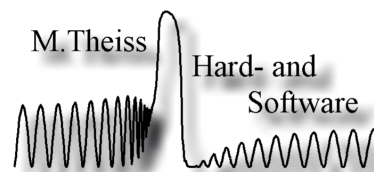


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CODE

Analysis, design, production control of thin films

by Wolfgang Theiss

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Foreword

This document gives a short summary of several talks and documents about spectrum simulation.

All the pictures are just screen shots, not prepared explicitly for this document. In between the pictures there are comments that should guide you from slide to slide.

Most of the slides in the talks are interactive pictures: You can vary slider positions and see what happens to the spectra. Unfortunately, in this static document these dynamical impressions cannot be reproduced.

In the graphs displaying optical constants the real part is drawn blue, the imaginary one is given in red.

In the case of spectrum fits, the measured spectra are always in red, the simulated spectra in blue.

All simulations have been performed with our SCOUT, CODE and SPRAY software products which are commercially available.

Aachen, March 2004

1 Overview

1.1 The company

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Software development for optical analysis and design

Consulting work in the field of optical spectroscopy

(material science, thin film analysis, optical design, production and process control)

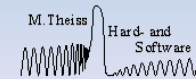
Wolfgang Theiss

Almost 20 years of experience in optical spectroscopy

Optical properties of homogeneous and inhomogeneous materials

Software development

Teaching (university, industry)



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1.2 The talk

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W.Theiss

M.Theiss Hard- and Software

Content

Software overview

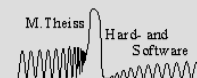
Customized views

Optical model

Computation of technical data

Fit and design

Production control



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1.3 The software

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Software overview

- Object oriented design
- Objects are collected in lists
- Object relations defined by drag&drop

Important objects (SCOUT and CODE software)

Optical modelling:	Materials, Layer stacks, Spectra
Global parameter connections:	Master parameters
Parameter fits:	Fit parameters, fit parameter sets
Customized user interfaces:	Views, view objects

CODE software only:

Computation of technical data:	Integral quantities
--------------------------------	---------------------

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2 Customized views

The appearance of the main window is defined by so-called views (user-defined):

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Customized views

- The main window shows a view
- You can define and switch between several views
- A 'View' is a collection of view objects

Static view objects display text, bitmaps or vector drawings

Dynamic view objects display object properties

Some view objects are buttons for actions

Some view objects modify object parameters

This talk will be full of view examples!

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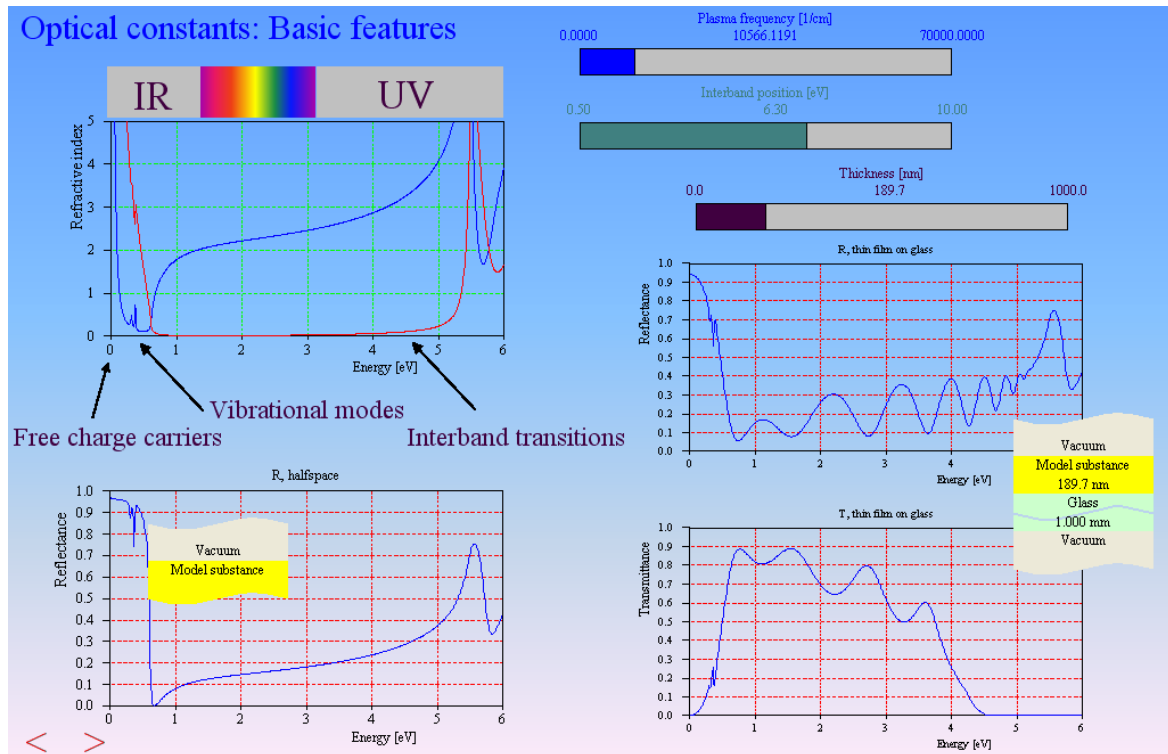
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3 Optical model

3.1 Material constants

3.1.1 Optical constants: Overview

Three basic types of excitations determine the optical constants of almost all materials:



Optical model

Material constants

How can we get flexible and realistic optical constant models?

Using combinations of

- Tauc-Lorentz model for interband transitions
- OJL model for interband transitions
- Kim oscillator model
- Classical and advanced Drude model
- and a constant, real refractive index

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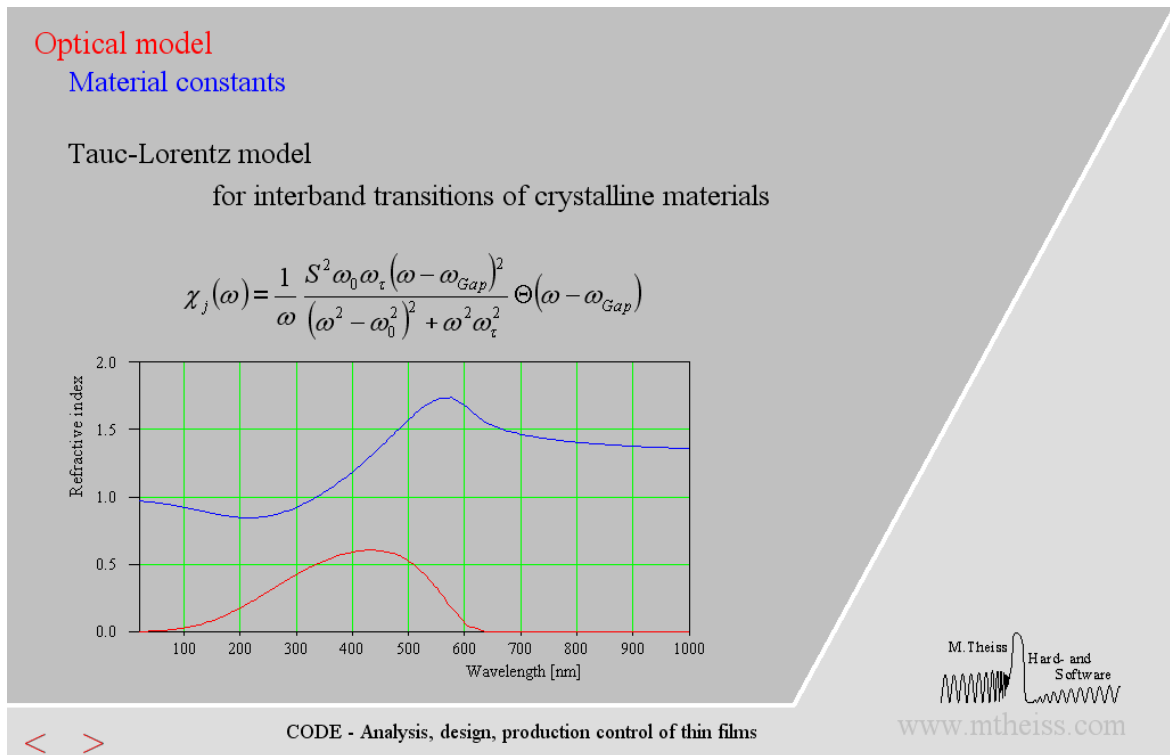
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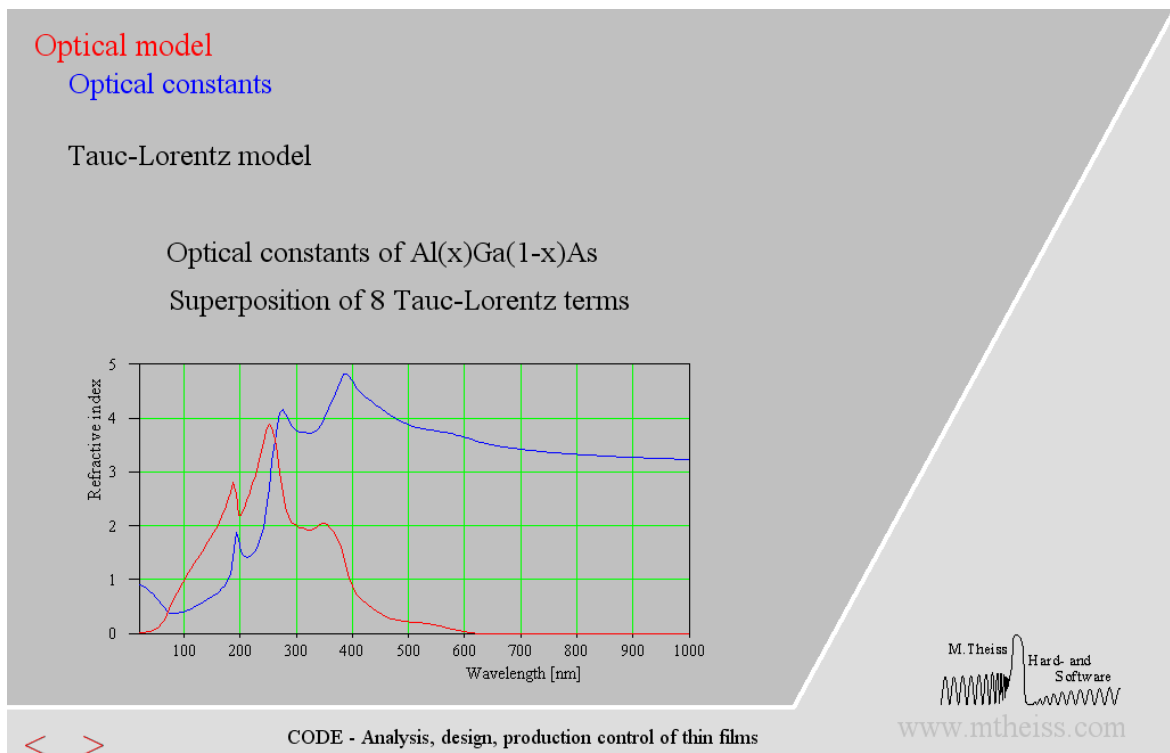
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3.1.2 Interband transitions

Interband transitions of crystalline materials can be described using the Tauc-Lorentz model:



Here is a typical example using the superposition of 8 interband transitions:



Amorphous materials have less rich featured, broad interband transitions which can often be described in good quality using a single OJL model:

Optical model
 Optical constants

OJL model
 for interband transitions of amorphous materials

Refractive index

Wavelength [nm]

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The theory behind the OJL model is summarized in the following page:

OJL model for interband transitions in amorphous materials

Density of states $N(E)$

Disorder creates localized states in the gap between valence and conduction band

Valence band

Conduction band

Energy E

No disorder

Strong disorder

Extended states

Localized 'tail states'

'Mobility edge'

Energy E

OJL model (S.K.O'Leary, S.R.Johnson, P.K.Lim, J. Appl. Phys., Vol. 82, No. 7, 1.October 1997):

