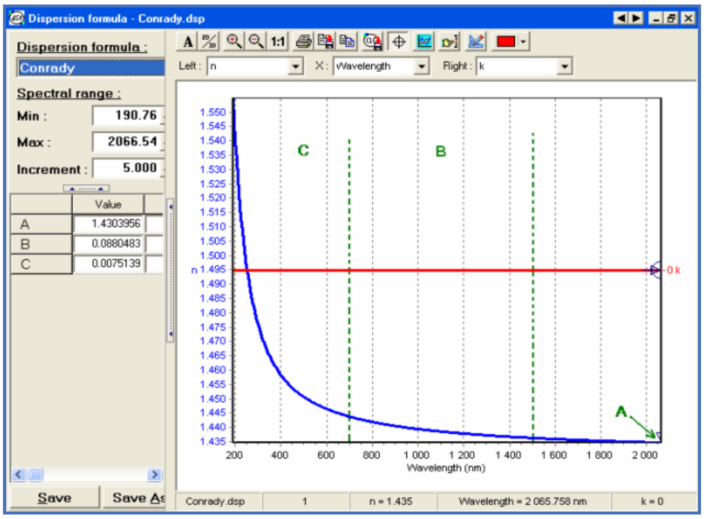
Conrady's equation cannot be easily applied to metals and semiconductors.

This empirical formula is not Kramers-Kronig consistent and therefore does not have any physical meaning.

Parameter setup

Conrady function has similar application to the *Cauchy Transparent formula*. It is useful for transparent materials with normal dispersion.

Conrady function



Dispersion formula - Conrady.dsp

Dispersion formula : Conrady

Spectral range :

Min : 190.76

Max : 2066.54

Increment : 5.000

	Value
A	1.4303956
B	0.0880483
C	0.0075139

Left : n

X : Wavelength

Right : k

Conrady.dsp | 1 | n = 1.435 | Wavelength = 2 065.758 nm | k = 0

Optical properties of SiO_2 given by the Conrady function

Application to materials

The Conrady model is used for transparent materials like insulators, glasses.

Materials	A	B	C	S.R (eV)
SiO_2	1.427	0.111	0.00513	0.7 - 6
TiO_2	2,500	-1.148	0.731	1.5 - 4

References

1. A. E. Conrady, Applied Optics and Optical Design, Dover (1960).

Appendix A6d: Sellmeier Dispersion Model

Theoretical model

Equation of Sellmeier Transparent

The Sellmeier formula (1871) is semi-empirical but it remains more accurate than the Cauchy dispersion law for characterizing the refractive index of a material across a wider spectral range. The transparent Sellmeier equation for the index of refraction looks like:

$$\boxed{n^2(\lambda) = A + B \times \frac{\lambda^2}{\lambda^2 - \lambda_0^2} \quad (1)}$$

without absorption:

$$\boxed{k(\lambda) = 0 \quad (2)}$$

Parameters of the Sellmeier Transparent function

3 parameters are used in the equation of the *Sellmeier Transparent model* to describe the refractive index variation.

Parameters describing the refractive index

- A ($1 \leq A$) is a dimensionless parameter that determines the value of the refractive index when when $\lambda \to \infty$ and B ~ 0. It represents the contribution of the ultraviolet term.
- B ($A \leq B$) is another dimensionless parameter that determines the shape of the refractive index in the visible range.
- λ_0 (in nm^2) is the resonance wavelength for which the refractive index diverges. The fit must be performed for wavelengths $\lambda \neq \lambda_0$ otherwise $n^2(\lambda) \to \infty$.

Equation of Sellmeier Absorbent

The Sellmeier Absorbent equation for the refractive index is written as follows:

$$\boxed{n^2(\lambda) = \frac{1+A}{1+\dfrac{10^4 \cdot B}{\lambda^2}} \quad (3)}$$

and the extinction coefficient is given by the relation below:

$$\boxed{k(\lambda) = \frac{C}{10^{-2} \cdot n \cdot D \cdot \lambda + \dfrac{10^2 \cdot E}{\lambda} + \dfrac{1}{\lambda^3}} \quad (4)}$$

Parameters of the Sellmeier Absorbent function

2 parameters describe the refractive index

- A is a dimensionless parameter that is linked to the amplitude of the refractive index. When $\lambda \to \infty$ then $n(\lambda) = \sqrt{1+A}$.
- B (in nm^2) has an influence on the curvature of the refractive index: if $B > 0$, n increases with λ and the bigger B is the more straight $n^2(\lambda)$ is. If $B < 0$, n decreases with λ.

3 parameters describe the extinction coefficient

- C is a dimensionless parameter that determines the strength of the absorption coefficient curve.
- D (nm^{-1}) and E (nm) are terms corresponding to a development series similar to that of Schott-Briot formula. Increasing D and E involves a decrease of the absorption coefficient.

Limitation of the model

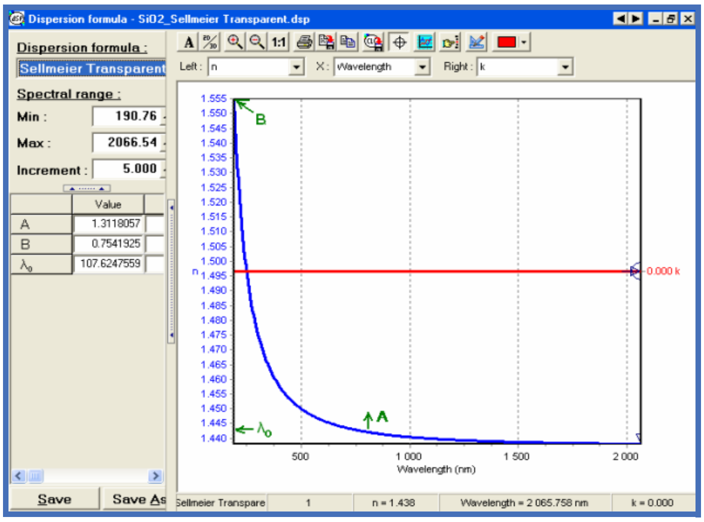
Sellmeier equations cannot be easily applied to metals and semiconductors.

These empirical relations are not Kramers-Kronig consistent and therefore do not have any physical meaning.

Parameter setup

The Sellmeier Transparent function behaves like the *Cauchy Transparent function*. It exhibits normal dispersion, so the refractive index decreases with increasing wavelengths.

