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

Developing optical production control methods for SCOUT

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.

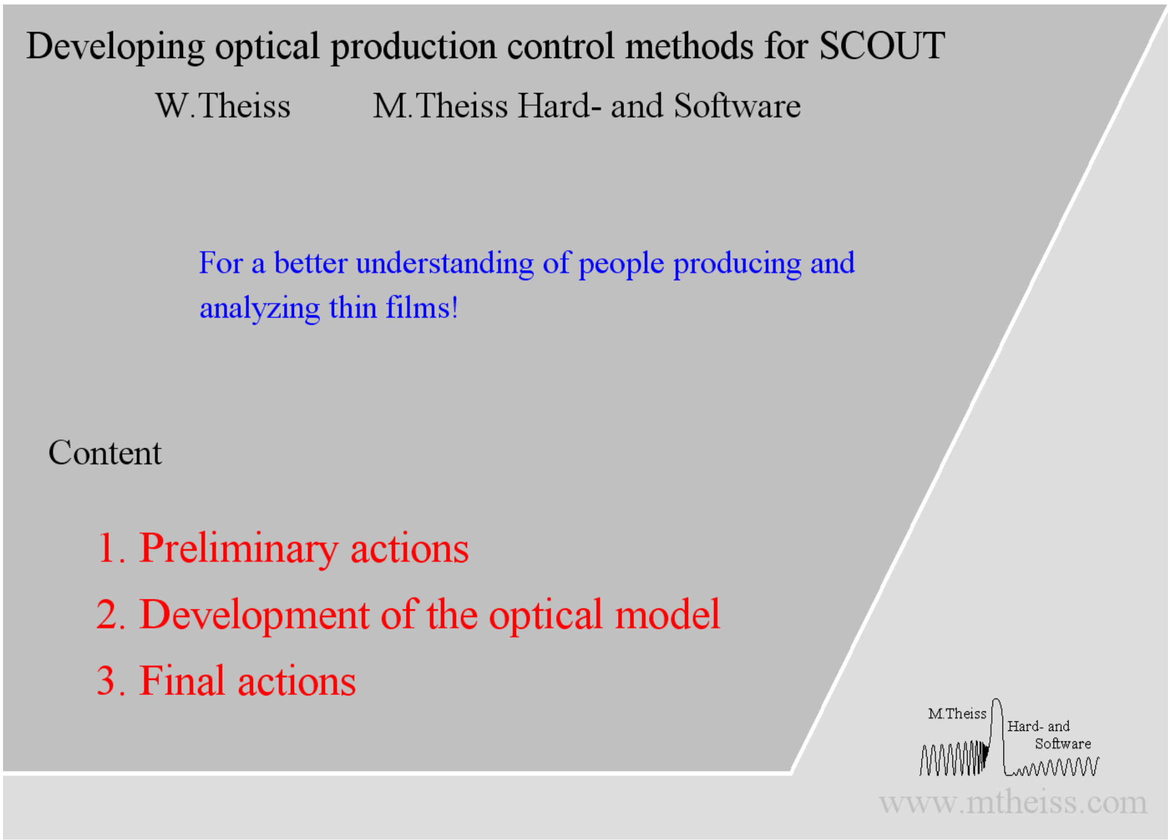
In the graphs displaying optical constants the real part is drawn blue, the imaginary one is given in red.
In the case of spectrum fits, the measured spectra are always in red, the simulated spectra in blue.

All simulations have been performed with our SCOUT software which is commercially available.

Aachen, October 2003

1 Overview

1.1 Title



Developing optical production control methods for SCOUT

W.Theiss M.Theiss Hard- and Software

For a better understanding of people producing and analyzing thin films!

Content

1. Preliminary actions
2. Development of the optical model
3. Final actions

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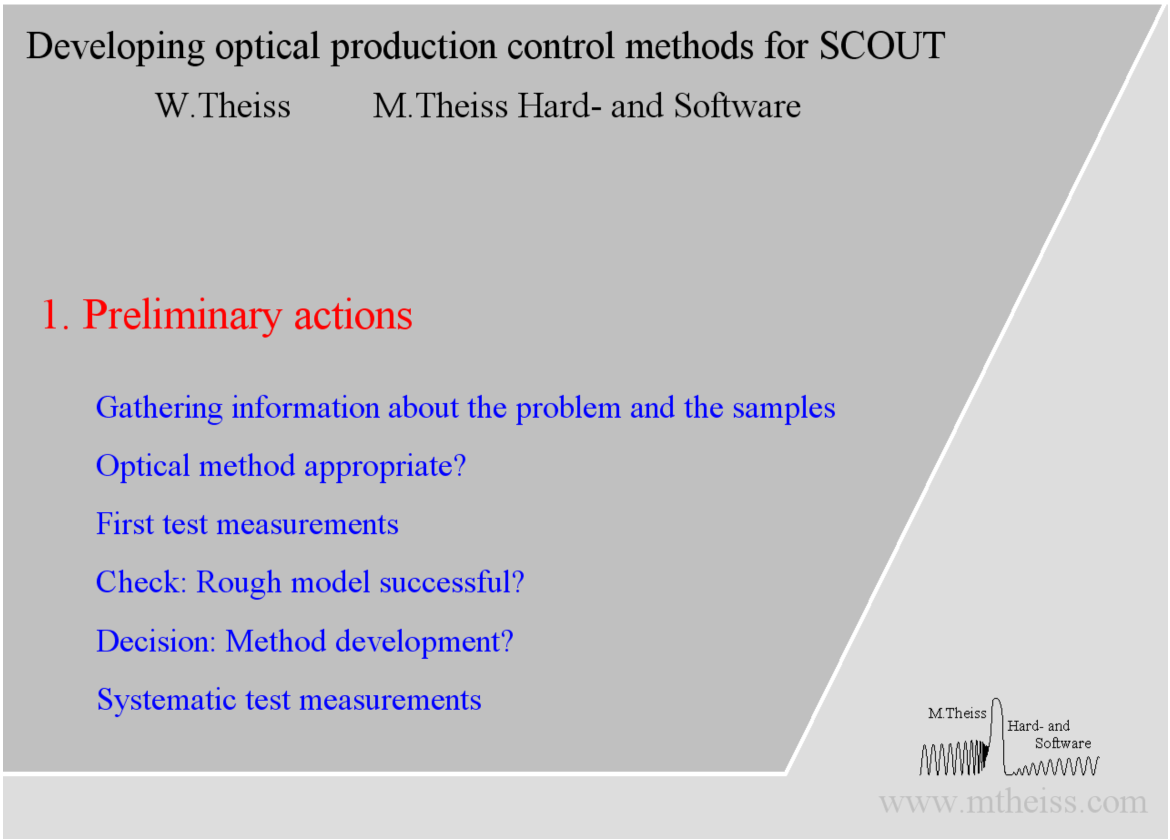
1.2 Introduction

A short introductory rush through the three main steps of the presentation:



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1. Preliminary actions

Gathering information about the problem and the samples

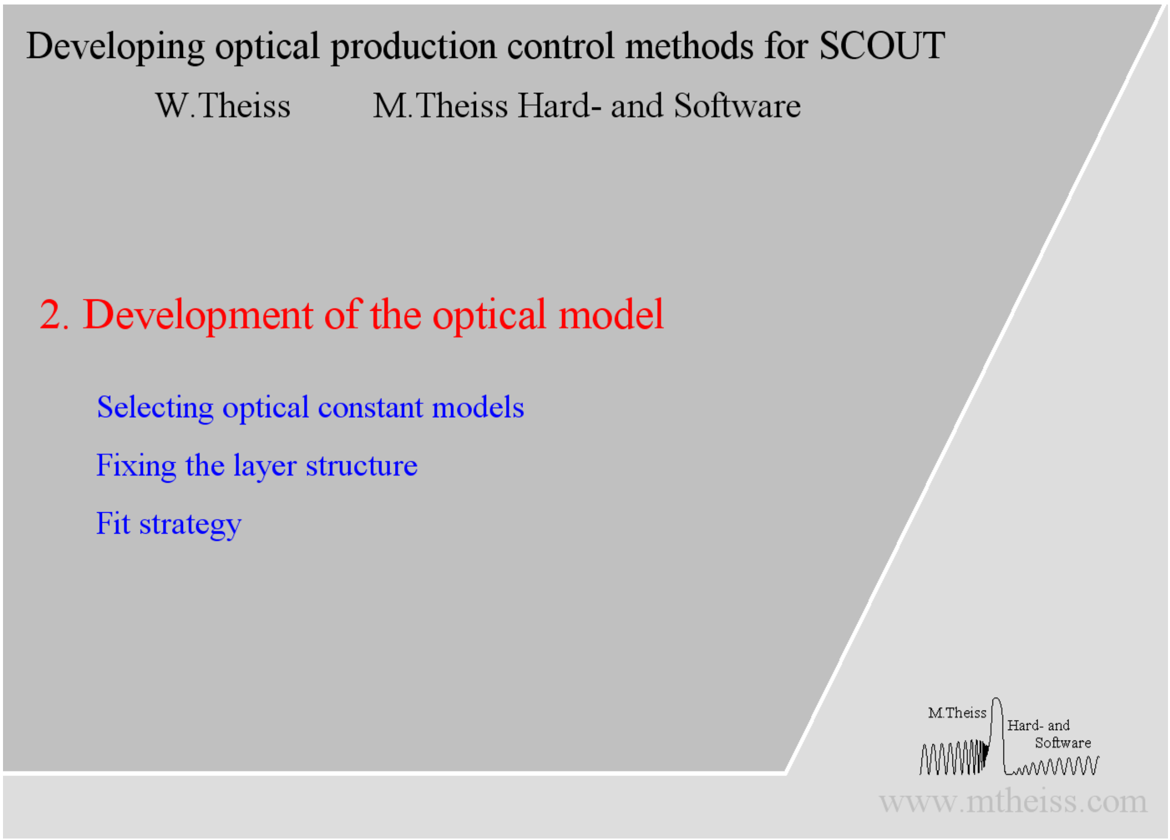
Optical method appropriate?

First test measurements

Check: Rough model successful?

Decision: Method development?

Systematic test measurements



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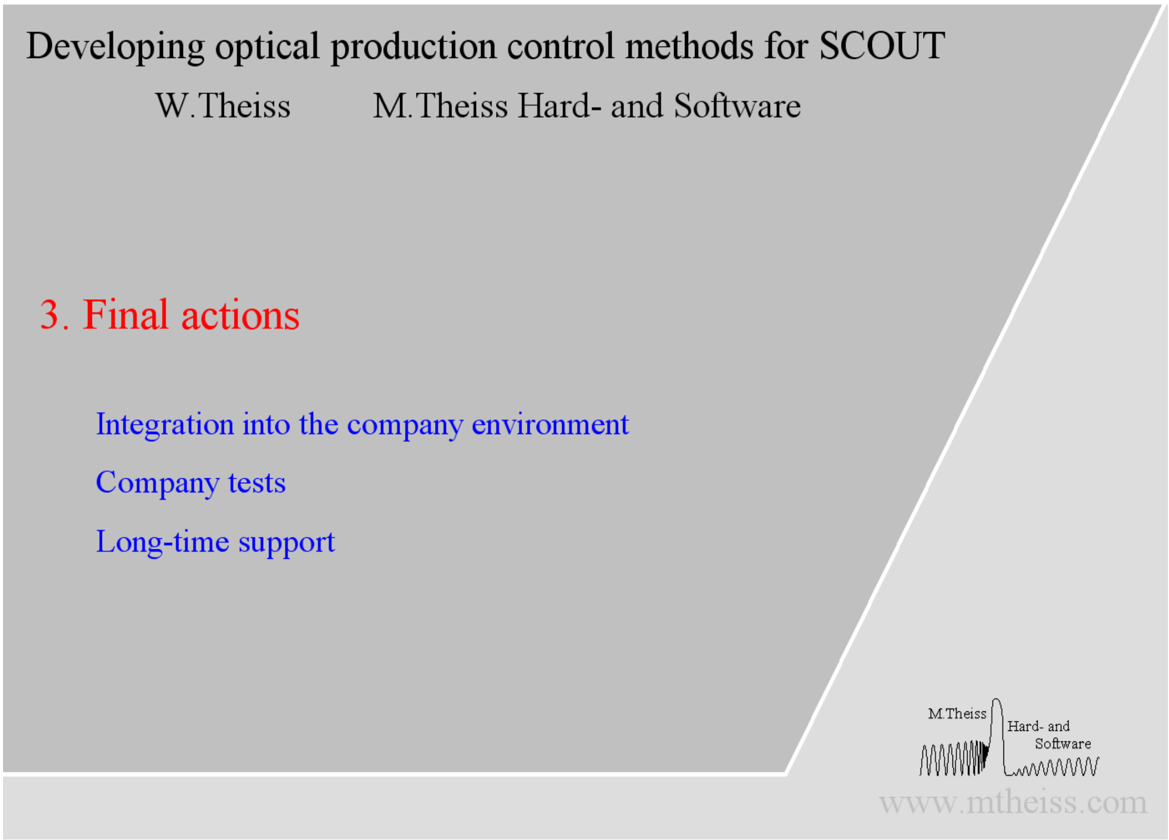
2. Development of the optical model

Selecting optical constant models

Fixing the layer structure

Fit strategy



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3. Final actions

Integration into the company environment

Company tests

Long-time support

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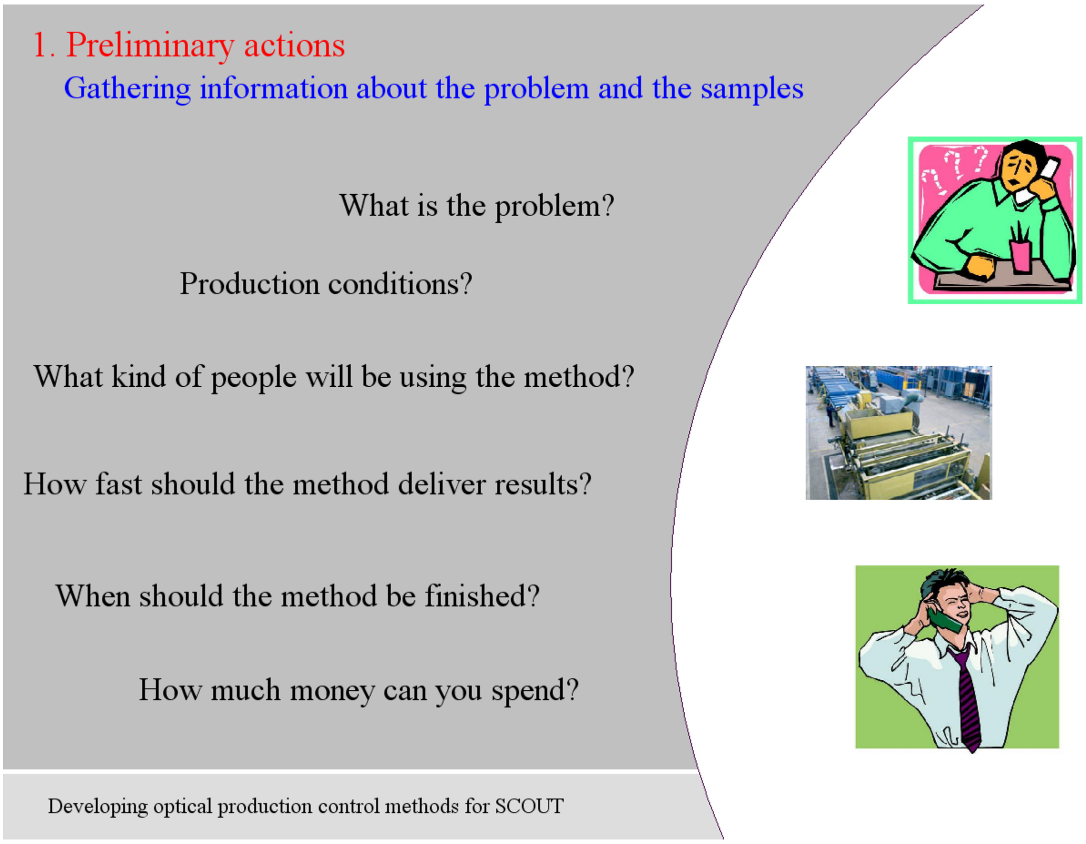
2 Preliminary actions

2.1 Gathering information

Get information about the problem to be solved and the circumstances of the development:



1. Preliminary actions

Gathering information about the problem and the samples

What is the problem?

Production conditions?

What kind of people will be using the method?

How fast should the method deliver results?

When should the method be finished?

How much money can you spend?

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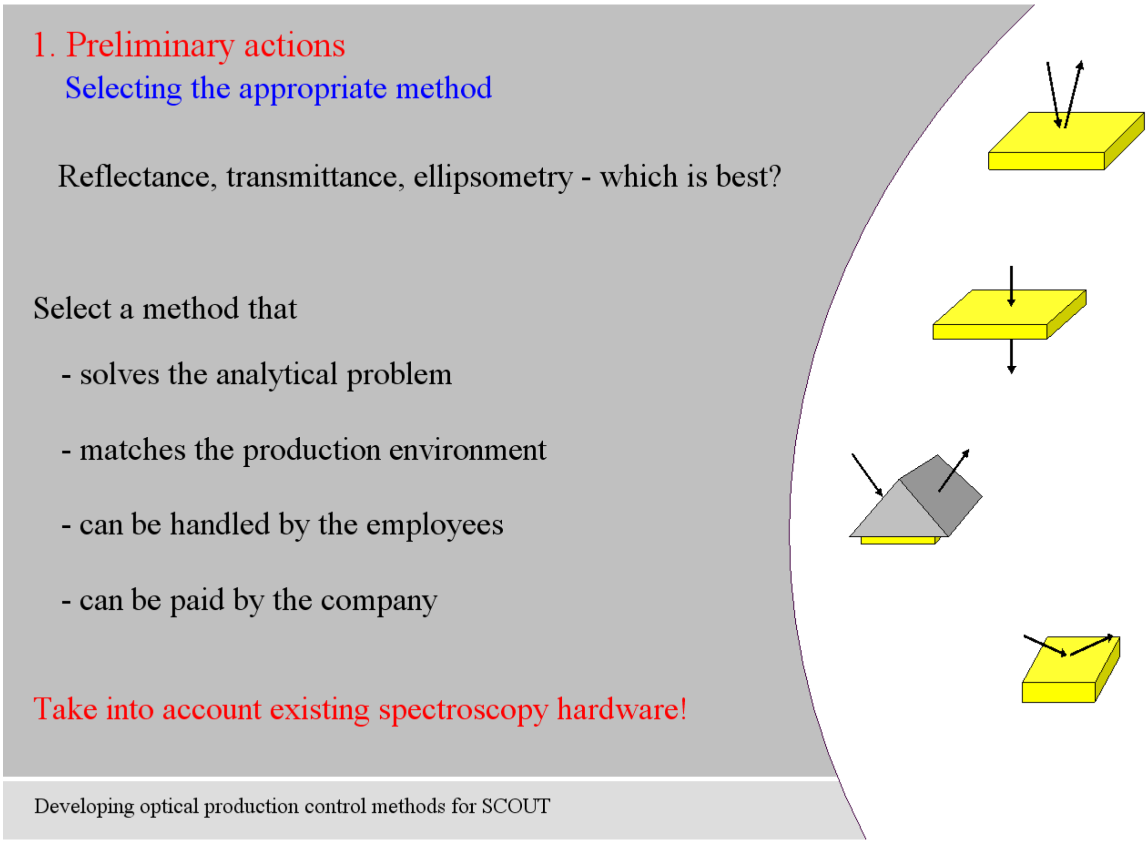
2.2 Selecting the appropriate method

Considering the goal of the method and the external conditions, the appropriate experimental technique is selected:



1. Preliminary actions

Selecting the appropriate method

Reflectance, transmittance, ellipsometry - which is best?

Select a method that

- solves the analytical problem
- matches the production environment
- can be handled by the employees
- can be paid by the company

Take into account existing spectroscopy hardware!