Parabolic bands and exponentially decaying tail states

Density of states $N(E)$

Valence band

Conduction band

$\sim \exp((E-E_c)/\gamma_c)$

$\sim \exp(-(E-E_v)/\gamma_v)$

E_v E_0 E_c

Energy E

Extended to extended

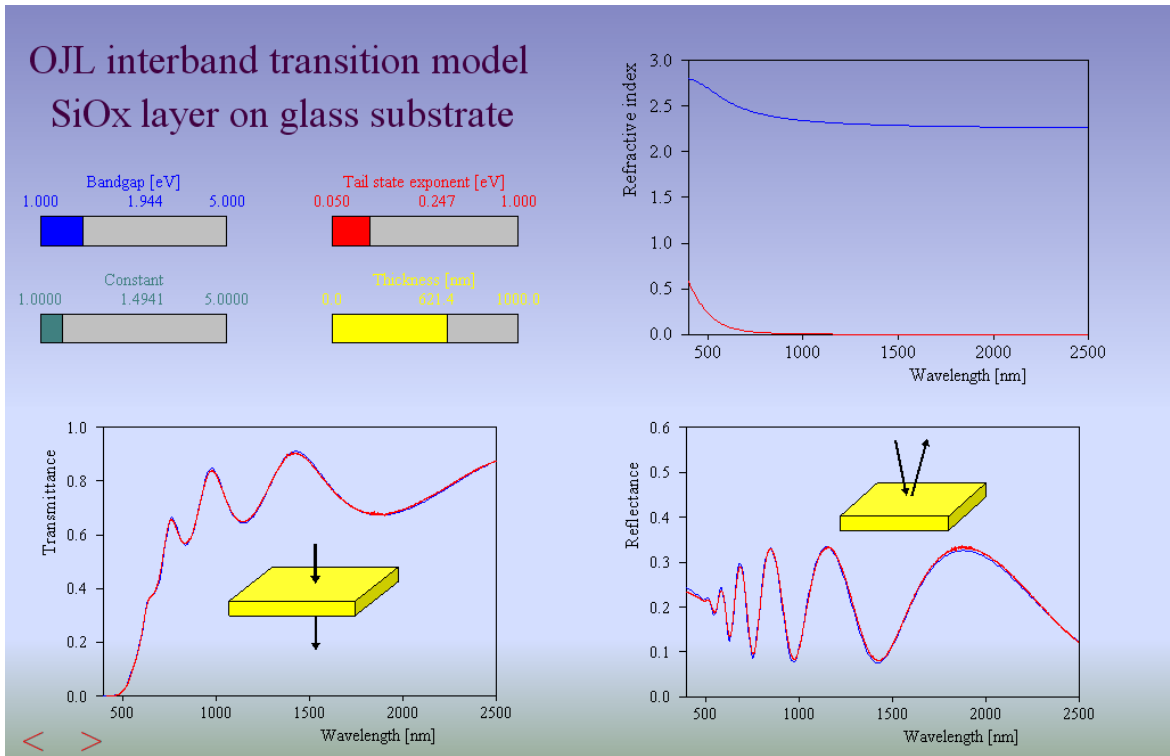
Localized to extended

Extended to localized

Localized to localized

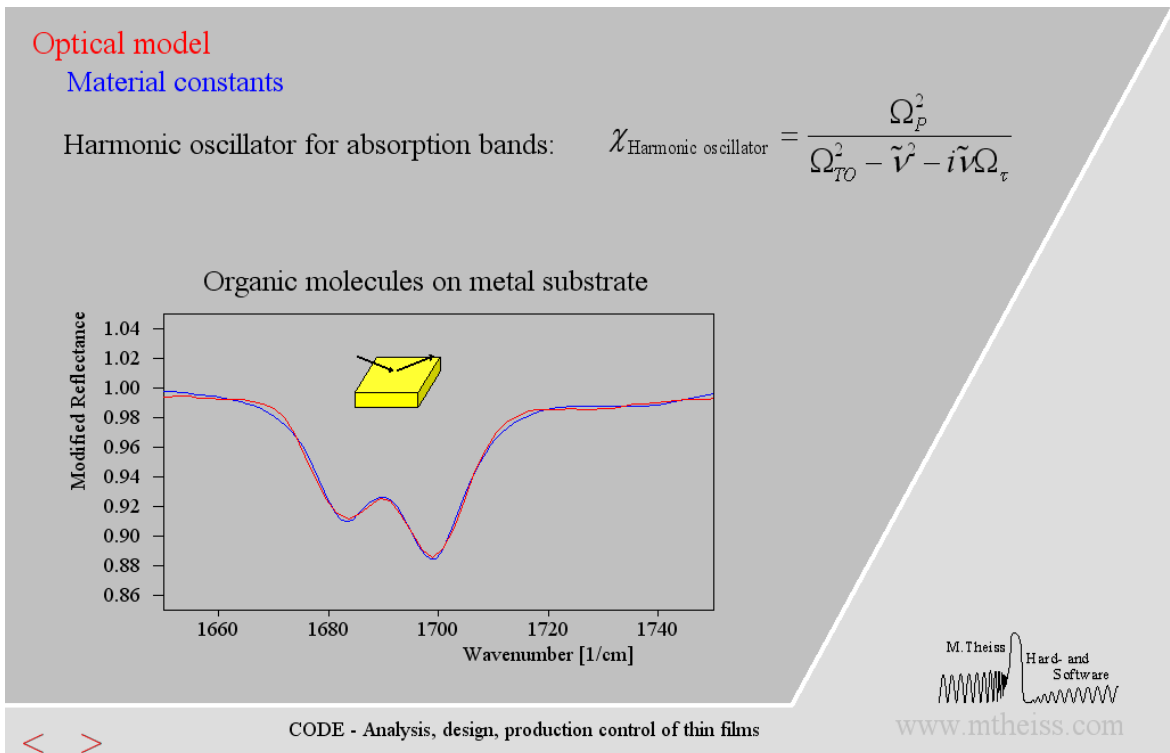
Energy E

Here is an example of a succesful application of the OJL model:



3.1.3 Vibrational modes

Vibrational modes and some electronic interband transitions can be modeled using oscillator terms. The simplest approach is the harmonic oscillator which leads to a Lorentzian line shape of the absorption band:



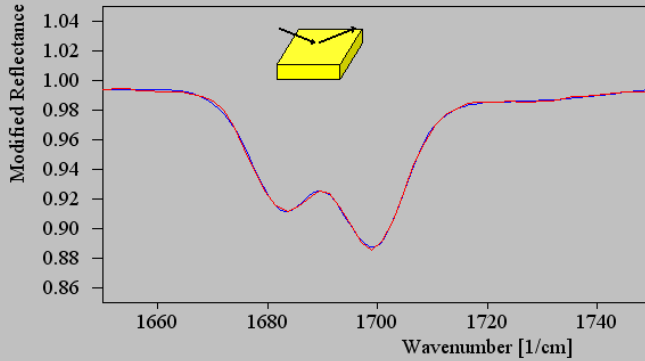
However, in most cases a Gaussian line shape is more realistic. In SCOUT and CODE this can be obtained using Kim oscillators:

Optical model
Material constants

Kim oscillator for absorption bands: from Gaussian to Lorentzian lineshape

$$\chi_{\text{Kim oscillator}} = \frac{\Omega_p^2}{\Omega_{TO}^2 - \tilde{\nu}^2 - i\tilde{\nu}\tau} \quad \text{with} \quad \tau(\tilde{\nu}) = \Omega_\tau \exp\left(-\frac{1}{1 + \sigma^2} \left(\frac{\tilde{\nu} - \Omega_{TO}}{\Omega_\tau}\right)^2\right)$$

Organic molecules on metal substrate

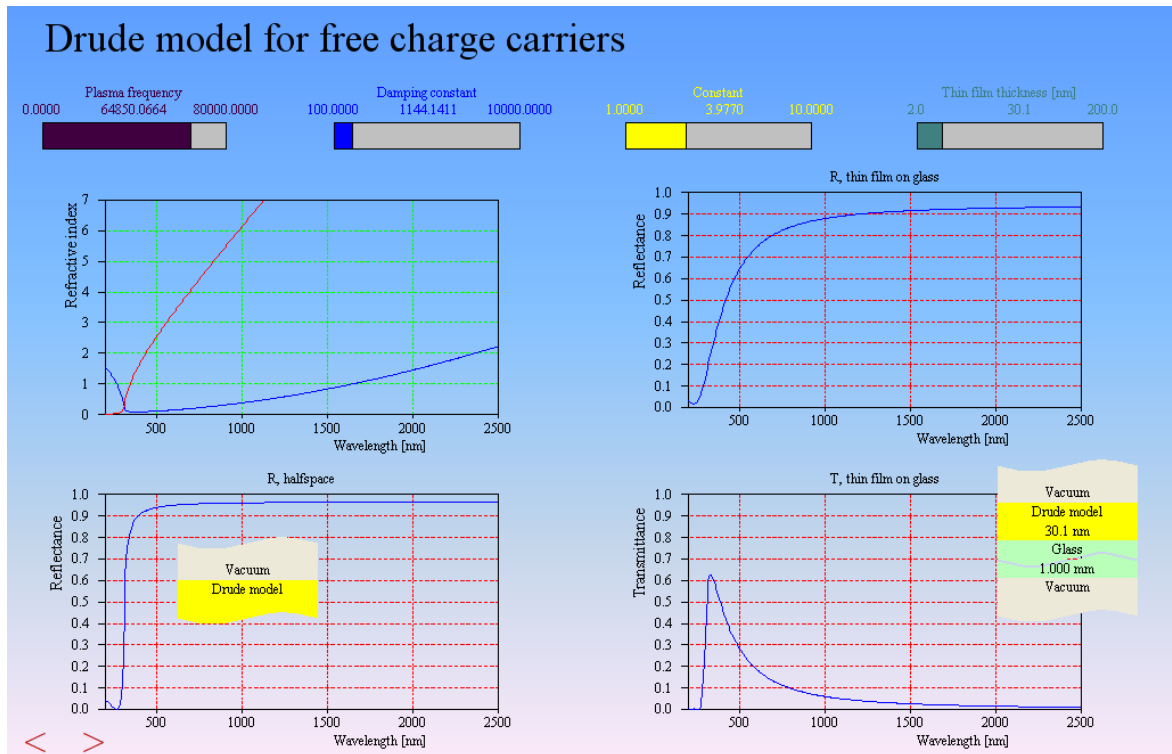


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3.1.4 Charge carriers

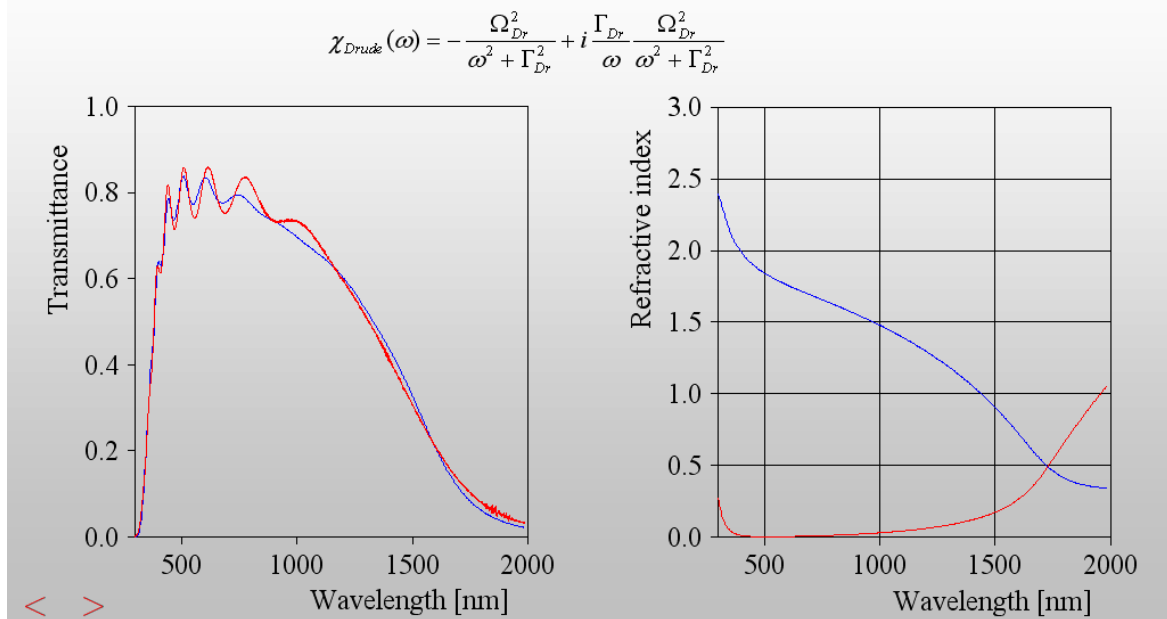
The interaction of free charge carriers like electrons or holes can be described with the Drude model. This model has two parameters only: The plasma frequency is proportional to the square root of the carrier density, the damping constant to the inverse of the mobility. Characteristic for the presence of many charge carriers (like in metals) is the large imaginary part of the refractive index. If it is larger than the real part, no wave propagation is possible in the material. This leads to a 'rejection' of incoming waves, i.e. to a high reflectance. Radiation penetrating a metal is absorbed very efficiently in a very thin film.