Sellmeier Transparent function



Dispersion formula - SiO2_Sellmeier Transparent.dsp

Dispersion formula : Sellmeier Transparent

Spectral range :

Min : 190.76

Max : 2066.54

Increment : 5.000

	Value
A	1.3118057
B	0.7541925
λ_0	107.6247559

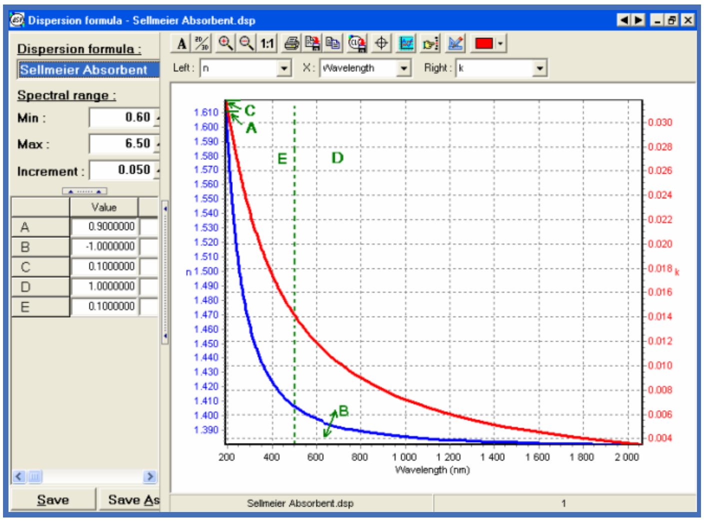
Left : n   X : Wavelength   Right : k

Sellmeier Transpare | 1 | n = 1.438 | Wavelength = 2 065.758 nm | k = 0.000

Optical properties of SiO_2 given by the Sellmeier Transparent function

The *Sellmeier Absorbent* function behaves like the *Cauchy Absorbing* function. This function also gives decreasing absorption and dispersion with increasing wavelength. Note that this is not physical in the presence of absorption as the Kramers-Kronig relation states that the refractive index should normally increase with increasing wavelength.

Sellmeier Absorbent function



Dispersion formula - Sellmeier Absorbent.dsp

Dispersion formula : Sellmeier Absorbent

Spectral range :

Min : 0.60

Max : 6.50

Increment : 0.050

	Value
A	0.9000000
B	-1.0000000
C	0.1000000
D	1.0000000
E	0.1000000

Left : n   X : Wavelength   Right : k

Sellmeier Absorbent.dsp | 1

Optical properties of a polymer given by the Sellmeier absorbent function

Application to materials

The Sellmeier model is used for transparent materials such as organics, insulators, glasses.

Valid spectral range

The Sellmeier equation mostly holds for wavelengths far from λ_0 in the range of transparency.

References

1. http://en.wikipedia.org/wiki/Sellmeier_equation
2. http://www.schott.com/optics_devices/english/download/tie-29_refractive_index_v2.pdf

Appendix A6e: Fixed Index Dispersion Formula

Theoretical model

The Fixed index dispersion formula is given by constant refractive index and extinction coefficient for any wavelength:

$$\boxed{\begin{cases} n(\lambda) = const. = n \\ k(\lambda) = const. = k \end{cases}}$$

The parameters of the equations

Only 2 parameters are needed to describe the model:

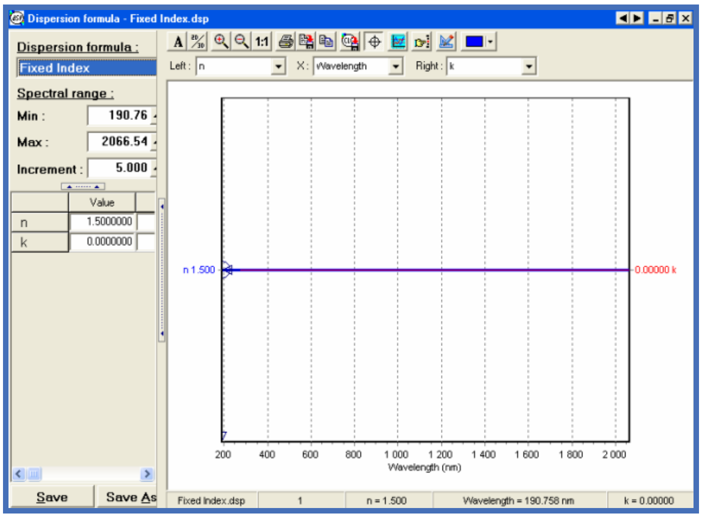
- *n* is the value of the refractive index.
- *k* is the value of the extinction coefficient.

Limitation of the model

This formula strictly describes the vacuum. The Fixed index equation does not apply to metals and semiconductors.

Parameter setup

Fixed index function



Dispersion formula - Fixed Index.dsp

Dispersion formula : Fixed Index

Spectral range :

Min : 190.76

Max : 2066.54

Increment : 5.000

	Value
n	1.5000000
k	0.0000000

Left : n
X : Wavelength
Right : k

Fixed Index.dsp | 1 | n = 1.500 | Wavelength = 190.758 nm | k = 0.00000

Fixed Index formula given a refractive index equal to 1.5

Application to materials

The *Fixed index* model is applicable to non dispersive materials like air. It is often used when the measurement is performed in different ambient media (liquids).

It can be used to decrease the number of fitting parameters when the material dispersion can be neglected.

Appendix A7: Forouhi-Bloomer alias Amorphous Dispersion Formula

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured data are used to describe a model where each layer refers to a given material. The model uses mathematical relations called dispersion formulae that help to evaluate the thickness and optical properties of the material by adjusting specific fit parameters.

This application note deals with the original Forouhi & Bloomer dispersion formula also known as «Amorphous» (name used in the DeltaPsi2 software). We recommend the use of the updated «New Amorphous» formulation, please refer to the corresponding technical note.

Forouhi-Bloomer alias «Amorphous» theoretical model

The Forouhi-Bloomer formulation (1986, 1988) is applicable to amorphous semiconductors and dielectrics and is based on the quantum-mechanical theory of absorption. It takes into account the optical band gap in the inter-band region. It is supposed that the valence and conduction bands are parabolic and are separated by a forbidden band whose width is E_g. Peaks that can be seen in the optical spectrum correspond to transitions of electrons between two states. For an amorphous material, a single peak is present in the optical spectrum which refers to the transition between the bonding state in the valence band and the anti-bonding state in the conduction band.

For crystalline semiconductors dielectrics and metals, several peaks can be observed, indicating the transitions occurring between the critical-point in the valence and conduction bands.

In the interband region, metals, semiconductors and dielectrics have similar structure in their optical functions. Thus, the same physical processes are involved for these three types of materials.

Optical properties depend on inter-band transitions of electrons that are related to photon absorption.

The equation of $\alpha(\omega)$ below derives from the quantum expression of the absorption.