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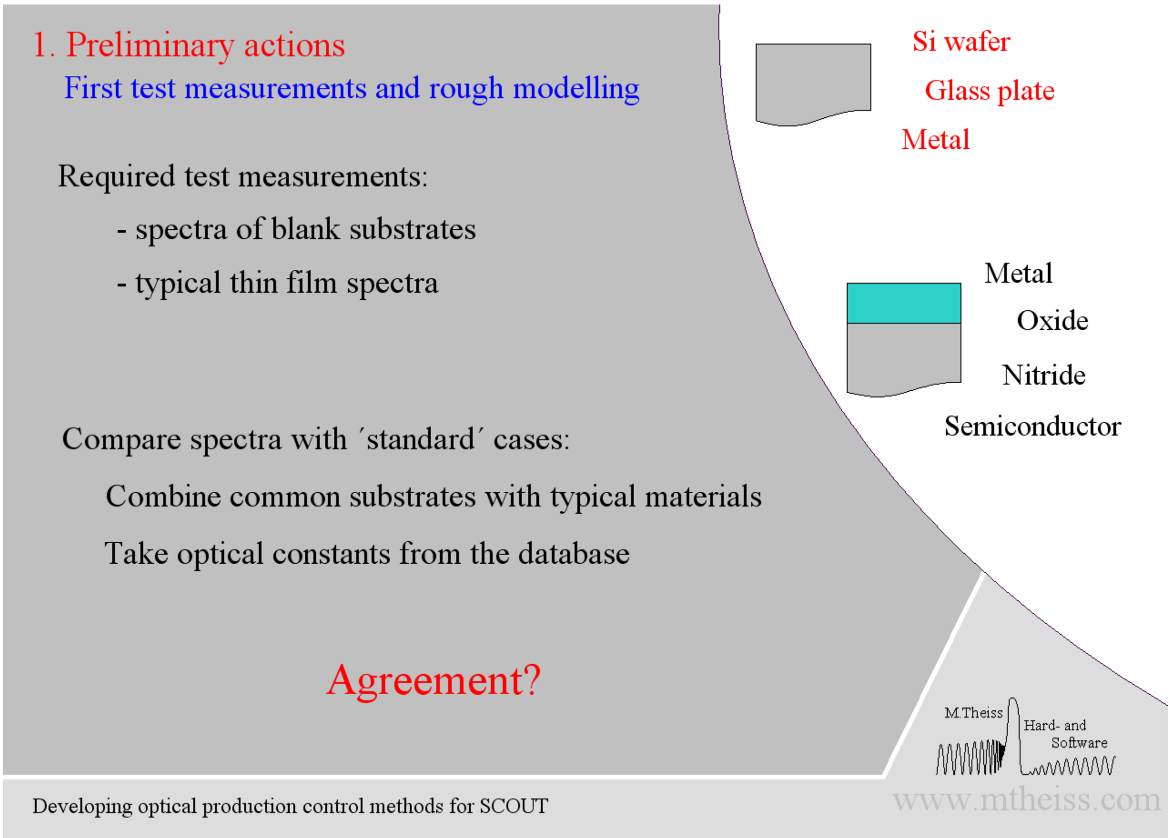
2.3 First test measurements and rough optical modelling

Do first test measurements: Investigate a blank substrate, and - if possible - a seris of thin film spectra covering the expected variety of cases in the production.

Verify that measured substrate spectra agree with simulated ones. This is an important check of the spectrometer hardware and the measurement procedure.

Can we successfully describe the thin film test measurements with preliminary, simple optical models?
Identify the type of material by comparison to known cases: Metal, semiconductor, oxide or nitride?



1. Preliminary actions

First test measurements and rough modelling

Required test measurements:

- spectra of blank substrates
- typical thin film spectra

Compare spectra with ´standard´ cases:

Combine common substrates with typical materials

Take optical constants from the database

Agreement?

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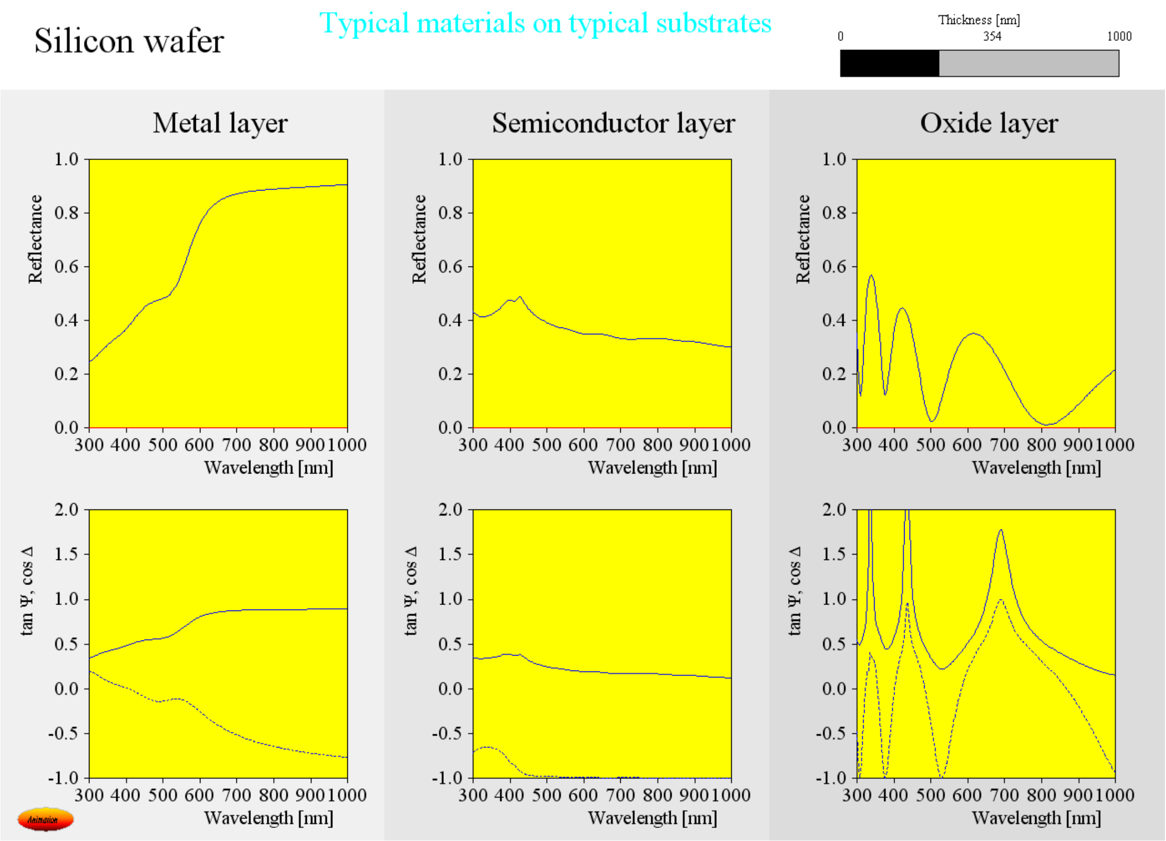
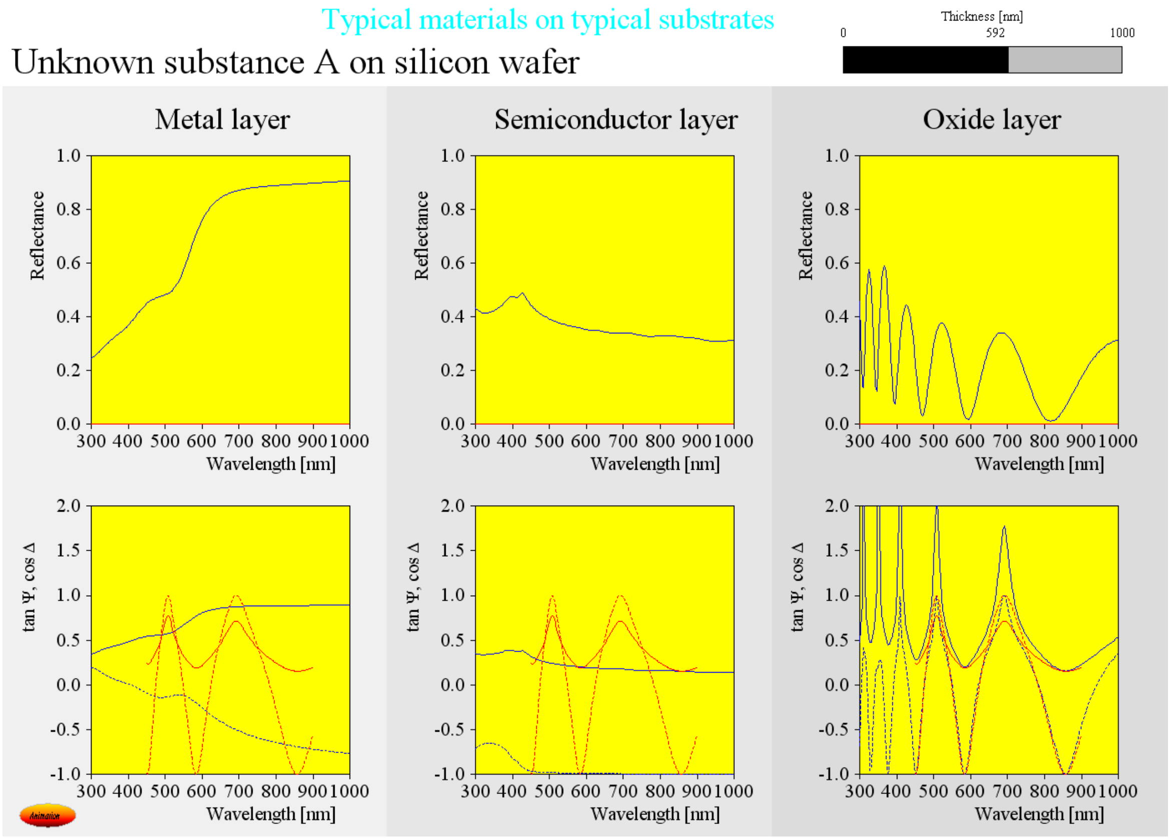
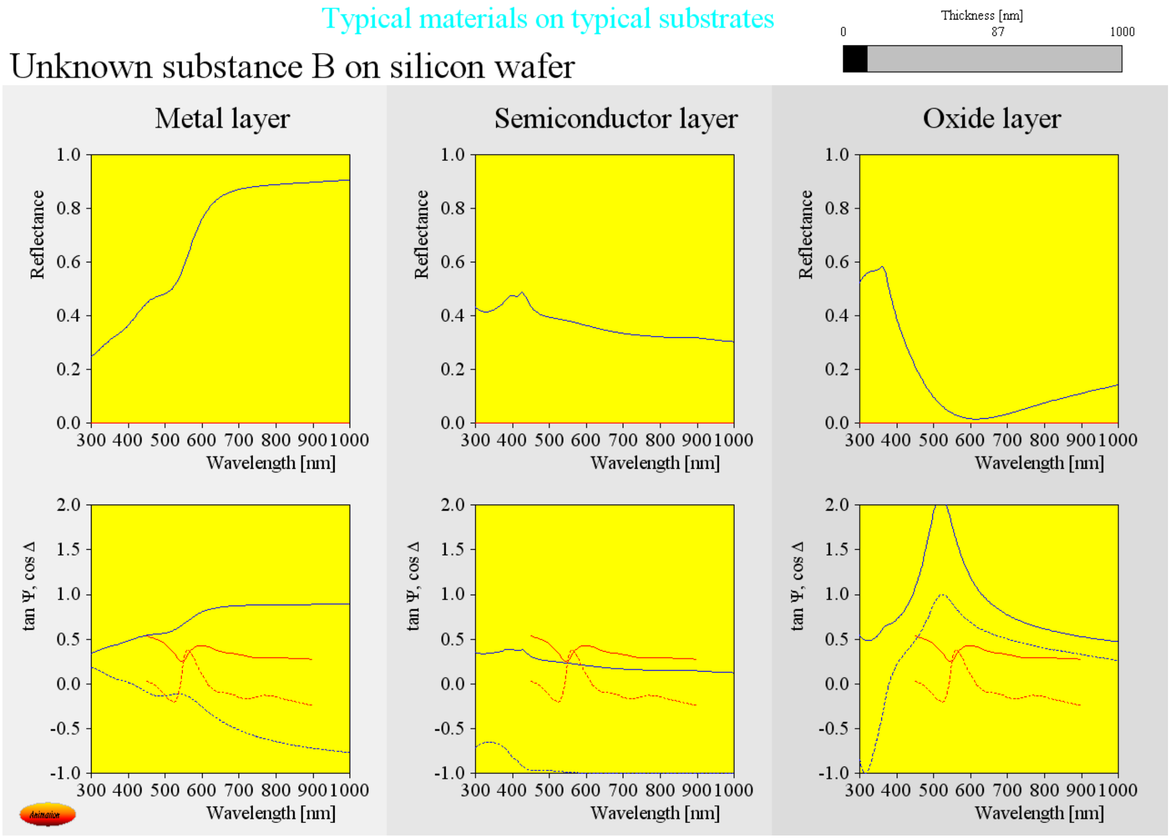
The following graphs show spectra of typical metal, semiconductor and oxide thin films on a silicon wafer substrate. The top pictures display the reflectance, the bottom ones show ellipsometry spectra:



We now load measured ellipsometry data for an unknown substance on silicon. A rough comparison shows that the material behaves like a typical oxide. Very likely an adjustable ´oxide model´ will lead to a succesful simulation (this will be verified later on):

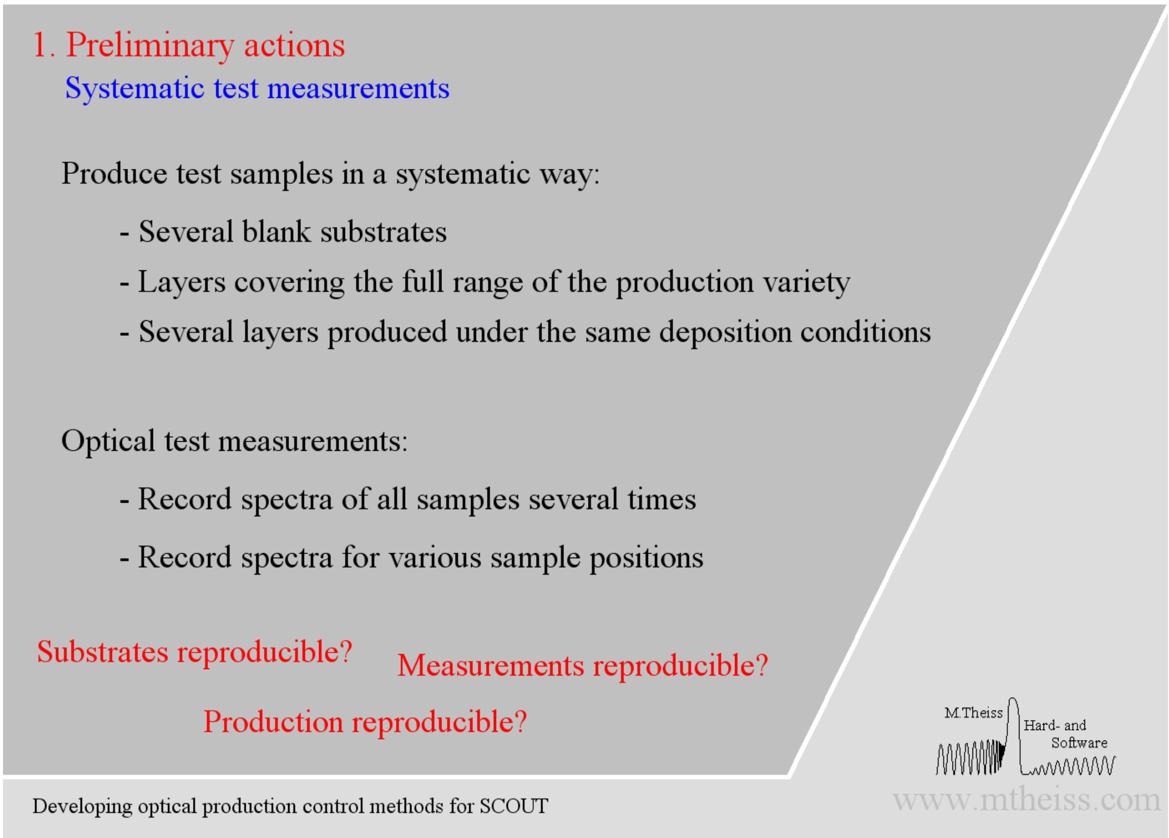


For another test material there is no convincing agreement with any of the typical cases. In this case a new type of optical constant model has to be developed:



2.4 Systematic test measurements

In case of succesful pre-liminary tests: Decide to realize the method and continue with systematic test measurements.



1. Preliminary actions

Systematic test measurements

Produce test samples in a systematic way:

- Several blank substrates
- Layers covering the full range of the production variety
- Several layers produced under the same deposition conditions

Optical test measurements:

- Record spectra of all samples several times
- Record spectra for various sample positions

Substrates reproducible? Measurements reproducible?

Production reproducible?

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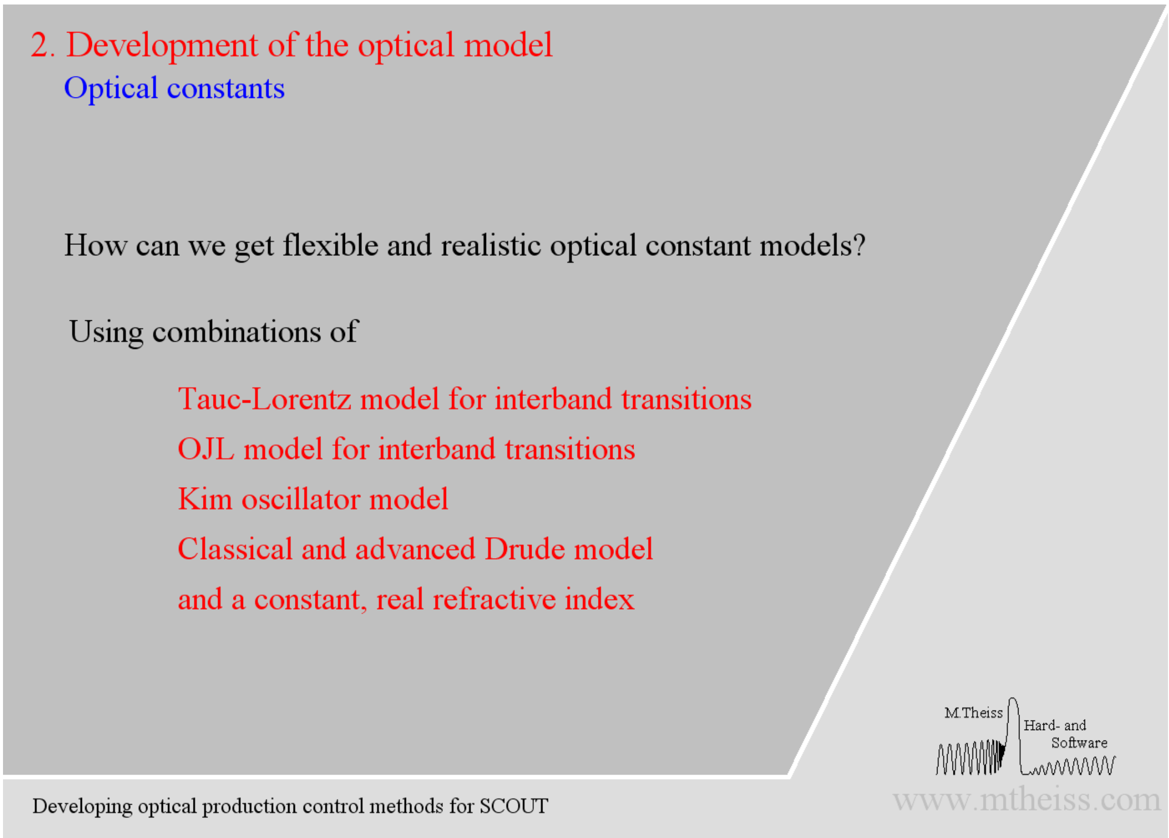
3 Development of the optical model

3.1 Optical constants

Having gathered enough information and data the optical model for the given analytical problem can be developed.

The basis of any spectrum simulation method are correct optical constants. In most cases of optical process control models with adjustable parameters are required.