The following example shows that the simple Drude model does not always perform excellently:

Drude model

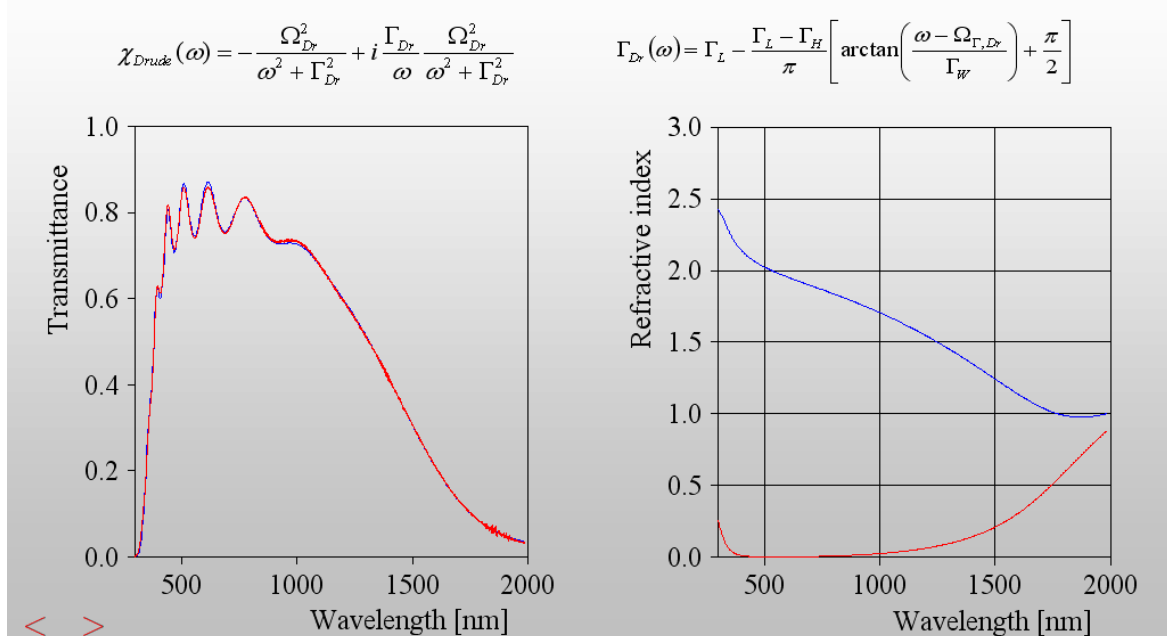
ITO on glass: constant + OJL interband transition + Drude model



In cases like this you can try an extension of the Drude model which features a frequency-dependent damping constant. Electron scattering at charged donor or acceptor atoms may lead to a characteristic frequency dependence of the damping constant in the Drude model:

Extended Drude model

ITO on glass: Constant + OJL interband transition + extended Drude model



3.1.5 Master model

Sometimes the optical constants of a material vary systematically with a compositional parameter like oxygen content in a non-stoichiometric oxide or the concentration of an atomic species in a ternary system. This can be described conveniently in SCOUT and CODE using so-called master models which provide for every parameter a user-defined formula to express its dependence on the master quantity:

Optical model
Material constants

Master model: Control many slave parameters by one master parameter

Optical constants of Al(x)Ga(1-x)As Al content x
0.0000 0.3057 1.0000

Superposition of 8 Tauc-Lorentz terms

Refractive index

Wavelength [nm]

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3.2 Layer stacks

3.2.1 Computation of reflectance and transmittance

Single layer treatment using geometric series:

Reflection and Transmission of a single layer

Taking into account multiple reflections:

amplitude reflection coefficient

$$r_{a,b} = r_{a,b} + \frac{\tau_{a,b} \phi r_{b,c} \phi \tau_{b,a}}{1 - r_{b,c} \phi r_{b,a} \phi}$$

amplitude transmission coefficient

$$t_{a,b} = \frac{\tau_{a,b} \phi \tau_{b,c}}{1 - r_{b,c} \phi r_{b,a} \phi}$$

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Multilayers are processed applying the single layer expressions many times:

Reflection and Transmission of multilayers

Formalism for complex layer stacks:
reduce the stack repeatedly by the last layer

$$r_{x,y} = r_{x,y} + \frac{\tau_{x,y} \phi \rho_{y,z} \phi \tau_{y,x}}{1 - \rho_{y,z} \phi \rho_{y,x} \phi}$$

$$t_{x,y} = \frac{\tau_{x,y} \phi \tau_{y,z}}{1 - \rho_{y,z} \phi \rho_{y,x} \phi}$$

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3.2.2 Coherent/incoherent superposition

CODE has a very efficient algorithm to compute R and T of partially coherent superposition of waves:

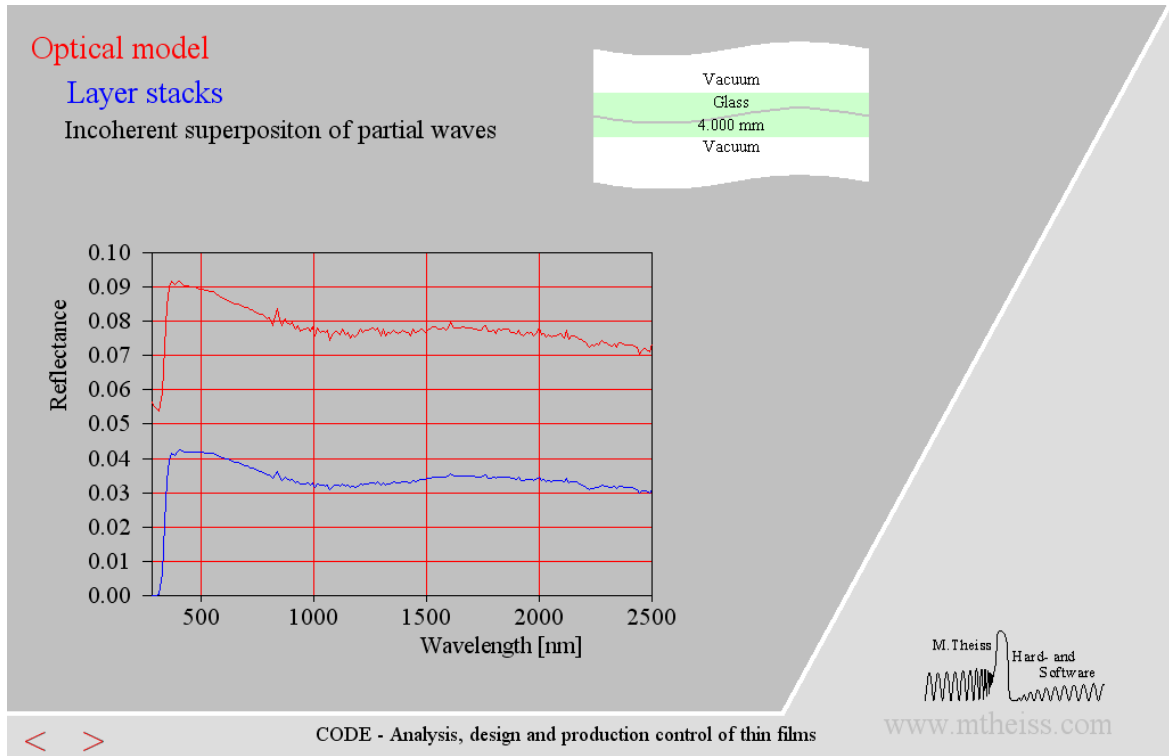
Thickness variation

Thickness distribution

Thickness variation

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For thick layers the incoherent contributions to R and T can be computed individually. Red curve in the following graph: All reflection orders superimposed. Blue curve: Backside reflection only:



3.2.3 What is the correct layer stack?


Optical model
Layer structure

Is the layer structure known and well-defined?
 Can we find a good optical model with the expected layer structure?
 If not, are we allowed to introduce additional layers to the model?

Typical cases:

- Surface roughness
- Mixing of adjacent materials at interfaces
- Depth inhomogeneity

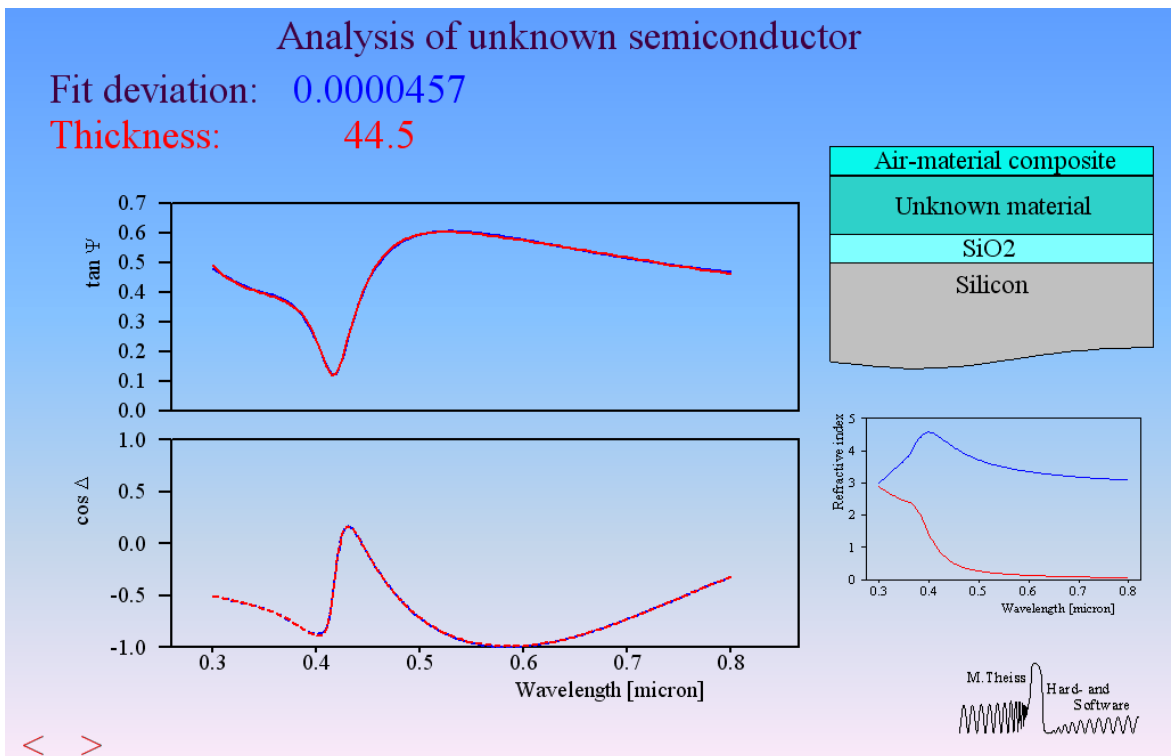
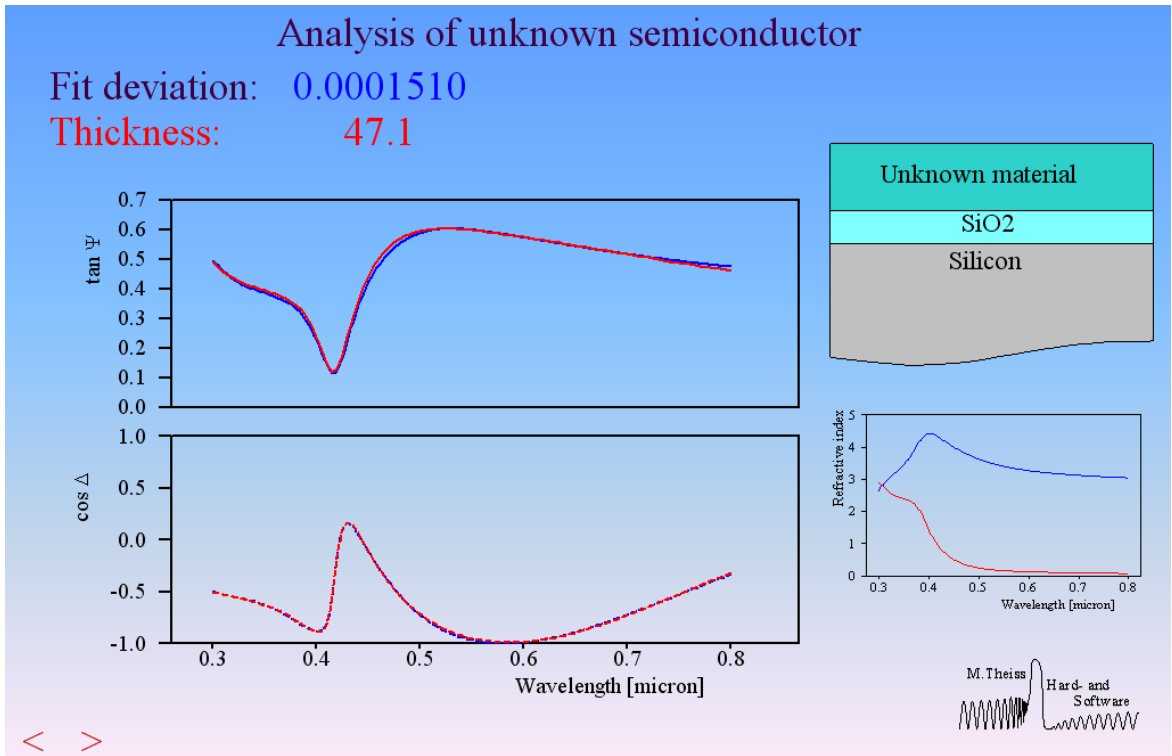
Do the additional layers influence the final results?
 Should the use of additional layers be reported to the producer?
 Should information about the additional layers be part of the results?