Equation of $\alpha(\omega)$

$$\alpha(\omega) = \lim_{\Delta x \to 0}\left[-\frac{1}{I}\cdot\frac{\Delta I}{\Delta x}\right] = \frac{\Theta(\omega)\cdot\Phi(\omega)}{I_0} = \frac{2\cdot\omega\cdot k}{c} \quad (1)$$

where:

- $\Theta(\omega)$ is the total number of ways a photon, of energy ω is removed from the incident intensity in a unit volume and a layer of infinitesimal thickness Δx; $\Theta(\omega)$ varies with the type (amorphous, dielectric, metallic) of the material considered.
- $\Phi(\omega)$ is the transition probability rate at which a photon is absorbed from the incident intensity in the frequency range $[\omega\ ;\ \omega + d\omega]$.
- I_0 is the incident photon intensity.

With $\Phi(\omega)$ defined as:

The equation of $\Phi(\omega)$ is deduced from first-order time-dependant perturbation theory for direct and finite electron transitions. $\Phi(\omega)$ depends on the dipole position matrix element squared between initial final states and also on the lifetime of the excited state through the following equation. For an amorphous material, the expression of $\Phi(\omega)$ is given by:

$$\Phi(\omega) = \frac{4\pi\hbar}{3c} e^2\, \omega\, I_0 \left|\left\langle \sigma^* \middle| \vec{x} \middle| \sigma \right\rangle\right|^2 \left\{ \frac{\gamma}{\left(E_{\sigma^*} - E_\sigma - \hbar\cdot\omega\right)^2 + \frac{\hbar^2\cdot\gamma^2}{4}} \right\} \quad (2.1)$$

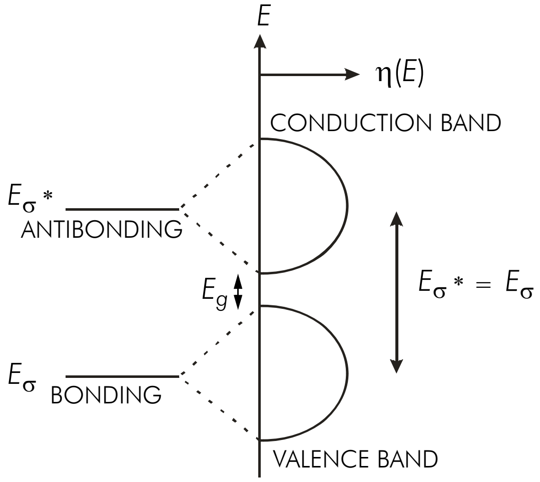


Fig. 1 Orbital states of the energies of the energies E_σ and E_σ (Ref. 2)*

where:

- e is the electron charge
- c is the light speed in vacuum
- $\hbar$ is the Planck constant
- $E=h\omega$ is the photon energy
- E_σ is the energy of the initial state
- $E_\sigma{}^*$ is the energy of the final excited state
- $\left|\langle\sigma^*|\vec{x}|\sigma\rangle\right|$ is the dipole matrix element squared between the bonding and anti-bonding states.

In the case of crystalline semiconductors, dielectrics and metals, $\Phi(\omega)$ is the sum over the number of types of transitions.

$$\Phi(\omega)=\frac{4\cdot\pi\cdot\hbar}{3\cdot c}\cdot e^2\cdot\omega\cdot I_0\cdot\sum_{j=1}^{N}\left|\left\langle\vec{k}^{\,c}_{crit}\middle|\vec{x}\middle|\vec{k}^{\,v}_{crit}\right\rangle\right|_j^2\times\ldots$$

$$\times\left\{\frac{\gamma_j}{\left\{\left[E_c\left(\vec{k}_{crit}\right)-E_v\left(\vec{k}_{crit}\right)\right]_j-\hbar\cdot\omega\right\}+\dfrac{\hbar^2\cdot\gamma_j^2}{4}}\right\} \quad (2.2)$$

where:

- the sum over N refers to the sum over the number of observed peaks associated with the transitions.
- $\left|\left\langle\vec{k}^{\,c}_{crit}\middle|\vec{x}\middle|\vec{k}^{\,v}_{crit}\right\rangle\right|_j^2$ is the dipole matrix element squared between the i^{th} critical-point state in the valence band and the i^{th} critical-point state in the conduction band.

With Θ(ω) defined as:

$\Theta(\omega)$ is proportional to the number of possible transitions for a given photon of energy $\hbar\omega$ to be removed. $\Theta(\omega)$ depends on the product of the number of occupied electron states in the valence band times the number of unoccupied electron states in the conduction band. The densities of states in the valence and conduction bands are assumed to have a parabolic shape.

Therefore, $\Theta(\omega)$ is written as

$$\Theta(\omega)\propto\int dE_v\,\eta_v(E_v)\cdot\eta_c(E_v+\hbar\omega) \quad (3.1)$$

where:

- $\eta_v(E)=cst\times\left(E_v^{top}-E\right)^{1/2}$ (3.2) is the density of states in the valence band.
- $\eta_c(E)=cst\times\left(E-E_c^{bottom}\right)^{1/2}$ (3.3) is the density of states in the conduction band.
- the band gap energy is $E_g=E_c^{bottom}-E_v^{top}$ (3.4).

For amorphous and crystalline materials the final expression of $\Theta_a(\omega)$ is

$$\Theta_a(\omega)=\Theta_c(\omega)=cst\times\left(\hbar\cdot\omega-E_g\right)^2 \quad (3.5)$$

For metals $E_g=0$, $\Theta m(\omega)$ has the following expression:

$$\Theta_m(\omega)=cst\times(\hbar\cdot\omega)^2 \quad (3.6)$$

Equation of k(ω)

Knowing the equations of $\Theta(\omega)$, $\Phi(\omega)$ and $\alpha(\omega)$ it is then possible to determine $k(\omega)$:

$$k(\omega)=\frac{c}{2\omega}\alpha(\omega)=\frac{c}{2\omega}\frac{1}{I_0}\Phi(\omega)\Theta(\omega) \quad (4.1)$$

By neglecting all the second order processes and replacing all $\Theta_a(\omega)$ and $\Phi_a(\omega)$ by their respective expressions the corresponding extinction coefficient is derived through these equations:

The final equation for the extinction coefficient of amorphous materials is written as:

$$\boxed{k(E)=\begin{cases}\dfrac{A\cdot\left(E-E_g\right)^2}{E^2-B\cdot E+C} & ;\text{ for } E>E_g\\ 0 & ;\text{ for } E\le E_g\end{cases} \quad (4.2)}$$

with

$$\begin{cases}A=cst\cdot\left|\langle\sigma^*|x|\sigma\rangle\right|^2\times\gamma\\ B=2\cdot\left(E_{\sigma*}-E_\sigma\right)\\ C=\left(E_{\sigma*}-E_\sigma\right)^2+\dfrac{\hbar^2\cdot\gamma^2}{4}\end{cases} \quad (4.3)$$