2. Development of the optical model

Optical 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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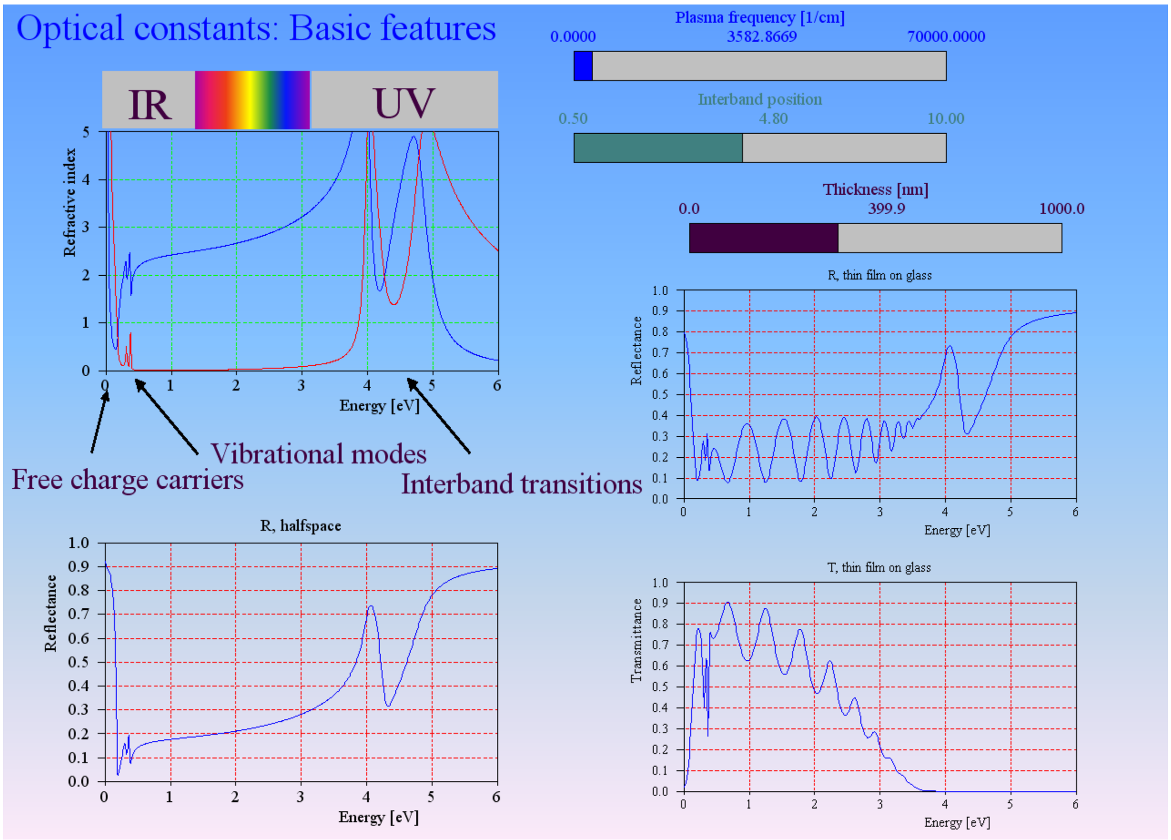
With these models we can successfully treat the three basic excitations: Interband transitions, vibrational modes and the acceleration of free charge carriers (electrons, holes).

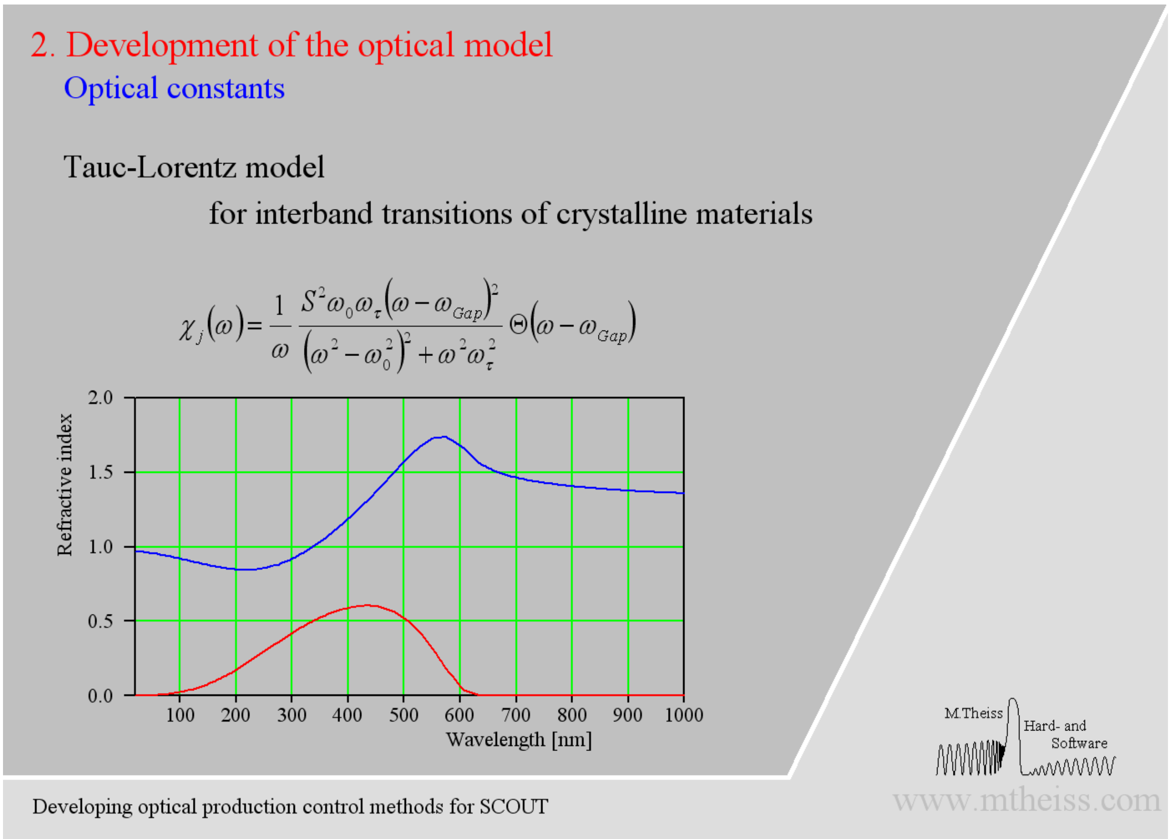


Optical constants: Basic features

Models for the individual excitation types are suggested in the following sections.

3.1.1 Interband transitions

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



2. Development of the optical model

Optical constants

Tauc-Lorentz model

for interband transitions of crystalline materials

$$\chi_j(\omega)=\frac{1}{\omega}\frac{S^2\omega_0\omega_\tau\left(\omega-\omega_{Gap}\right)^2}{\left(\omega^2-\omega_0^2\right)^2+\omega^2\omega_\tau^2}\Theta\left(\omega-\omega_{Gap}\right)$$

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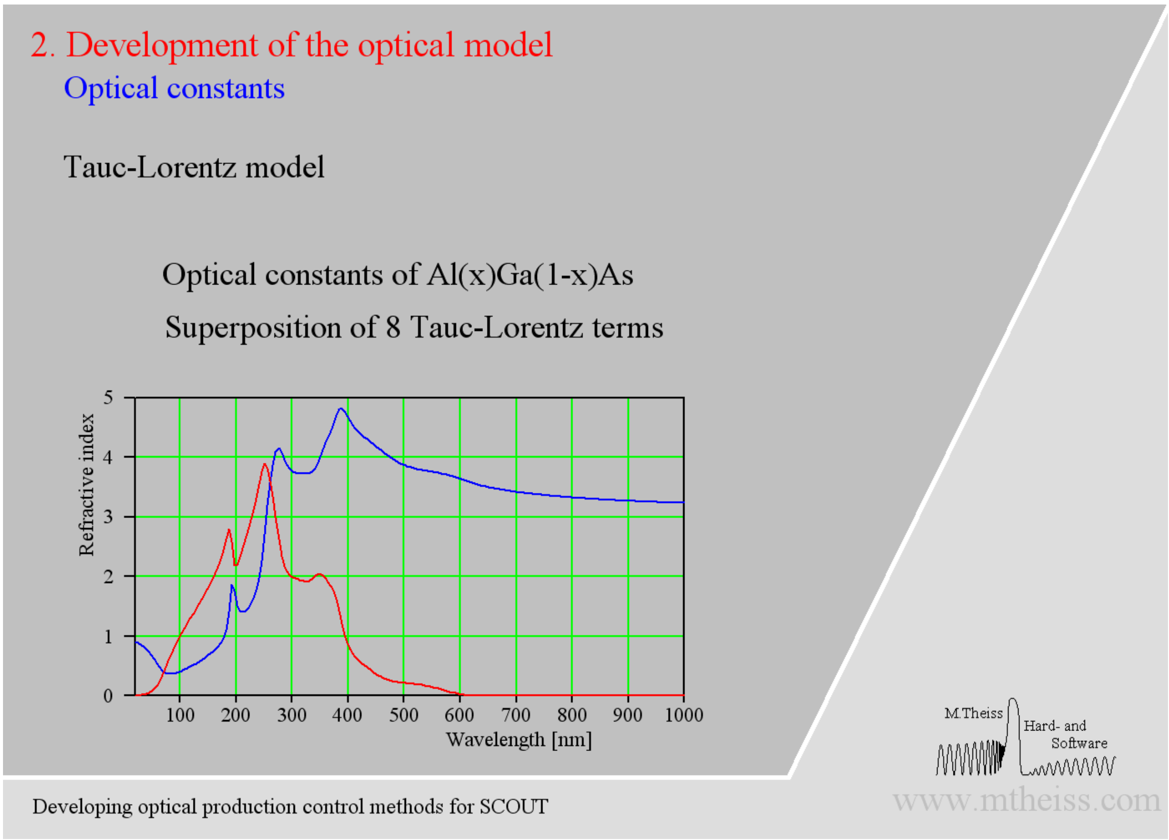
Here is a typical example using the superposition of 8 interband transitions:



2. Development of the optical model

Optical constants

Tauc-Lorentz model

Optical constants of Al(x)Ga(1-x)As

Superposition of 8 Tauc-Lorentz terms

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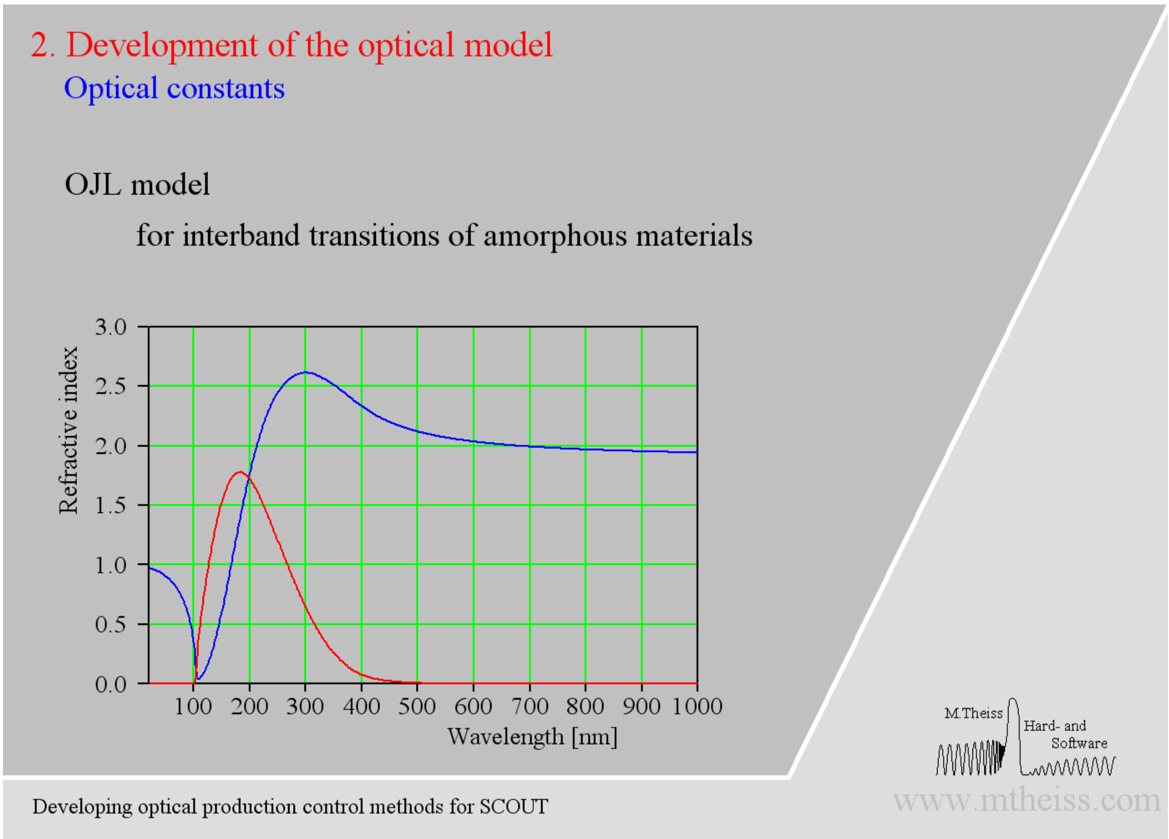
Amorphous materials have less rich featured, broad interband transitions which can often be described in good quality using a single OJL model:



2. Development of the optical model

Optical constants

OJL model

for interband transitions of amorphous materials

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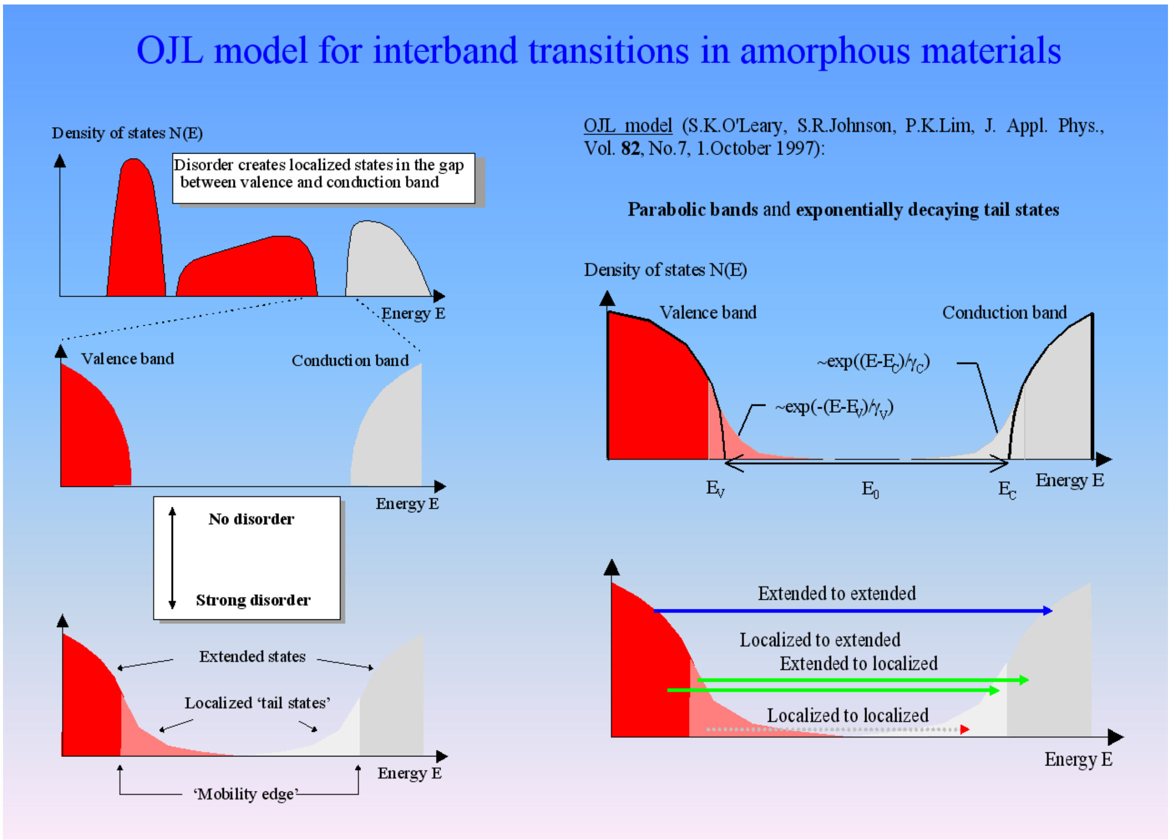
The theory behind the OJL model is summarized in the following page:

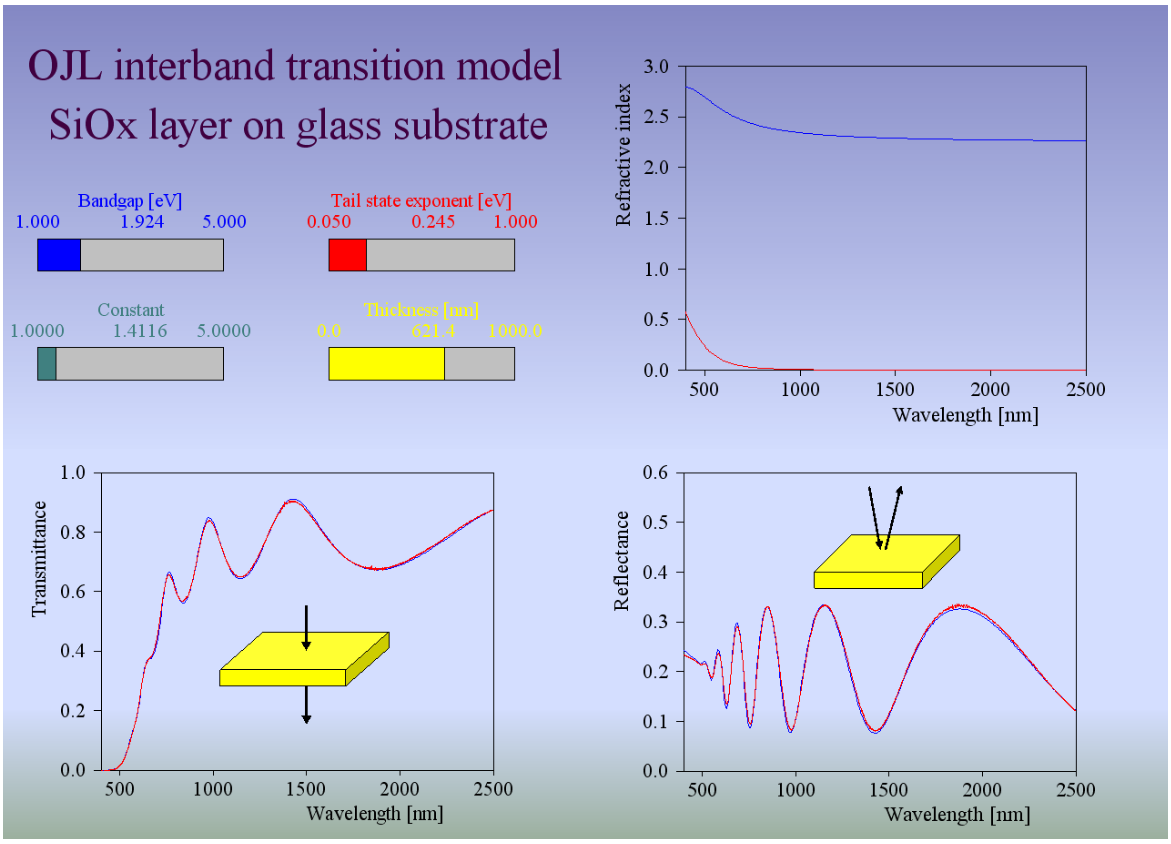


OJL model for interband transitions in amorphous materials

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

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



OJL interband transition model

SiOx layer on glass substrate

Bandgap [eV] 1.000 1.924 5.000

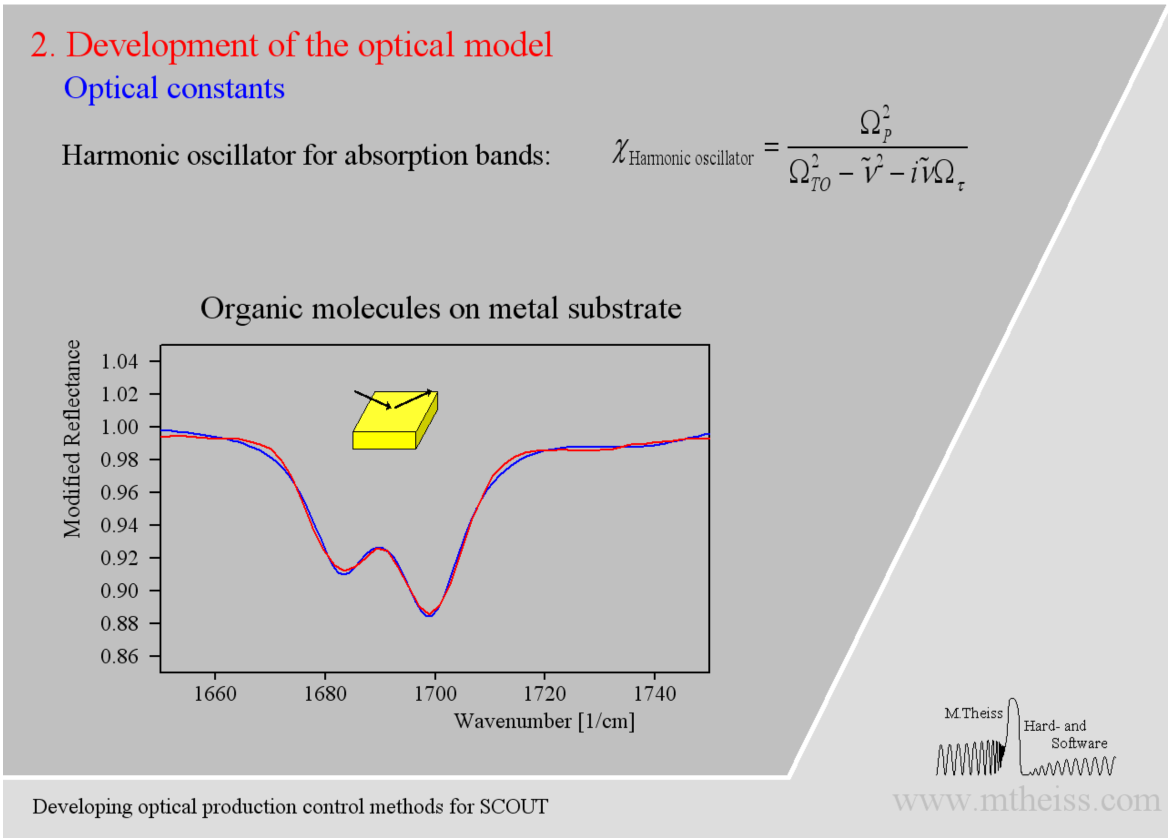
Tail state exponent [eV] 0.050 0.245 1.000