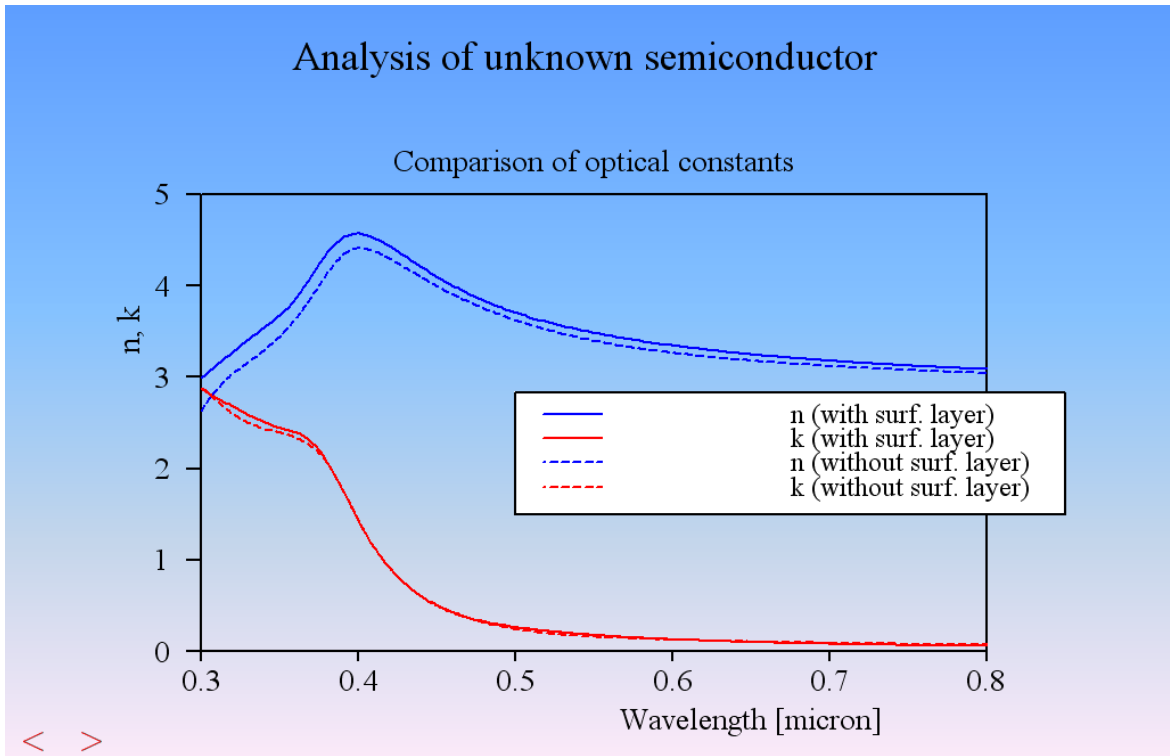


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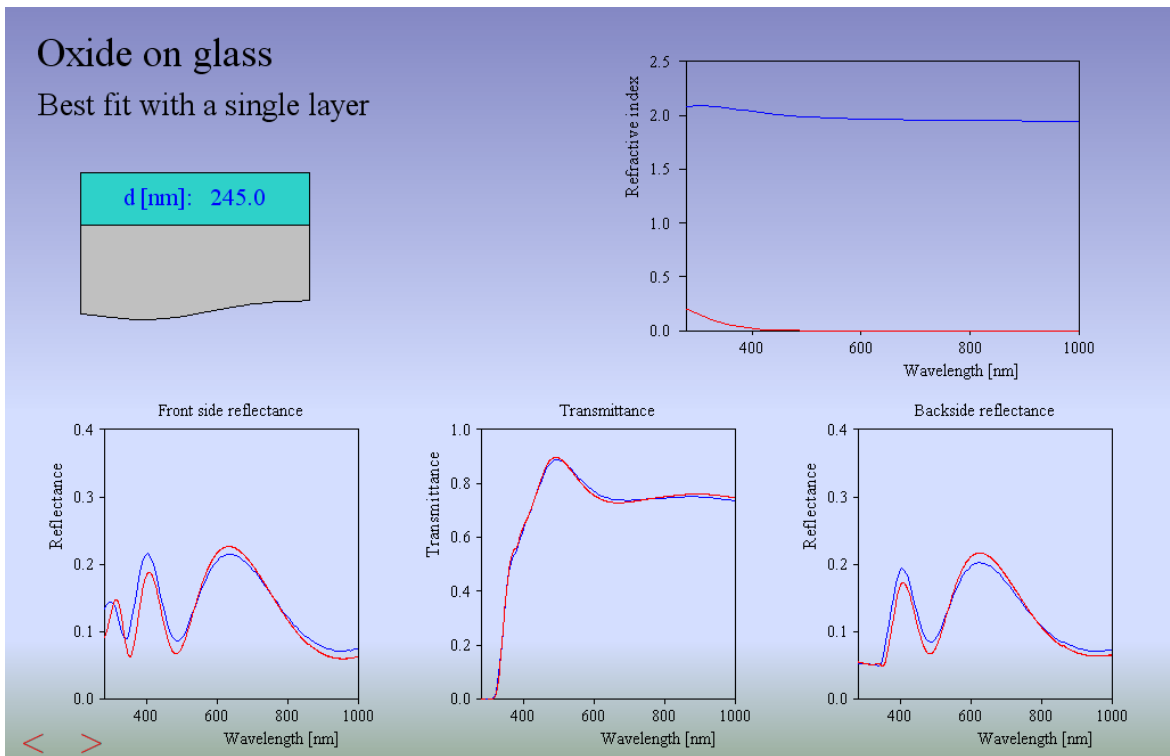
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Example: The next graphs show the influence of the introduction of a surface layer to the results of a `single layer analysis`. It is not easy to decide if the differences are significant if the roughness is always the same. However, if the roughness changes from sample to sample it should definitely be part of the model and part of the exported results.

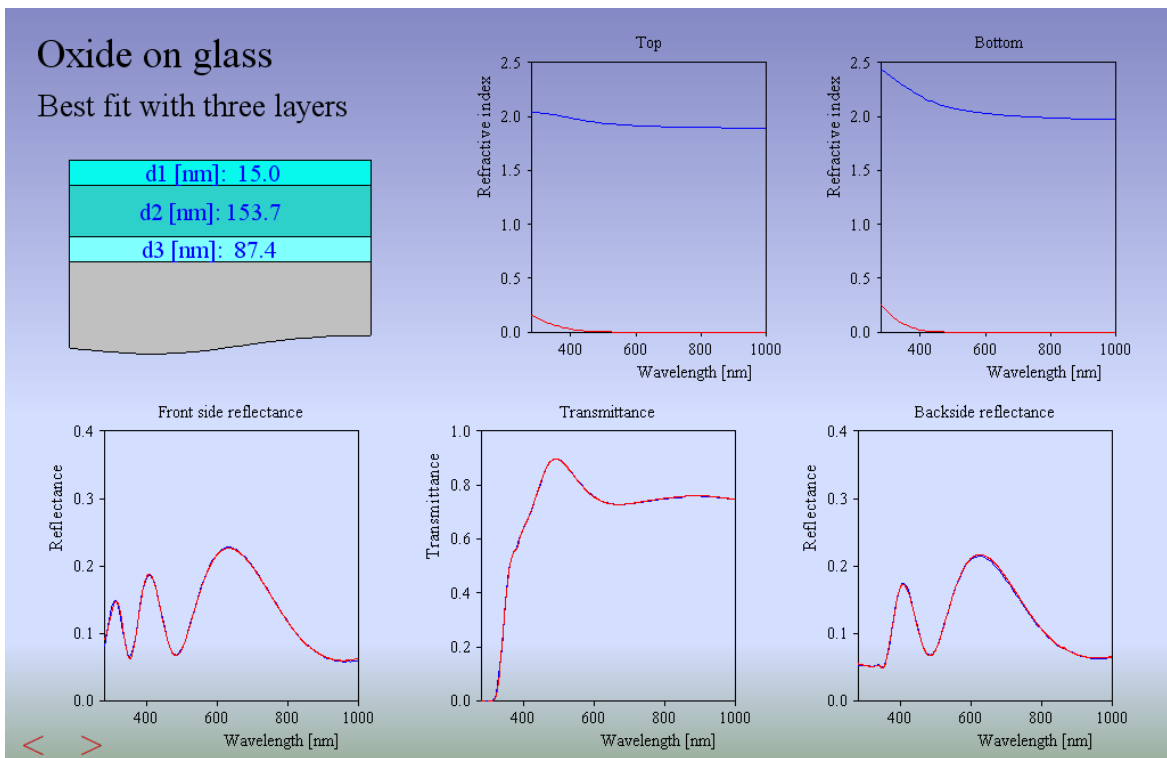
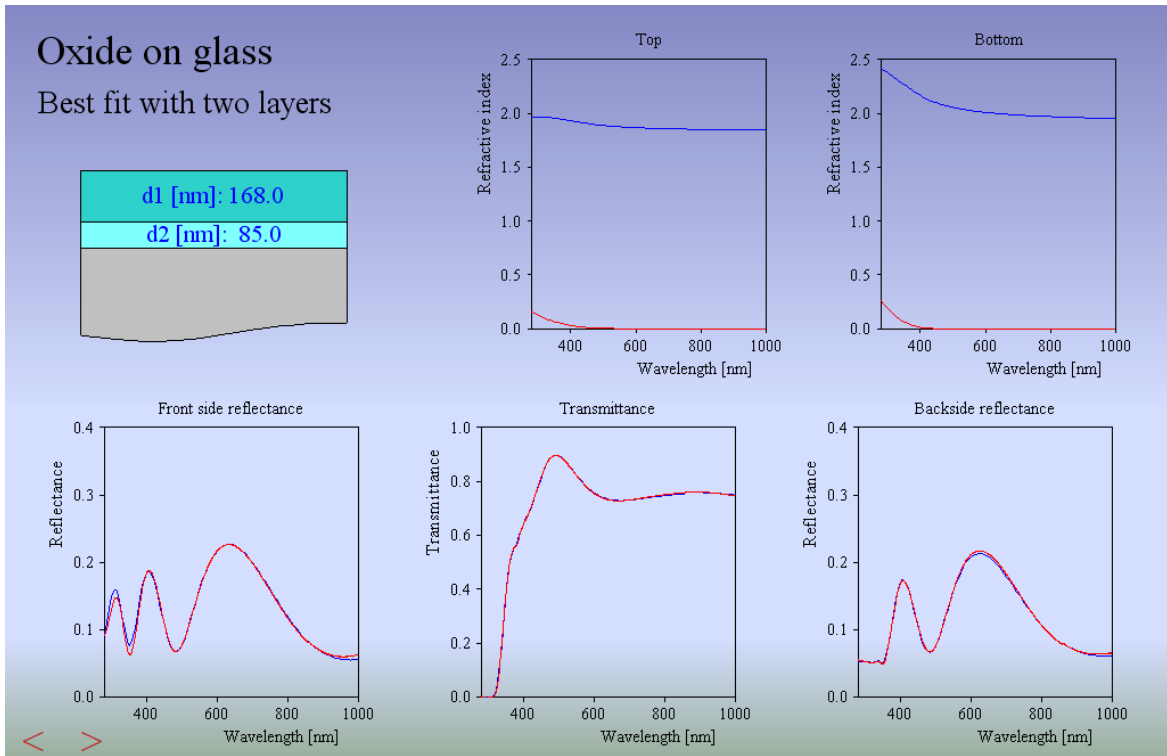