The final expression for the extinction coefficient of crystalline materials is written this way:

$$\boxed{k(E)=\begin{cases}\displaystyle\sum_{j=1}^{N}\frac{A_j\times\left(E-E_g\right)^2}{E^2-B_j\cdot E+C_j} & ;\text{ for } E>E_g\\ 0 & ;\text{ for } E\le E_g\end{cases} \quad (4.4)}$$

where A_j, B_j and C_j are given by:

$$\begin{cases} A_j = \gamma_j \cdot cst \cdot \left| \left\langle \vec{k}^{\,c}_{crit} \middle| \vec{x} \middle| \vec{k}^{\,v}_{crit} \right\rangle \right|_j^2 \\ B_j = 2 \cdot \left[E_c\left(\vec{k}_{crit}\right) - E_v\left(\vec{k}_{crit}\right) \right]_j \\ C_j = \left[E_c\left(\vec{k}_{crit}\right) - E_v\left(\vec{k}_{crit}\right) \right]_j^2 + \dfrac{\hbar^2 \cdot \gamma_j^2}{4} \end{cases} \quad (4.5)$$

The final expression for the extinction coefficient of metals is written as:

$$\boxed{k(E) = \begin{cases} \displaystyle\sum_{j=1}^{N} \frac{A_j \times E^2}{E^2 - B_j \cdot E + C_j} & ;\ \text{for E} > \text{E}_\text{g} \\ 0 & ;\ \text{for E} \le \text{E}_\text{g} \end{cases} \quad (4.6)}$$

where A_j, B_j and C_j are given by:

$$\begin{cases} A_j = \gamma_j \cdot cst \cdot \left| \left\langle \vec{k}^{\,c}_{crit} \middle| \vec{x} \middle| \vec{k}^{\,v}_{crit} \right\rangle \right|_j^2 \\ B_j = 2 \cdot \left[E_c\left(\vec{k}_{crit}\right) - E_v\left(\vec{k}_{crit}\right) \right]_j \\ C_j = \left[E_c\left(\vec{k}_{crit}\right) - E_v\left(\vec{k}_{crit}\right) \right]_j^2 + \dfrac{\hbar^2 \cdot \gamma_j^2}{4} \end{cases} \quad (4.7)$$

Crystalline semiconductors and metals may have several peaks present in the structure of the extinction coefficient which reveals the presence of several oscillators. The number of oscillators determines the name of the dispersion formula as shown below:

Formula	Number of oscillators	Number of parameters
Amorphous	N=1	5
Double Amorphous	N=2	8
Triple Amorphous	N=3	11
Quatre Amorphous	N=4	14

Equation of n(ω)

Then Kramers-Kronig (K-K) relation is used to determine the refractive index through a Hilbert transform of k(*E*):

$$n(E) - n(\infty) = \frac{1}{\pi} \cdot P \cdot \int_{-\infty}^{+\infty} \frac{k(E') - k(\infty)}{E' - E} dE' \quad (5.1)$$

where P is the Cauchy principal value containing the residuals of the integrand at poles located on the lower half of the complex plane and along the real axis.

The derivation of K-K yields the final expression for the refractive index:

In the case of an amorphous material:

$$\boxed{n(E) = \sqrt{\varepsilon_\infty} + \frac{B_0 \cdot E + C_0}{E^2 - B \cdot E + C} \quad (5.2)}$$

where

$$\begin{cases} B_0 = \dfrac{A}{Q} \cdot \left(\dfrac{-B^2}{2} + B \cdot E_g - E_g^2 + C \right) \\ C_0 = \dfrac{A}{Q} \cdot \left(\left(E_g^2 + C\right) \cdot \dfrac{B}{2} - 2 \cdot E_g \cdot C \right) \\ Q = \dfrac{1}{2} \cdot \sqrt{4 \cdot C - B^2} \end{cases} \quad (5.3)$$

In the case of a crystalline semiconductors and metals:

$$\boxed{n(E) = \sqrt{\varepsilon_\infty} + \sum_{j=1}^{N} \frac{B_{0j} \cdot E + C_{0j}}{E^2 - B_j \cdot E + C_j} \quad (5.4)}$$

where:

$$\begin{cases} B_{0j} = \dfrac{A_j}{Q_j} \left(-\dfrac{B_j^2}{2} + E_g \cdot B_j - E_g^2 + C_j \right) \\ C_{0j} = \dfrac{A_j}{Q_j} \left(\left(E_g^2 + C_j\right) \cdot \dfrac{B_j}{2} - 2 \cdot E_g \cdot C_j \right) \\ Q_j = \dfrac{1}{2} \cdot \sqrt{4 \cdot C_j - B_j^2} \end{cases} \quad (5.5)$$

The parameters of the equation

Parameter describing the refractive index

The term ε(∞) is an additional parameter corresponding to the high-frequency dielectric constant. It is at least superior to one and equal to the value of the dielectric function when $\omega \rightarrow \infty$.

At least 4 parameters describe the extinction coefficient.

- *A, B, C* are positive non zero parameters referring to the electronic structure of the material. For crystalline semiconductors, dielectrics and metals the subscript «*j*» (*j* = 1, 2, 3) for the parameters A_j, B_j, C_j refers to the number of oscillators.
- A_j (in eV) is related to the dipole matrix squared and gives the strength (amplitude) of the extinction coefficient peak. Due to correlation between *A* and *C*, the higher *A* is the higher the absorption peak and the smaller its width *C* is. Generally, $0<A_j<2$.
- $B_j/2$ (in eV) is approximately the energy at which the extinction coefficient is maximum (peak of absorption). As the value of *B* increases the absorption peak is shifted towards the UV region. Generally, $3<B_j<30$.
- C_j (in eV^2) is related to the broadening term of the absorption peak. It depends on the energy difference between different states and on the lifetime of transition. If there is no lifetime contribution in the expression of *B* then $C_j \geq B^2/4$. The larger C_j is the larger the absorption peak but the smaller its amplitude. Generally, $3<C_j<150$.
- E_g (in eV) is the energy band gap. It is equal to the minimum of energy required for a transition from the valence band to the conduction band. It is the energy from which the absorption starts to be non-zero: $k(E \geq E_g) \geq 0$. $E_g<B$ for all cases.