Constant 1.0000 1.4116 5.0000

Thickness [nm] 0.0 621.4 1000.0

3.1.2 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:



2. Development of the optical model

Optical constants

Harmonic oscillator for absorption bands:

$$\chi_{\text{Harmonic oscillator}} = \frac{\Omega_p^2}{\Omega_{TO}^2 - \tilde{\nu}^2 - i\tilde{\nu}\Omega_\tau}$$

Organic molecules on metal substrate

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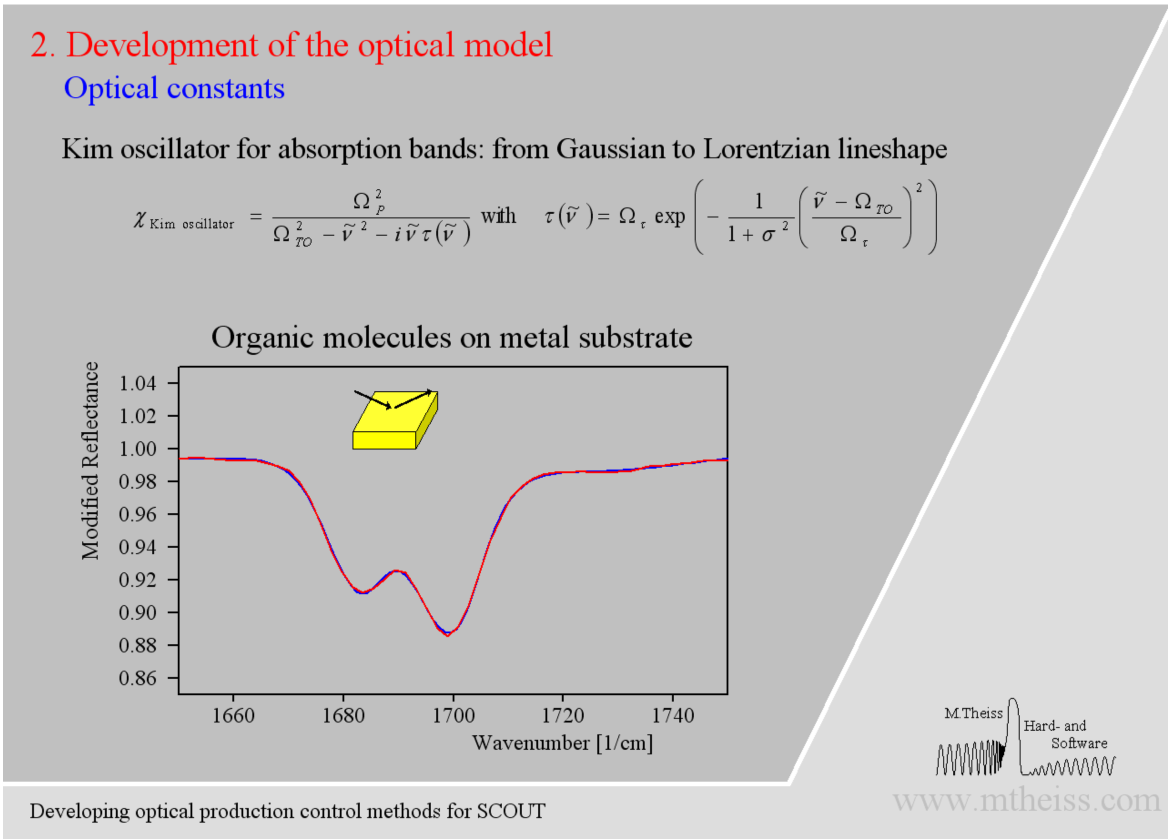
However, in most cases a Gaussian line shape is more realistic. In SCOUT this can be obtained using Kim oscillators:



2. Development of the optical model

Optical constants

Kim oscillator for absorption bands: from Gaussian to Lorentzian lineshape

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

Organic molecules on metal substrate

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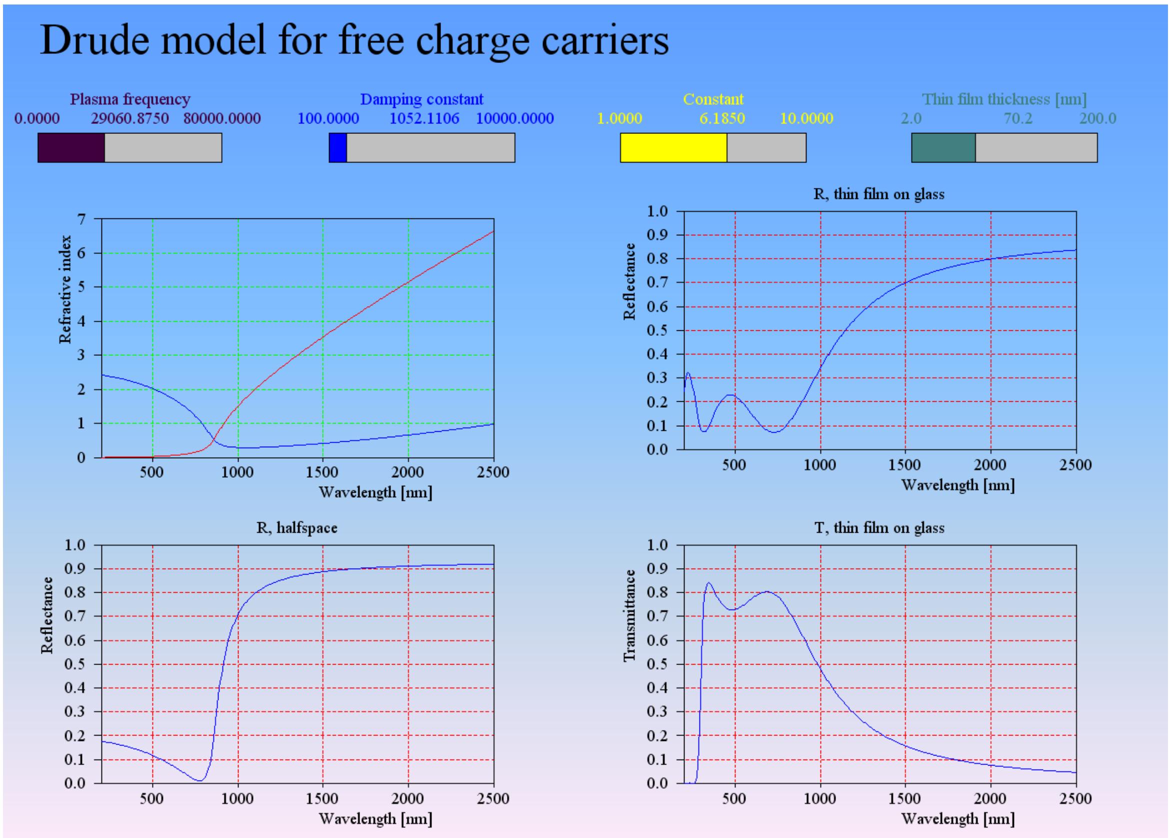
3.1.3 Charge carriers

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.



Drude model for free charge carriers

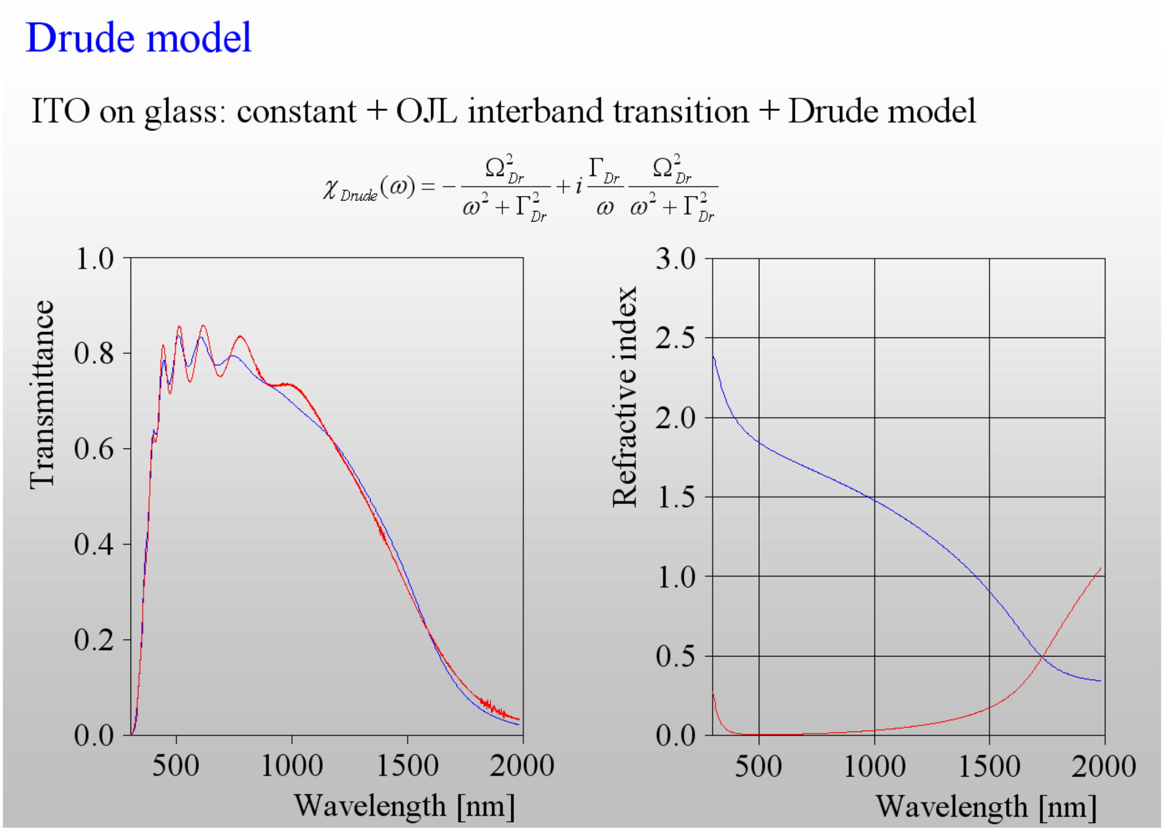
Plasma frequency: 0.0000 29060.8750 80000.0000

Damping constant: 100.0000 1052.1106 10000.0000

Constant: 1.0000 6.1850 10.0000

Thin film thickness [nm]: 2.0 70.2 200.0

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

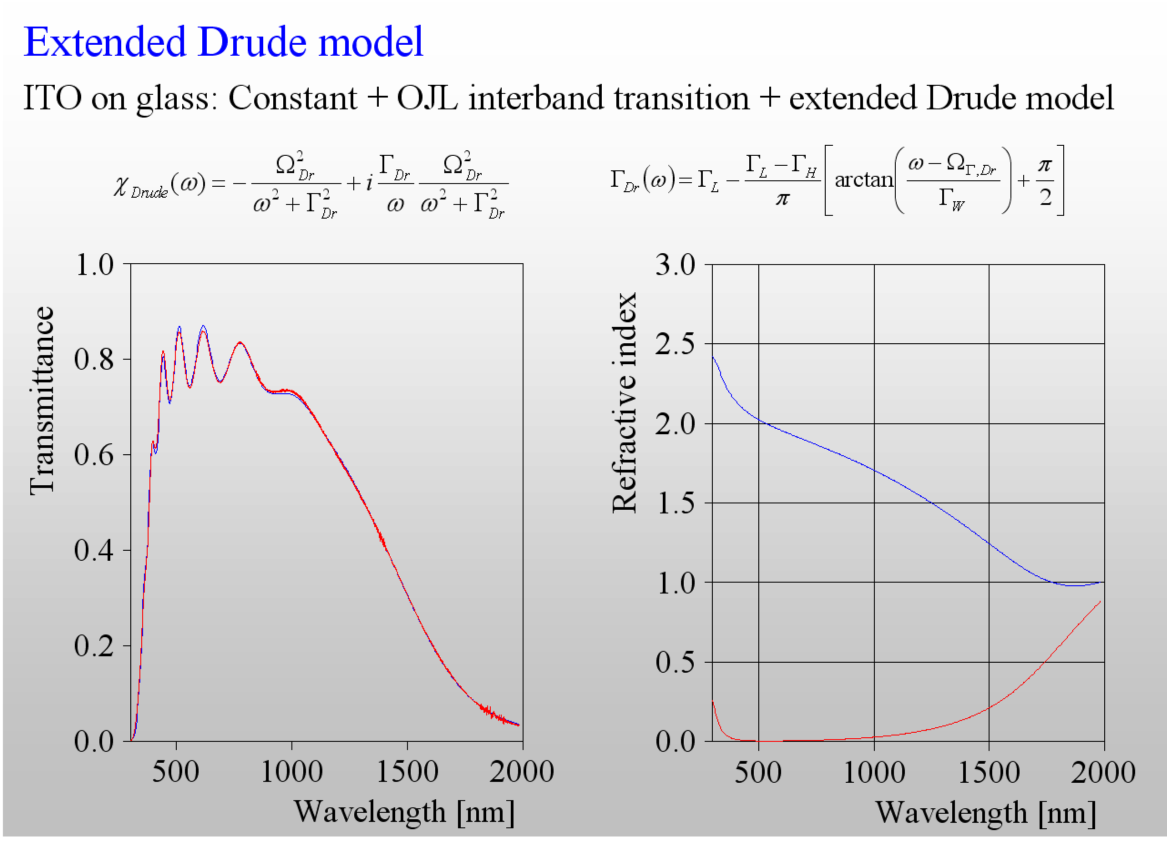


Drude model

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

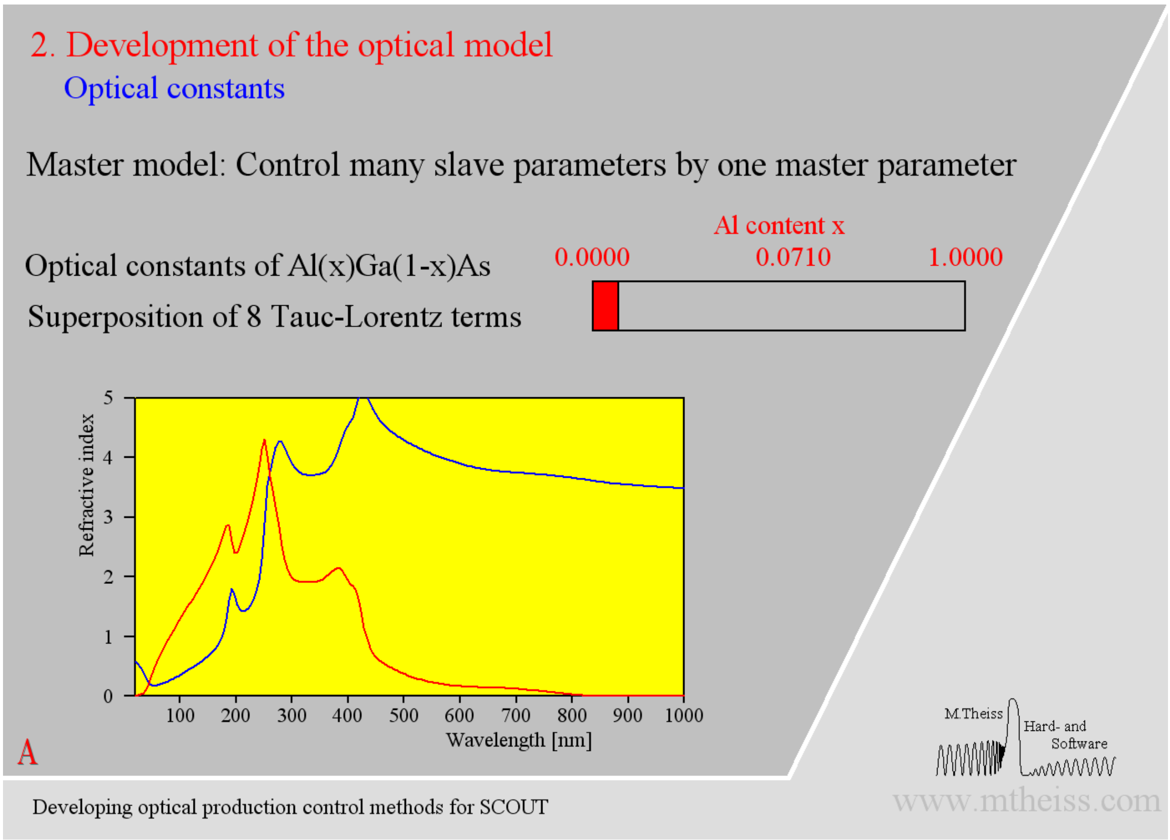
ITO on glass: Constant + OJL interband transition + extended Drude model

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

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

3.1.4 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 using so-called master models which provide for every parameter a user-defined formula to express its dependence on the master quantity:



2. Development of the optical model

Optical constants

Master model: Control many slave parameters by one master parameter

Optical constants of Al(x)Ga(1-x)As

Superposition of 8 Tauc-Lorentz terms

Al content x

0.0000 0.0710 1.0000

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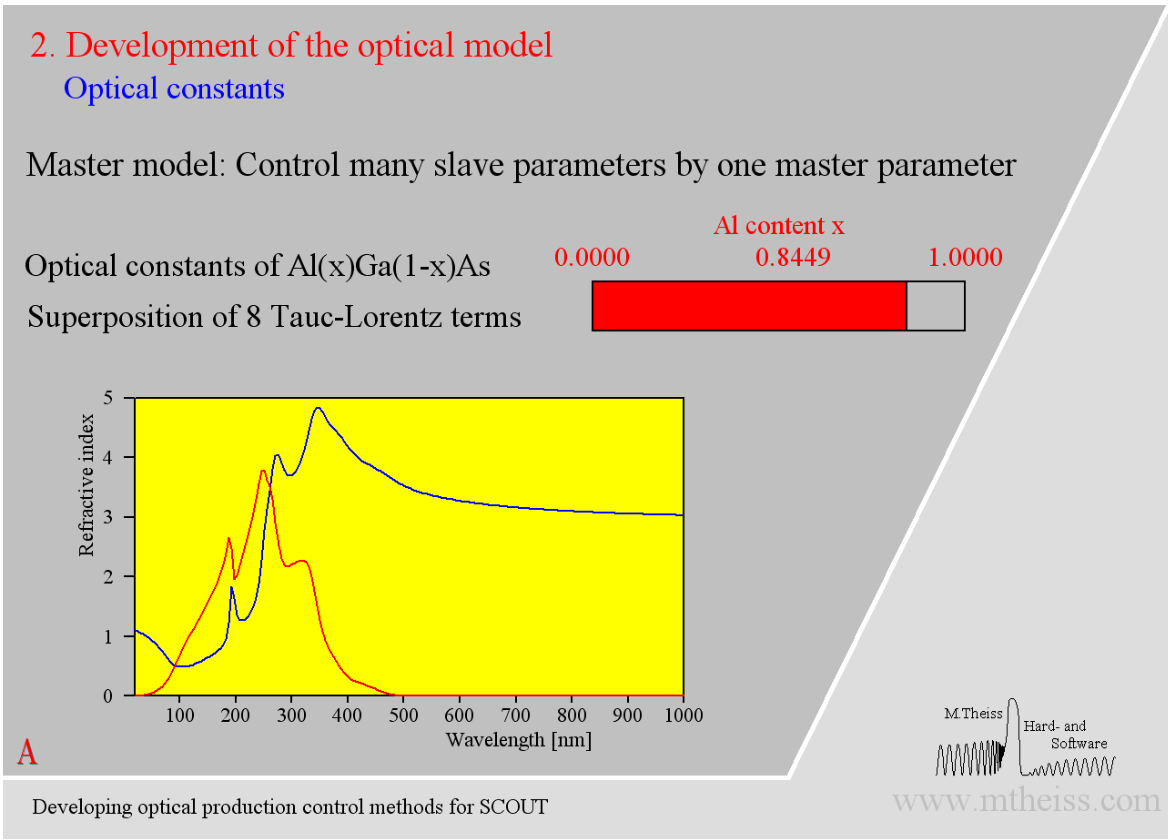

