M.Theiss Hard- and Software for Optical Spectroscopy
Dr.-Bernhard-Klein-Str. 110, D-52078 Aachen
Phone: (49) 241 5661390 Fax: (49) 241 9529100
E-mail: theiss@mtheiss.com Web: www.mtheiss.com

CODE
Analysis, design, production control of thin films

by Wolfgang Theiss

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Table of Contents

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.

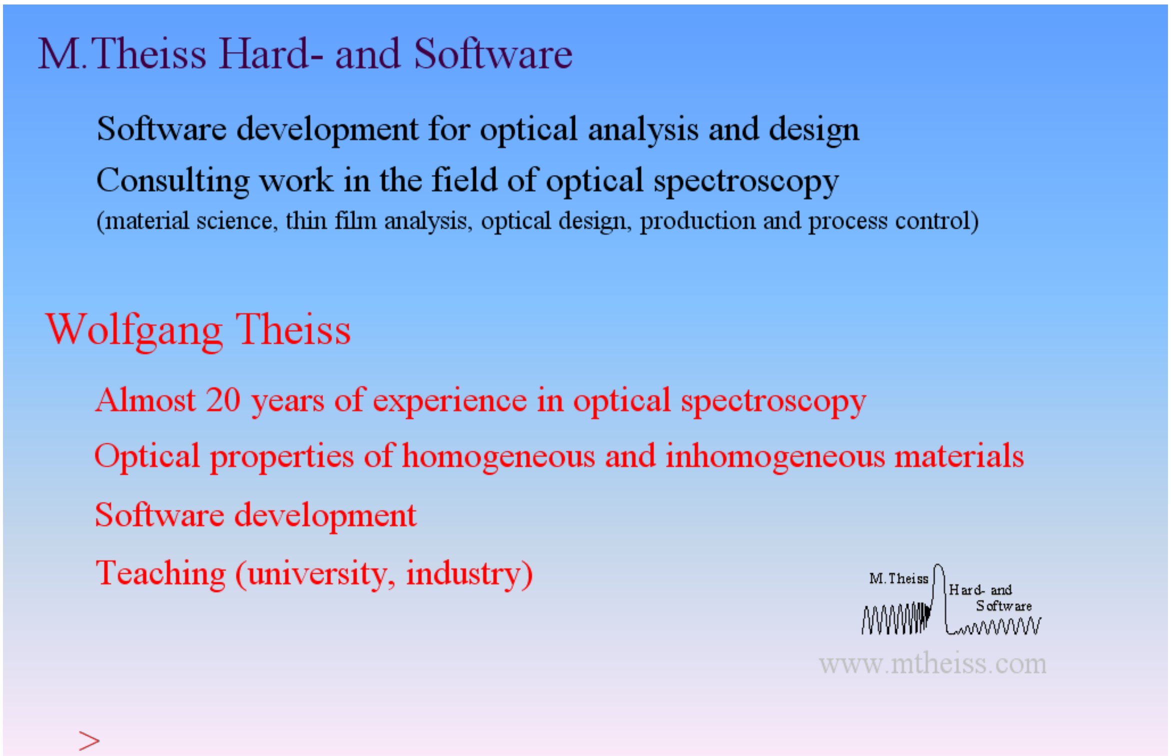
In the graphs displaying optical constants the real part is drawn blue, the imaginary one is given in red.
In the case of spectrum fits, the measured spectra are always in red, the simulated spectra in blue.

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

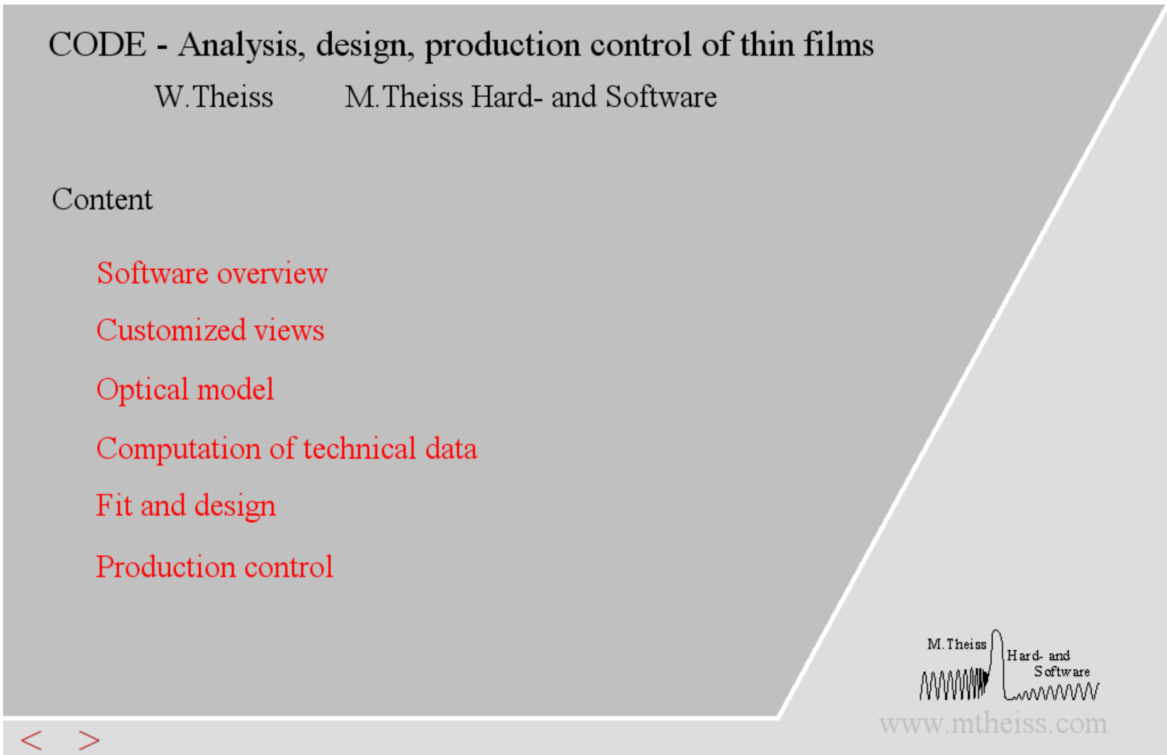
Aachen, March 2004

1 Overview

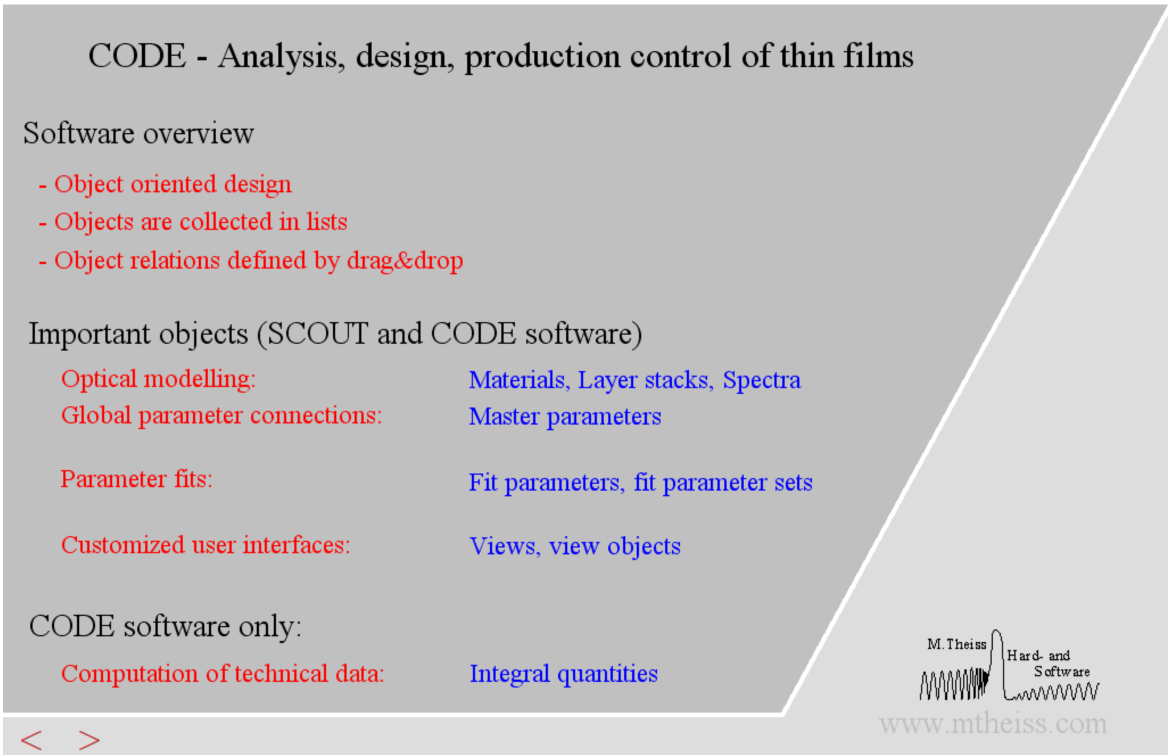
1.1 The company



1.2 The talk

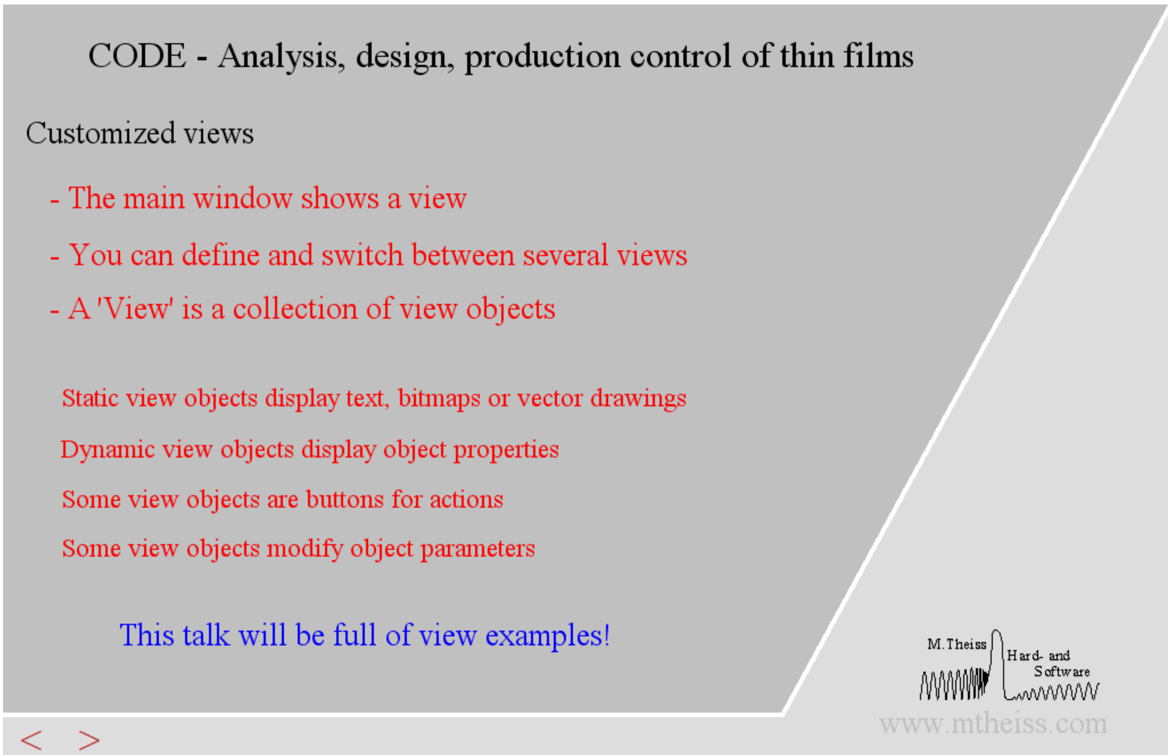


1.3 The software



2 Customized views

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

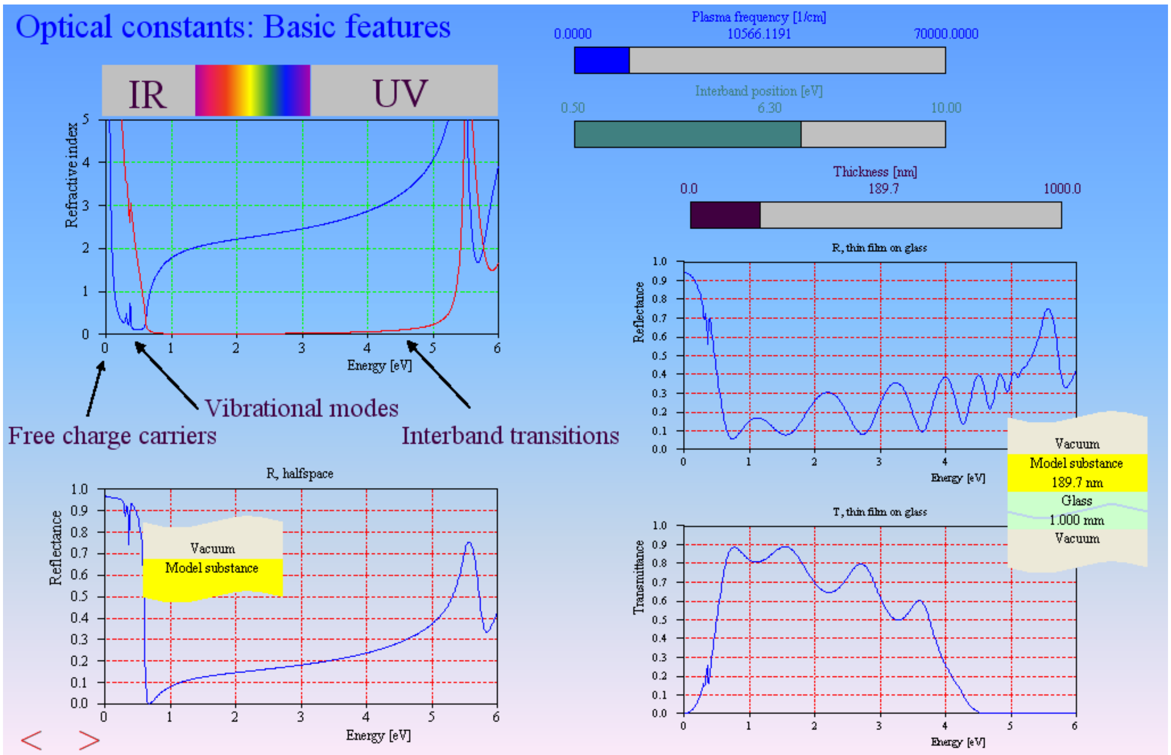


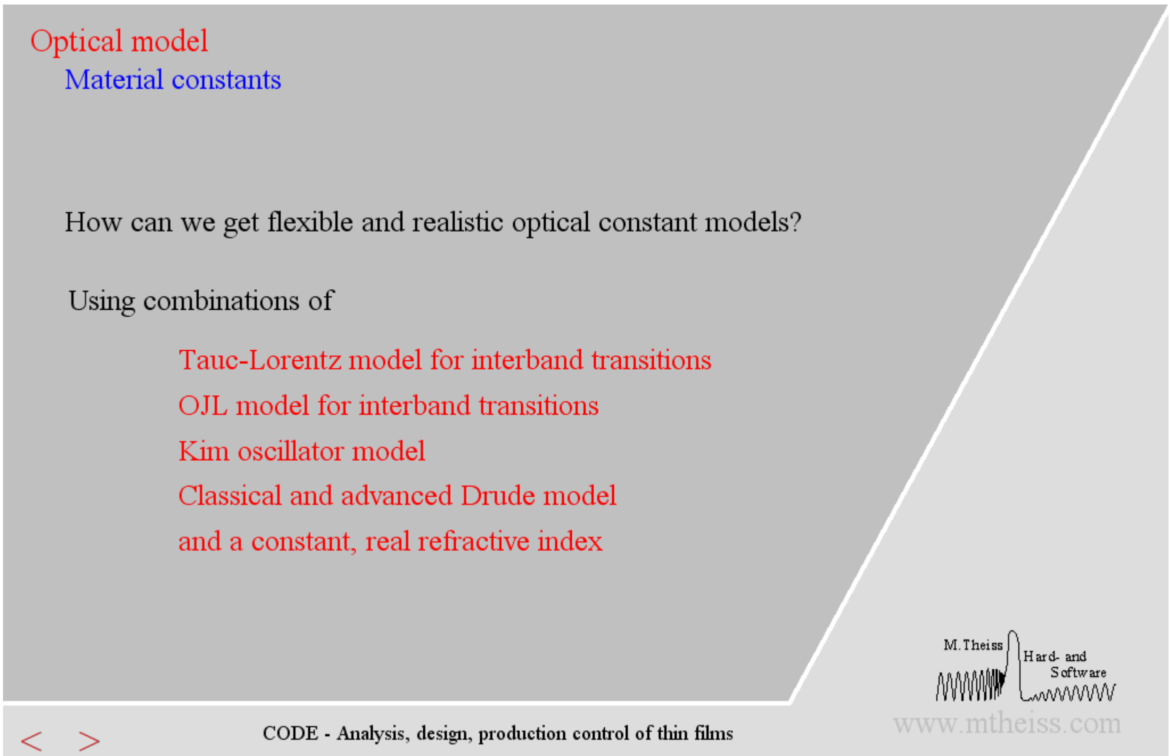
3 Optical model

3.1 Material constants

3.1.1 Optical constants: Overview

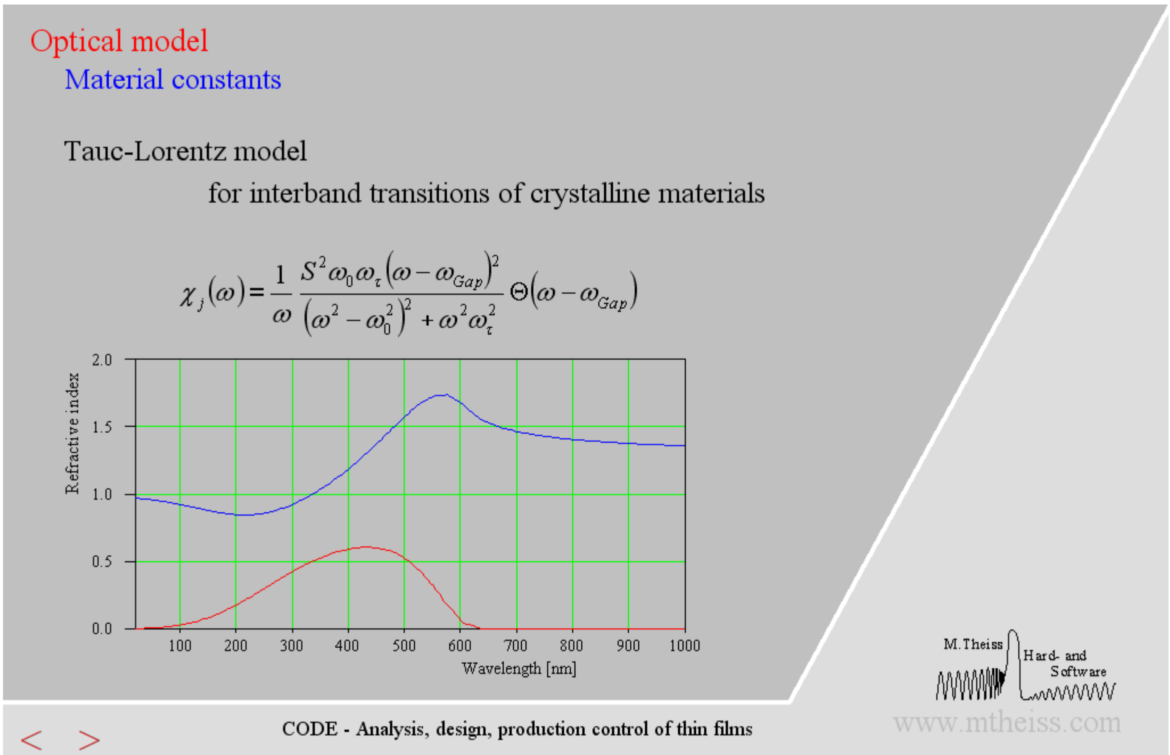
Three basic types of excitations determine the optical constants of almost all materials:



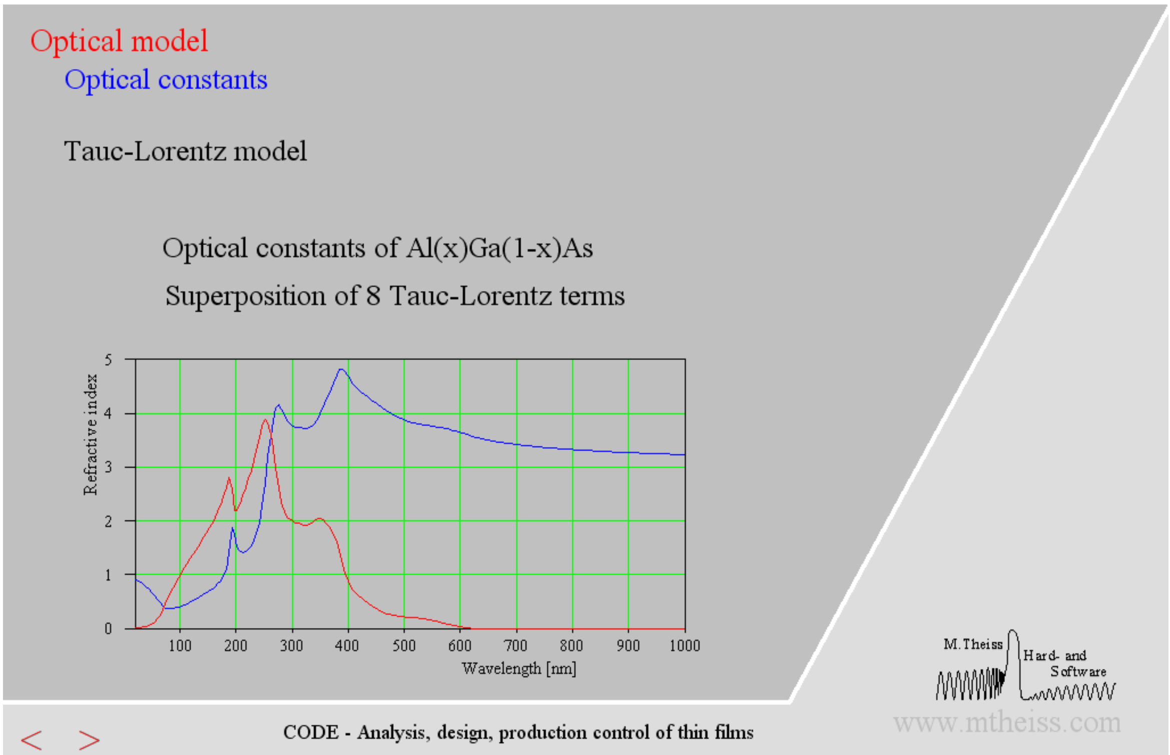


3.1.2 Interband transitions

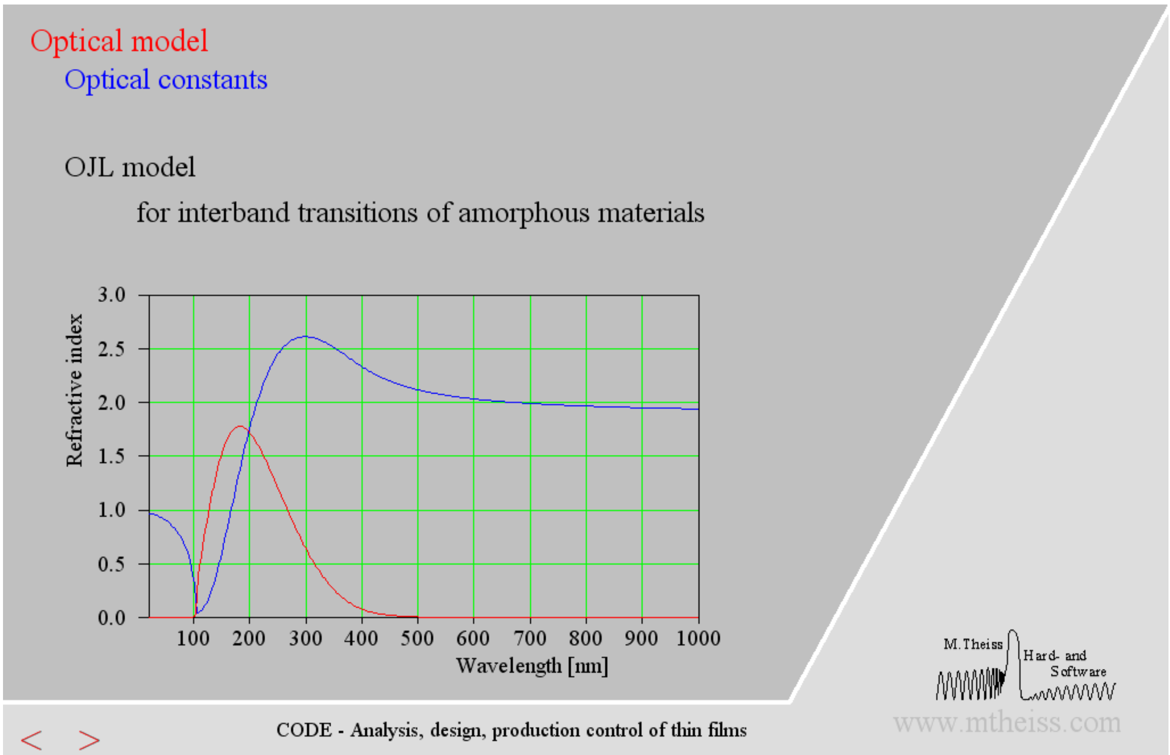
Interband transitions of cystalline materials can be descibed using the Tauc-Lorentz model:



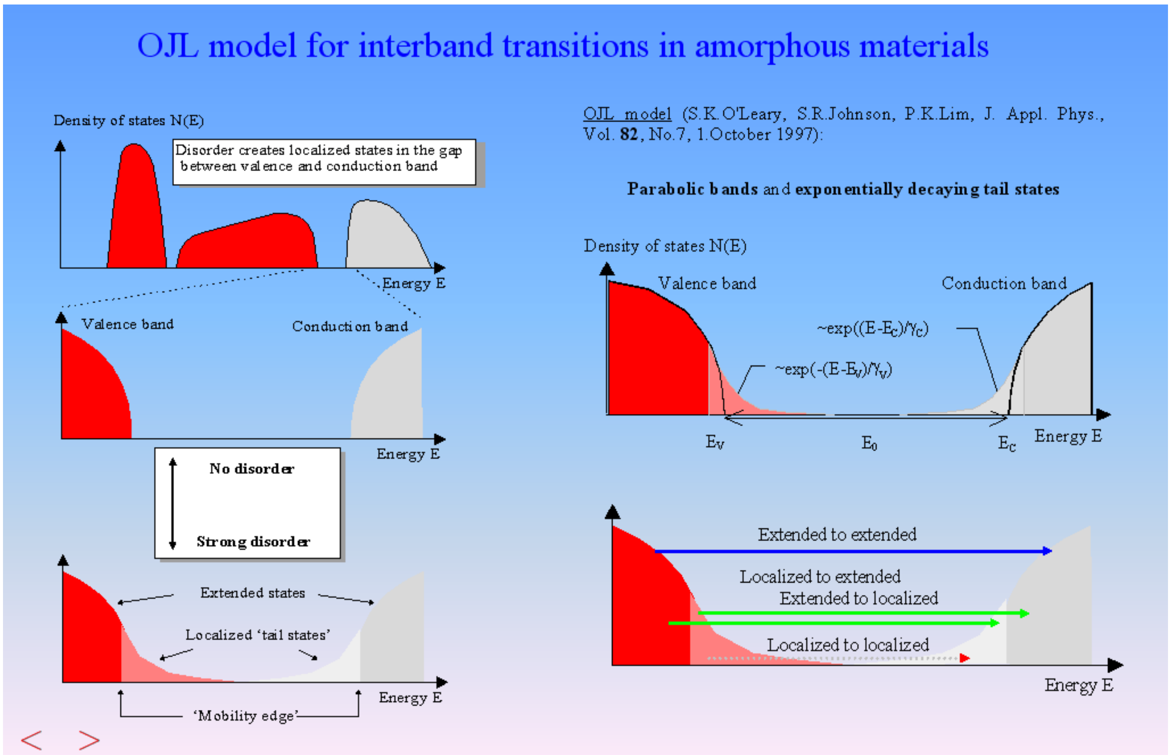
Here is a typical example using the superposition of 8 interband transitions:



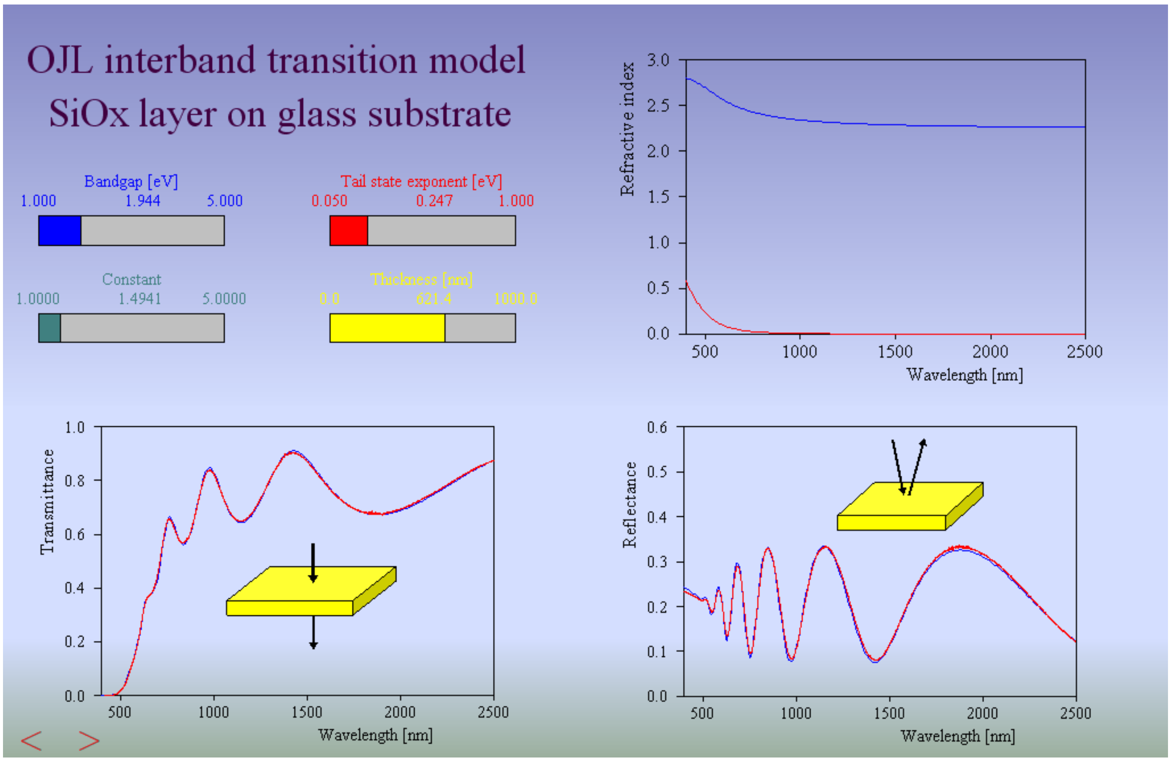
Amorphous materials have less rich featured, broad interband transitions which can often be described in good quality using a single OJL model:



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

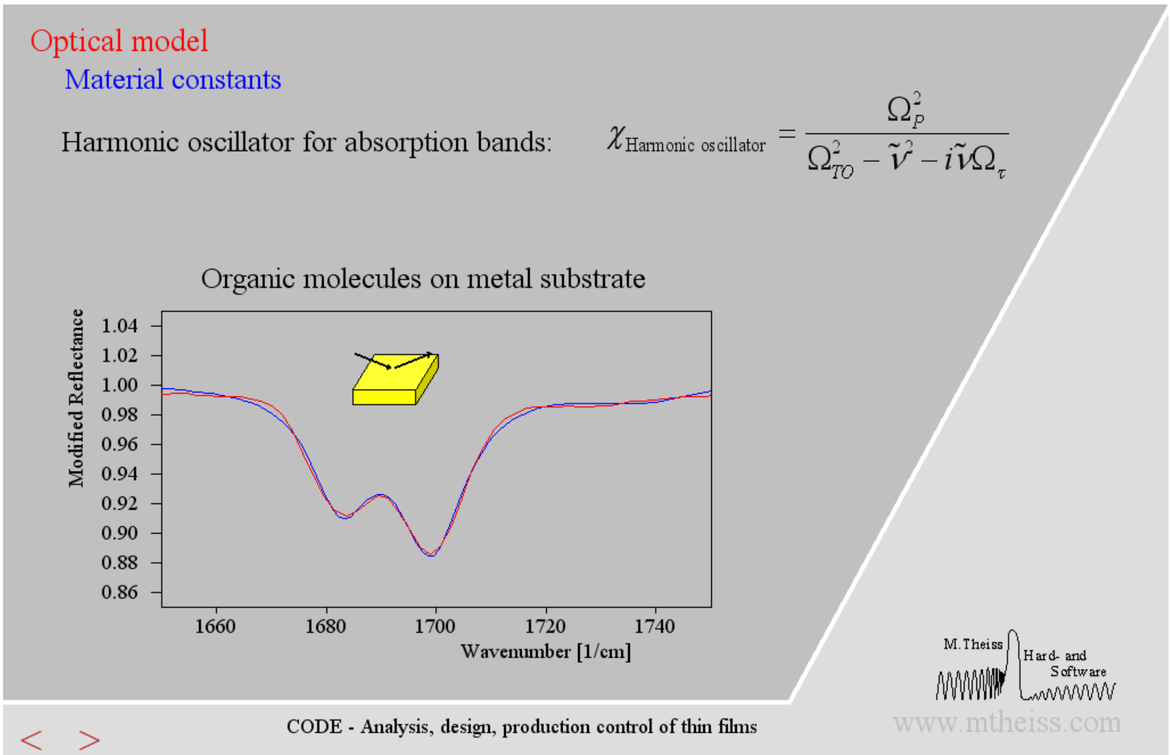


Here is an example of a succesful application of the OJL model:

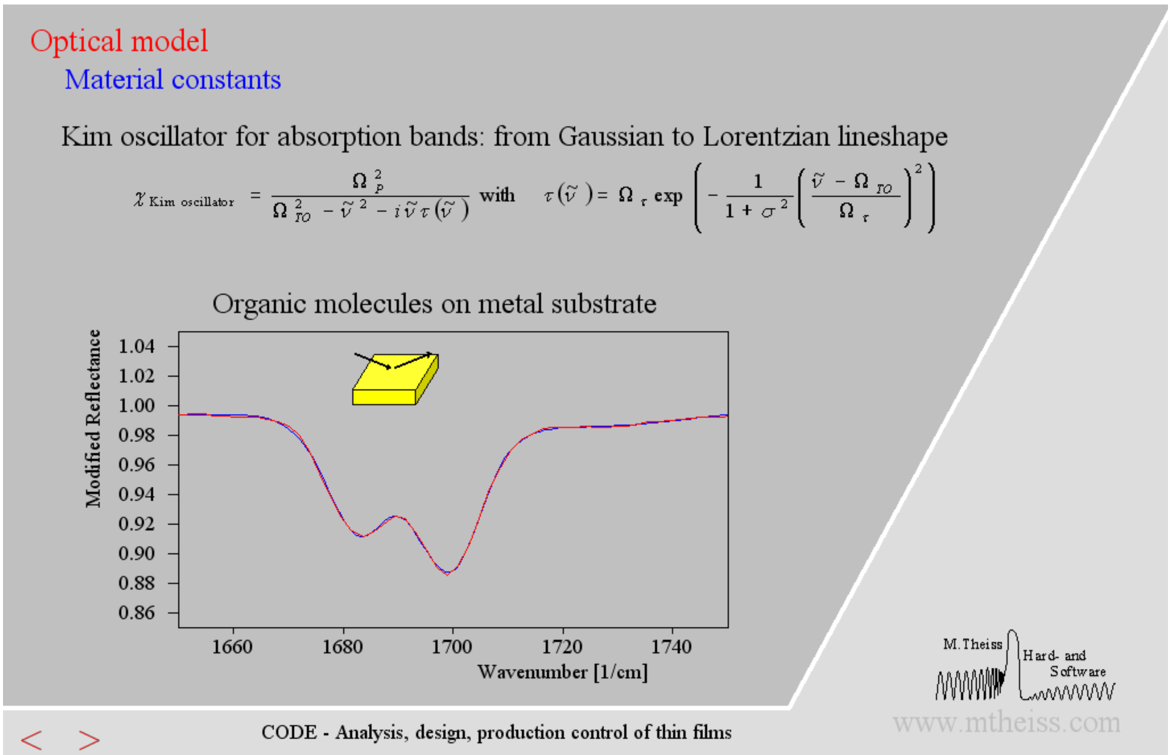


3.1.3 Vibrational modes

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:

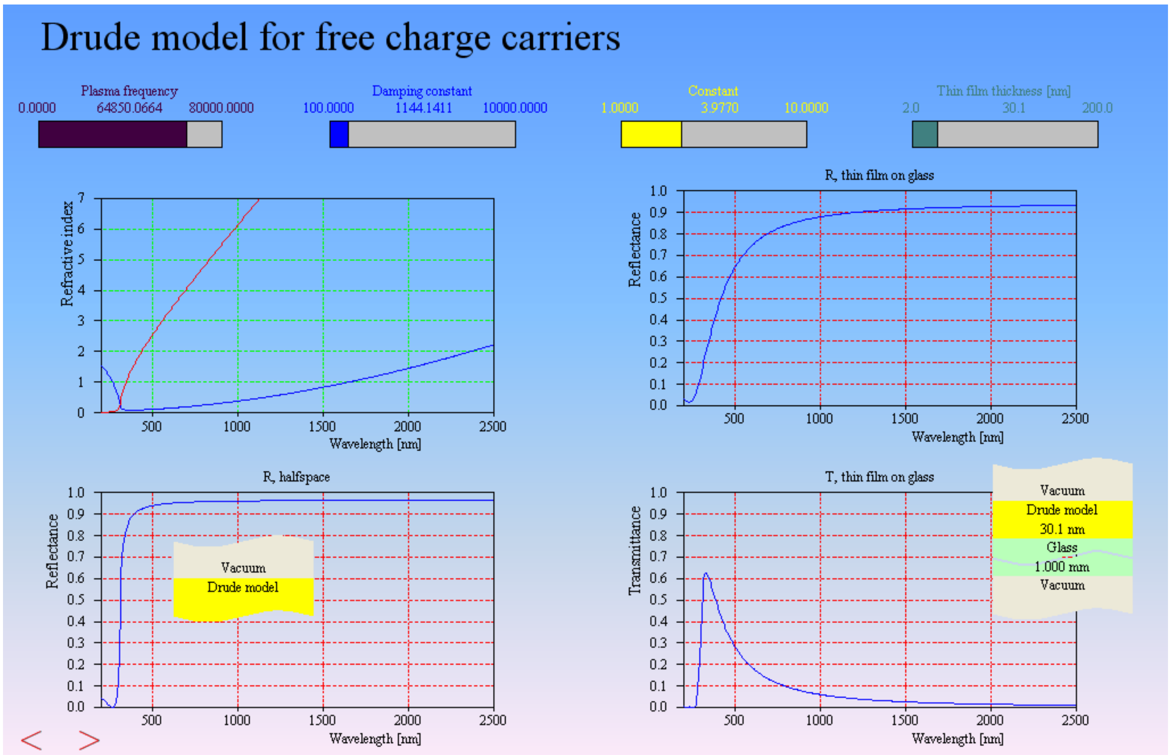


However, in most cases a Gaussian line shape is more realistic. In SCOUT and CODE this can be obtained using Kim oscillators:



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.

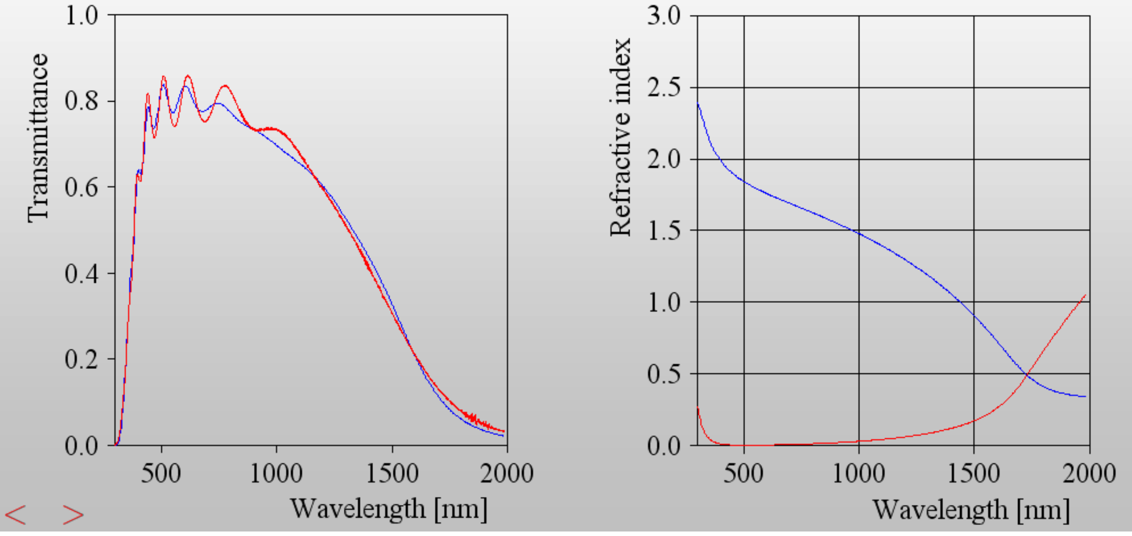


The following example shows that the simple Drude model does not always perform excellently:

Drude model

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

$$\chi_{Drude}(\omega) = -\frac{\Omega_{Dr}^2}{\omega^2 + \Gamma_{Dr}^2} + i\frac{\Gamma_{Dr}}{\omega}\frac{\Omega_{Dr}^2}{\omega^2 + \Gamma_{Dr}^2}$$

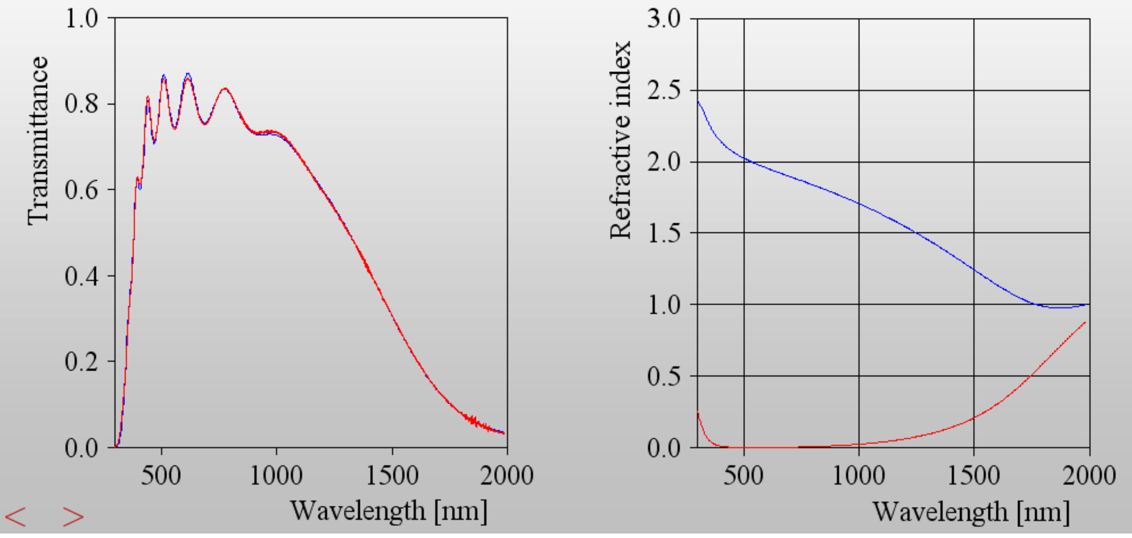


In cases like this you can try an extension of the Drude model which features a frequency-dependent damping constant. Electron scattering at charged donor or acceptor atoms may lead to a characteristic frequency dependence of the damping constant in the Drude model:

Extended Drude model

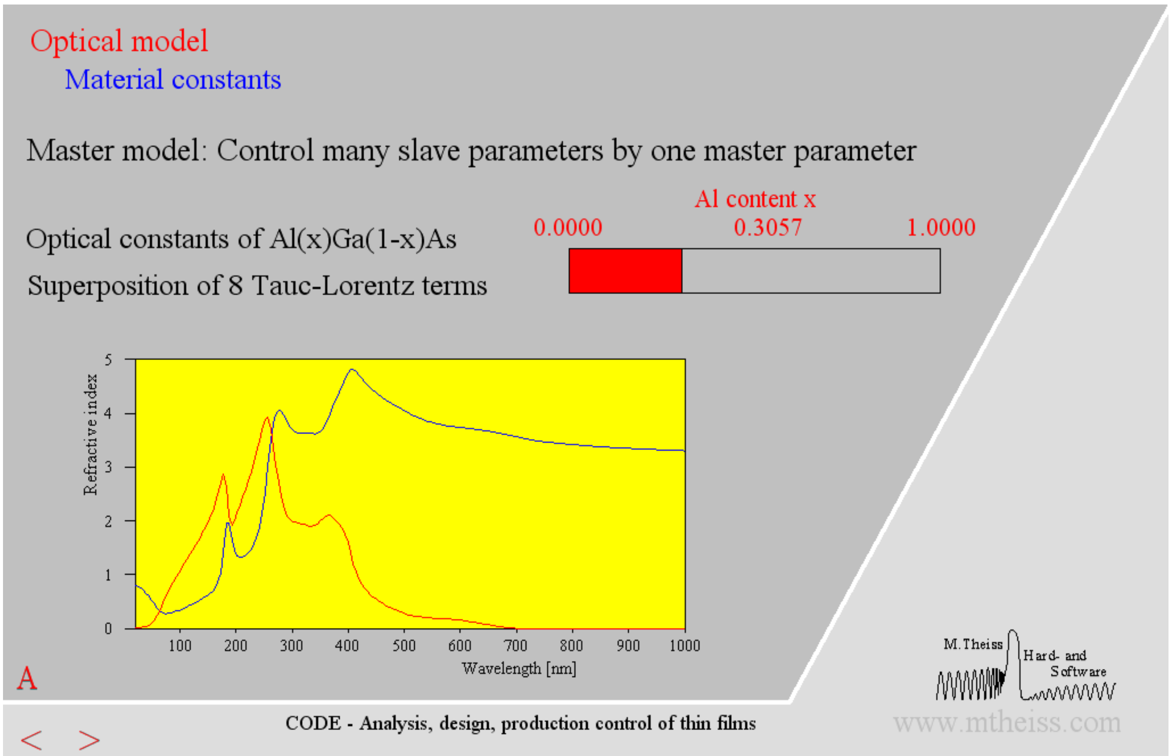
ITO on glass: Constant + OJL interband transition + extended Drude model

$$\chi_{Drude}(\omega) = -\frac{\Omega_{Dr}^2}{\omega^2 + \Gamma_{Dr}^2} + i\frac{\Gamma_{Dr}}{\omega}\frac{\Omega_{Dr}^2}{\omega^2 + \Gamma_{Dr}^2} \qquad \Gamma_{Dr}(\omega) = \Gamma_L - \frac{\Gamma_L - \Gamma_H}{\pi}\left[\arctan\left(\frac{\omega - \Omega_{\Gamma,Dr}}{\Gamma_W}\right) + \frac{\pi}{2}\right]$$



3.1.5 Master model

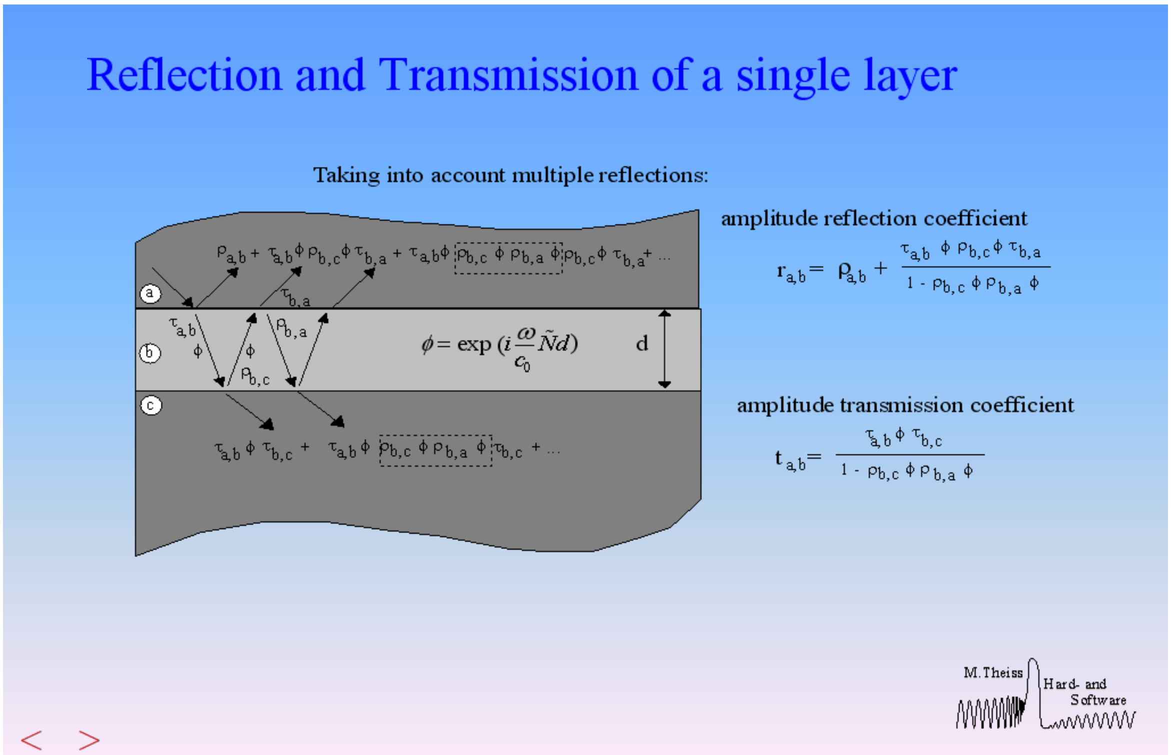
Sometimes the optical constants of a material vary systematically with a compositional parameter like oxygen content in a non-stochiometric oxide or the concentration of an atomic species in a ternary system. This can be described conveniently in SCOUT and CODE using so-called master models which provide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



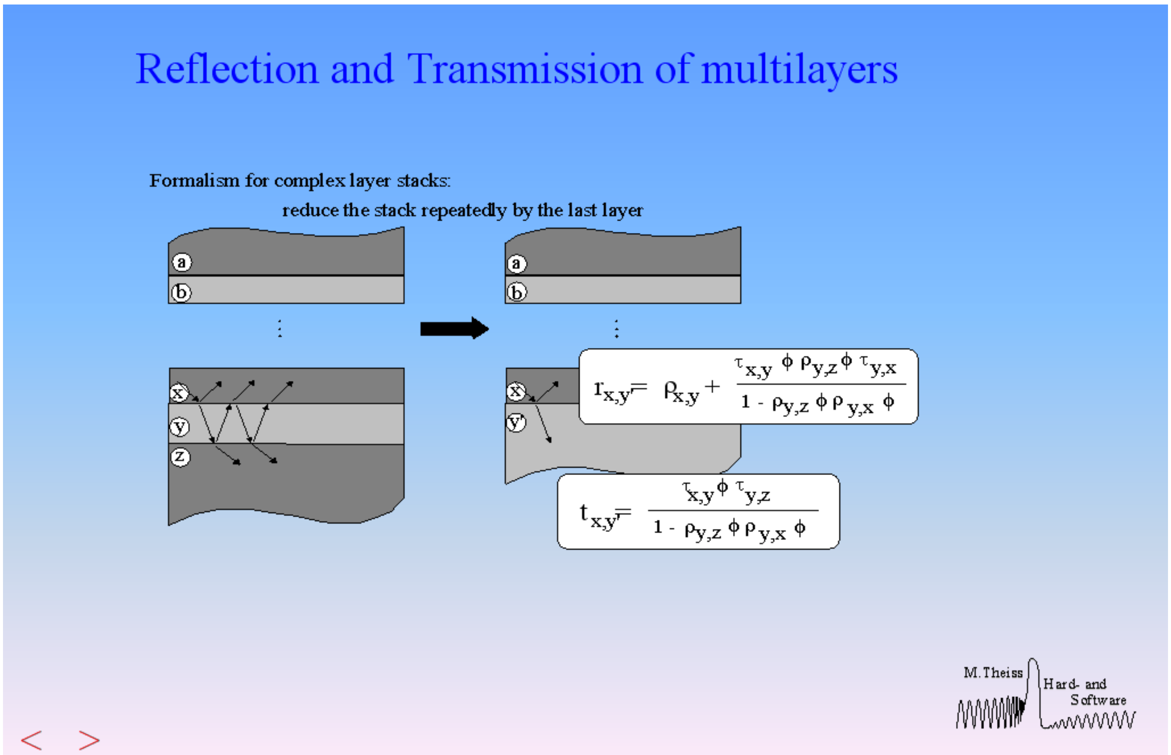
3.2 Layer stacks

3.2.1 Computation of reflectance and transmittance

Single layer treatment using geometric series:

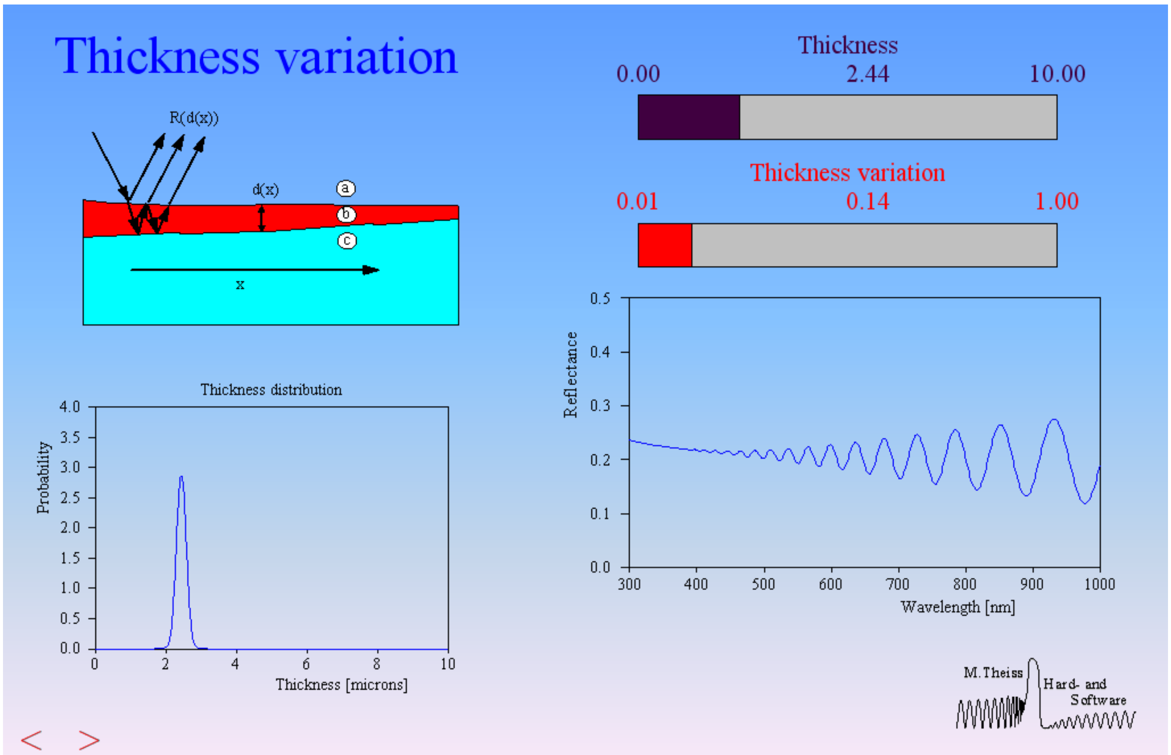


Multilayers are processed applying the single layer expressions many times:

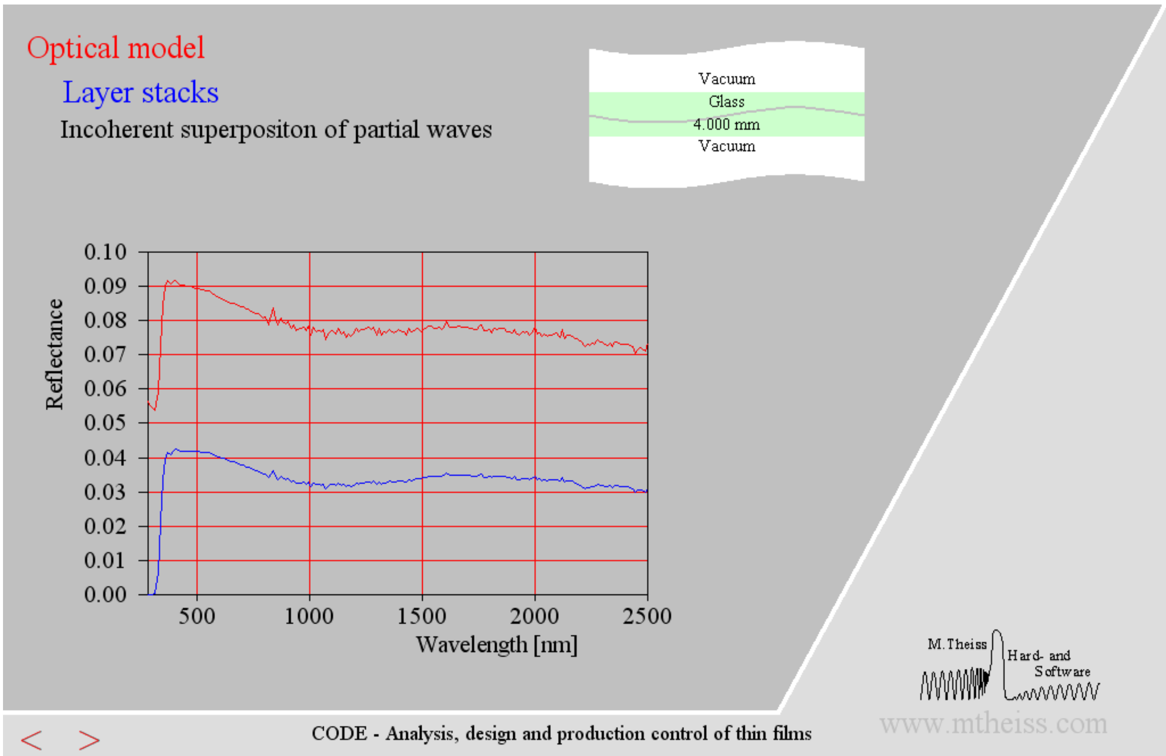


3.2.2 Coherent/incoherent superposition

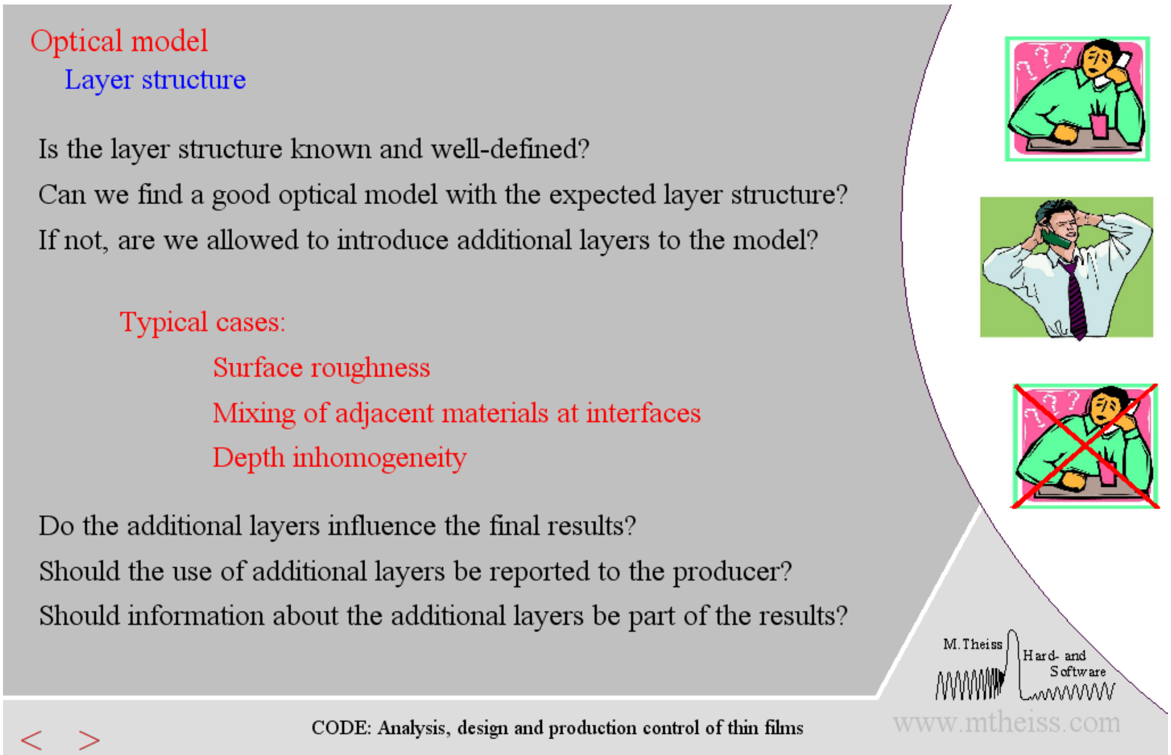
CODE has a very efficient algorithm to compute R and T of partially coherent superposition of waves:



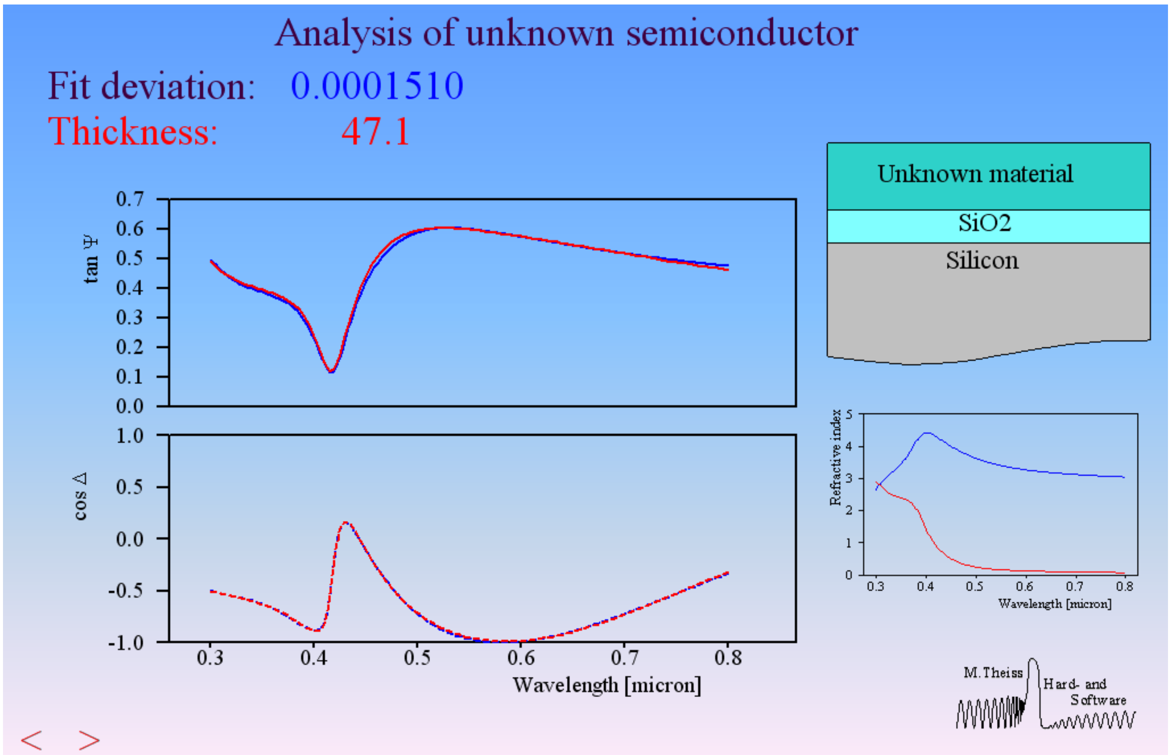
For thick layers the incoherent contributions to R and T can be computed individually. Red curve in the following graph: All reflection orders superimposed. Blue curve: Backside reflection only:



3.2.3 What is the correct layer stack?



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.


Analysis of unknown semiconductor
Fit deviation: 0.0001510
Thickness: 47.1
Unknown material
SiO2
Silicon
tan Ψ
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
cos Δ
1.0
0.5
0.0
-0.5
-1.0
0.3 0.4 0.5 0.6 0.7 0.8
Wavelength [micron]
Refractive index
Wavelength [micron]
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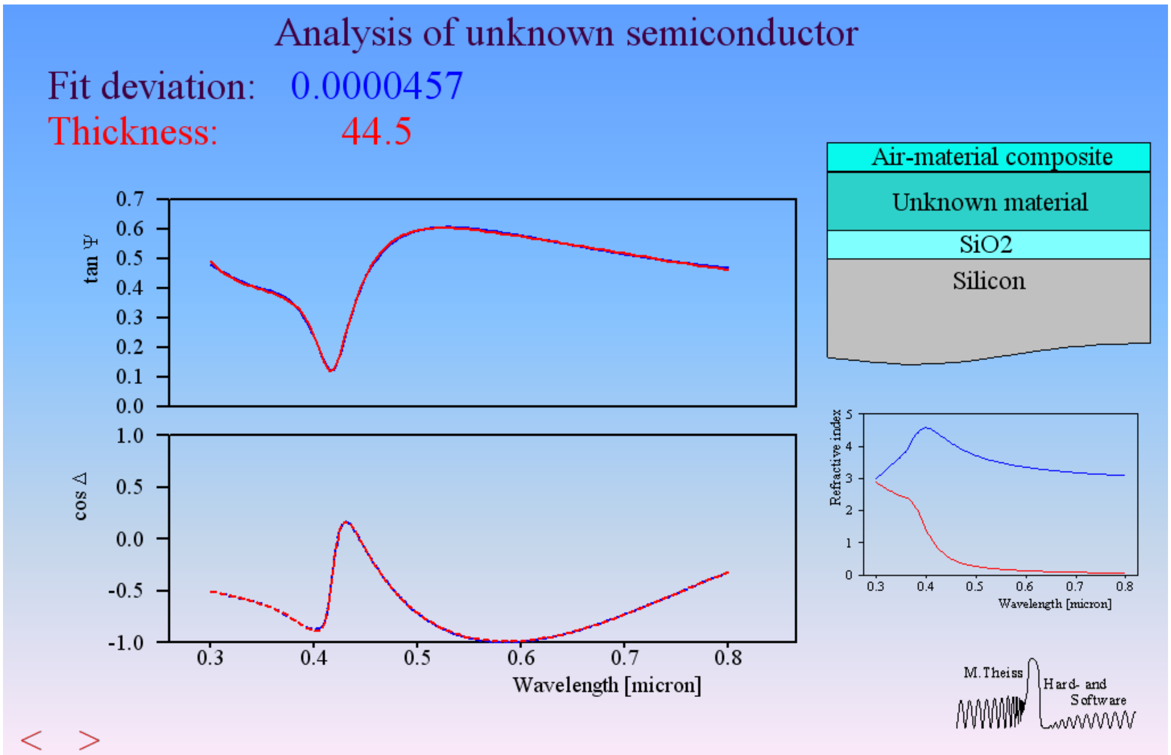
Analysis of unknown semiconductor
Fit deviation: 0.0000457
Thickness: 44.5
Air-material composite
Unknown material
SiO2
Silicon
tan Ψ
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
cos Δ
1.0
0.5
0.0
-0.5
-1.0
0.3 0.4 0.5 0.6 0.7 0.8
Wavelength [micron]
Refractive index
Wavelength [micron]
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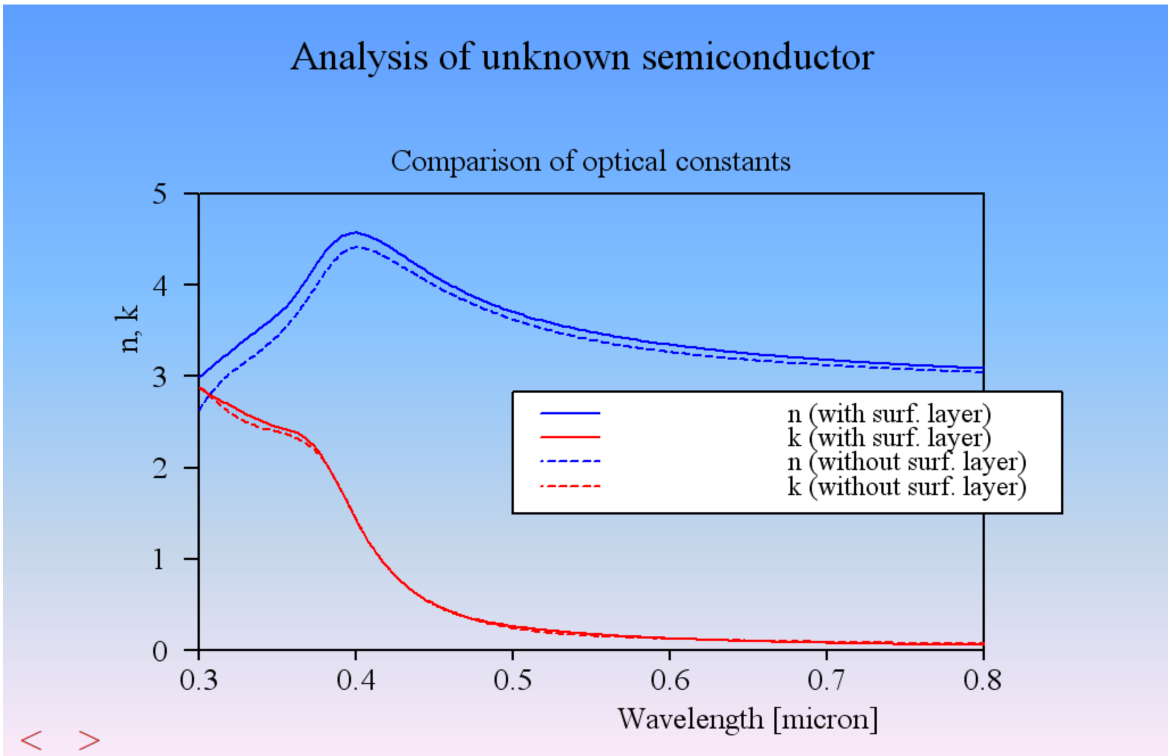
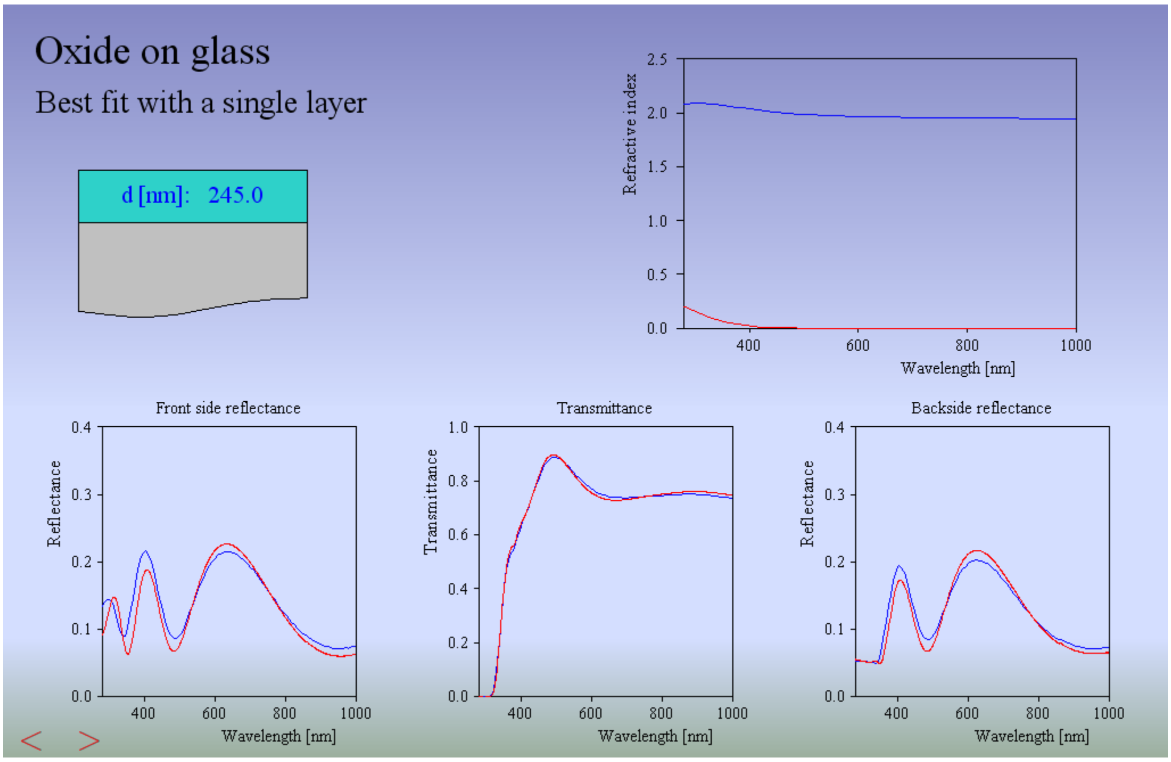
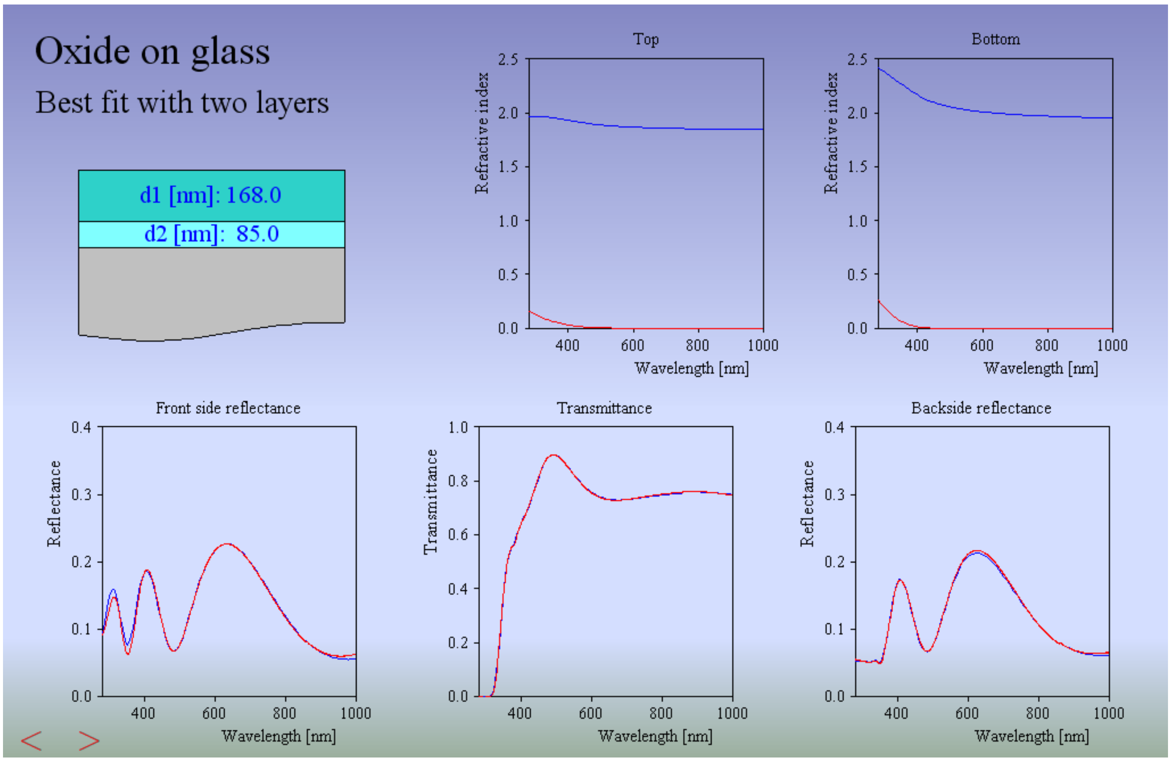
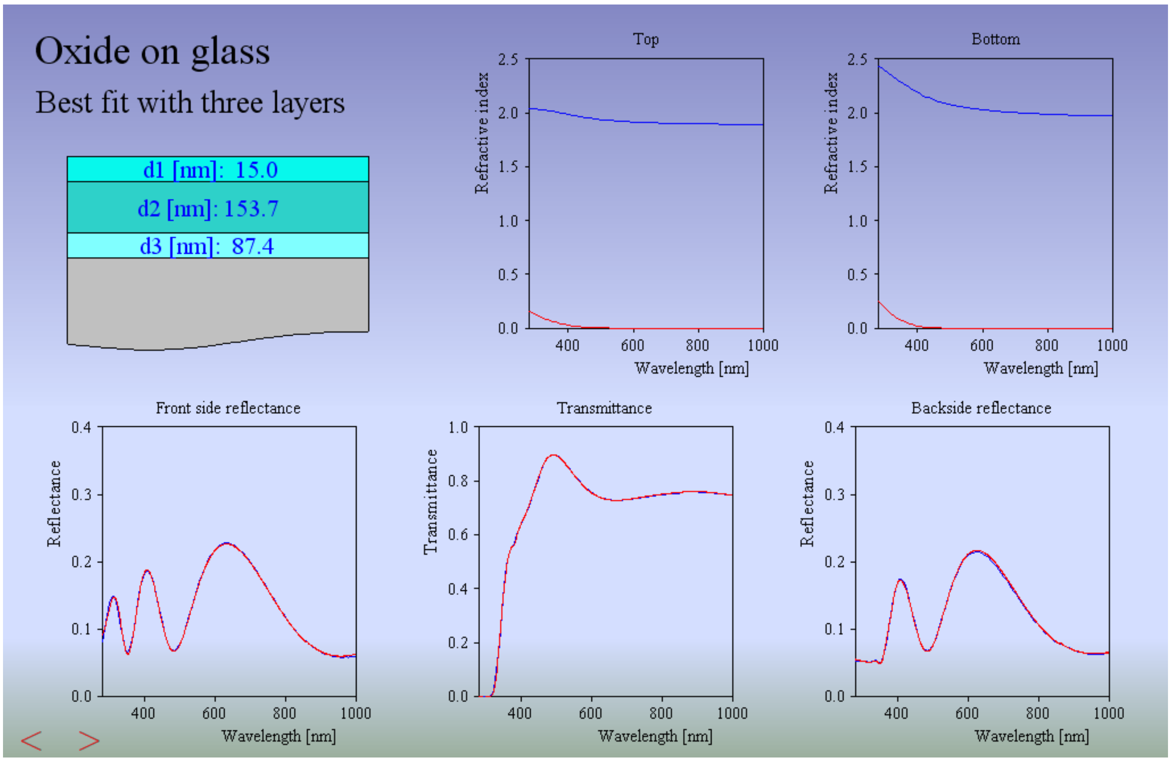