Limitation of the model

The Forouhi-Bloomer dispersion has some drawbacks due to the generation of unphysical results. Thus according to Jellison & Modine (Ref. 4):

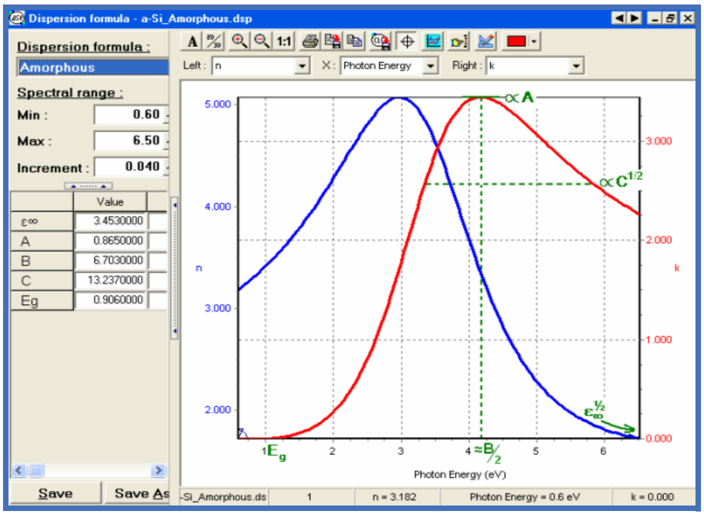
- The Forouhi-Bloomer model accuracy is rather bad below the band gap.
- After the fit, several energy gaps in the Forouhi-Bloomer equations might be negative.
- The limit of $k(E) \rightarrow$ cst as $E \rightarrow \infty$ is inconsistent with what is predicted by experiments, that is $k(E) \rightarrow 0$.
- Forouhi-Bloomer does not respect time reversal symmetry because $k(E) \neq k(-E)$.
- The *B* and *C* parameters are often correlated.

Parameter set up

Note that:

- The graphs below show the different contributions (in red dashed lines) to the imaginary part of the triple Amorphous dielectric function (red bold line).
- The sign « ∝ » before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

Amorphous function



Dispersion formula - a-Si_Amorphous.dsp

Dispersion formula : Amorphous

Spectral range :

Min : 0.60

Max : 6.50

Increment : 0.040

	Value
ε∞	3.4530000
A	0.8650000
B	6.7030000
C	13.2370000
Eg	0.9060000

Left : n

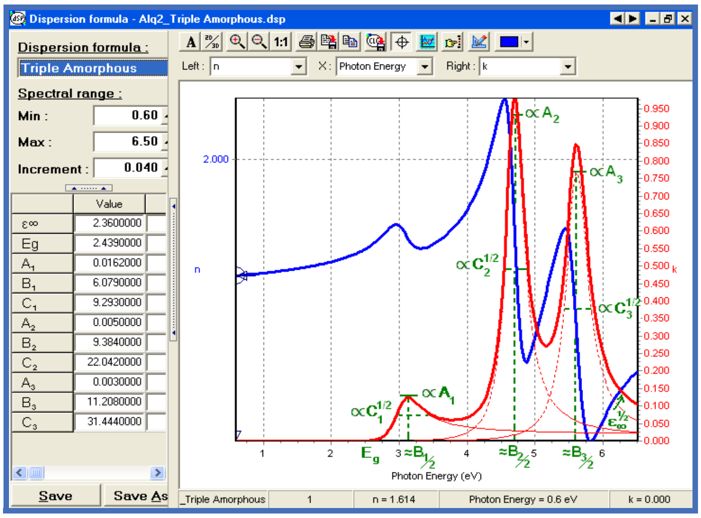
X : Photon Energy

Right : k

-Si_Amorphous.ds | 1 | n = 3.182 | Photon Energy = 0.6 eV | k = 0.000

Optical properties of a-Si given by the Amorphous function

Triple Amorphous function



Dispersion formula - Alq2_Triple Amorphous.dsp

Dispersion formula : Triple Amorphous

Spectral range :

Min : 0.60

Max : 6.50

Increment : 0.040

	Value
ε∞	2.3600000
Eg	2.4390000
A_1	0.0162000
B_1	6.0790000
C_1	9.2930000
A_2	0.0050000
B_2	9.3840000
C_2	22.0420000
A_3	0.0030000
B_3	11.2080000
C_3	31.4440000

Left : n

X : Photon Energy

Right : k

_Triple Amorphous | 1 | n = 1.614 | Photon Energy = 0.6 eV | k = 0.000

Optical properties of Alq3 given by Triple Amorphous function

Applications to materials

The amorphous model works particularly well for amorphous materials exhibiting an absorption in the visible and/or FUV range (absorbing dielectrics, semiconductors, polymers).

Materials following the Amorphous model

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

Materials	ε℘	A	B	C	Eg	S. R. (eV)
AlN	2.472	0.066	17.670	80.000	0.809	1.5 - 3
AlInGaP	5.521	0.0229	6.714	11.282	2.046	0.75 - 3
a-C	2.275	0.194	7.342	28.634	0.132	1.5 - 3.5
a-GaAs	4.766	0.407	5.872	9.605	1.418	0.6 - 3
a-Si	3.453	0.865	6.703	13.237	0.906	0.6 - 5
a-Si:H	3.710	1.090	6.670	12.720	1.270	0.6 - 5
a-SiGe	1.037	0.63	8.085	19.125	- 0.894*	0.8 - 3
SiN	3.569	0.225	13.491	48.649	4.299	0.6 - 6
TaOx	3.443	0.294	10.925	30.523	3.801	1.4 - 5
TiOx	4.470	0.470	8.300	17.799	3.190	0.6 - 5
WO_x	3.962	0.060	7.756	15.175	2.895	1.5 - 4.5
ZnSe	5.521	0.022	6.714	11.282	2.046	0.6 - 3

Materials following the Triple Amorphous model

Materials	ε℘	Eg	A_1	B_1	C_1	A_2
Alq2	2.360	2.439	0.005	9.384	22.042	0.0162

Materials	B_2	C_2	A_3	B_3	C_3	S. R. (eV)
Alq2	6.079	9.293	0.003	11.208	31.444	0.75 - 4

Materials following the Quatre Amorphous model

Materials	ε℘	Eg	A_1	B_1
GaAs	4.324	1.253	0.000	5.870
GaP	4.148	0.932	0.002	7.470
Ge	4.879	0.784	0.144	4.526
InGaP	4.996	1.296	0.040	6.681
c-Si	5.664	2.065	0.011	6.860

Materials	C_1	A_2	B_2	C_2
GaAs	8.618	0.148	6.248	10.037
GaP	13.967	0.024	7.946	15.957
Ge	5.280	0.304	6.789	12.694
InGaP	11.297	0.164	3.395	3.124
c-Si	11.778	0.054	7.361	13.625

Materials	A_3	B_3	C_3	A_4
GaAs	0.116	9.790	24.412	0.018
GaP	0.090	10.249	26.699	0.005
Ge	0.013	8.710	19.046	0.014
InGaP	0.114	8.033	16.913	0.098
c-Si	0.153	8.632	18.817	0.047