2. Development of the optical model

Optical constants

Master model: Control many slave parameters by one master parameter

Optical constants of Al(x)Ga(1-x)As

Superposition of 8 Tauc-Lorentz terms

Al content x

0.0000 0.8449 1.0000

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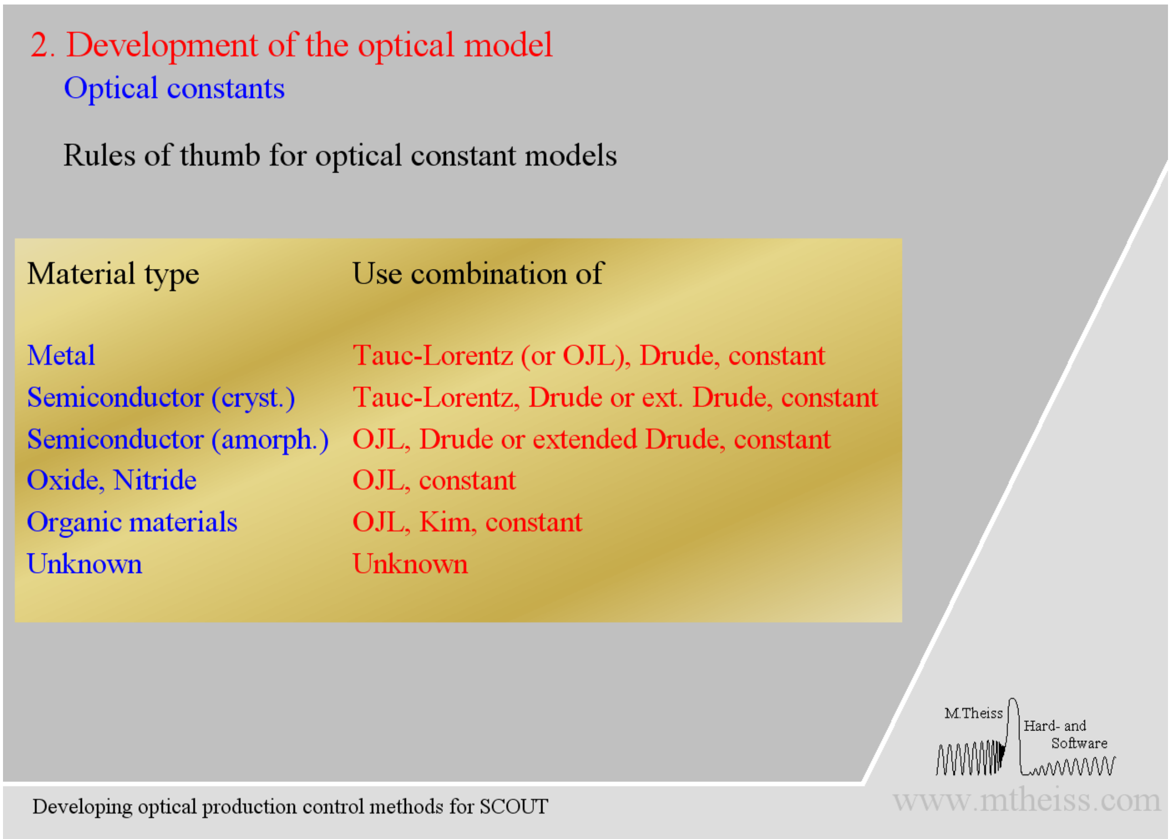
3.1.5 'Rules of thumb'

Use the following rules of thumb to find appropriate models for optical constants:



2. Development of the optical model

Optical constants

Rules of thumb for optical constant models

Material type	Use combination of
Metal	Tauc-Lorentz (or OJL), Drude, constant
Semiconductor (cryst.)	Tauc-Lorentz, Drude or ext. Drude, constant
Semiconductor (amorph.)	OJL, Drude or extended Drude, constant
Oxide, Nitride	OJL, constant
Organic materials	OJL, Kim, constant
Unknown	Unknown

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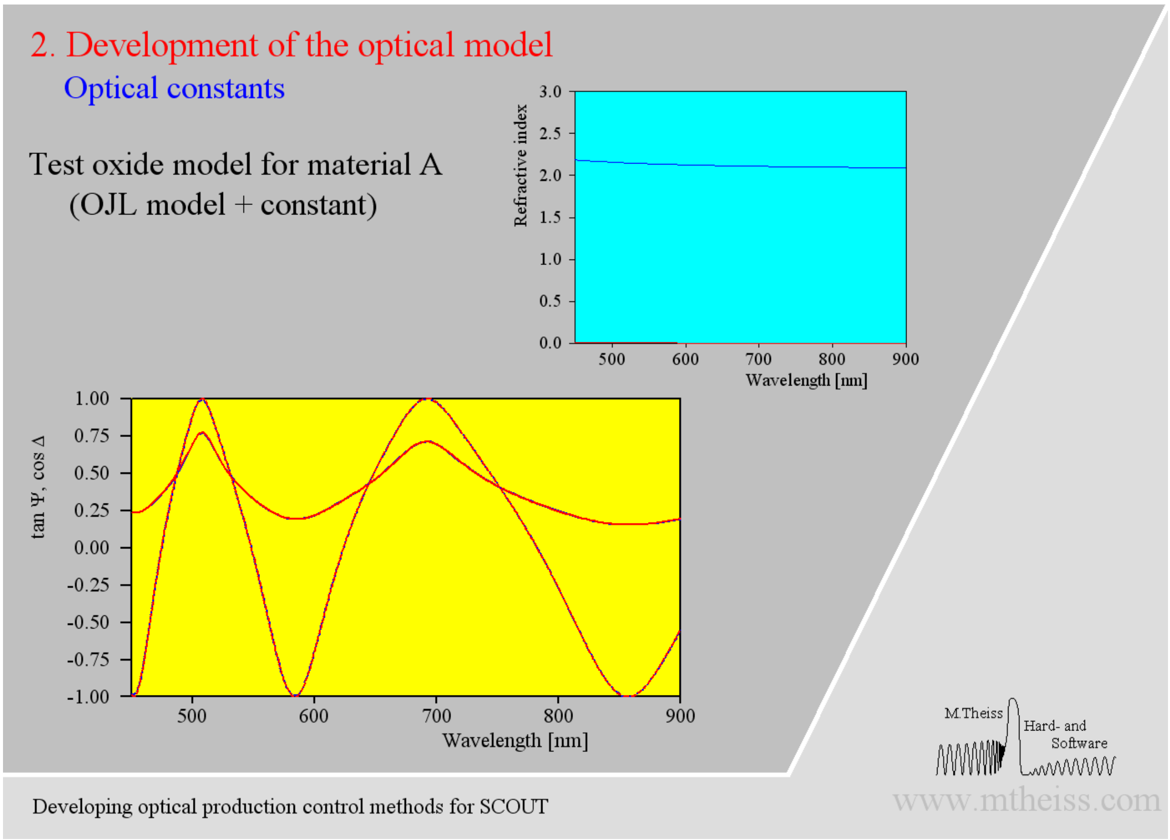
3.1.6 Substance A: Test oxide model

The optical properties of the unknown substance A (see above) can be described easily using the suggested oxide model:



2. Development of the optical model

Optical constants

Test oxide model for material A
(OJL model + constant)

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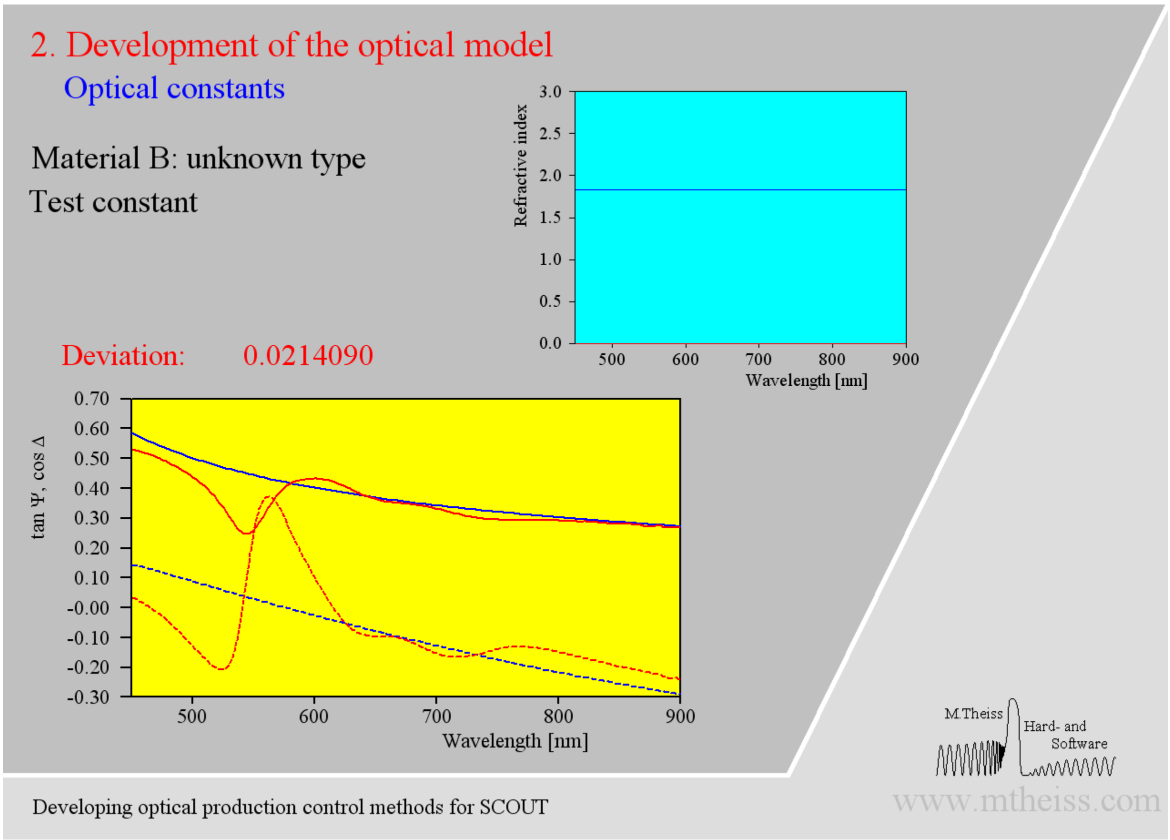
3.1.7 Substance B: Develop a new model

None of the standard cases seemed to be applicable for substance B (see above). Hence we have to develop a new model from scratch. In the following we assume that the layer thickness is about 40 nm (let's assume that we have got this rough number from the producer).
The simplest model would be just a constant. Varying the constant and the layer thickness the following 'agreement' of model and measurement is found:



2. Development of the optical model

Optical constants

Material B: unknown type

Test constant

Deviation: 0.0214090

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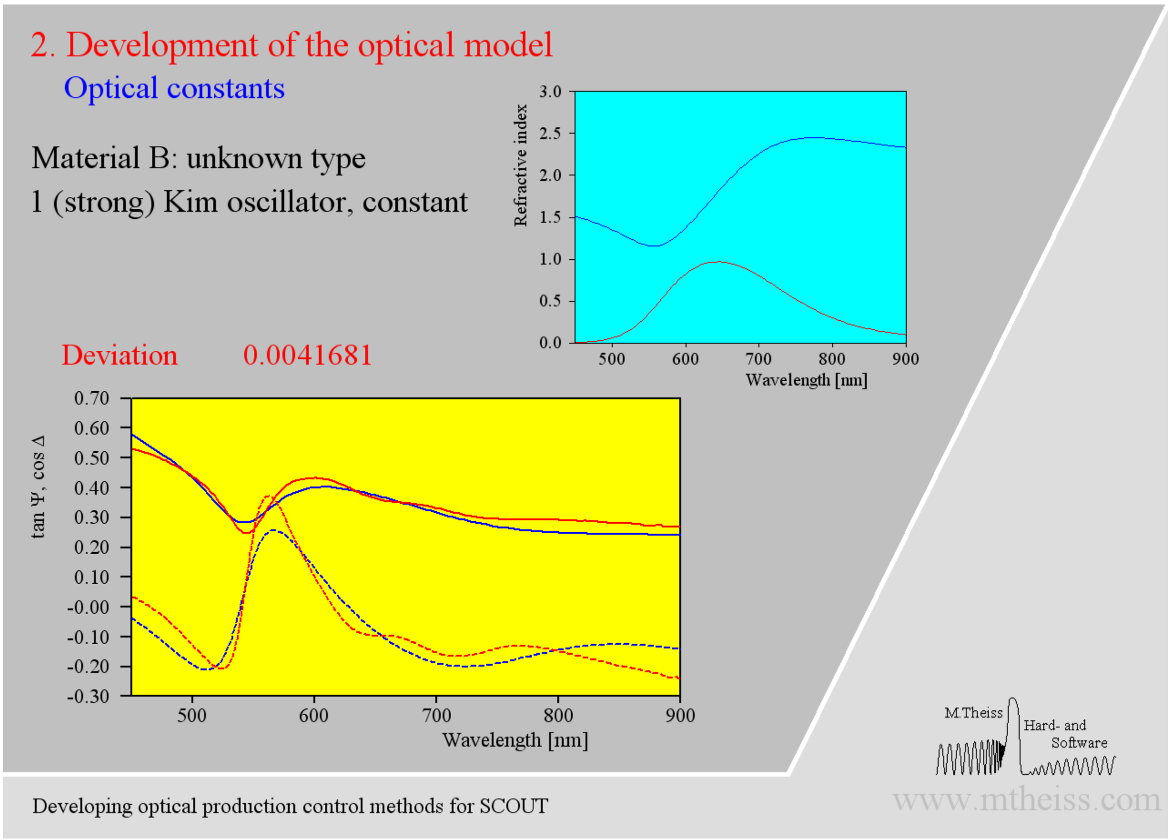
The spectral features do not look like interference fringes, so a rather strong dispersion of the refractive index and a strong absorption may be responsible for the observed structures.
Test a strong Kim oscillator (combined with a constant):



2. Development of the optical model

Optical constants

Material B: unknown type

1 (strong) Kim oscillator, constant

Deviation 0.0041681

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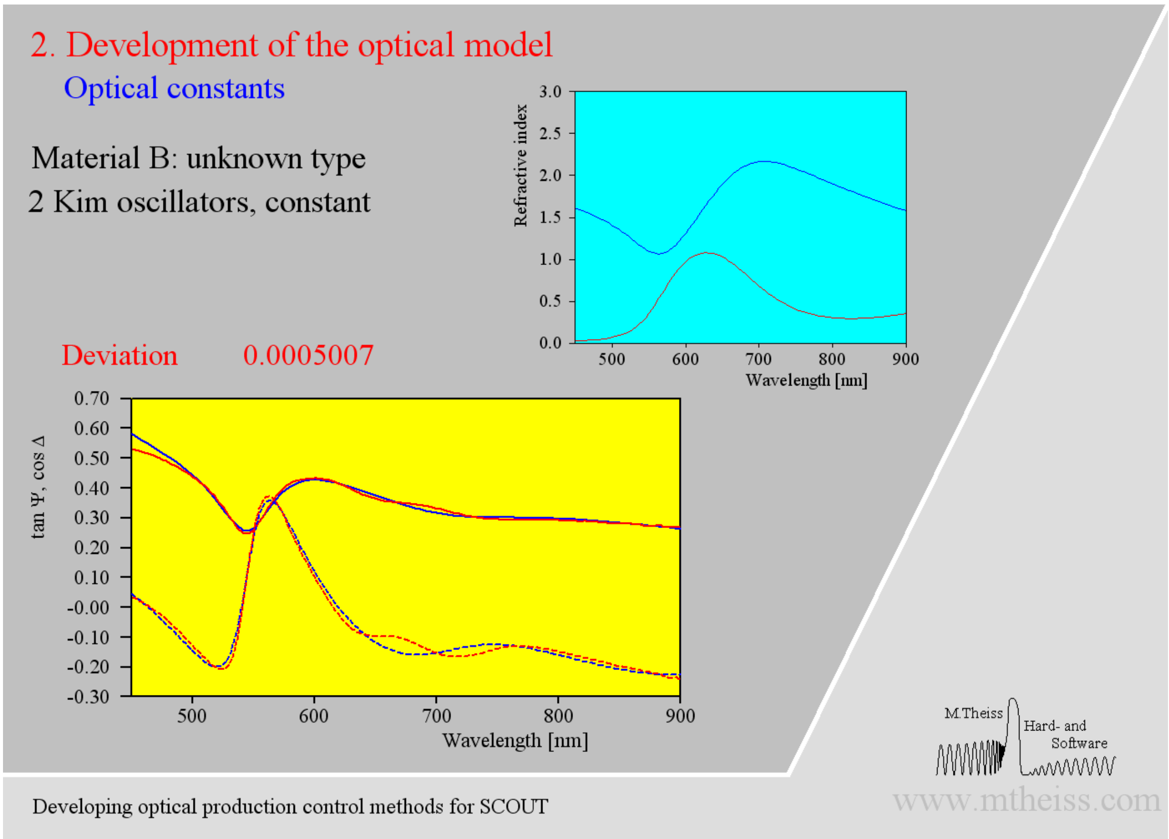
This looks promising. However, there are more structures in the measurement. Let's see if a second oscillator can help to improve the model. Although the second oscillator has been positioned around 750 nm initially, the fit algorithm moved it into the infrared in order to reduce the difference of model and measurement above 800 nm wavelength:



2. Development of the optical model

Optical constants

Material B: unknown type

2 Kim oscillators, constant

Deviation 0.0005007

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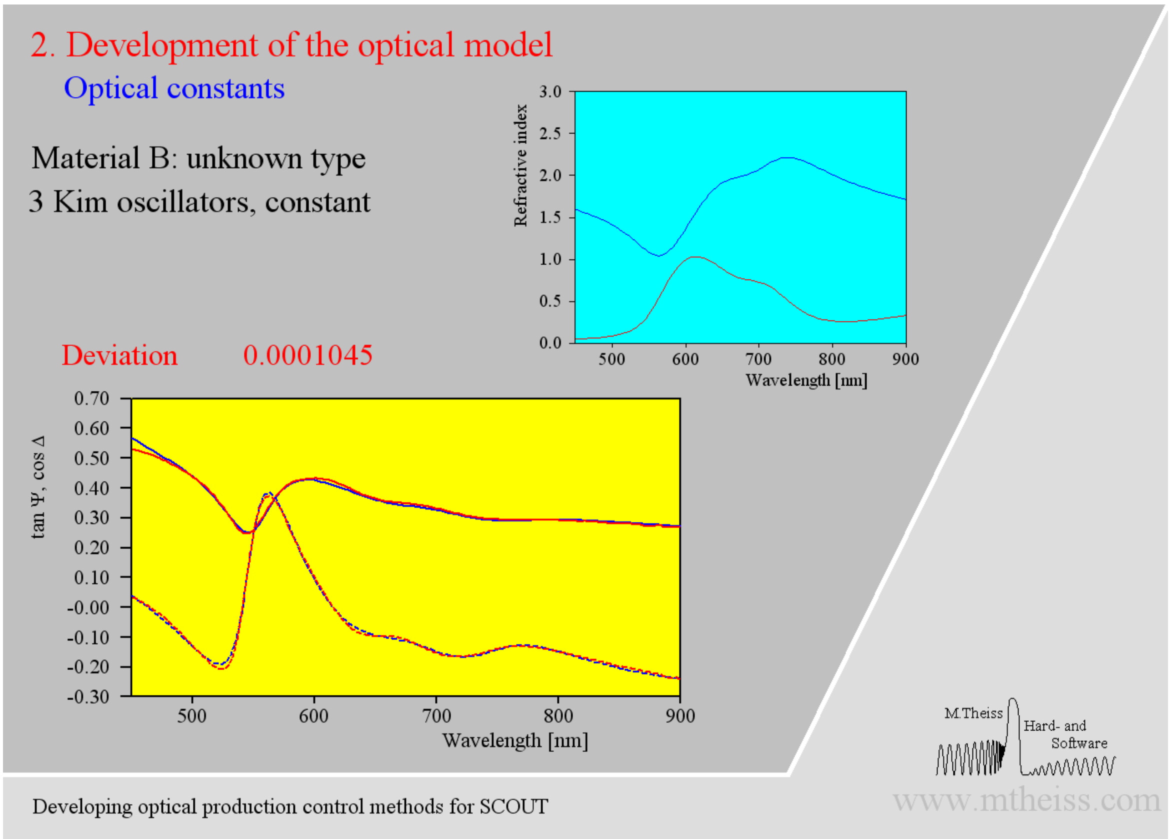
Still there is a large structural mismatch between 650 and 750 nm wavelength. Again, another Kim oscillator is introduced in order to fix this problem:



2. Development of the optical model

Optical constants

Material B: unknown type

3 Kim oscillators, constant

Deviation 0.0001045

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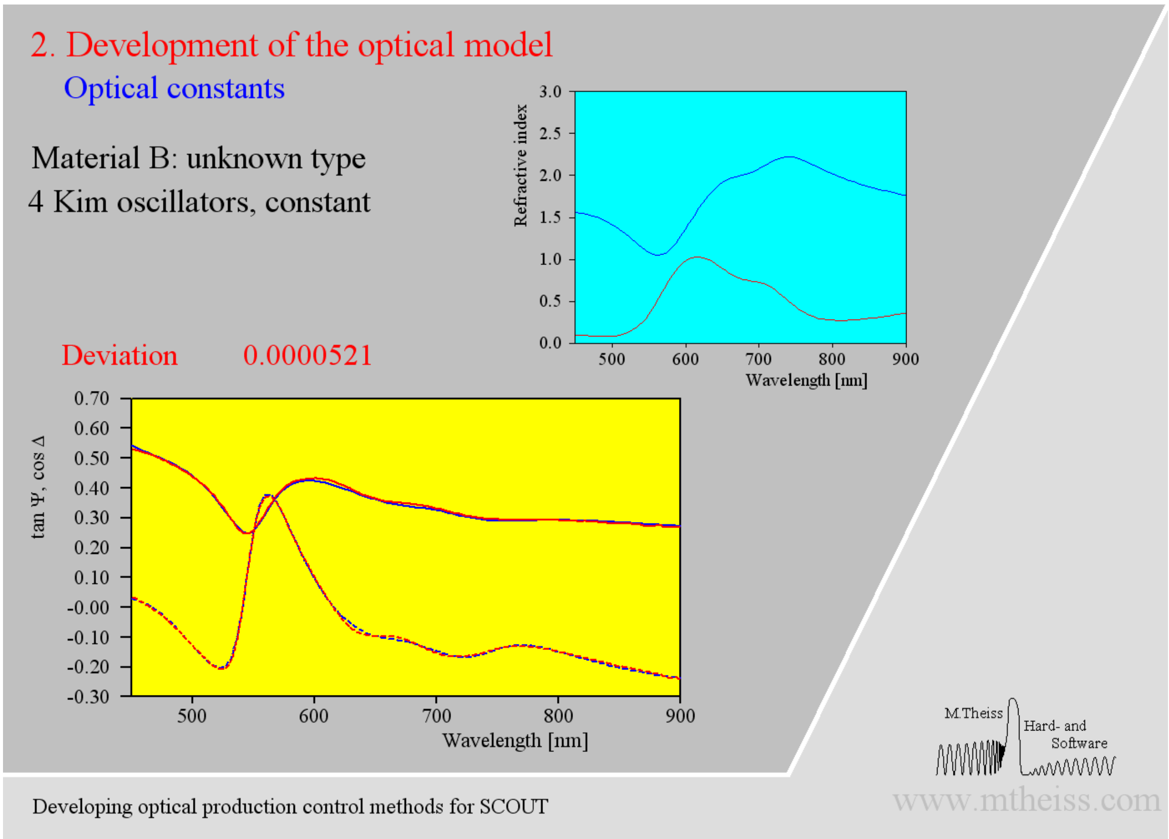
This is a real breakthrough. Only minor differences have to be removed. A Kim oscillator placed in the blue is now added which is going to improve the model for small wavelengths:



2. Development of the optical model

Optical constants

Material B: unknown type

4 Kim oscillators, constant

Deviation 0.0000521

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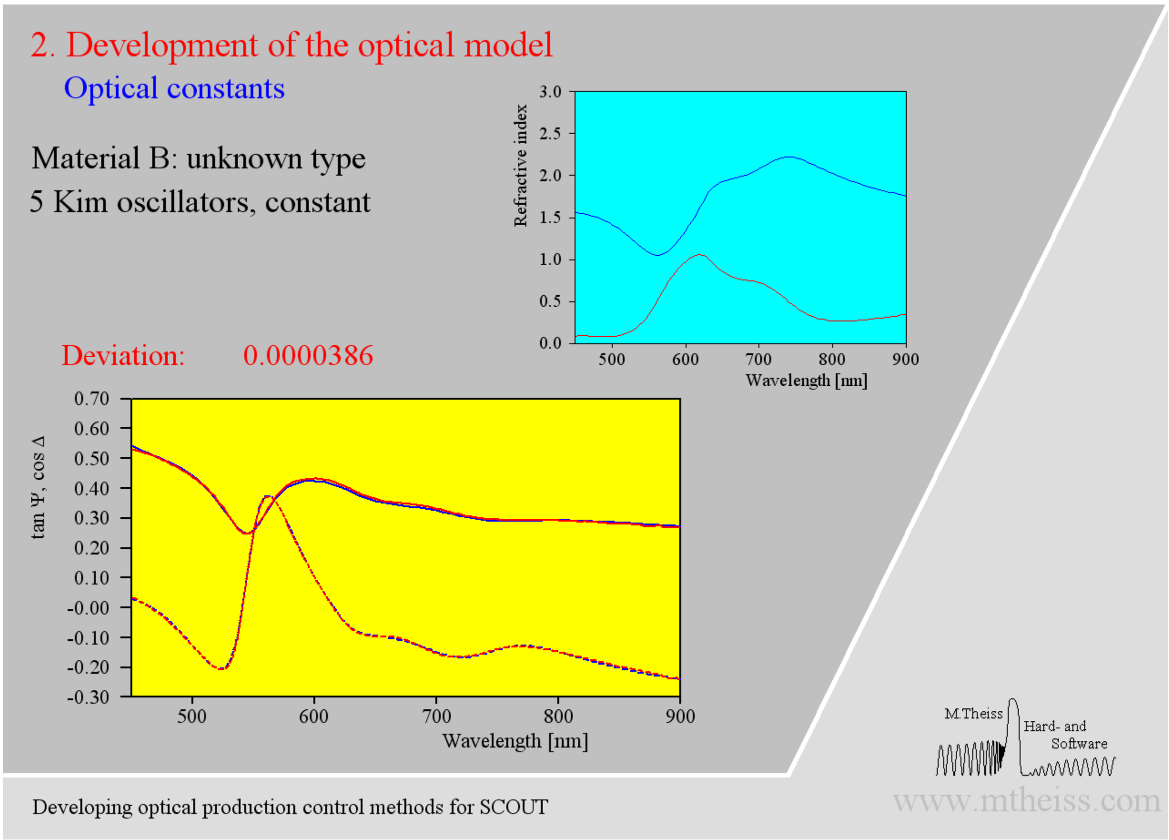
It's not easy to stop now because every additional oscillator turned out to be useful (and it seems to be a nice game). Let's do it one more time in the spectral range around 650 nm:



2. Development of the optical model

Optical constants

Material B: unknown type

5 Kim oscillators, constant

Deviation: 0.0000386

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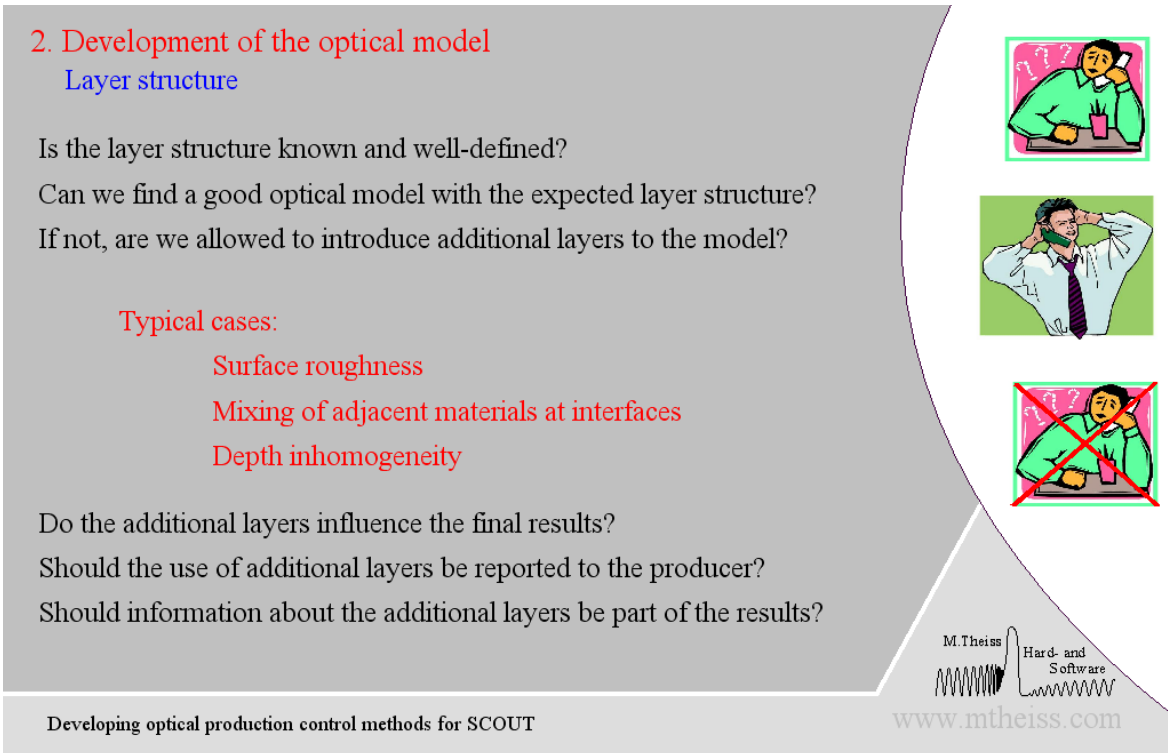
This seems to be good enough now. It would be important to check the obtained optical constants in other situtations. Other thicknesses could be prepared, and other substrates or different optical methods like reflectance or transmittance could be used in order to verify the validity of the result of the analysis.

3.2 Layer structure

In addition to the setup of optical constant models (see above) the structure of the layer stack must be questioned in some cases. Often layers additional to the ones reported by the producer must be introduced.



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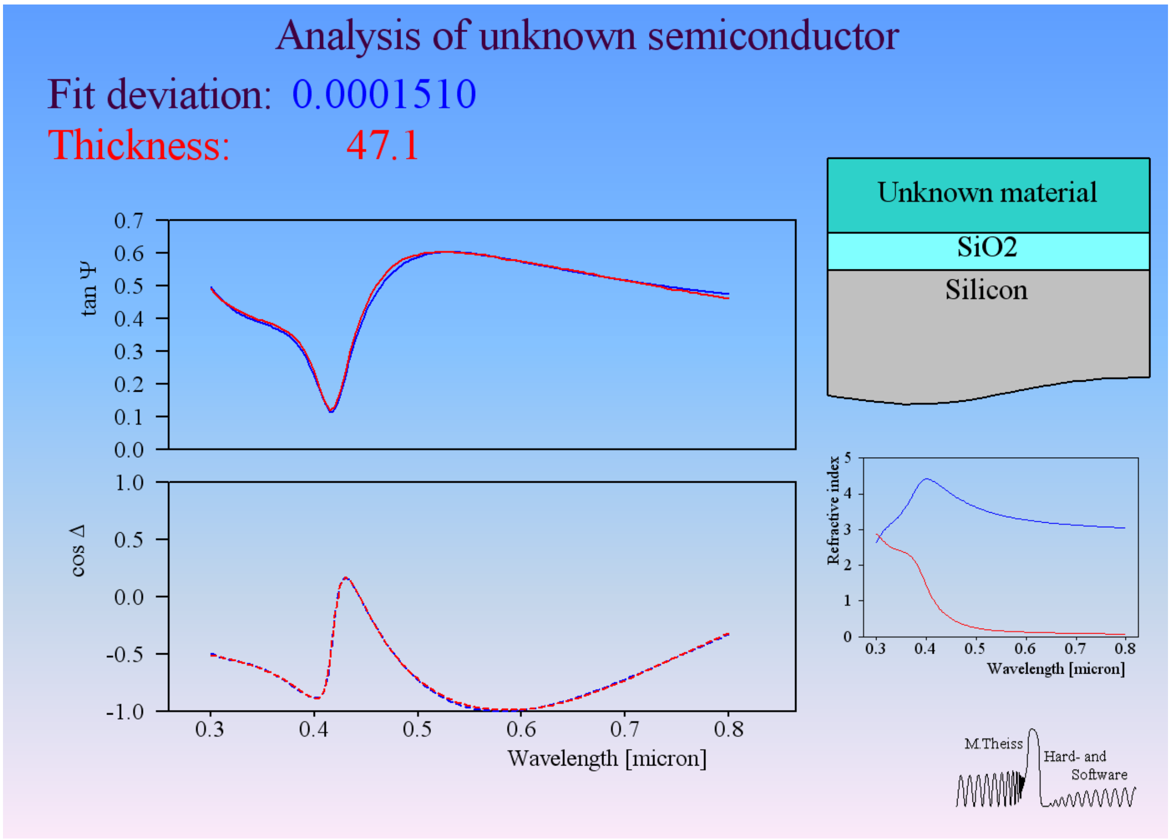
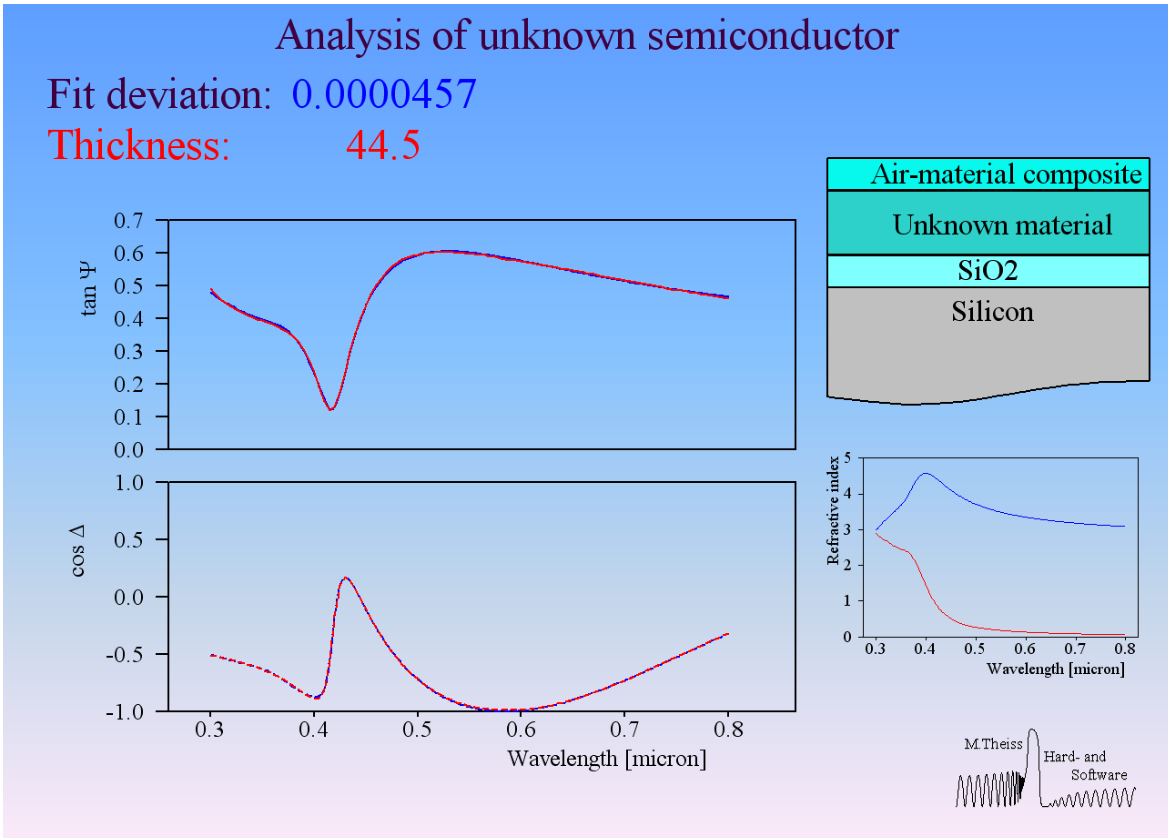
Example: The next graphs show the influence of the introduction of a surface layer to the results of a `single layer analysis´. It is not easy to decide if the differences are significant if the roughness is always the same. However, if the roughness changes from sample to sample it should definitely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