Here is another example: A customer asked for the optical constants of a single layer deposited on glass with a sputtering device. It turned out that even advanced optical constant models could not describe the optical properties of the layer properly.

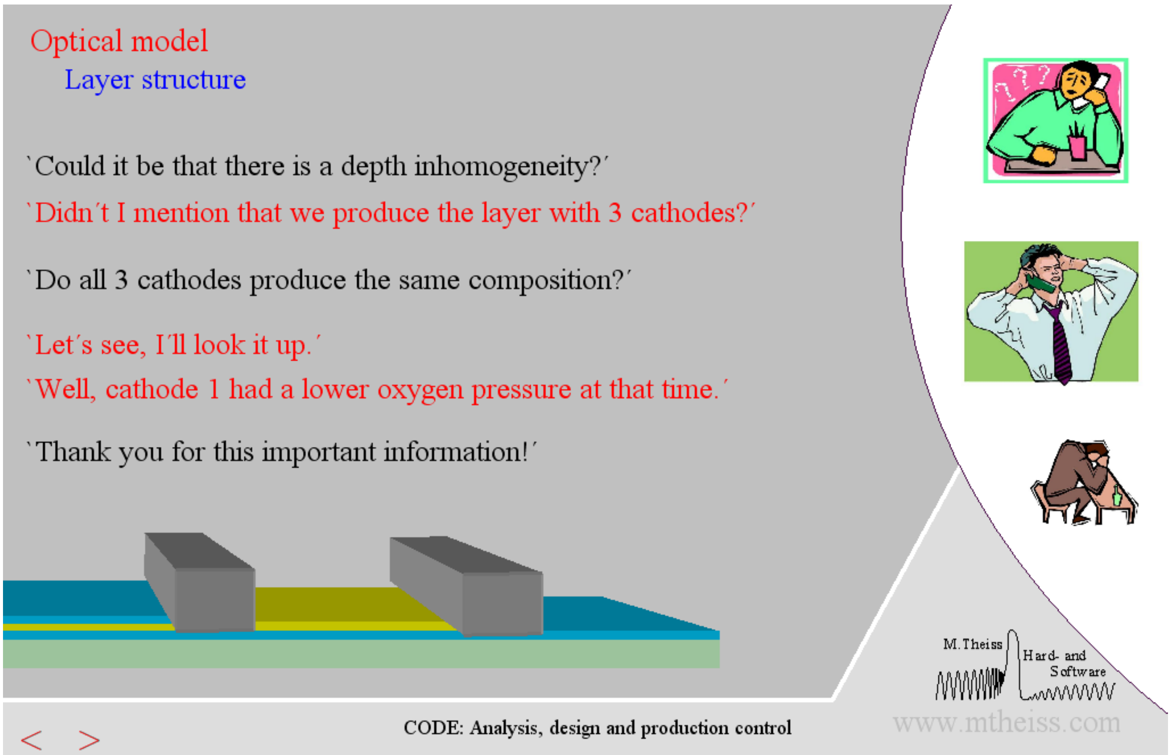


Only introducing a depth inhomogeneity (and a surface layer) could solve the problem:

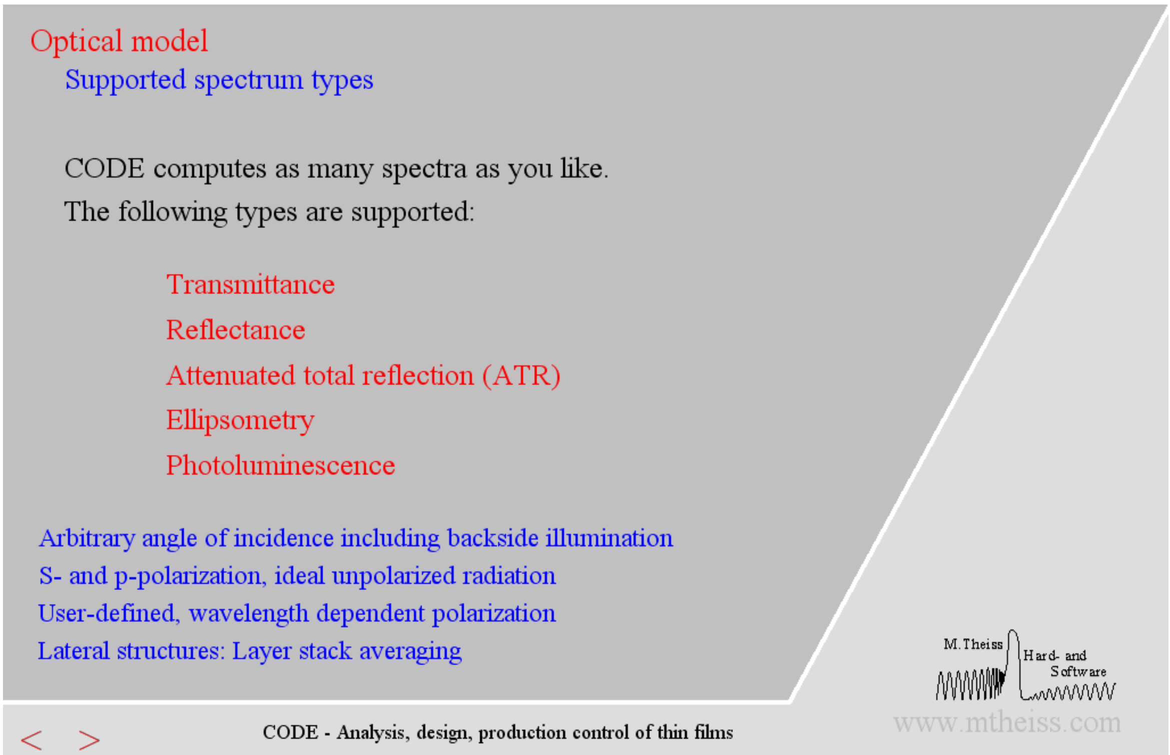




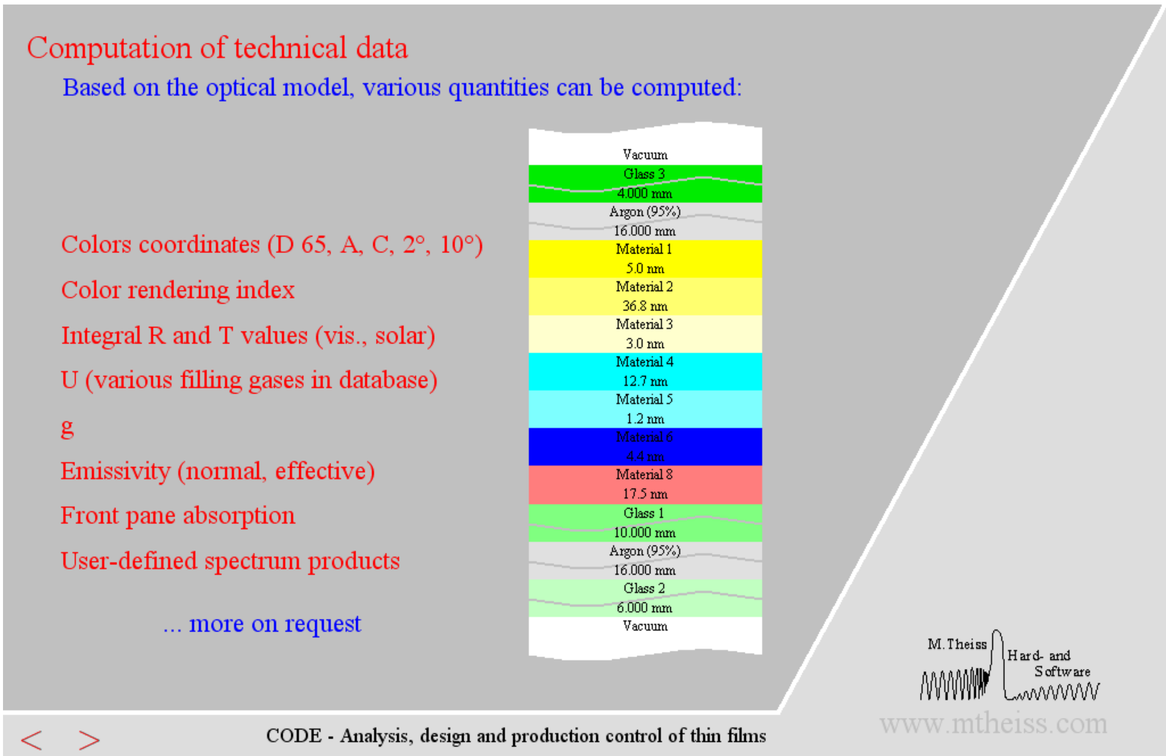
Communication with the producer finally verified the assumptions made in the successful fit:

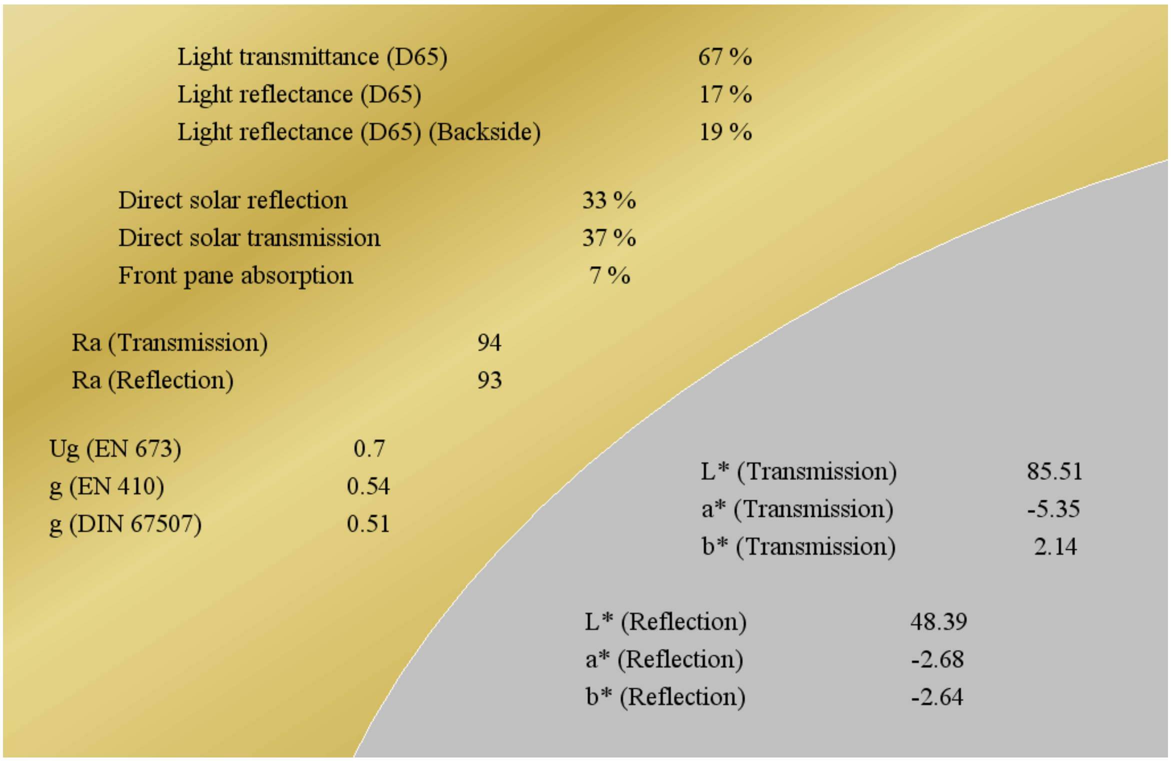


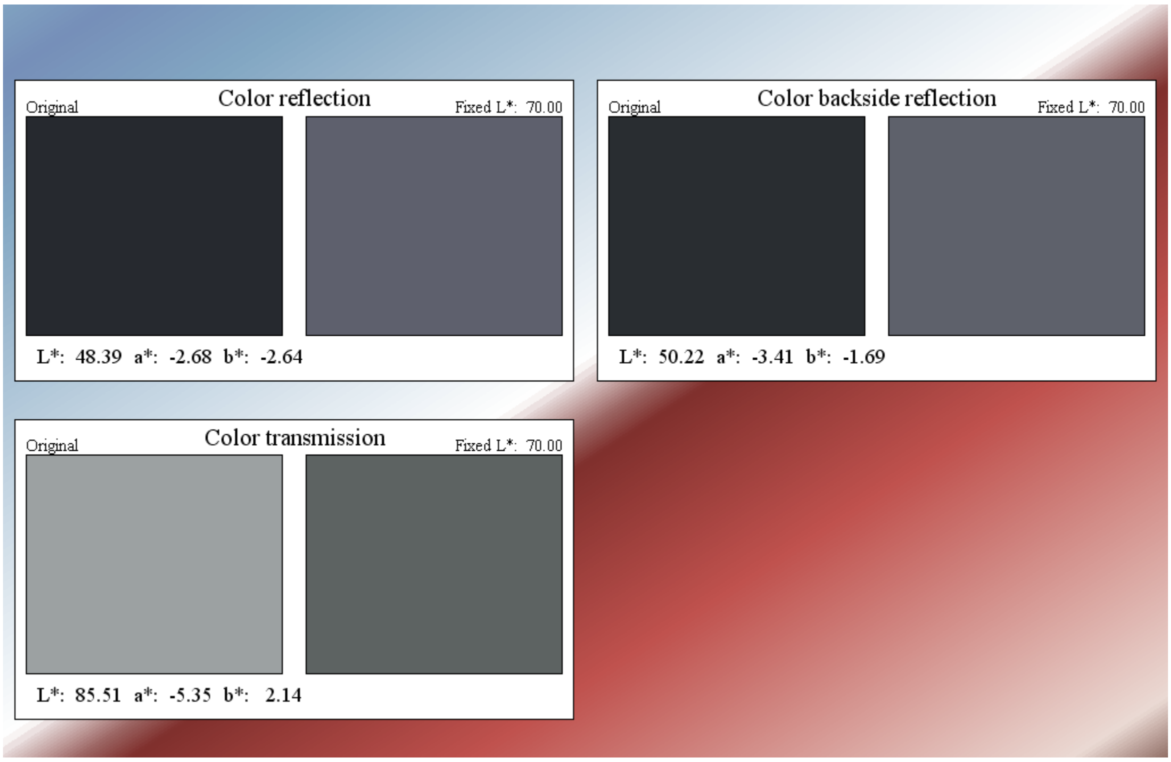
3.3 Spectrum types

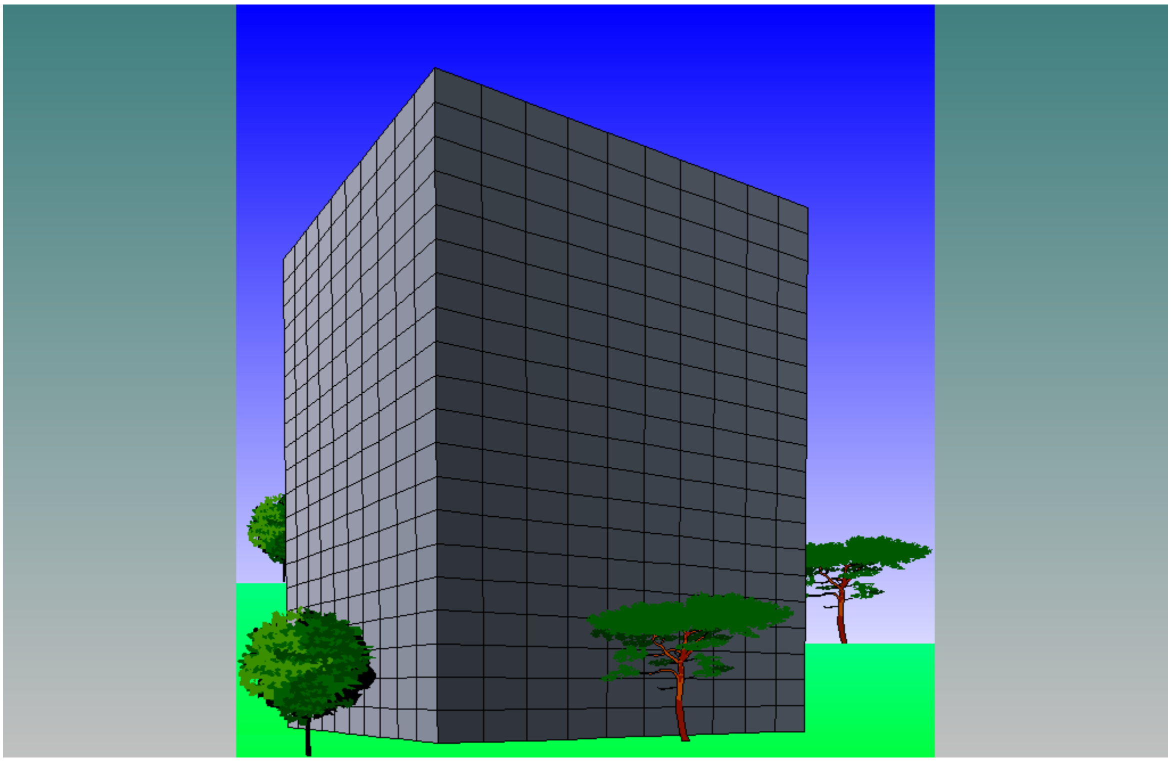


4 Computation of technical data

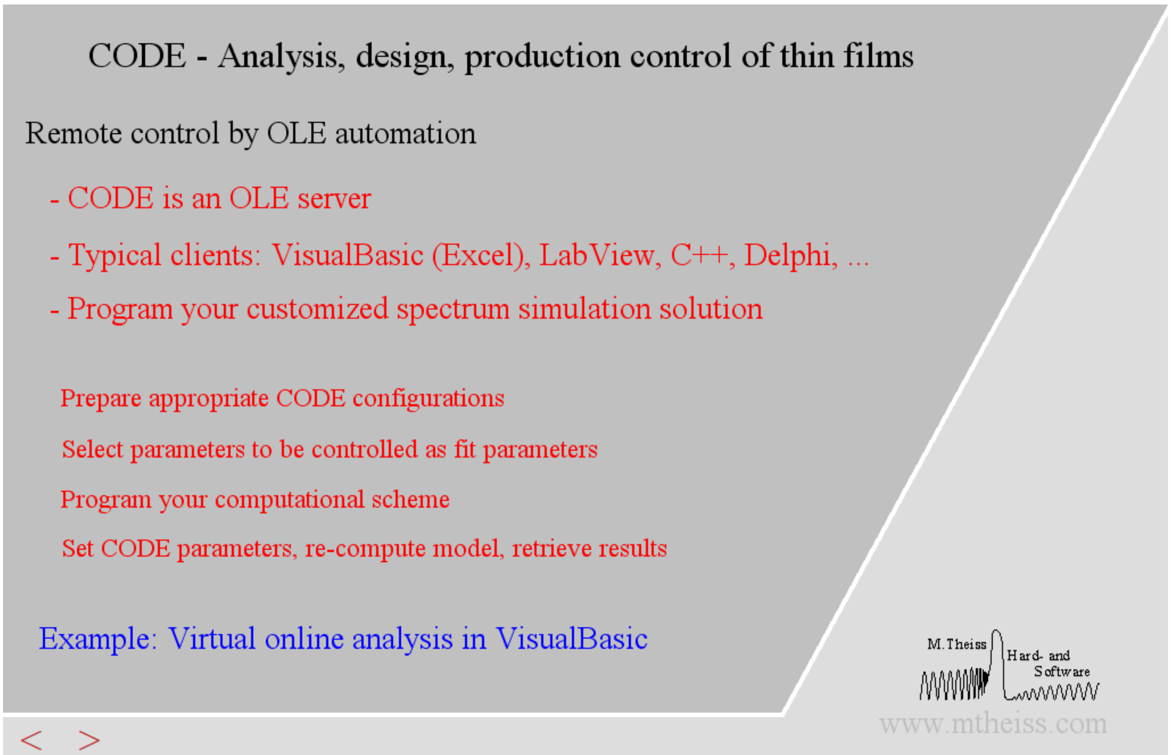





Original
Color reflection
Fixed L*: 70.00
L*: 48.39 a*: -2.68 b*: -2.64
Original
Color backside reflection
Fixed L*: 70.00
L*: 50.22 a*: -3.41 b*: -1.69
Original
Color transmission
Fixed L*: 70.00
L*: 85.51 a*: -5.35 b*: 2.14

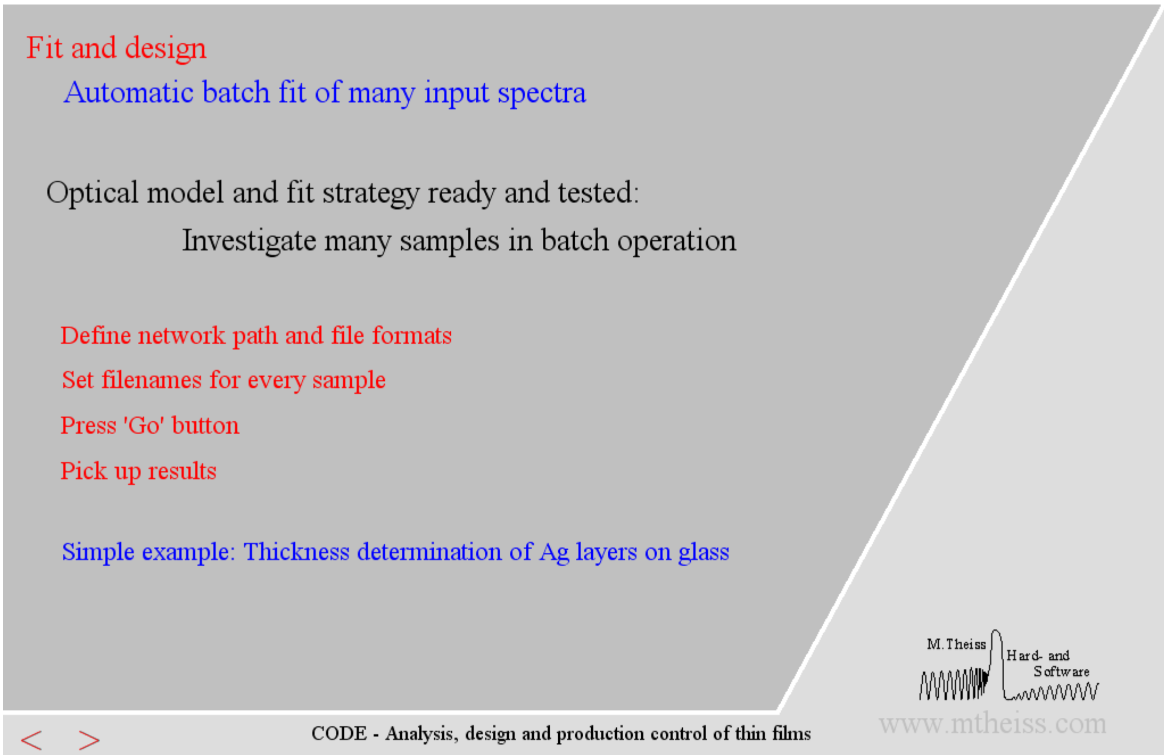


5 Remote control by OLE automation

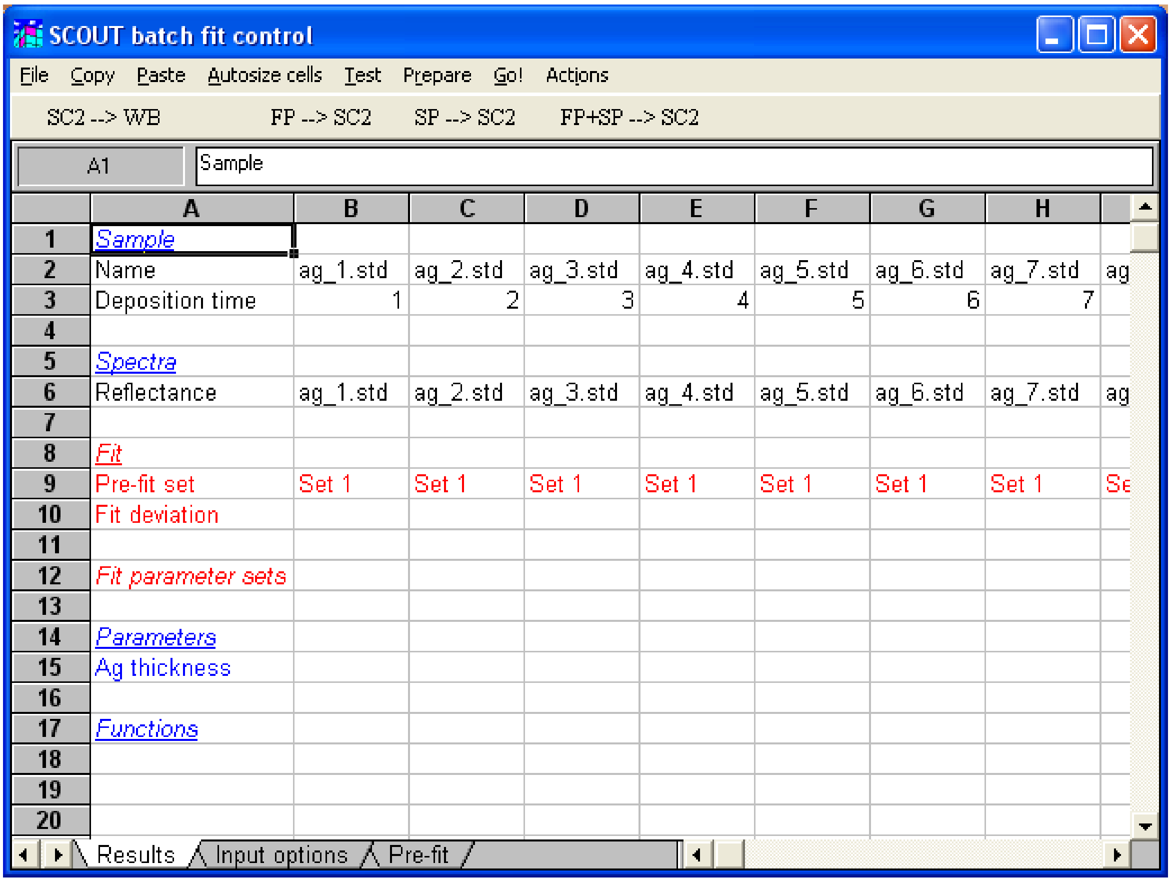


The Excel example shows how spectra can be sent to SCOUT which are then automatically fitted. The results are passed back to an Excel worksheet.

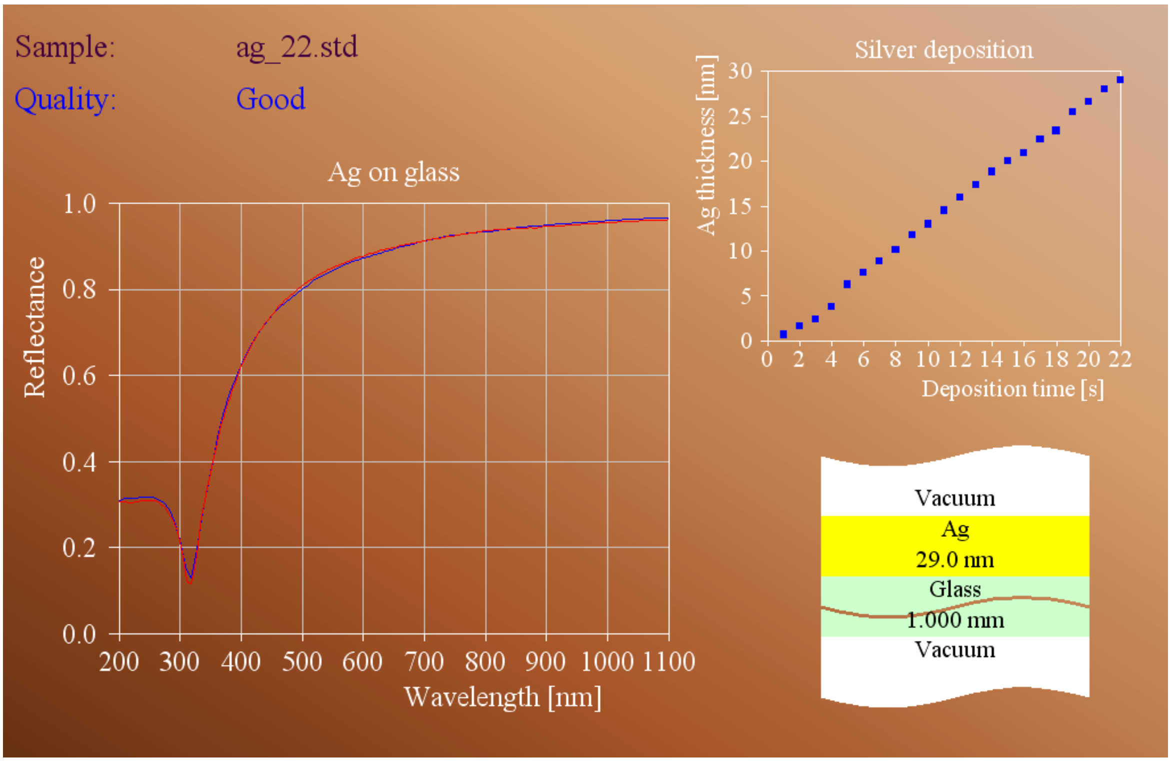
6 Batch processing



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:



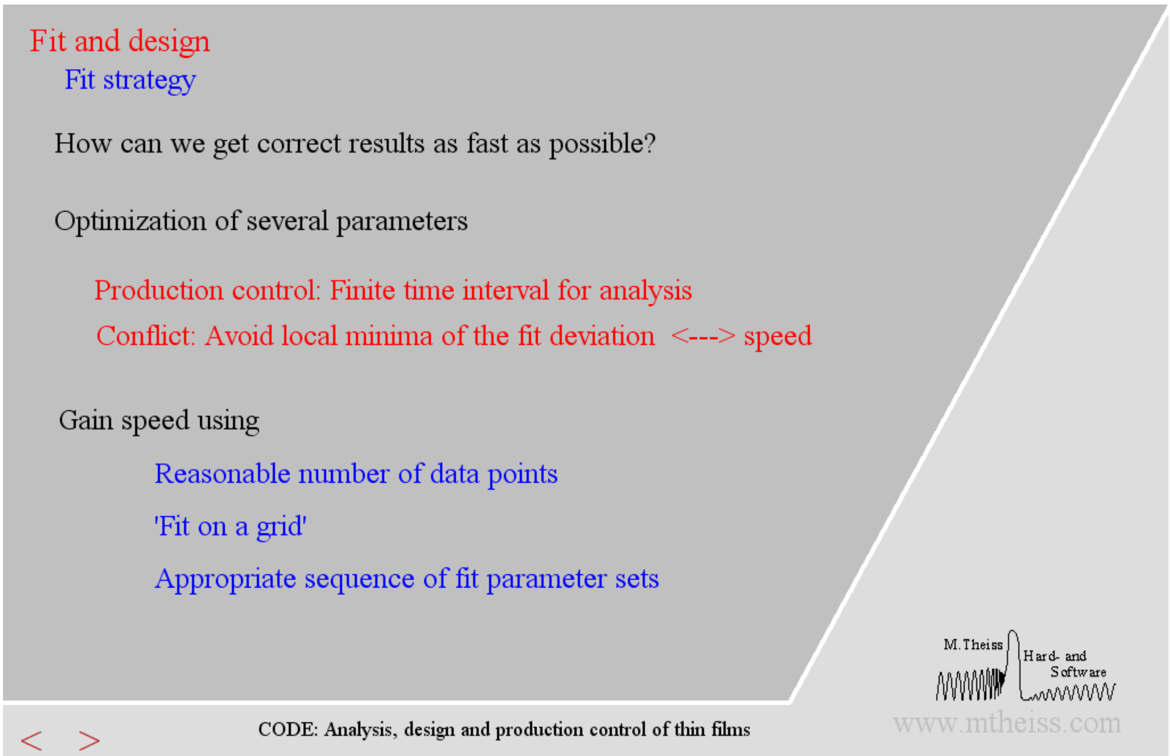
The results can be displayed directly in a view:



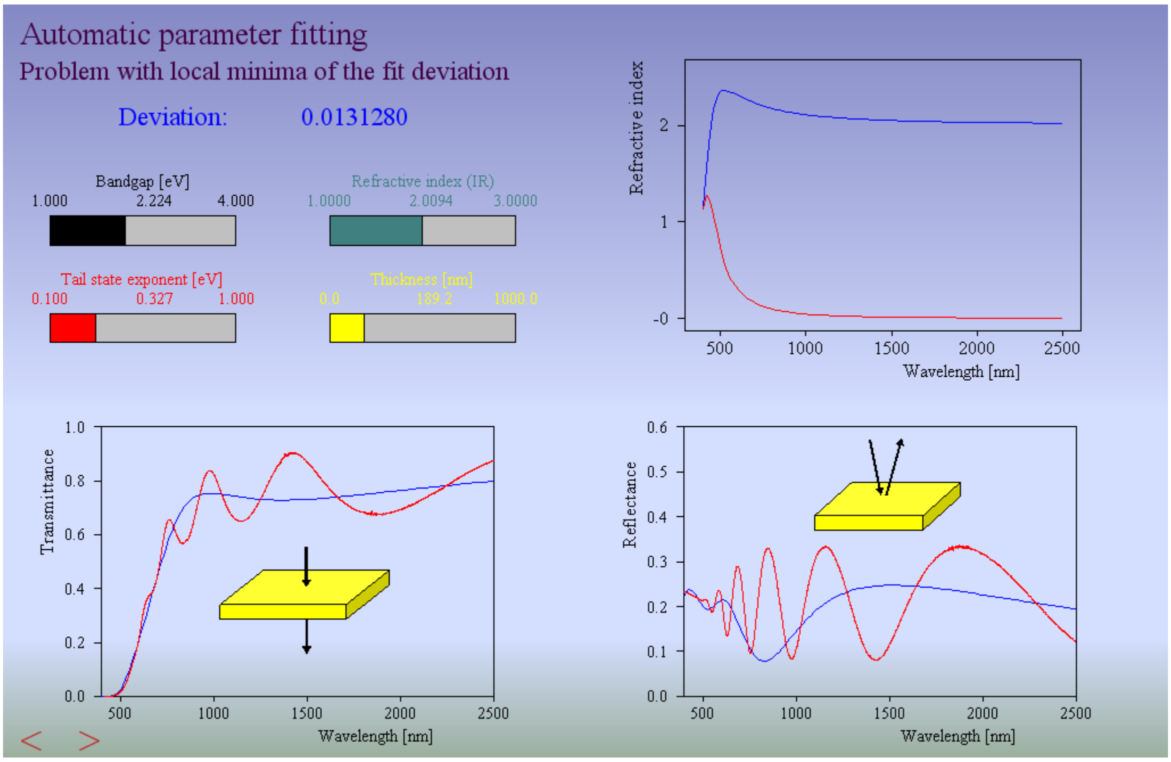
7 Analysis and design

7.1 Fit strategy

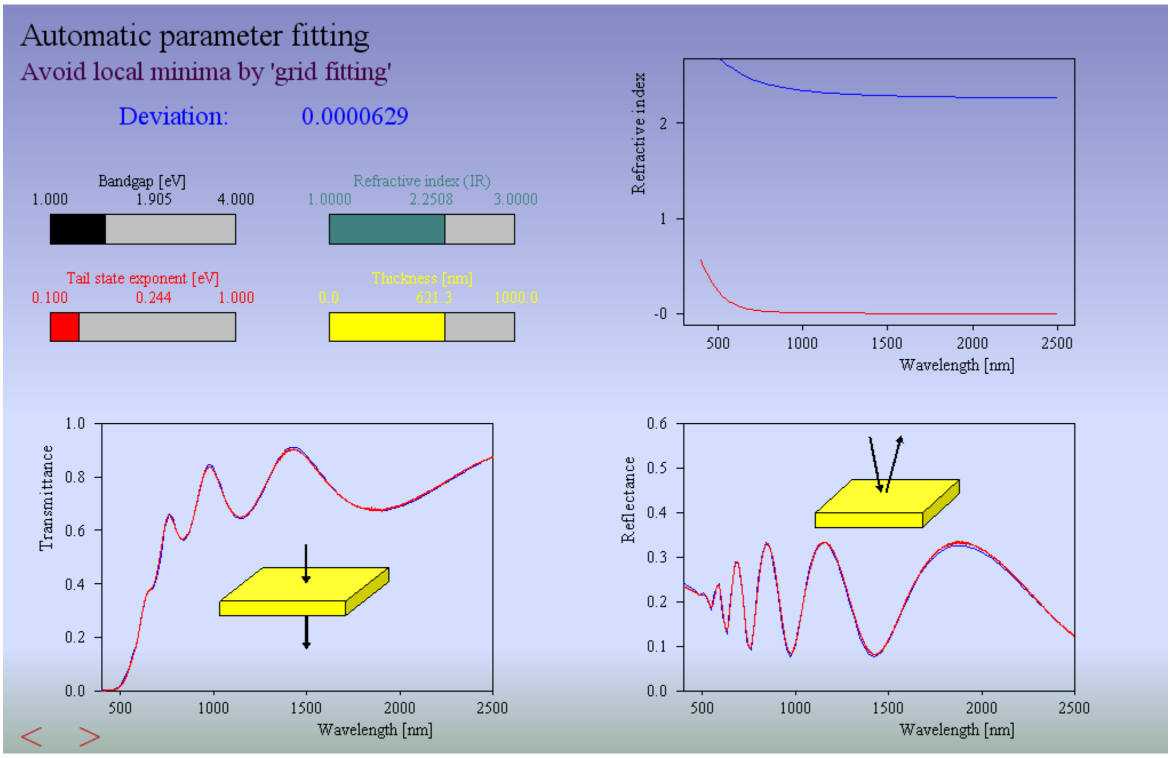
Once the optical model is ready, one must be decide which parameters may vary from sample to sample. These parameters must be determined following a fit strategy that leads to stable and reproducible results in the specified time frame.



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.



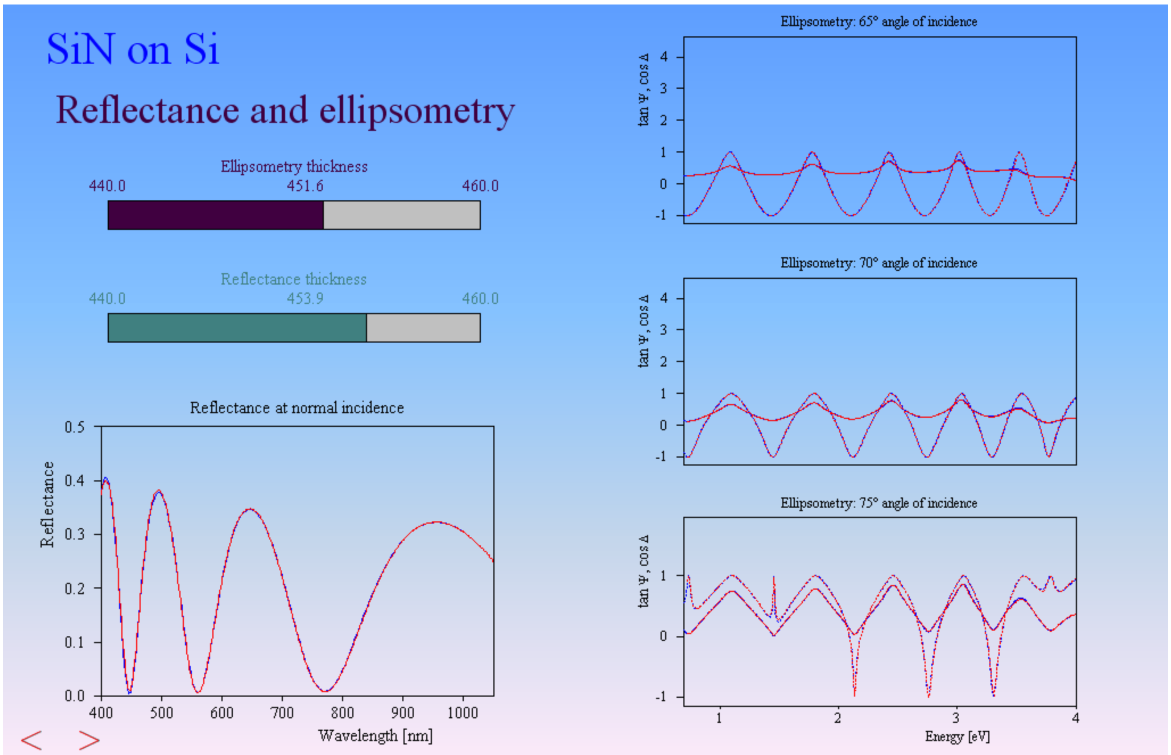
Using the 'grid fit' feature of SCOUT this problem can be overcome very efficiently: Before the multiple parameter fit is started, the right fringe order is found by trying several thickness values (equally spaced in a user-defined thickness range) and taking the best result as starting value for the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



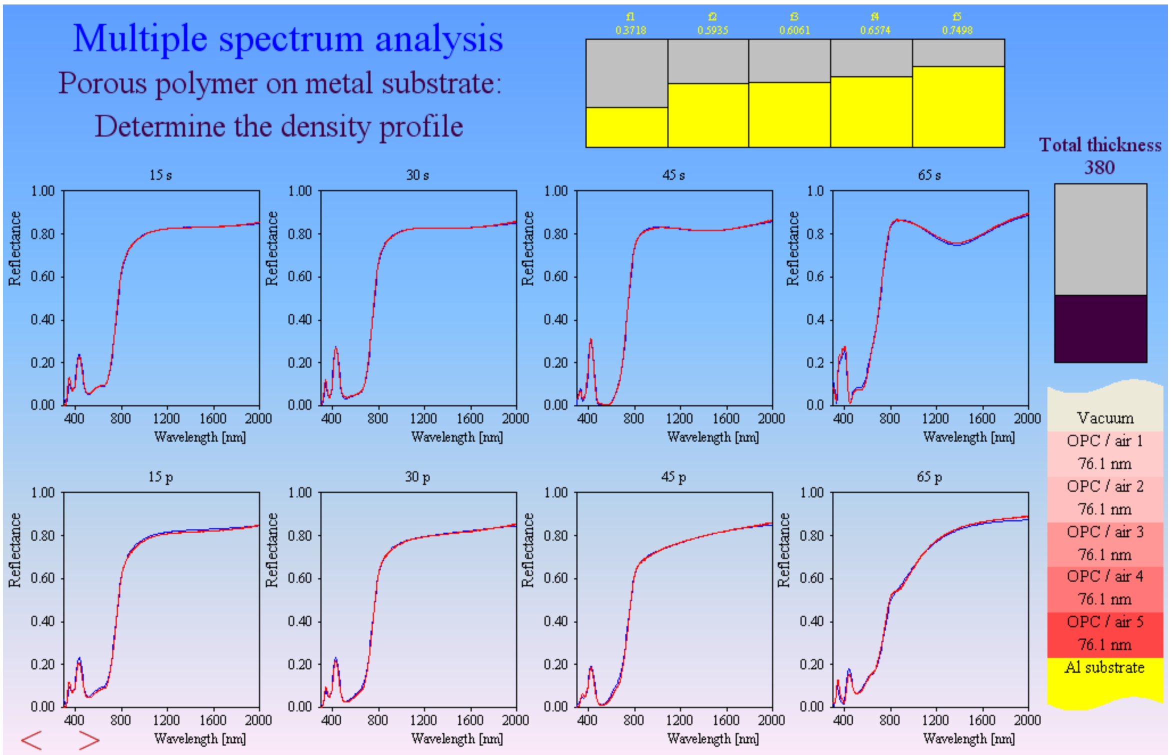
In many cases advanced fit strategies using so-called fit parameter sets are successful: Separate the fit parameters into groups which are optimized one after the other. You can, for example, fit the thickness and the refractive index of a material in a spectral region where the layer is transparent. 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

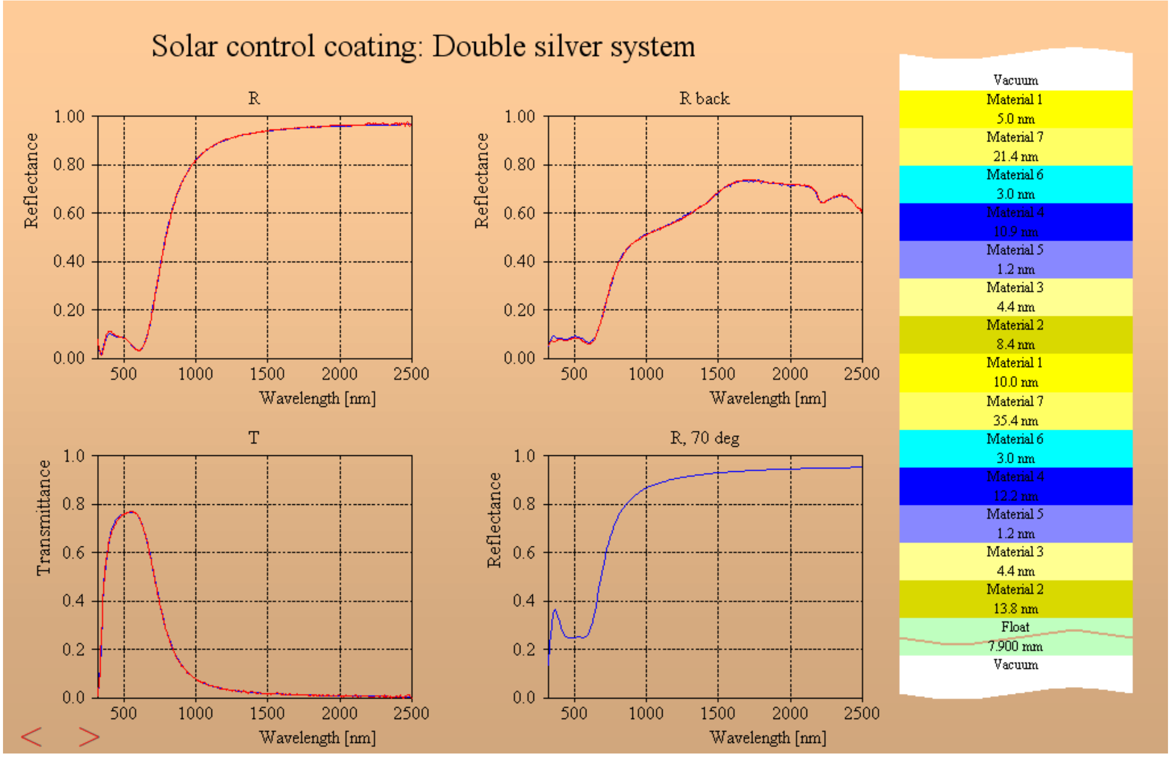
Fitting three ellipsometry and a reflectance spectrum. Since the investigated sample spot is not exactly the same in both experiments two different layer stacks are used in the model:



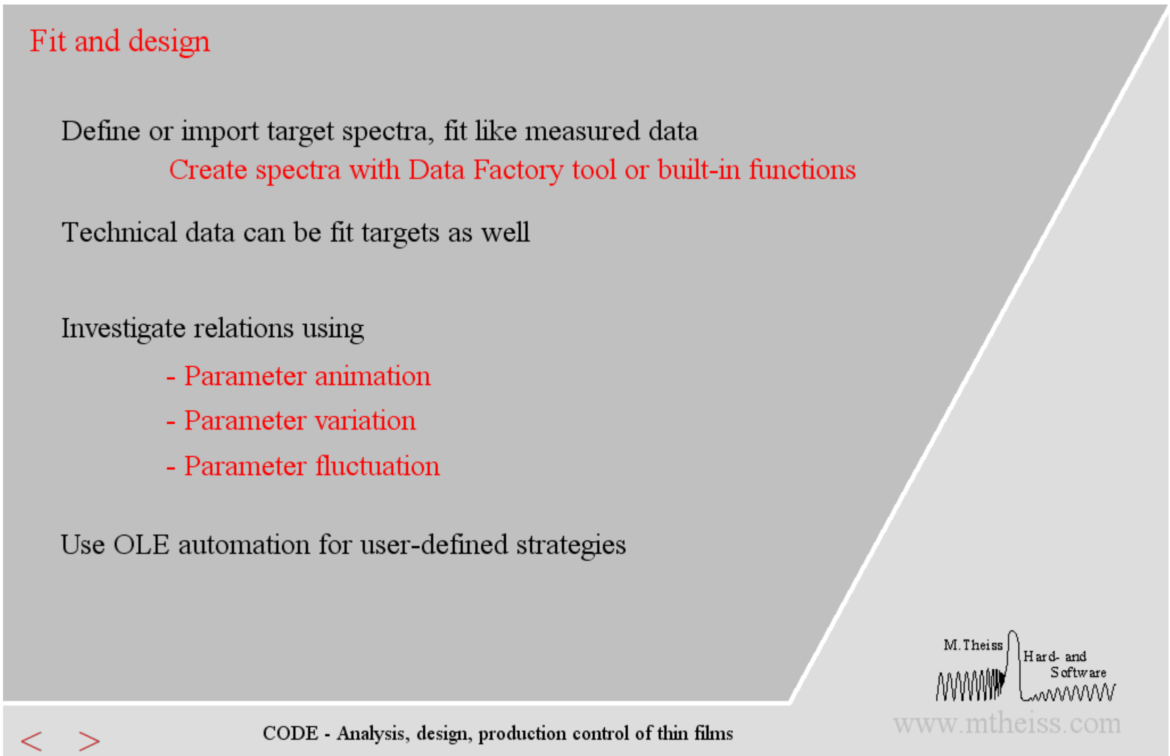
Here 8 spectra are fitted simultaneously:



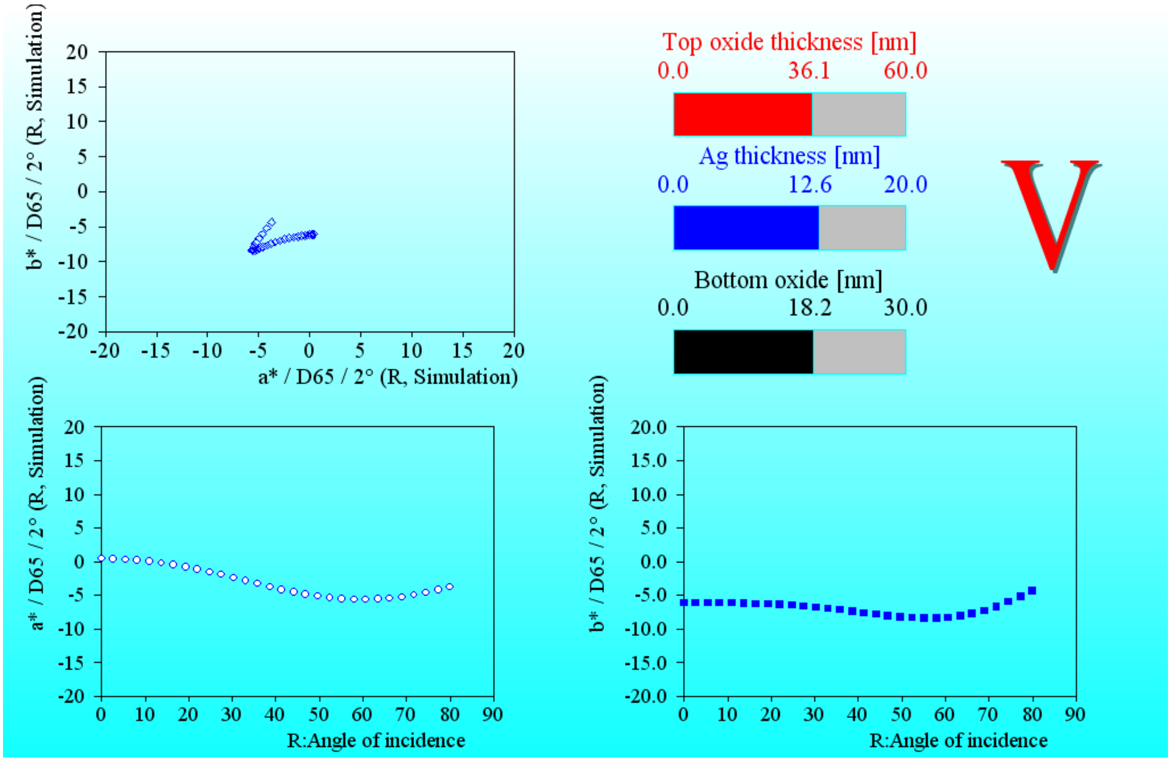
Quantitative description of a solar control coating:



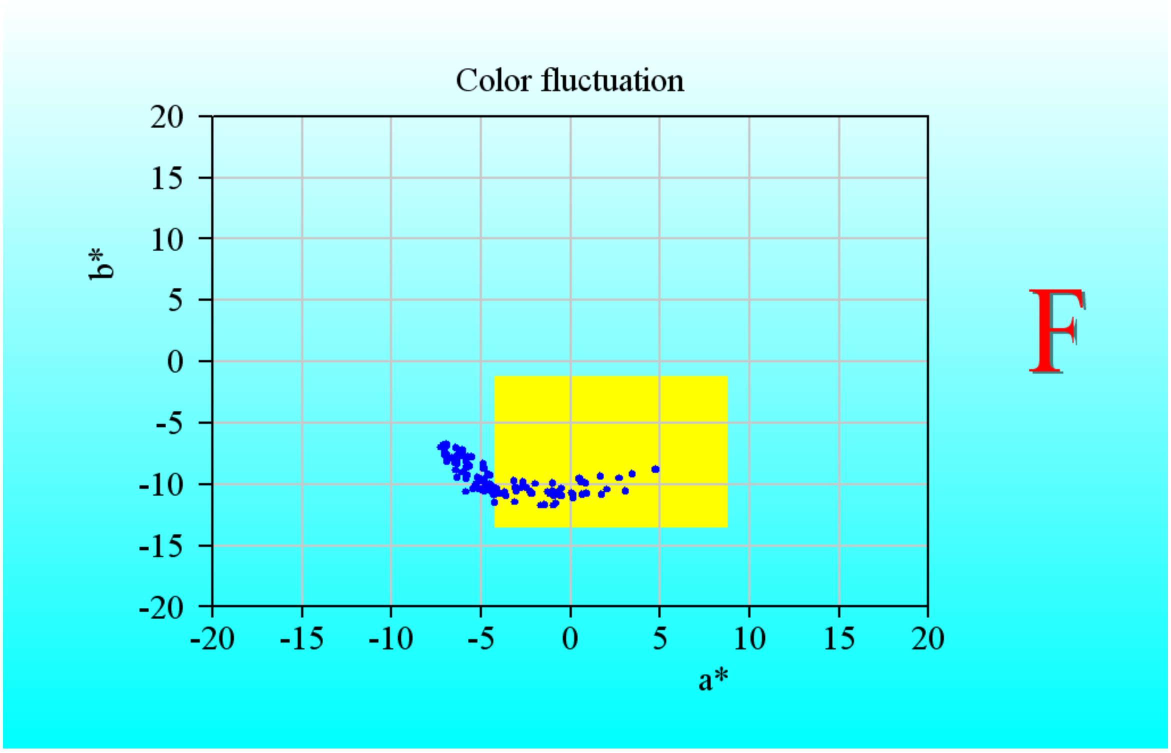
7.3 Design



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:

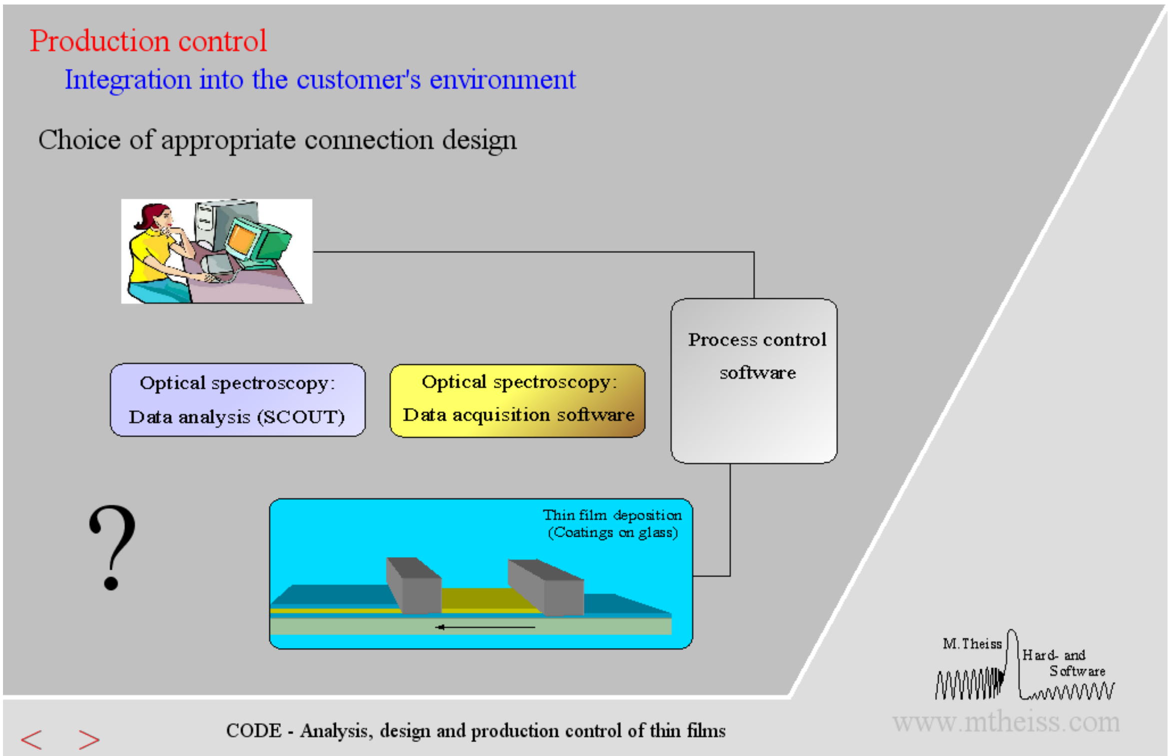


The parameter fluctuation feature computes the variation of technical data and spectra in the presence of random parameter fluctuations. This can be used to simulate the effect of production tolerances, for example:

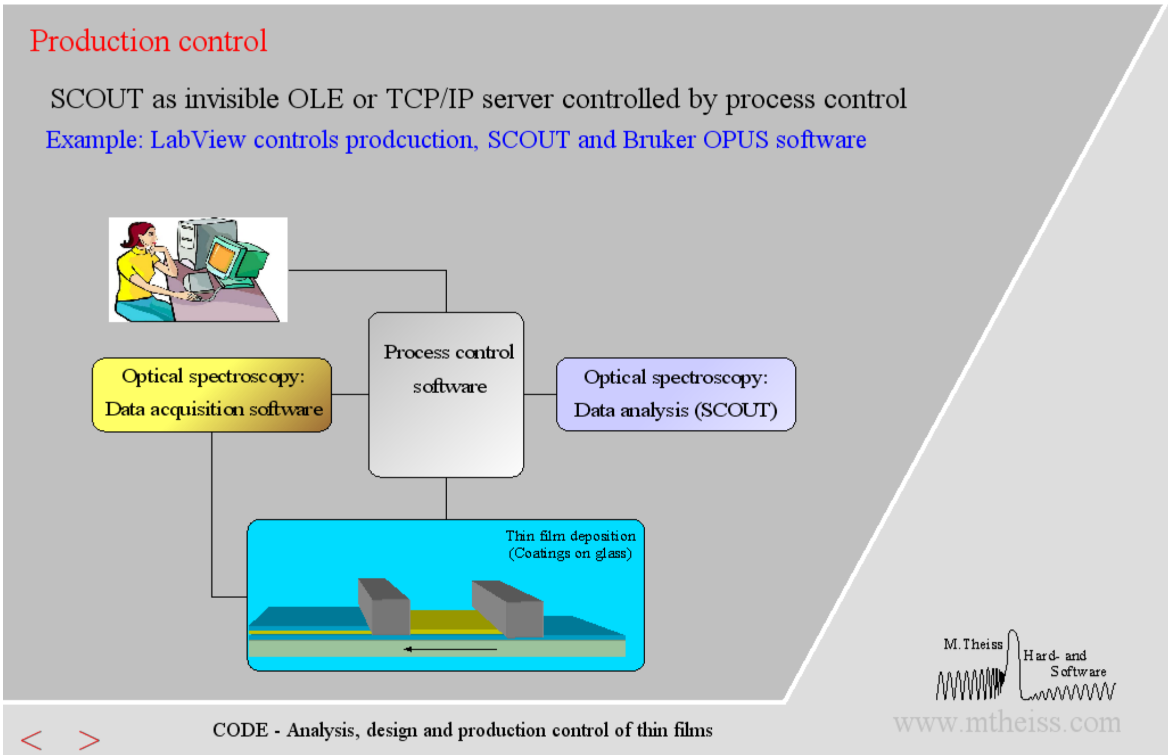


8 Production control schemes

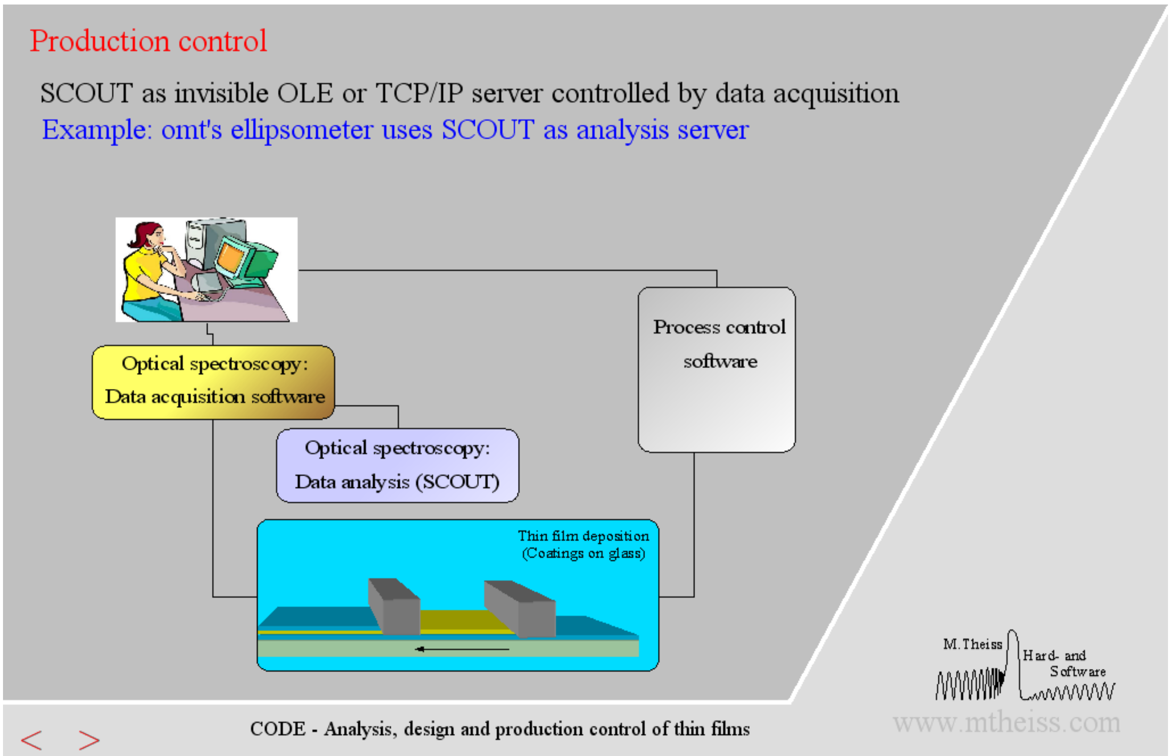
Now the method must be brought to the factory. The first question is how the various programs involved in the problem should be connected:



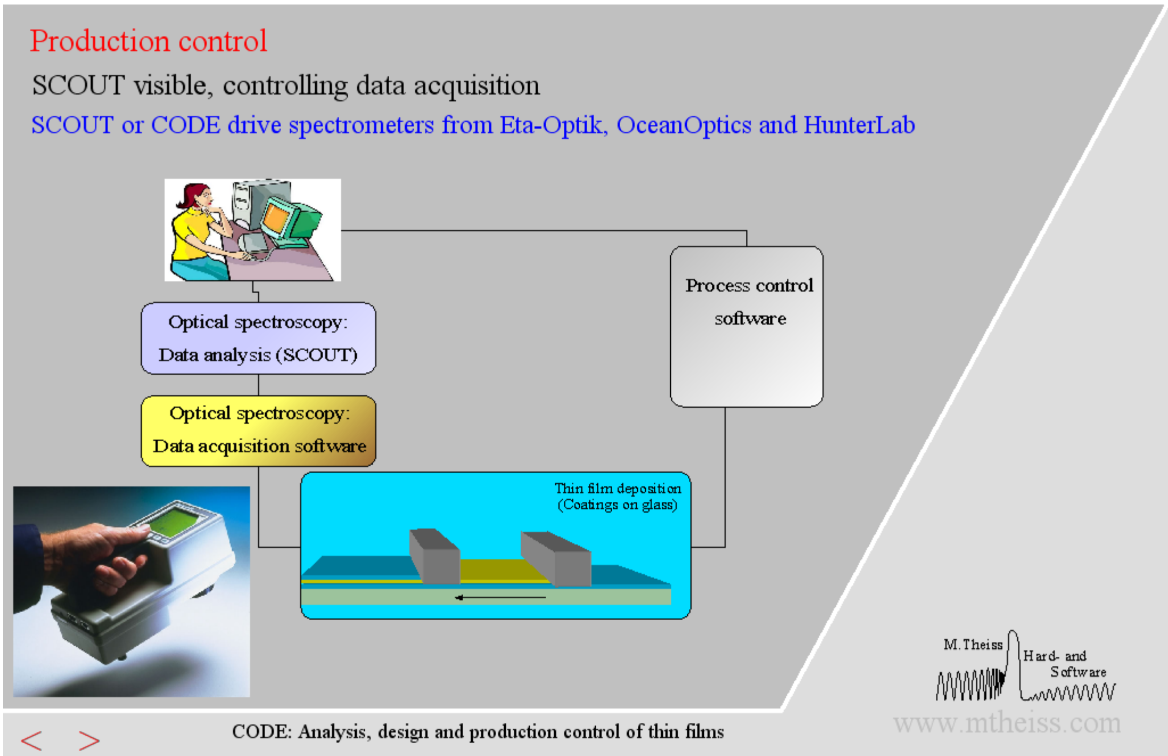
With SCOUT, several options are possible. The following example shows a configuration where both SCOUT and the data acquisition are controlled by the process control software. SCOUT can be accessed as OLE server or by TCP/IP communication.



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, consultance work