Materials	B_4	C_4	S. R. (eV)
GaAs	12.450	40.969	0.6 - 3
GaP	12.719	40.528	0.6 - 3
Ge	9.997	25.250	1.5 - 3
InGaP	13.008	39.464	0.6 - 3
c-Si	10.314	26.859	0.6 - 3

References

1. E. D. Palik, Handbook of Optical Constants of Solids II, Chap. 7.
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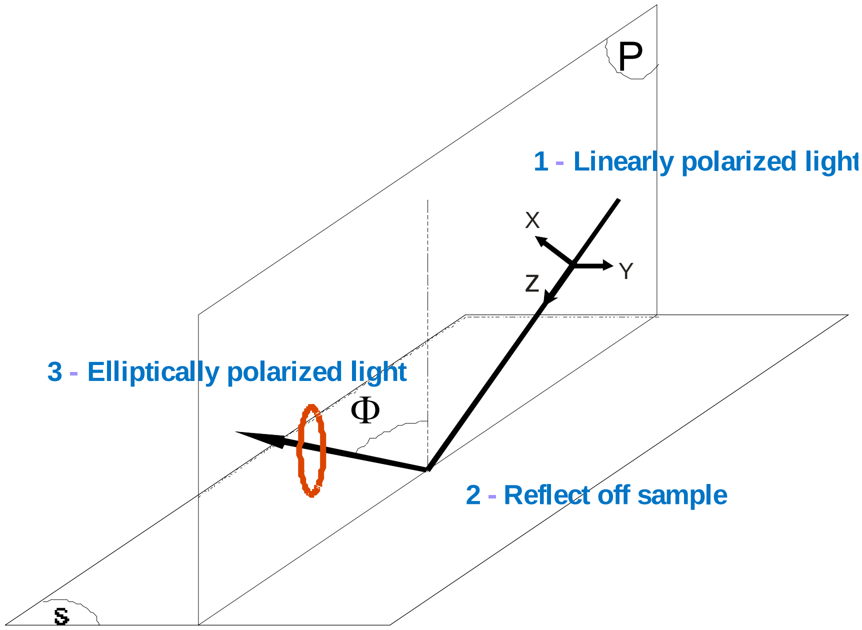
3. A. R. Forouhi, I. Bloomer, Phys. Rev. B 38, 1865 (1988).
4. G.E Jellison, F. A. Modine, Phys. Rev. , 69(3), 371-374 (1996).

Appendix B Propagation of Polarized Light: Jones and Mueller Formalism

The two most important mathematical descriptions of polarization are the Jones and the Mueller Formalism. The Jones formalism ia applicable only to completely polarized waves, but it can deal with coherent beams. The Mueller formalism instead is applicable also to partially polarized light, however, it can deal only with incoherent beams.

B1 Jones formalism

During a reflection under non normal incidence, the plane of incidence is defined by the incident beam and the normal direction on the sample:



The propagation vector of the light is z, the electromagnetic field can be described by two components, one perpendicular to the plane of incidence (s) and one parallel to the plane of incidence (p). These two axis define an orthogonal basis to describe the light polarization. A representation of the electric field vector is then:

Jones vector for an arbitrarily polarized beam

$$\vec{\mathrm{E}} = \mathrm{E}_s\vec{s} + \mathrm{E}_p\vec{p}$$

or written as a ***Jones vector***:

$$\vec{\mathrm{E}} = \begin{bmatrix} \mathrm{E}_s(t) \\ \mathrm{E}_p(t) \end{bmatrix}$$

$\mathrm{E}_p(t)$ and $\mathrm{E}_s(t)$ are the instantaneous scalar components of $\vec{\mathrm{E}}$.

By preserving the phase information it is possible to handle coherent waves:

$$\vec{E} = \begin{bmatrix} E_{0s} e^{i\varphi_s} \\ E_{0p} e^{i\varphi_p} \end{bmatrix}$$

If for example $E_{op} = E_{0s}$ and $_p = _s$ we get:

$$\vec{E} = E_{0p} e^{i\varphi_p} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Representing a light polarized linearly at 45°.

Since absolute amplitudes and phases are usually not interesting the irradiance can be normalized to unity so that we get:

$$\vec{E}_{45^\circ} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

and also:

$$\vec{E}_p = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \text{ and } \vec{E}_s = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

For right-circular light we have $E_{op} = E_{0s}$ and but the s-component is leading the p-component by 90°:

$$\vec{E}_R = \begin{bmatrix} E_{0s} e^{i\varphi s} \\ E_{0p} e^{i(\varphi_p - \pi/2)} \end{bmatrix}$$

Dividing by $E_{0s} e^{i\varphi s}$ yields:

$$\begin{bmatrix} 1 \\ e^{-i\pi/2} \end{bmatrix} = \begin{bmatrix} 1 \\ -i \end{bmatrix}$$

So that the normalized Jones-vectors for right-circular and respectively left-circular polarized light are:

$$\vec{E}_R = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} \text{ and } \vec{E}_L = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$$

One refers to two polarization states as being orthogonal when their Jones vectors are orthogonal. $\vec{E}_R$ and $\vec{E}_L$ form such a set, as do $\vec{E}_p$ and $\vec{E}_s$.

Any polarization state can be described by a linear combination of the vectors of such an orthonormal set.

An optical element transforms an incident beam represented by $\vec{E}_i$ into a transmitted beam $\vec{E}_t$. This can be described now mathematically using a 2 x 2 matrix:

$$\vec{E}_t = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \vec{E}_t = A\vec{E}_t$$

With the ***Jones matrix*** A. The effect of *n* optical elements can then simply be determined by matrix multiplication:

$$\vec{\mathrm{E}}_t = A_n \cdots A_2 A_1 \vec{\mathrm{E}}_t$$

Examples for Jones matrices:

Horizontal linear polarizer:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

Vertical linear polarizer:

$$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Linear polarizer at 45°:

$$\frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

Linear polarizer at -45°:

$$\frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

QWP, fast axis vertical:

$$e^{i\pi/4}\begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$$

QWP, fast axis horizontal:

$$e^{i\pi/4}\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$$

Circular polarizer right:

$$\frac{1}{2}\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$$

Circular polarizer left:

$$\frac{1}{2}\begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}$$

B2 Mueller formalism

Stokes vector for an arbitrarily polarized beam

All possible states of polarization, including partial polarization, can be described by a set of three real numbers. If we include the total light intensity we have four real, measurable quantities, the ***Stokes parameters*** S_0, S_1, S_2, S_3 forming the ***Stokes vector***:

$$\vec{\mathrm{S}} = \begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix} = \begin{bmatrix} I_0 \\ I_x - I_y \\ I_{\pi/4} - I_{-\pi/4} \\ I_R - I_L \end{bmatrix}$$

where:

$I_0 =$ total light intensity

$I_x =$ intensity through a linear polarizer at 0°

$I_y =$ intensity through a linear polarizer at 90°

$I_{\pi/4} =$ intensity through a linear polarizer at 45°

$I_{-\pi/4} =$ intensity through a linear polarizer at -45°

$I_R =$ intensity through a right circular polarizer

$I_L =$ intensity through a left circular polarizer

and $I_0 = I_x + I_y = I_{\pi/4} + I_{-\pi/4} = I_R + I_L$.