Here is another example: A customer asked for the optical constants of a single layer deposited on glass with a sputtering device. It turned out that even advanced optical constant models could not describe the optical properties of the layer properly.



Only introducing a depth inhomogeneity (and a surface layer) could solve the problem:



Communication with the producer finally verified the assumptions made in the successful fit:

Optical model
Layer structure

'Could it be that there is a depth inhomogeneity?'

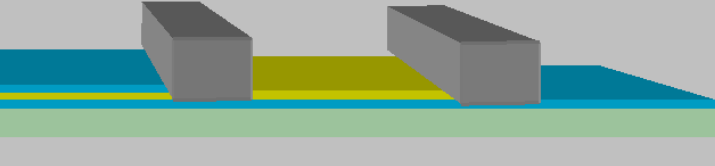

'Didn't I mention that we produce the layer with 3 cathodes?'

'Do all 3 cathodes produce the same composition?'

'Let's see, I'll look it up.'

'Well, cathode 1 had a lower oxygen pressure at that time.'

'Thank you for this important information!'

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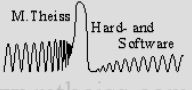
3.3 Spectrum types

Optical model
Supported spectrum types

CODE computes as many spectra as you like.
The following types are supported:

- Transmittance
- Reflectance
- Attenuated total reflection (ATR)
- Ellipsometry
- Photoluminescence

Arbitrary angle of incidence including backside illumination
S- and p-polarization, ideal unpolarized radiation
User-defined, wavelength dependent polarization
Lateral structures: Layer stack averaging



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4 Computation of technical data

Computation of technical data

Based on the optical model, various quantities can be computed:

Colors coordinates (D 65, A, C, 2°, 10°)

Color rendering index

Integral R and T values (vis., solar)

U (various filling gases in database)

g

Emissivity (normal, effective)

Front pane absorption

User-defined spectrum products

... more on request



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Light transmittance (D65)	67 %
Light reflectance (D65)	17 %
Light reflectance (D65) (Backside)	19 %

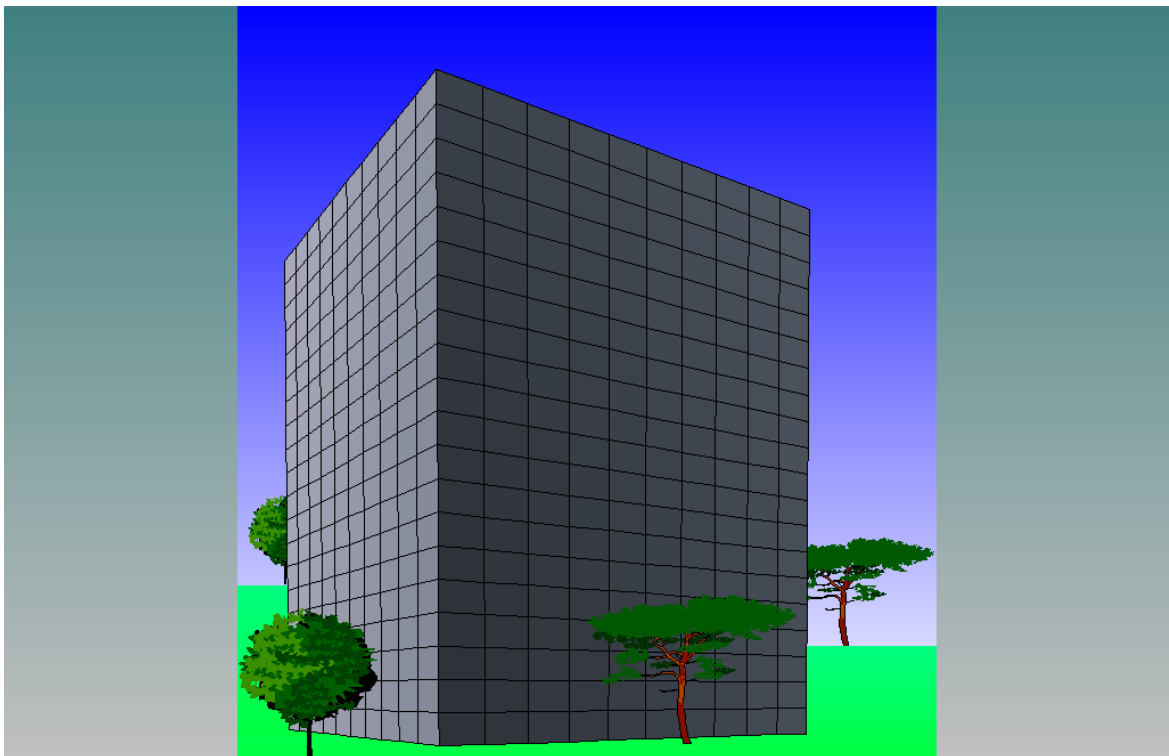
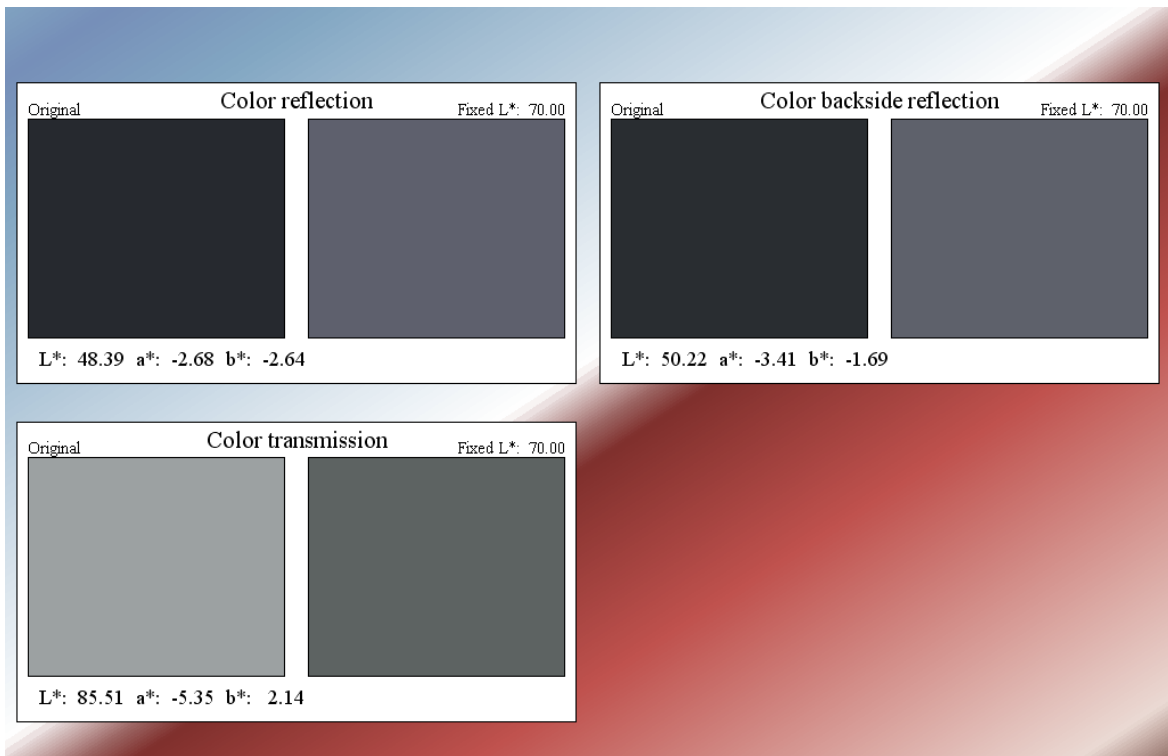
Direct solar reflection	33 %
Direct solar transmission	37 %
Front pane absorption	7 %

Ra (Transmission)	94
Ra (Reflection)	93

Ug (EN 673)	0.7
g (EN 410)	0.54
g (DIN 67507)	0.51

L* (Transmission)	85.51
a* (Transmission)	-5.35
b* (Transmission)	2.14

L* (Reflection)	48.39
a* (Reflection)	-2.68
b* (Reflection)	-2.64



5 Remote control by OLE automation

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Remote control by OLE automation

- CODE is an OLE server
- Typical clients: VisualBasic (Excel), LabView, C++, Delphi, ...
- Program your customized spectrum simulation solution

Prepare appropriate CODE configurations

Select parameters to be controlled as fit parameters

Program your computational scheme

Set CODE parameters, re-compute model, retrieve results

Example: Virtual online analysis in VisualBasic

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The Excel example shows how spectra can be sent to SCOUT which are then automatically fitted. The results are passed back to an Excel worksheet.

6 Batch processing

Fit and design

Automatic batch fit of many input spectra

Optical model and fit strategy ready and tested:

Investigate many samples in batch operation

- Define network path and file formats
- Set filenames for every sample
- Press 'Go' button
- Pick up results

Simple example: Thickness determination of Ag layers on glass

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CODE can analyze series of input spectra automatically in a batch process. Enter the filenames and the import filter to be used and start the batch fit operation in the batch control window:

SCOUT batch fit control

File Copy Paste Autosize cells Test Prepare Go! Actions

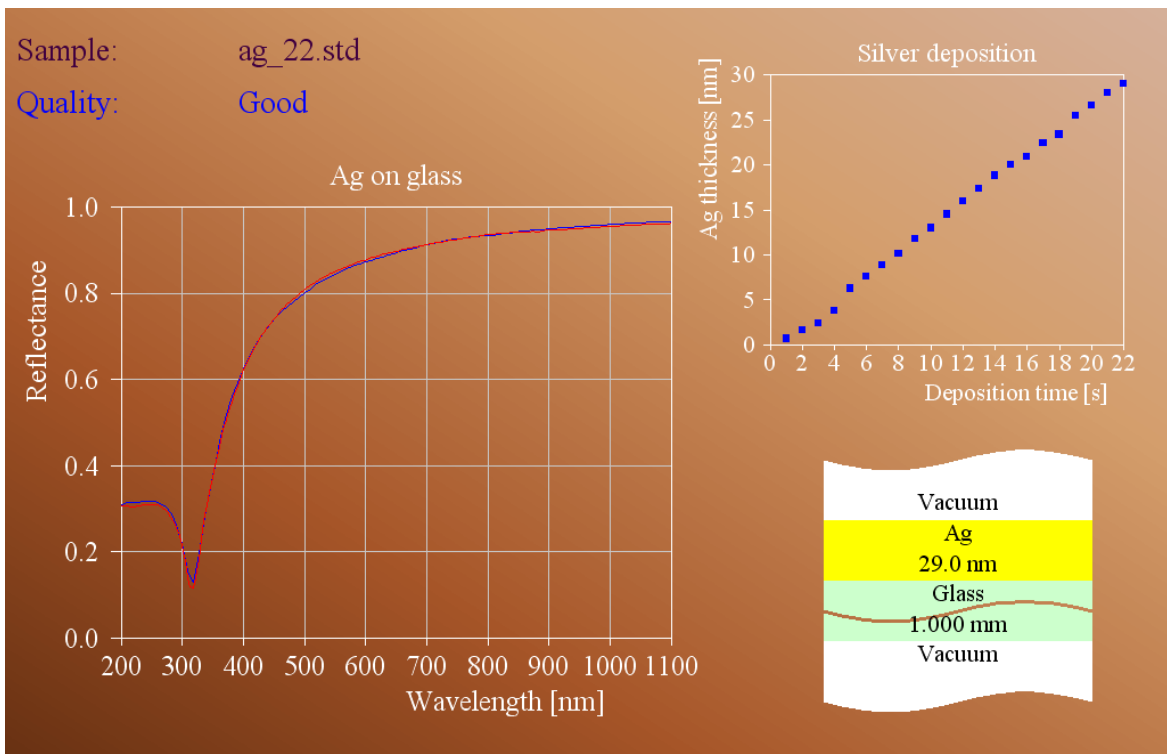
SC2 --> WB FP --> SC2 SP --> SC2 FP+SP --> SC2

A1 Sample

	A	B	C	D	E	F	G	H	
1	Sample								
2	Name	ag_1.std	ag_2.std	ag_3.std	ag_4.std	ag_5.std	ag_6.std	ag_7.std	ag
3	Deposition time	1	2	3	4	5	6	7	
4									
5	Spectra								
6	Reflectance	ag_1.std	ag_2.std	ag_3.std	ag_4.std	ag_5.std	ag_6.std	ag_7.std	ag
7									
8	Fit								
9	Pre-fit set	Set 1	Set 1	Set 1	Set 1	Set 1	Set 1	Set 1	Se
10	Fit deviation								
11									
12	Fit parameter sets								
13									
14	Parameters								
15	Ag thickness								
16									
17	Functions								
18									
19									
20									

Results Input options Pre-fit

The results can be displayed directly in a view:



7 Analysis and design

7.1 Fit strategy

Once the optical model is ready, one must decide which parameters may vary from sample to sample. These parameters must be determined following a fit strategy that leads to stable and reproducible results in the specified time frame.

Fit and design
Fit strategy

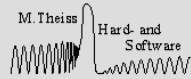
How can we get correct results as fast as possible?

Optimization of several parameters

Production control: Finite time interval for analysis
Conflict: Avoid local minima of the fit deviation <----> speed

Gain speed using

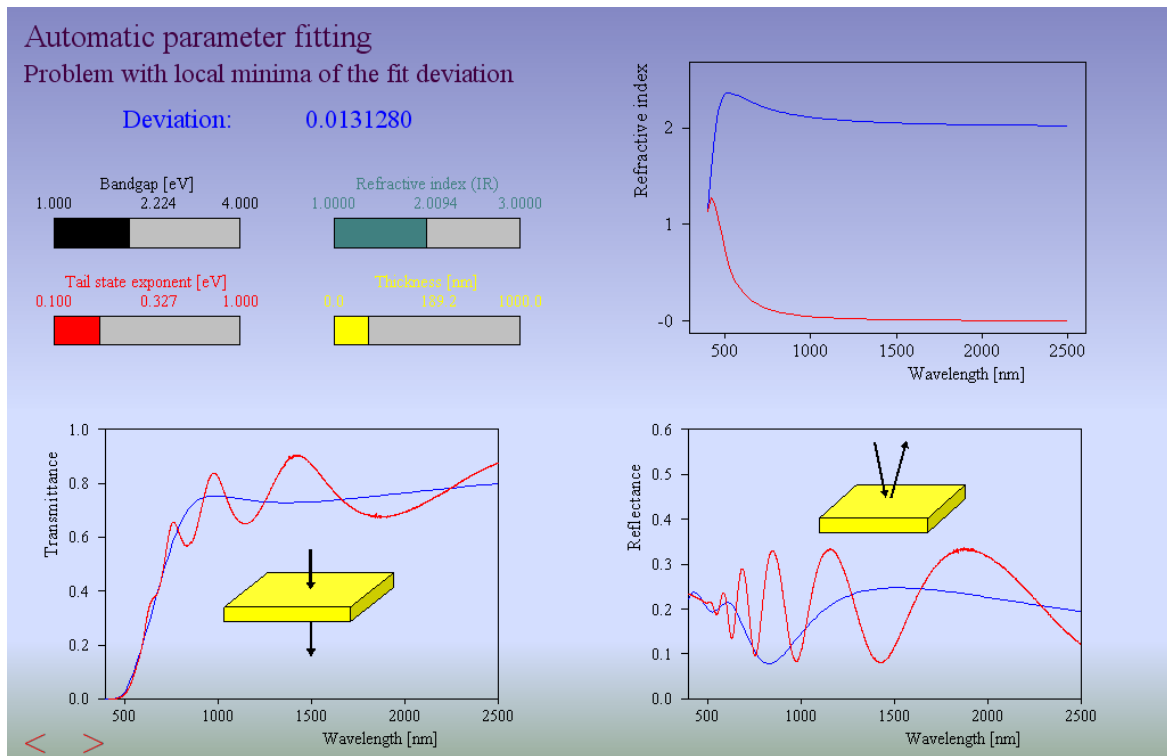
- Reasonable number of data points
- 'Fit on a grid'
- Appropriate sequence of fit parameter sets

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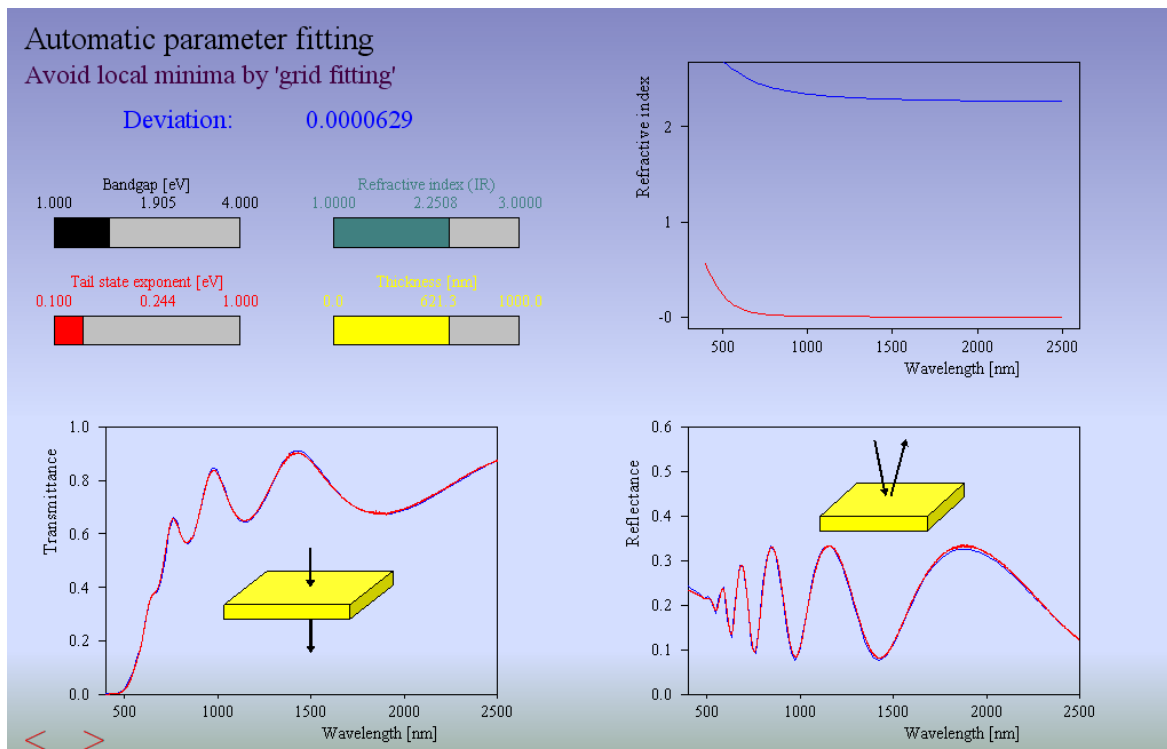
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Multiple parameter optimization is a common problem of numerical mathematics. One of the main issues is to avoid that algorithms get stuck in local minima of the fit deviation. Methods like simulated annealing or genetic algorithms which overcome the local minimum problem are much too slow to be used for production control.

Here is an example of a SCOUT fit running into a local fit deviation minimum: A start value of the layer thickness far away from the correct value drove the model into the wrong interference fringe order.



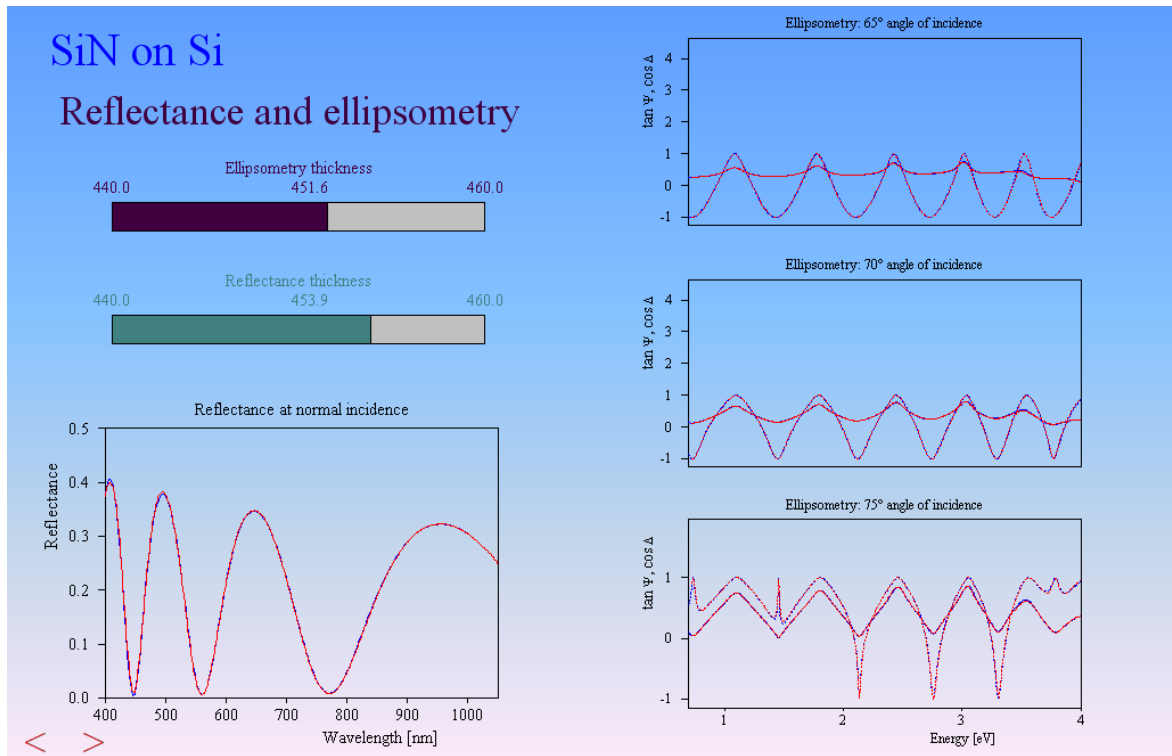
Using the 'grid fit' feature of SCOUT this problem can be overcome very efficiently: Before the multiple parameter fit is started, the right fringe order is found by trying several thickness values (equally spaced in a user-defined thickness range) and taking the best result as starting value for the thickness.