Analysis of unknown semiconductor

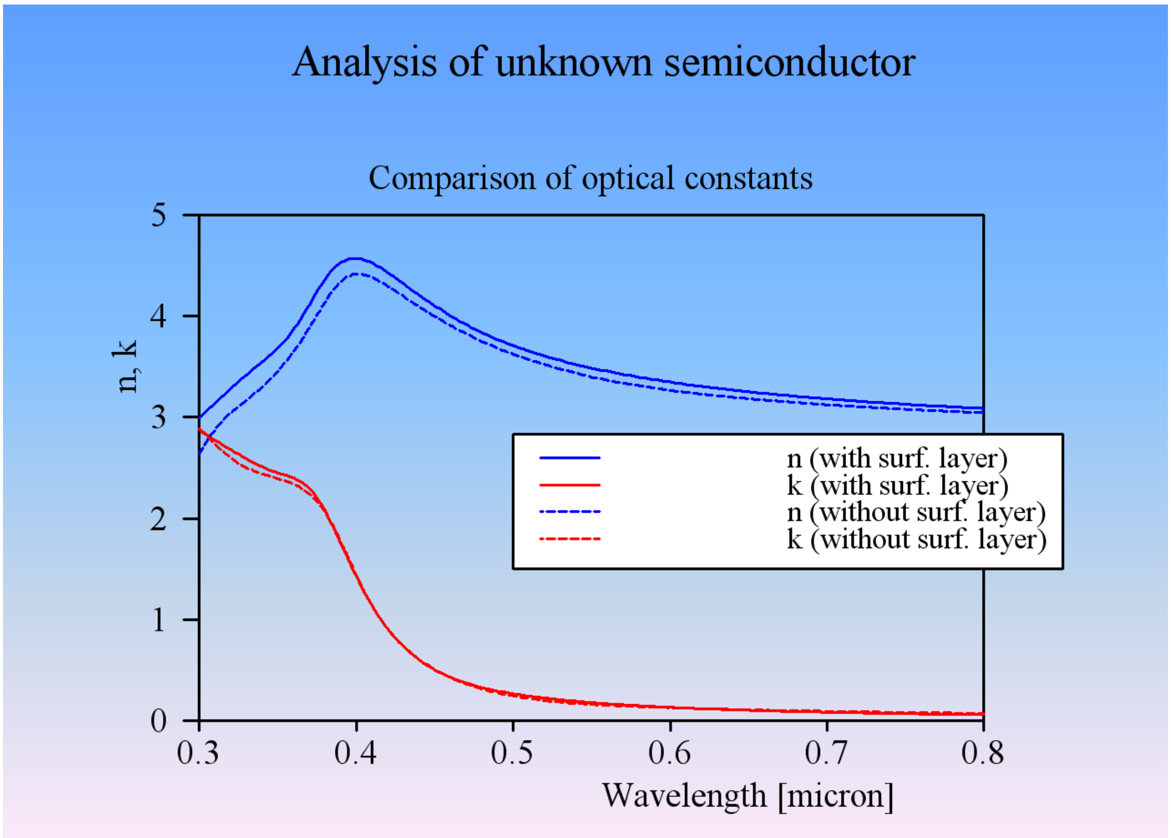
Fit deviation: 0.0001510

Thickness: 47.1


Analysis of unknown semiconductor

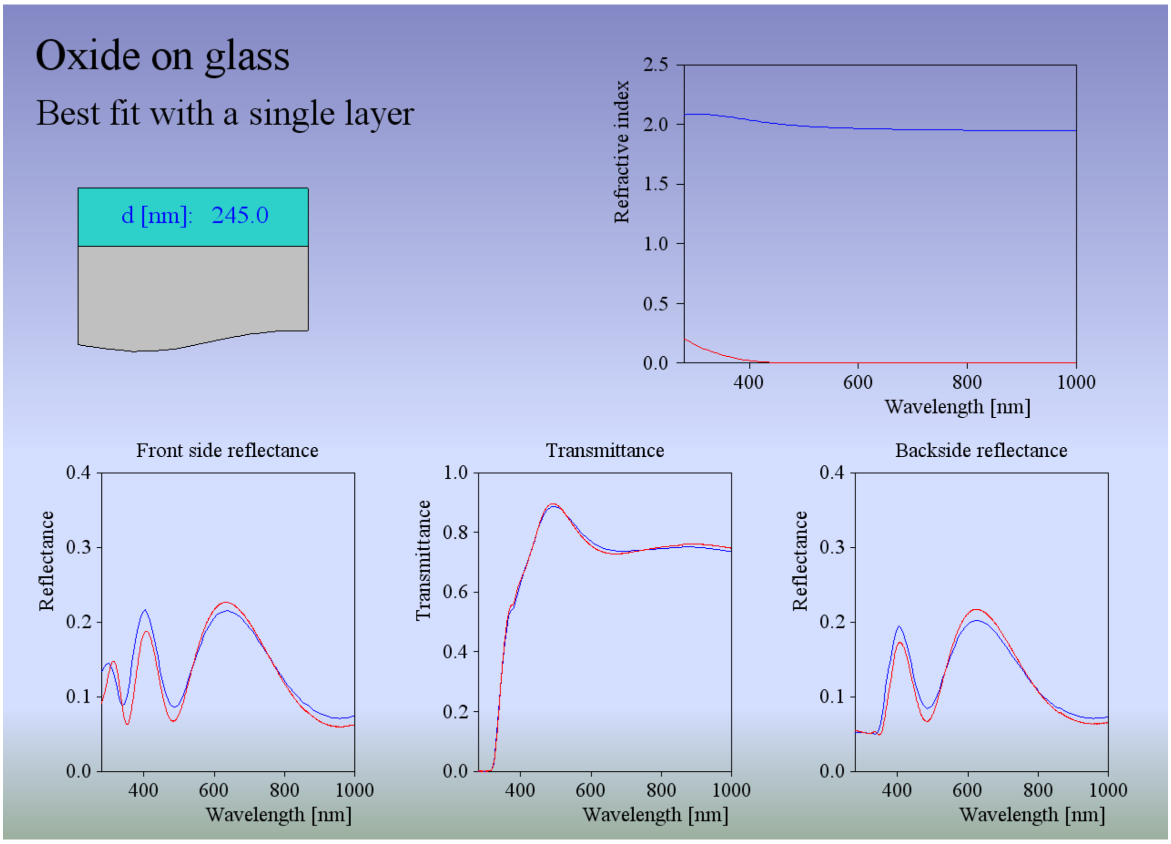
Fit deviation: 0.0000457

Thickness: 44.5


Analysis of unknown semiconductor

Comparison of optical constants

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.

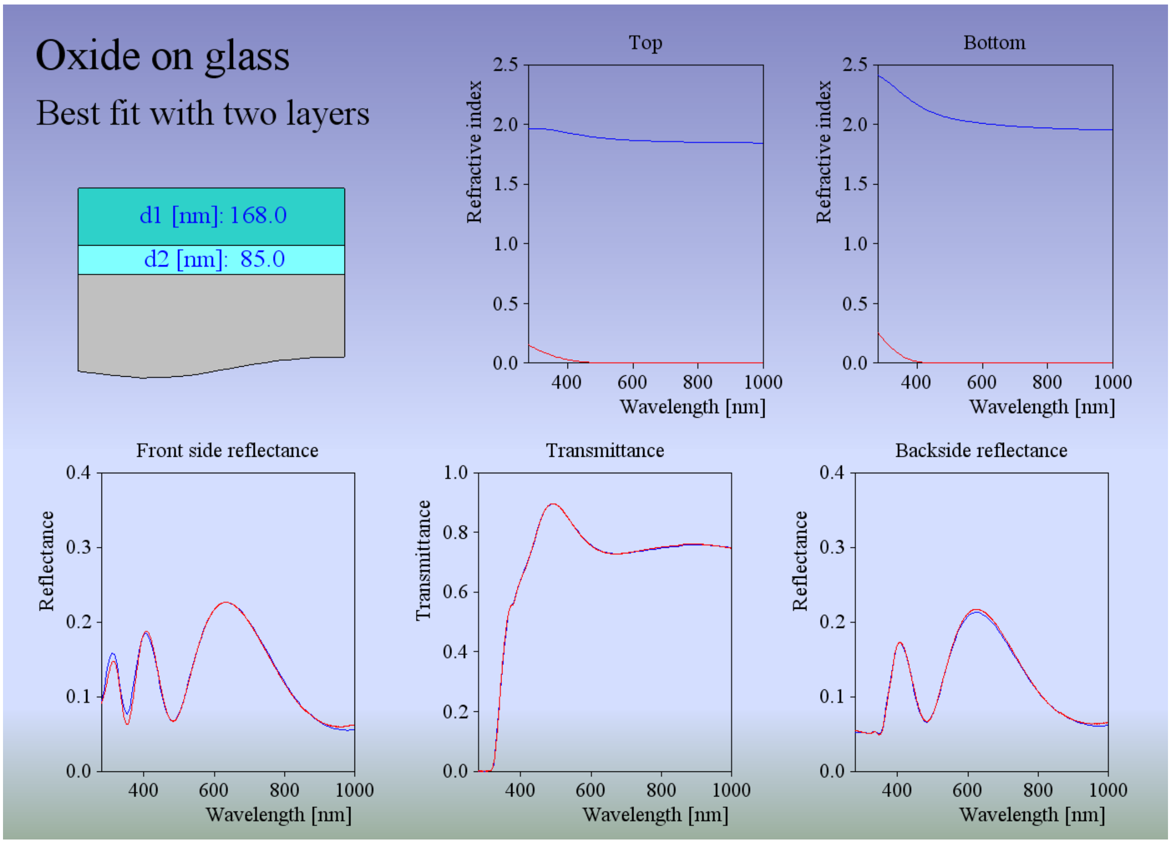


Oxide on glass

Best fit with a single layer

d [nm]: 245.0

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

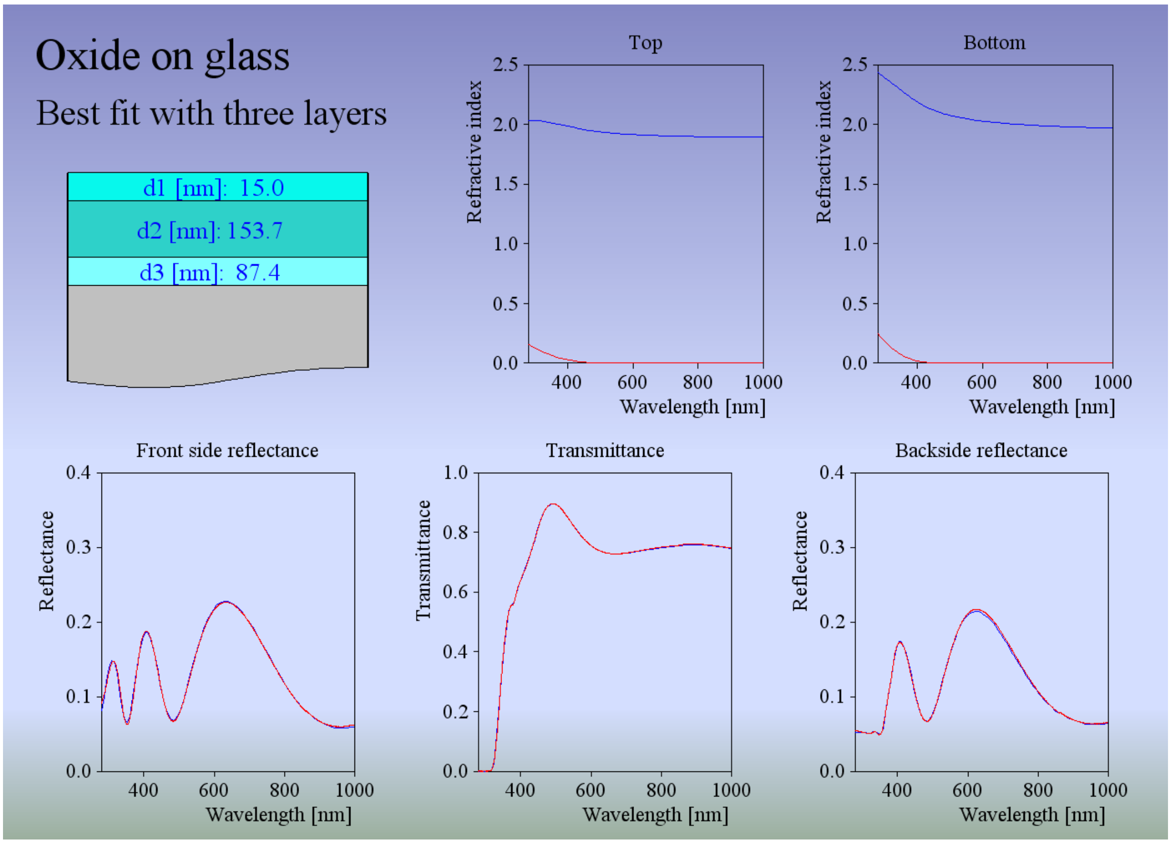


Oxide on glass

Best fit with two layers

d1 [nm]: 168.0

d2 [nm]: 85.0

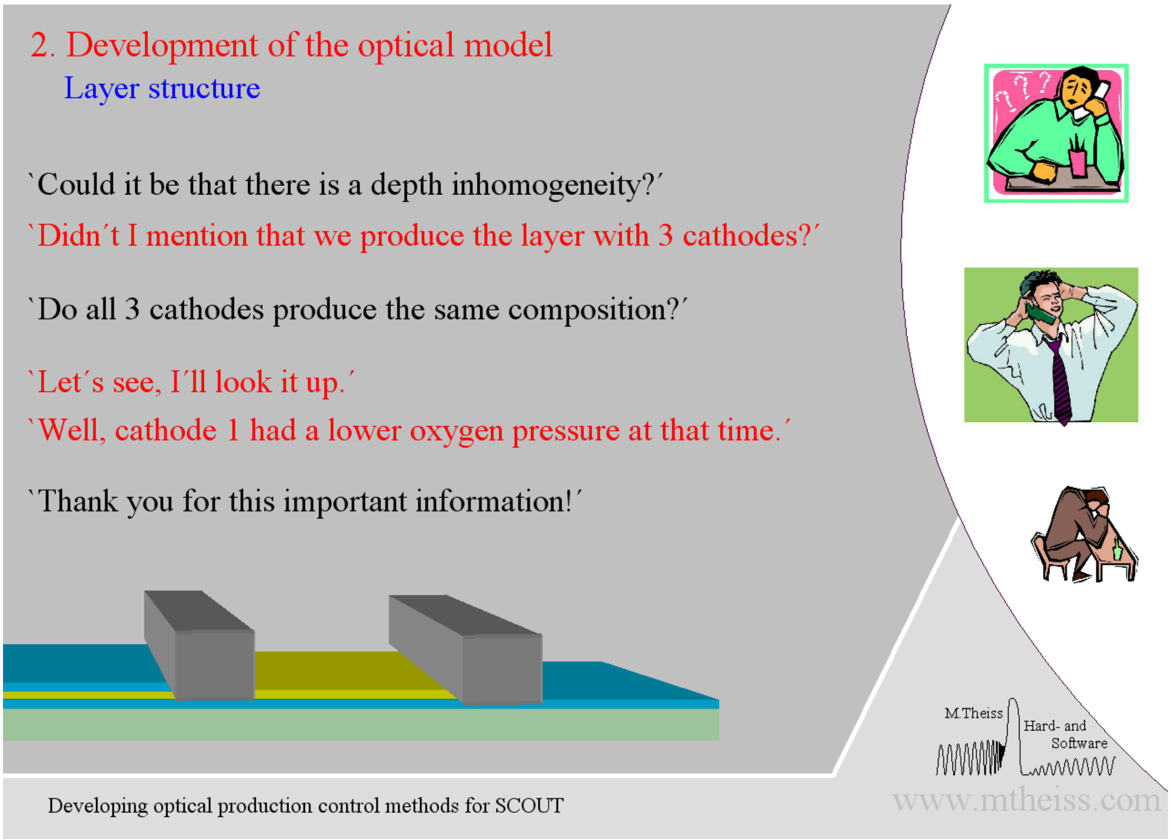


Oxide on glass

Best fit with three layers

d1 [nm]: 15.0
d2 [nm]: 153.7
d3 [nm]: 87.4

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



2. Development of the 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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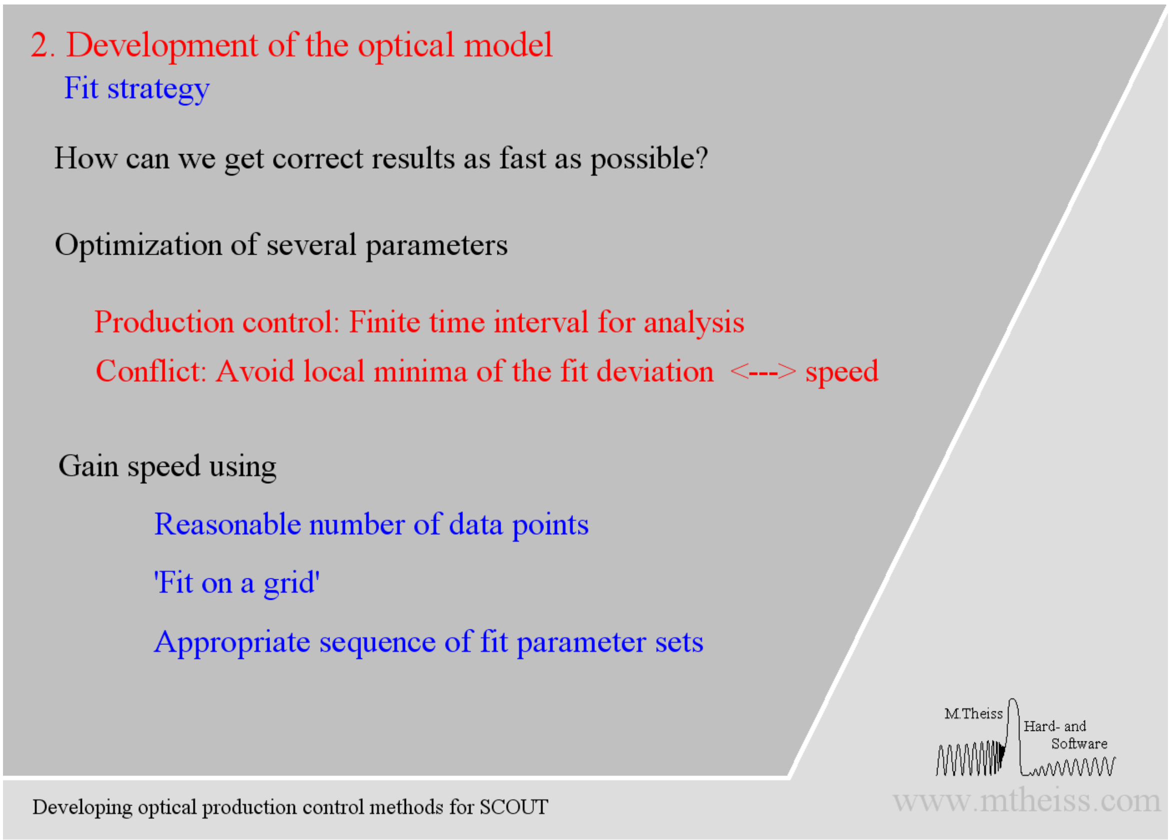
3.3 Fit strategy

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.



2. Development of the optical model

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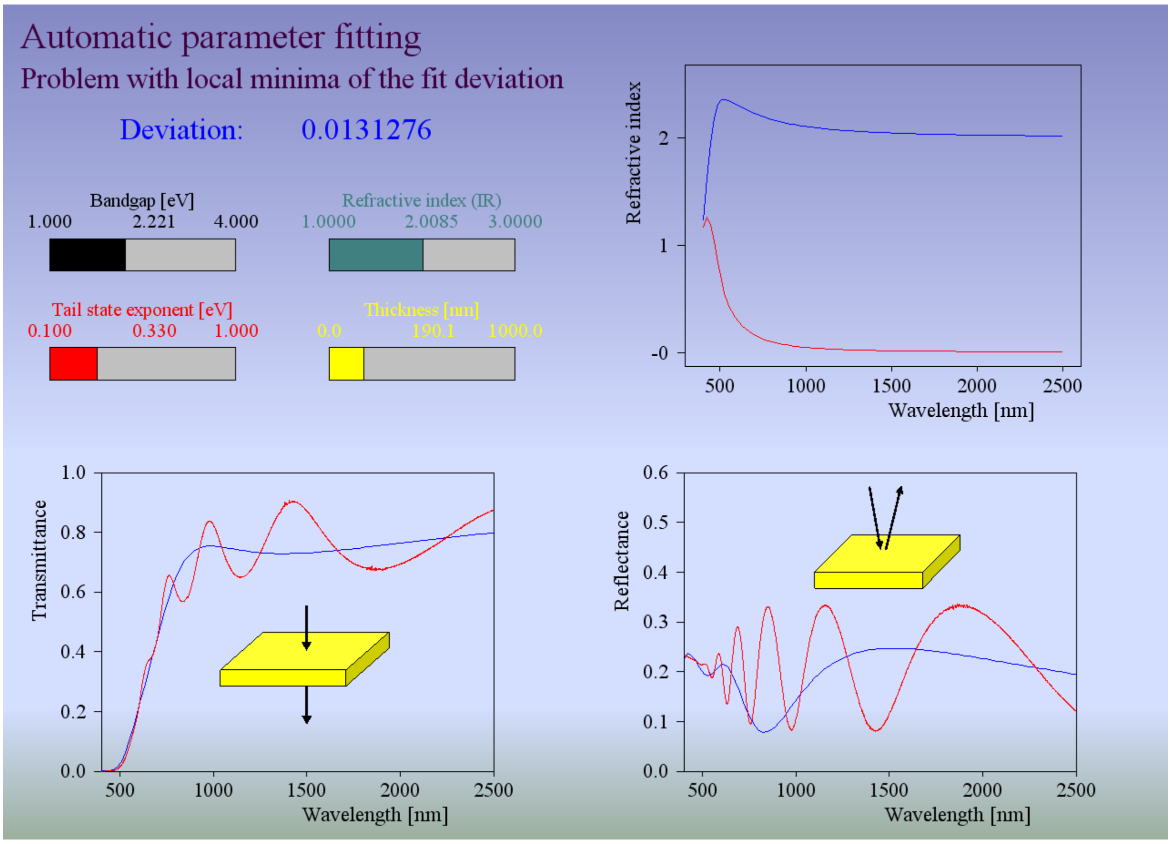
Multiple parameter optimization is a common problem of numerical mathematics. One of the main issues is to avoid that algorithms get stuck in local minima of the fit deviation. Methods like simulated annealing or genetic algorithms which overcome the local minimum problem are much too slow to be used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



Automatic parameter fitting

Problem with local minima of the fit deviation

Deviation: 0.0131276

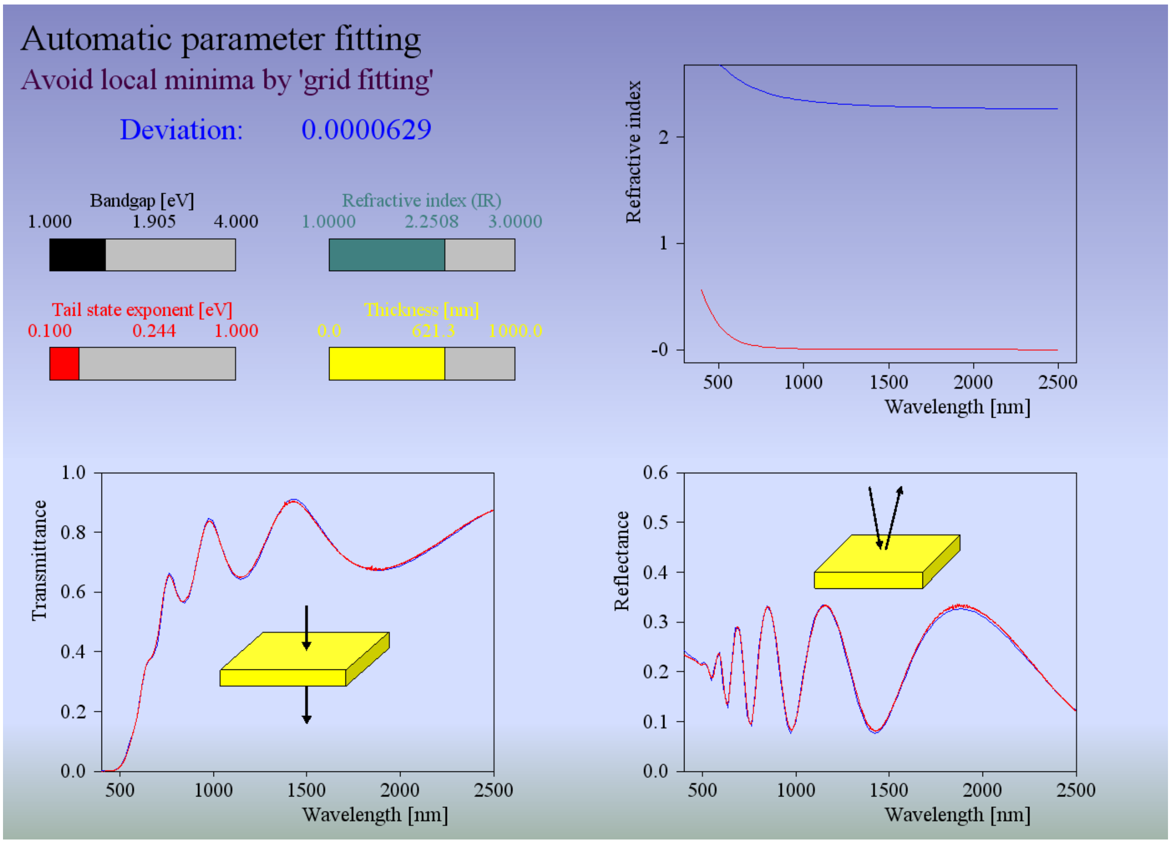
Bandgap [eV] 1.000 2.221 4.000

Refractive index (IR) 1.0000 2.0085 3.0000

Tail state exponent [eV] 0.100 0.330 1.000

Thickness [nm] 0.0 190.1 1000.0

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.