It is often convenient to normalize the Stokes parameters by dividing each one by the S_0. The set of parameters for natural light is then:

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Examples for Stokes vectors:

horizontally polarized: $\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ vertically polarized: $\begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}$

linearly polarized at 45°: $\begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ linearly polarized at -45°: $\begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}$

right circular polarized: $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ left circular polarized: $\begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix}$

For completely polarized light we must have:

$$S_0^2 = S_1^2 + S_2^2 + S_3^2$$

Furthermore, for partially polarized light we can now calculate the degree of polarization by:

$$Deg_{Pol} = \sqrt{S_1^2 + S_2^2 + S_3^2} / S_0$$

Also in the Mueller formalism we have a matrix method to deal with the vectors representing the state of polarization. These Mueller, 4 x 4 matrices are applied in much the same way as are the Jones matrices:

with

$$\vec{\mathrm{S}}_t = M\vec{\mathrm{S}}_i$$

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix}$$

Examples for Mueller matrices:

Horizontal linear polarizer:

$$\frac{1}{2}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Vertical linear polarizer:

$$\frac{1}{2}\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Linear polarizer at 45°:

$$\frac{1}{2}\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Linear polarizer at -45°:

$$\frac{1}{2}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

QWP, fast axis vertical:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

QWP, fast axis horizontal:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

Circular polarizer right:

$$\frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

Circular polarizer left:

$$\frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$

Appendix C Deduction of Psi and Delta from raw data

The measured intensity of a phase-modulated ellipsometer can be written as:

$$I(t) = I\,[I_0 + I_s \sin(\delta_0 + A_m \sin \omega t) + I_c \cos(\delta_0 + A_m \sin \omega t)] \qquad (1)$$

with the amplitude of modulation A_m and the frequency of modulation ω. I is a pre-factor (lamp intensity, sample reflectivity, transmission of optical elements), which is omitted during later calculations. δ_0 is the rest-birefringence of the modulator.

The factors I_0, I_s and I_c contain the azimuth of the polarizer P, the modulator M and the analyzer A in respect to the plane of incidence and the ellipsometric angles ψ and Δ:

$$I_0 = 1 + \cos 2A \cos 2M \cos 2(P - M) - \{\cos 2A + \cos 2M \cos 2(P - M)\} \cos 2\psi \qquad (1a)$$

$$I_s = \sin 2(P - M) \sin 2A \sin 2\psi \sin \Delta \qquad (1b)$$

$$I_c = \sin 2(P - M) \{\sin 2M (\cos 2\psi - \cos 2A) + \sin 2A \cos 2M \sin 2\psi \cos \Delta\} \qquad (1c)$$

We make the following transformation:

$$\sin(\delta_0 + A_m \sin \omega t) = \sin\delta_0 \cos(A_m \sin \omega t) + \cos\delta_0 \sin(A_m \sin \omega t)$$

(and analogous for the cos-Term)

and the following series expansion:

$$\sin(A_m \sin \omega t) = 2\,J_1(A_m) \sin \omega t + \ldots$$

$$\cos(A_m \sin \omega t) = J_0(A_m) + 2\,J_2(A_m) \cos 2\omega t + \ldots$$

whereby $J_n(A_m)$ is the n-th Bessel-function of A_m.

these terms will be used again in equation (1).

The detected signal can as well be written as:

$$S(t) = S_0 + S_1 e^{it} + S_2 e^{2it} + \ldots \qquad (2)$$

Where again ω = modulation frequency of the photoelastic modulator.
By Fourier-analysis we get the coefficients S_0, S_1 and S_2.
A comparison of equations (1) and (2) yields:

$$S_0 = I\,[I_0 + J_0(A_m)\,(I_c \cos \delta_0 + I_s \sin \delta_0)] \qquad (3a)$$

$$S_1 = I\,[2\,J_1(A_m)\,(I_s \cos \delta_0 - I_c \sin \delta_0)] \qquad (3b)$$

$$S_2 = I\,[2\,J_2(A_m)\,(I_c \cos \delta_0 + I_s \sin \delta_0)] \qquad (3c).$$

and further by normalization

$$S_{\omega} \equiv \frac{S_1}{S_0} \qquad \textbf{(4a)}$$

and

$$S_{2\omega} \equiv \frac{S_2}{S_0} \qquad \textbf{(4b)}$$

*I*s and *I*c can now be calculated by inversion of the equations from *S* and S_2 (whereby I_0 = 1 in the given configurations). The values for A_m and δ_0 are determined during the calibration of the system.

$$\mathrm{Is} = \frac{\dfrac{S_{\omega}}{2T_1J_1(A_m)}\cos\delta_0 + \dfrac{S_{2\omega}}{2T_2J_2(A_m)}\sin\delta_0}{1 - J_0(A_m)\dfrac{S_{2\omega}}{2T_2J_2(A_m)}}$$

$$\mathrm{Ic} = \frac{\dfrac{S_{2\omega}}{2T_2J_2(A_m)}\cos\delta_0 - \dfrac{S_{\omega}}{2T_1J_1(A_m)}\sin\delta_0}{1 - J_0(A_m)\dfrac{S_{2\omega}}{2T_2J_2(A_m)}}$$

(T_1 and T_2 the norms of the electronic transfer functions of the system for each harmonic)

All the measurement is funded on the determination of the values I_s and I_c, which are directly proportional to the ellipsometric angles and .