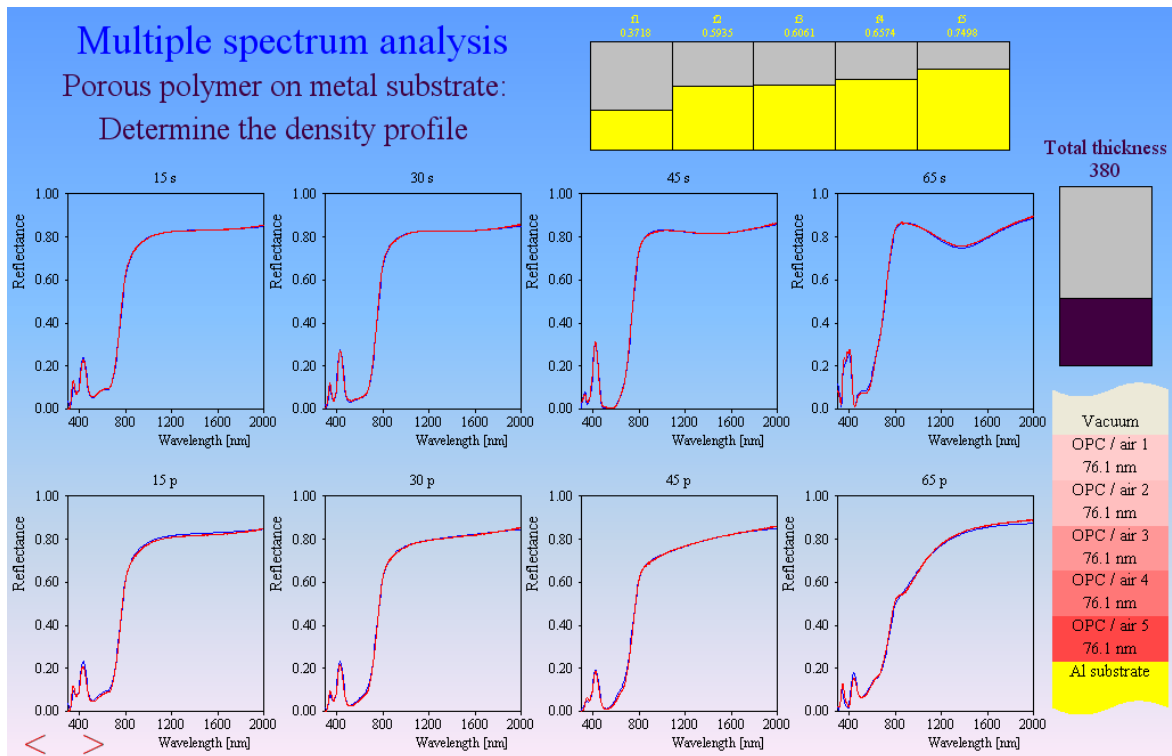
In many cases advanced fit strategies using so-called fit parameter sets are successful: Separate the fit parameters into groups which are optimized one after the other. You can, for example, fit the thickness and the refractive index of a material in a spectral region where the layer is transparent. Then freeze the parameters, and determine bandgap and other interband parameters in a spectral range with strong absorption. Then, in a final step, all parameters are optimized using the full width of the spectral data. Separating the problem into smaller pieces can speed up the optimization procedure significantly.

7.2 Examples

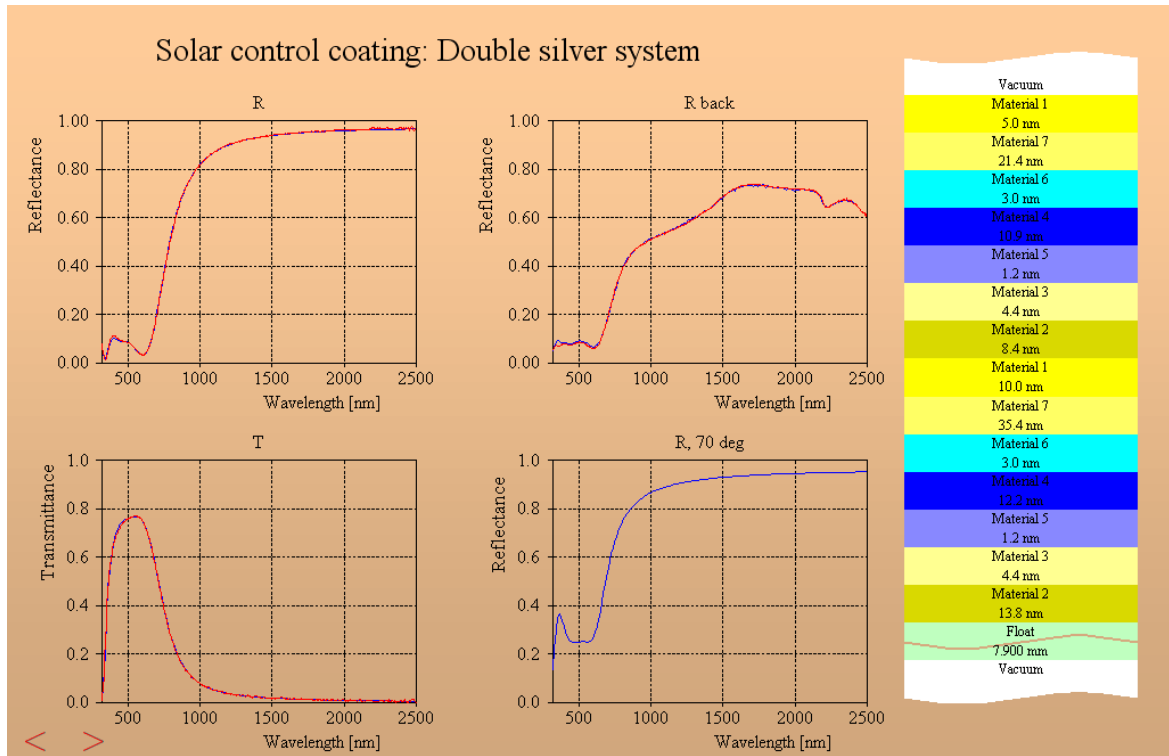
Fitting three ellipsometry and a reflectance spectrum. Since the investigated sample spot is not exactly the same in both experiments two different layer stacks are used in the model:



Here 8 spectra are fitted simultaneously:



Quantitative description of a solar control coating:



7.3 Design

Fit and design

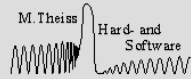
Define or import target spectra, fit like measured data
 Create spectra with Data Factory tool or built-in functions

Technical data can be fit targets as well

Investigate relations using

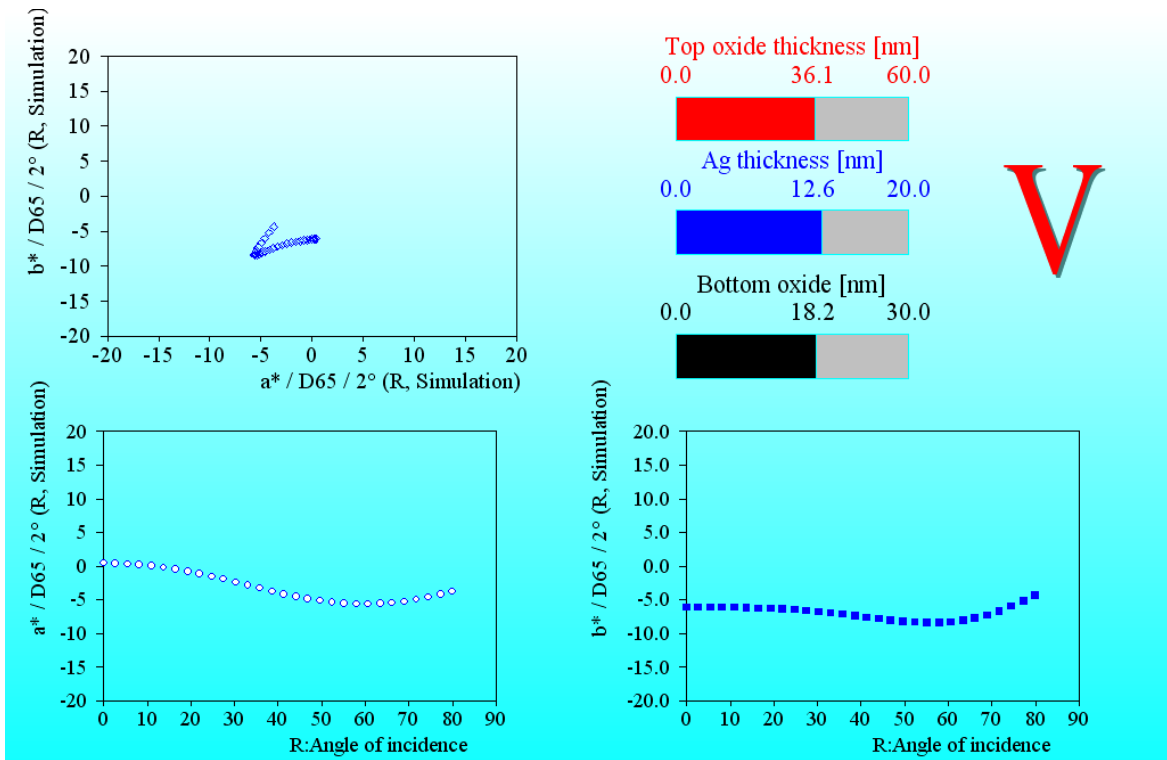
- Parameter animation
- Parameter variation
- Parameter fluctuation

Use OLE automation for user-defined strategies

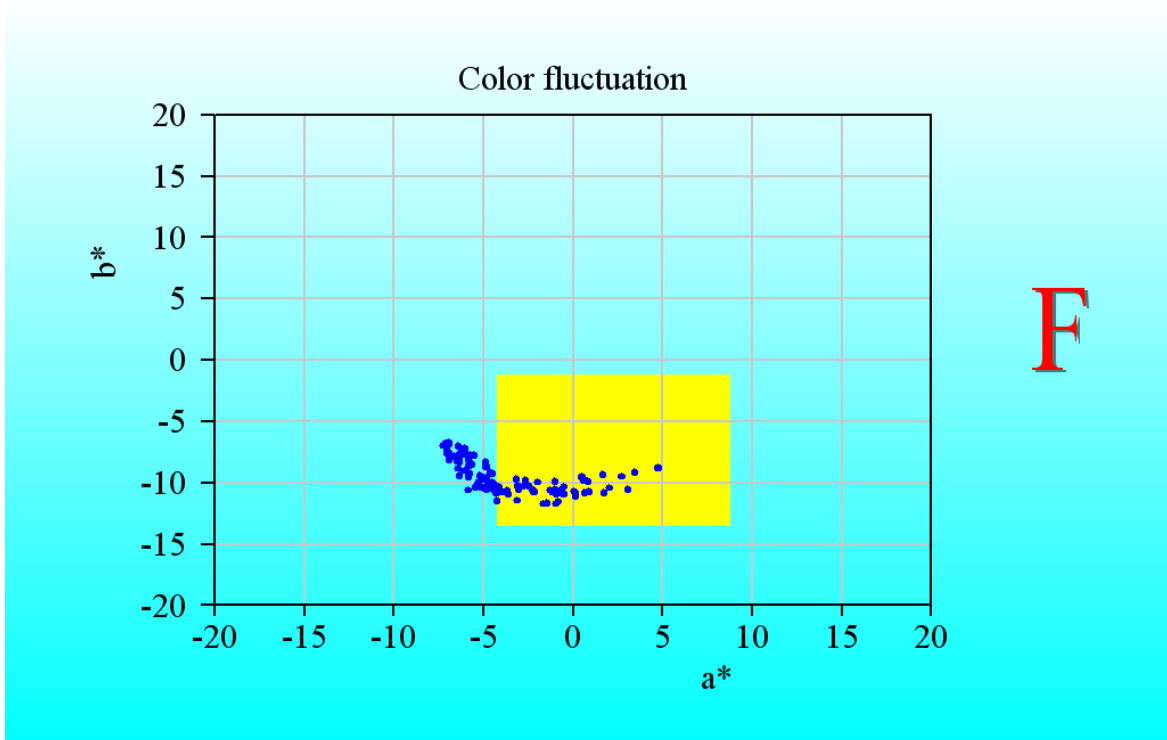
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Investigate the influence of the variation of a model parameter (e.g. a film thickness) on the coating properties using the parameter variation feature. Here the angle of incidence is varied and the color of a coating in reflection is inspected:

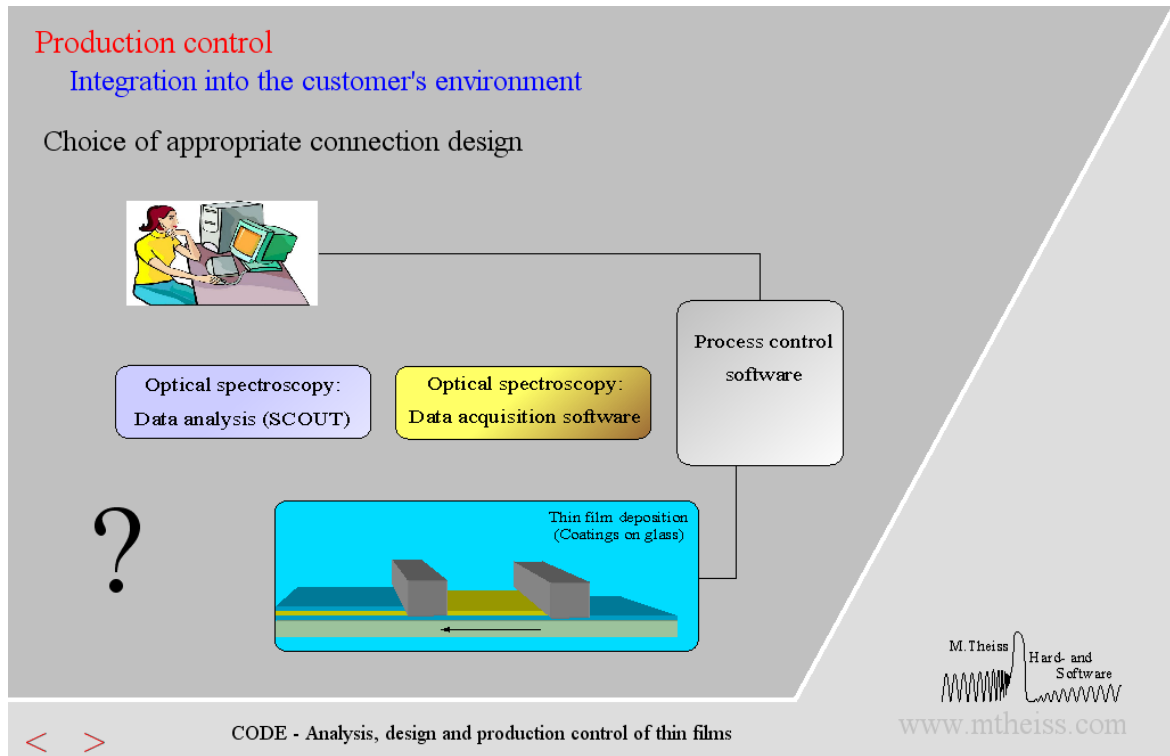


The parameter fluctuation feature computes the variation of technical data and spectra in the presence of random parameter fluctuations. This can be used to simulate the effect of production tolerances, for example:

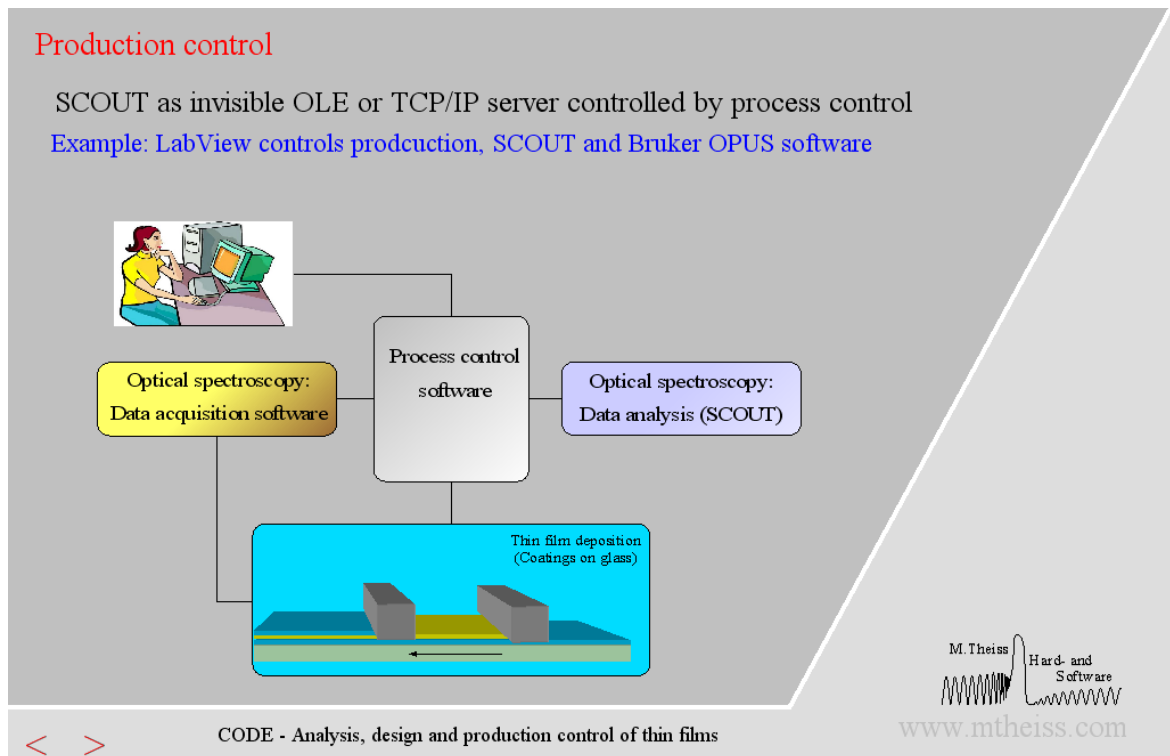


8 Production control schemes

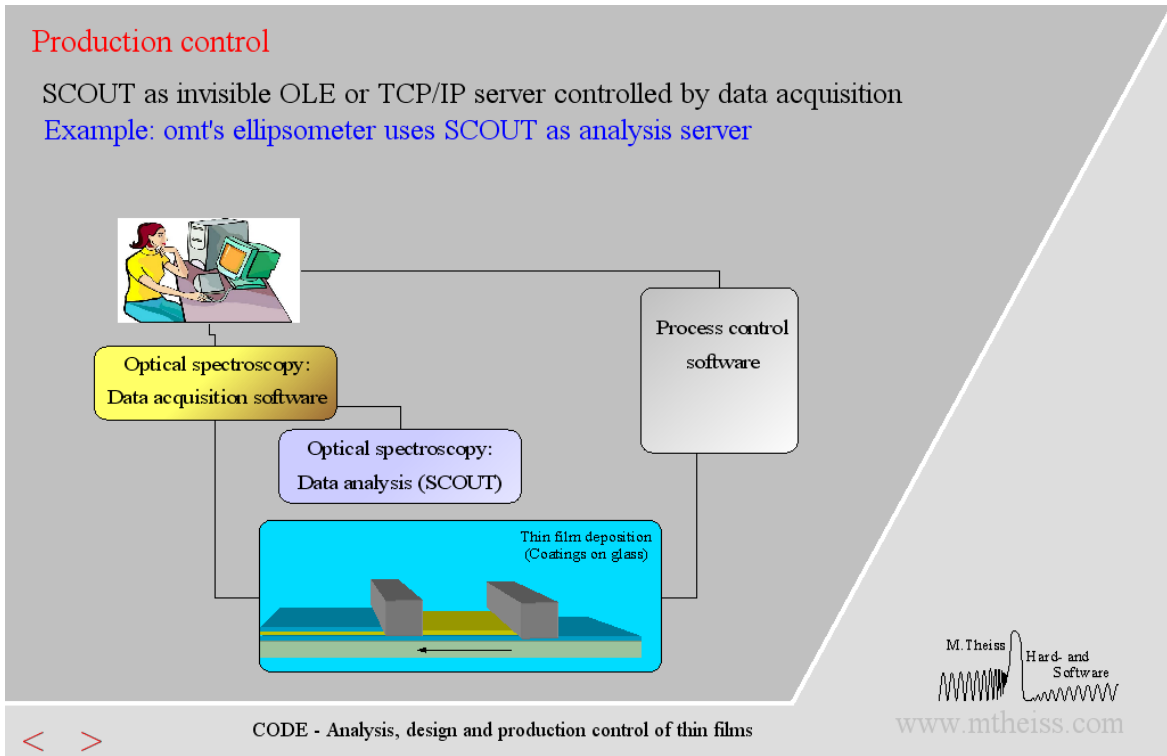
Now the method must be brought to the factory. The first question is how the various programs involved in the problem should be connected:



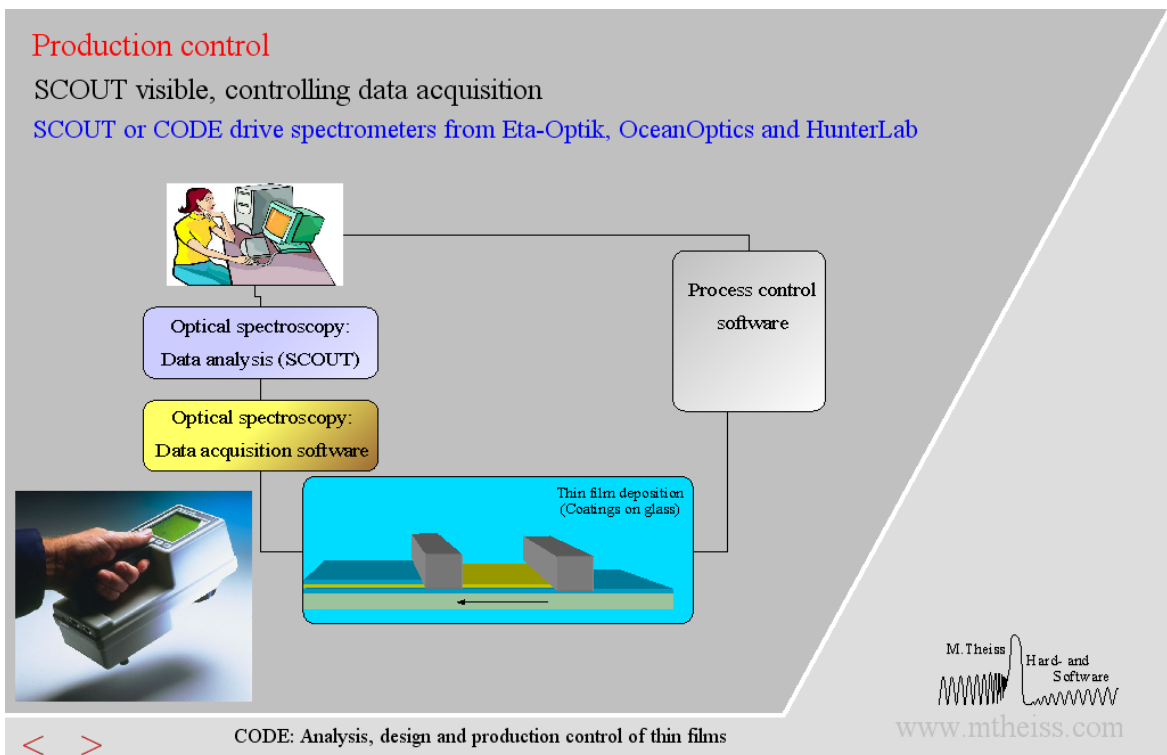
With SCOUT, several options are possible. The following example shows a configuration where both SCOUT and the data acquisition are controlled by the process control software. SCOUT can be accessed as OLE server or by TCP/IP communication.



The optical analysis can also be completely independent of the process control software:



SCOUT can also be used to control spectroscopic hardware and display results. In this case an appropriate user interface must be developed.



Once the decision concerning the factory configuration is made, the required hardware and software installations are to be done and the proper data exchange between all involved programs and computers must be established and verified.

9 Program development, training, consultancy work

CODE - Analysis, design, production control of thin films

If you miss something ...

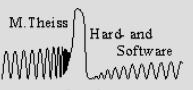
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Thank you for listening!

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