Automatic parameter fitting

Avoid local minima by 'grid fitting'

Deviation: 0.0000629

Bandgap [eV] 1.000 1.905 4.000

Refractive index (IR) 1.0000 2.2508 3.0000

Tail state exponent [eV] 0.100 0.244 1.000

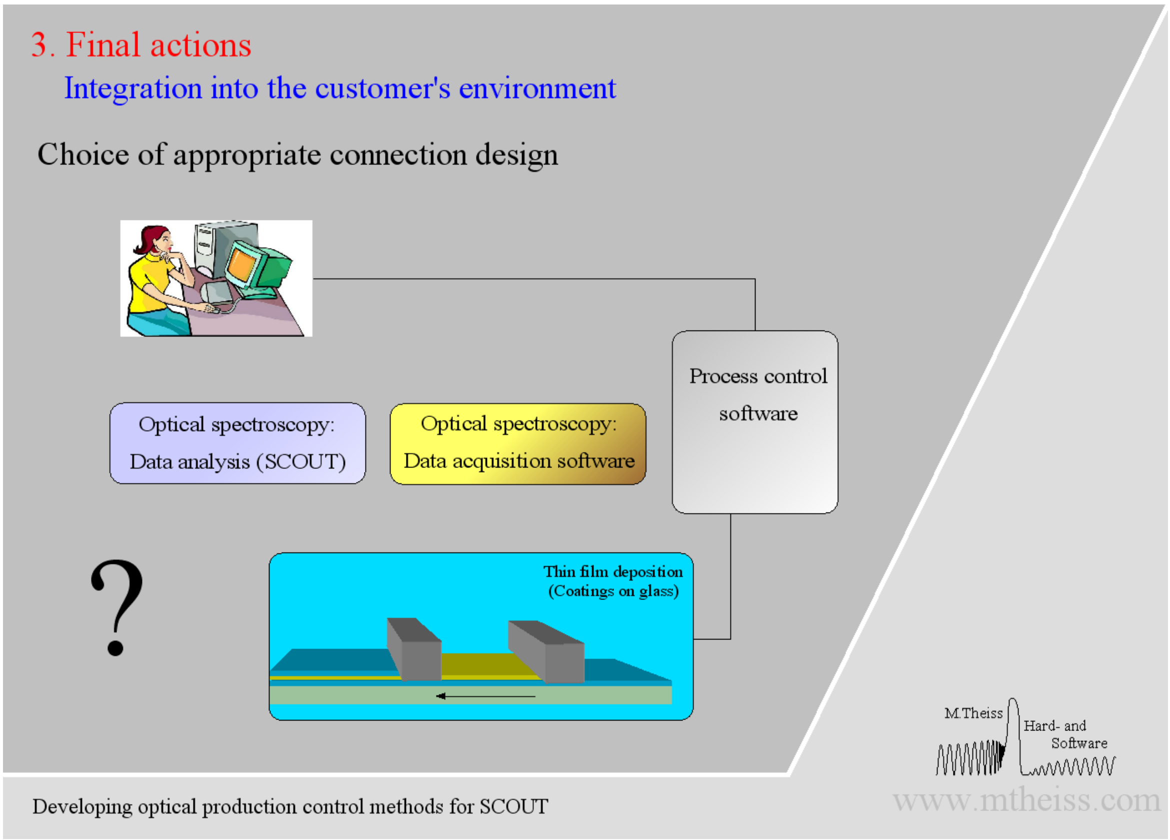
Thickness [nm] 0.0 621.3 1000.0

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.

4 Final actions

4.1 Integration into the customer's environment

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



3. Final actions

Integration into the customer's environment

Choice of appropriate connection design

Process control software

Optical spectroscopy: Data analysis (SCOUT)

Optical spectroscopy: Data acquisition software

?

Thin film deposition (Coatings on glass)

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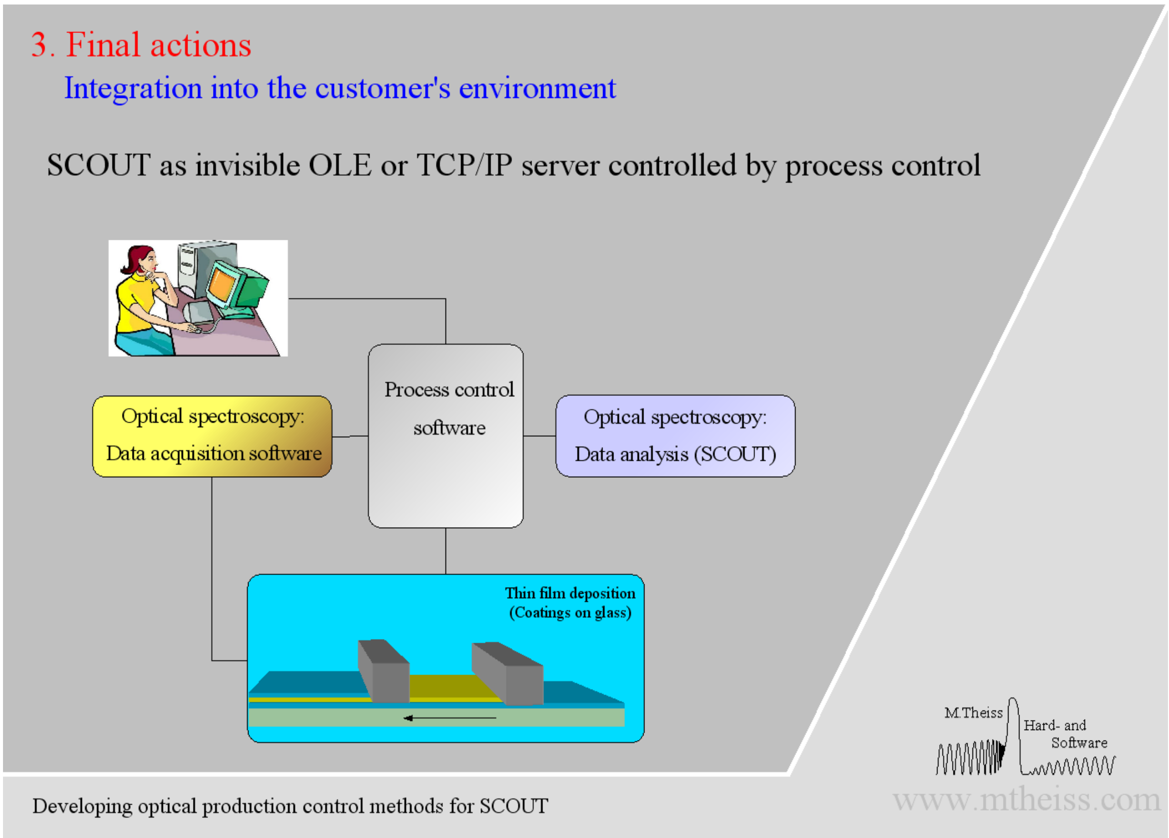
With SCOUT, several options are possible. The following example shows a configuration where both SCOUT and the data acquisition are controlled by the process control software. SCOUT can be accessed as OLE server or by TCP/IP communication.



3. Final actions

Integration into the customer's environment

SCOUT as invisible OLE or TCP/IP server controlled by process control

Process control software

Optical spectroscopy: Data acquisition software

Optical spectroscopy: Data analysis (SCOUT)

Thin film deposition (Coatings on glass)

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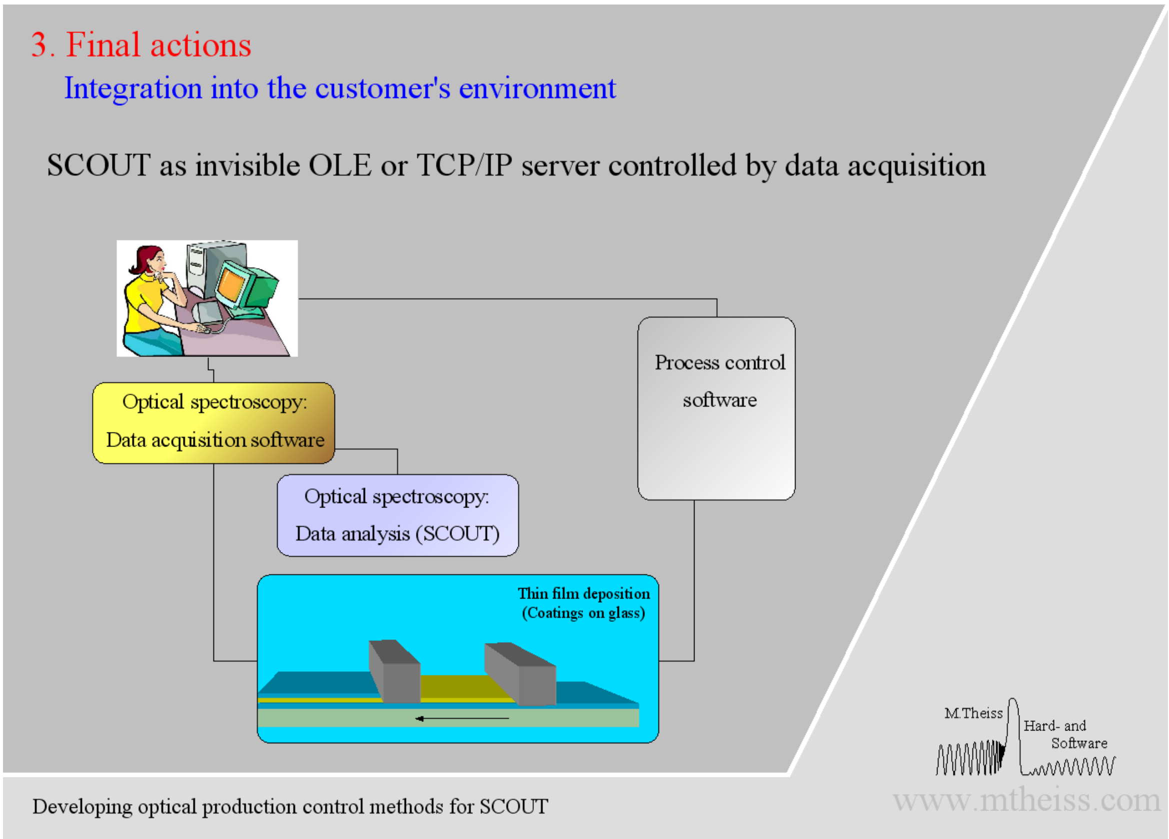
The optical analysis can also be completely independent of the process control software:



3. Final actions

Integration into the customer's environment

SCOUT as invisible OLE or TCP/IP server controlled by data acquisition

Process control software

Optical spectroscopy: Data acquisition software

Optical spectroscopy: Data analysis (SCOUT)

Thin film deposition (Coatings on glass)

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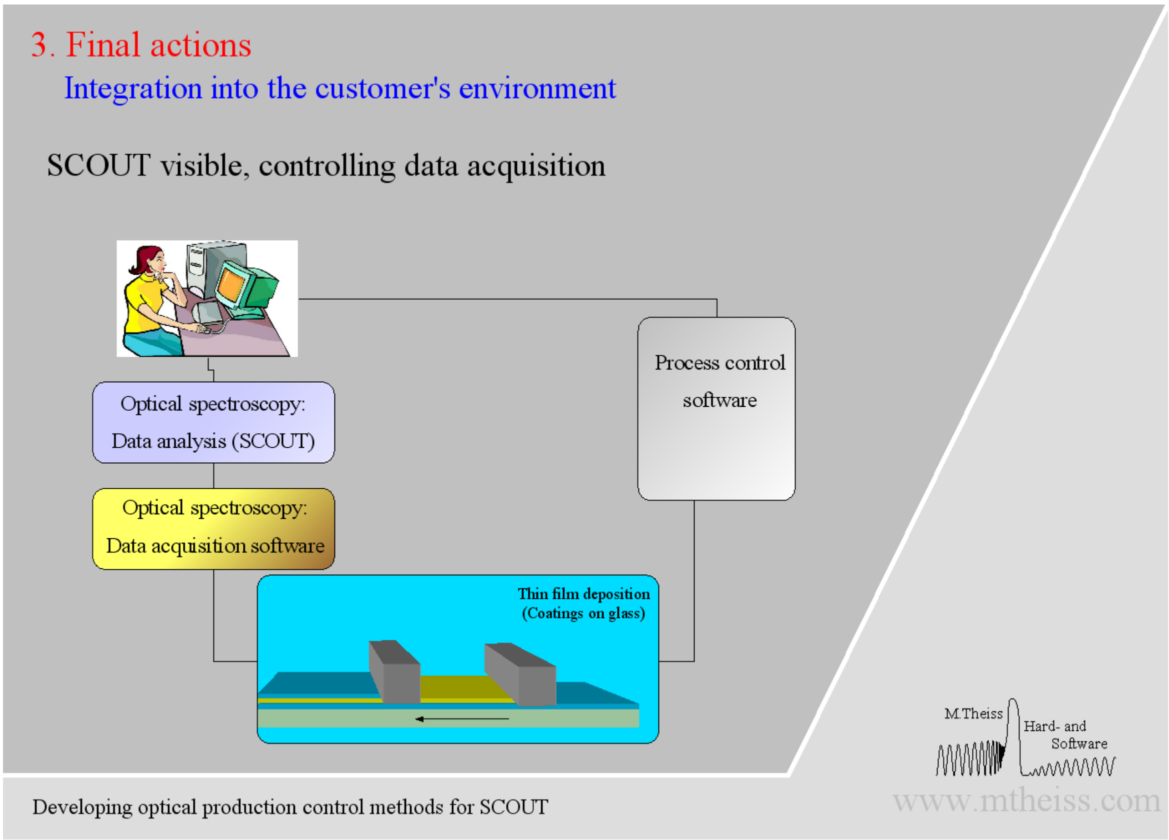
SCOUT can also be used to control spectroscopic hardware and display results. In this case an appropriate user interface must be developed.



3. Final actions

Integration into the customer's environment

SCOUT visible, controlling data acquisition

Optical spectroscopy:
Data analysis (SCOUT)

Optical spectroscopy:
Data acquisition software

Process control
software

Thin film deposition
(Coatings on glass)

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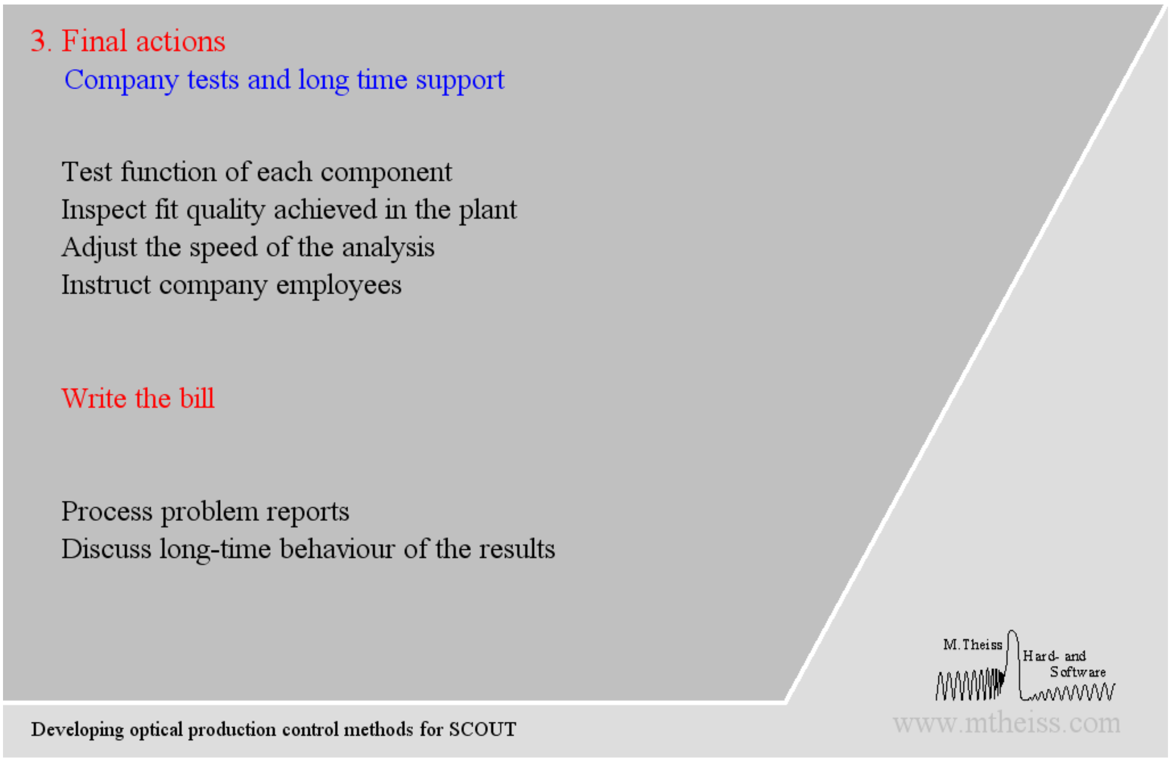
Once the decision concerning the factory configuration is made, the required hardware and software installations are to be done and the proper data exchange between all involved programs and computers must be established and verified.

4.2 Company tests and long-time support

Finally, the method must be tested and optimized in the plant during production. The long-time support contains the processing of error reports (bug fixing) and updates of the model and the user-interface.



3. Final actions

Company tests and long time support

Test function of each component
Inspect fit quality achieved in the plant
Adjust the speed of the analysis
Instruct company employees

Write the bill

Process problem reports
Discuss long-time behaviour of the results

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Developing optical production control methods for SCOUT