Summary: determination of the ellipsometric angles and from the detected signal:

$$\begin{pmatrix} S_0 \\ S_1 \\ S_2 \end{pmatrix} \longrightarrow \begin{pmatrix} S_{\omega} \\ S_{2\omega} \end{pmatrix} \longrightarrow \begin{pmatrix} \mathrm{Is} \\ \mathrm{Ic} \end{pmatrix} \longrightarrow \begin{pmatrix} \Psi \\ \Delta \end{pmatrix}$$

Examples for the last step:

configuration II (for example P = 45°, M = 0°, A = 45°):

I_0 = 1

I_s = sin2 sin

I_c = sin2 cos

configuration III (for example P = 90°, M = 45°, A = 45°):

I_0 = 1

I_s = sin2 sin

$I_{c'}$ = cos2

Measuring in these two configurations we already can determine a polarization factor for isotropic samples:

P = Is+Ic+Ic'

Appendix D Deduction of Mueller Matrix and Jones Matrix elements from UVISEL Data

D1 UVISEL data and Mueller matrix elements

The relations for the intensities I_0, I_s and I_c of a phase-modulated ellipsometer in the configuration ASMP (analyzer - sample - modulator - polarizer) with a sample represented by the corresponding Mueller-Matrix M are:

$$I_0 = M_{11} + M_{12} \cos 2A + M_{13} \sin 2A + \cos 2(P-M) \times$$
$$\times [\cos 2M (M_{21} + M_{22} \cos 2A + M_{23} \sin 2A) + \sin 2M (M_{31} + M_{32} \cos 2A + M_{33} \sin 2A)]$$

$$I_s = \sin 2(P-M) (M_{41} + M_{42} \cos 2A + M_{43} \sin 2A)$$

$$I_c = \sin 2(P-M) \times$$
$$\times [\cos 2M (M_{31} + M_{32} \cos 2A + M_{33} \sin 2A) - \sin 2M (M_{21} + M_{22} \cos 2A + M_{23} \sin 2A)]$$

whereby M_{ij} (i, j = 1, 2, 3, 4) the elements of the Mueller-Matrix of the sample.

P = azimuth of polarizer
M = azimuth of modulator
A = azimuth of analyzer

In the following we show the expressions for the most important configurations:
For a Polarizer setting of +45° (P-M = +45°) we get the following simplified expressions:

$$I_0 = M_{11} + M_{12} \cos 2A + M_{13} \sin 2A$$
$$I_s = M_{41} + M_{42} \cos 2A + M_{43} \sin 2A$$
$$I_c = \cos 2M (M_{31} + M_{32} \cos 2A + M_{33} \sin 2A) - \sin 2M (M_{21} + M_{22} \cos 2A + M_{23} \sin 2A)$$

and further:
for the “alignment” configuration (M = 0° or 90°, A = 0° or 90°) :

$$I_0 = M_{11} + (-1)^A M_{12}$$
$$I_s = M_{41} + (-1)^A M_{42}$$
$$I_c = (-1)^M [M_{31} + (-1)^A M_{32}]$$

for the “calibration” configuration I (M = ±45°, A = 0° or 90°) :

$$I_0 = M_{11} + (-1)^A M_{12}$$

$I_s = M_{41} + (-1)^A M_{42}$
$I_c = - (-1)^M [M_{21} + (-1)^A M_{22}]$

for the “measurement” configuration II (M = 0° or 90°, A = ±45°) :
$I_0 = M_{11} + (-1)^A M_{13}$
$I_s = M_{41} + (-1)^A M_{43}$
$I_c = (-1)^M [M_{31} + (-1)^A M_{33}]$

for the “measurement” configuration III (M = ±45°, A = ±45°) :
$I_0 = M_{11} + (-1)^A M_{13}$
$I_s = M_{41} + (-1)^A M_{43}$
$I_c = - (-1)^M [M_{21} + (-1)^A M_{23}]$.

(the factor $(-1)^E = +1$ for an element (A or M) with azimuth E = 0° or +45° and $(-1)^E = -1$ for E = 90° or -45°).

D2 Determination of the Mueller matrix elements

We measure in the following 8 configurations:

1. M = -45	A = -45	Ic = A	
2. M = -45°	A = 45	Ic = B	
3. M = 0	A = - 45	Ic = C	Is = D
4. M = 0	A = 45	Ic = E	Is = F
5. M = -45°	A = 0	Ic = G	
6. M = 0	A = 90	Ic = H	Is = I
7. M = 0	A = 0	Ic = J	
8. M = -45	A = 90	Ic = L	

in matrix formalism that means:

$$\begin{pmatrix} 0 & A & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -B & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & D & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & -E & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -F & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ -G & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ -J & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ L & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} M12 \\ M13 \\ M21 \\ M22 \\ M23 \\ M31 \\ M32 \\ M33 \\ M41 \\ M42 \\ M43 \end{pmatrix} \equiv \begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \\ G \\ H \\ I \\ J \\ L \end{pmatrix}$$

So that we can determine the following elements of the normalized (M11=1) mueller matrix: M12 ; M13 ; M21 ; M22 ; M23 ; M31 ; M32 ; M33 ; M41 ; M42 ; M43.

$$M_{UVISEL} = \begin{bmatrix} 1 & M_{12} & M_{13} & - \\ M_{21} & M_{22} & M_{23} & - \\ M_{31} & M_{32} & M_{33} & - \\ M_{41} & M_{42} & M_{43} & - \end{bmatrix}$$

Note that if one inverts the direction of light (i.e. PMSA instead of ASMP) t would be possible to measure M^T and thus further 3 elements: M_{14}, M_{24} and M_{34}. This means that theoretically it is possible to measure 14 of the 15 normalized elements of the Mueller matrix. Only M_{44} cannot be determined!

D3 Deduction of Jones matrix elements from the Mueller matrix elements

Non-depolarizing Mueller matrices are transformed into Jones matrices using the following relations:

Jones matrix: $J = \begin{bmatrix} j_{xx} & j_{xy} \\ j_{yx} & j_{yy} \end{bmatrix} = \begin{bmatrix} \rho_{xx} e^{i\phi_{xx}} & \rho_{xy} e^{i\phi_{xy}} \\ \rho_{yx} e^{i\phi_{yx}} & \rho_{yy} e^{i\phi_{yy}} \end{bmatrix}$

where the amplitudes are:

$$\rho_{xx} = \tfrac{1}{\sqrt{2}} \sqrt{M_{11} + M_{12} + M_{21} + M_{22}}$$

$$\rho_{xy} = \tfrac{1}{\sqrt{2}} \sqrt{M_{11} + M_{12} + M_{21} - M_{22}}$$

$$\rho_{yx} = \tfrac{1}{\sqrt{2}} \sqrt{M_{11} + M_{12} - M_{21} - M_{22}}$$

$$\rho_{yy} = \tfrac{1}{\sqrt{2}}\sqrt{M_{11} - M_{12} - M_{21} + M_{22}}$$

and the relative phases are:

$$\phi_{xy} - \phi_{xx} = \arctan\left(\frac{-M_{14} - M_{24}}{M_{13} + M_{23}}\right)$$

$$\phi_{yx} - \phi_{xx} = \arctan\left(\frac{M_{41} + M_{42}}{M_{41} + M_{32}}\right)$$

$$\phi_{yy} - \phi_{xx} = \arctan\left(\frac{M_{43} - M_{34}}{M_{33} + M_{43}}\right)$$

The phase ϕ_{xx} is not determined; it represents the absolute phase relative to which the other phases are determined.