M.Theiss, Hard- and Software for Optical Spectroscopy
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Main Software Products

Analyze optical spectra of layer stacks by spectrum simulation and parameter fits. Determine thicknesses, n and k, bandgaps, concentrations, frequencies ... Page 2

Analyze and design optical properties of thin film coatings. Optimize technical data like color coordinates, light reflectance, emissitivy, U, g, ... Page 13

SCORE computes the properties of window products based on panes, gases and coatings from your CODE database. Page 17

Automated, production oriented design of optical coatings using a genetic algorithm. Optimize material selections and layer thicknesses. Page 18

Simulate and optimize the performance of optical setups by spectral ray-tracing, including light scattering (Mie module) and fluorescence. Optimize light sources, probeheads, paints, printing devices,... Page 20

Creation, manipulation and transformation of spectra and other data sets.
Easy drag&drop exchange with our other software products. Page 24

Get digital data from scanned literature graphics. Manual and semi-automatic point selection. Page 25

M.Theiss Hard- and Software

SCOUT is a Windows 98/2000/NT/XP software for the analysis of optical spectra by comparison of measurements and models. The following quantities are simulated:

Reflectance, Transmittance, Absorbance, ATR, Ellipsometry, Photoluminescence
Electric field distribution, Local absorption

Model calculations based on

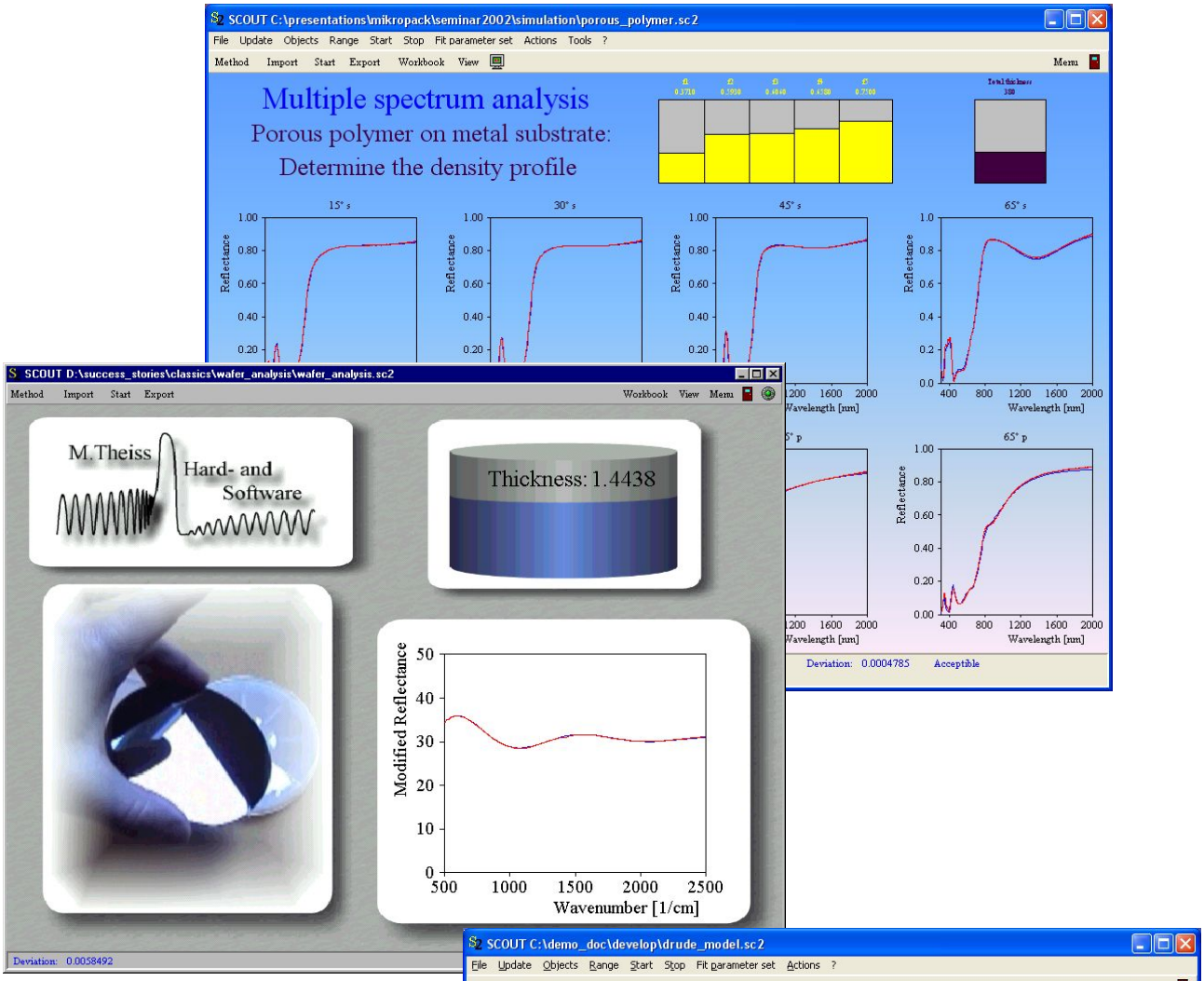
Optical constant models (Classical Drude model for free carriers, enhanced Drude model with frequency-dependent carrier damping, harmonic oscillators, extended oscillator model due to Brendel, extended oscillator model due to Kim, OJL interband transition model, Campi-Coriasso interband transition model, Tauc-Lorentz interband transition model, user-defined expressions for optical constants, imported dielectric functions)

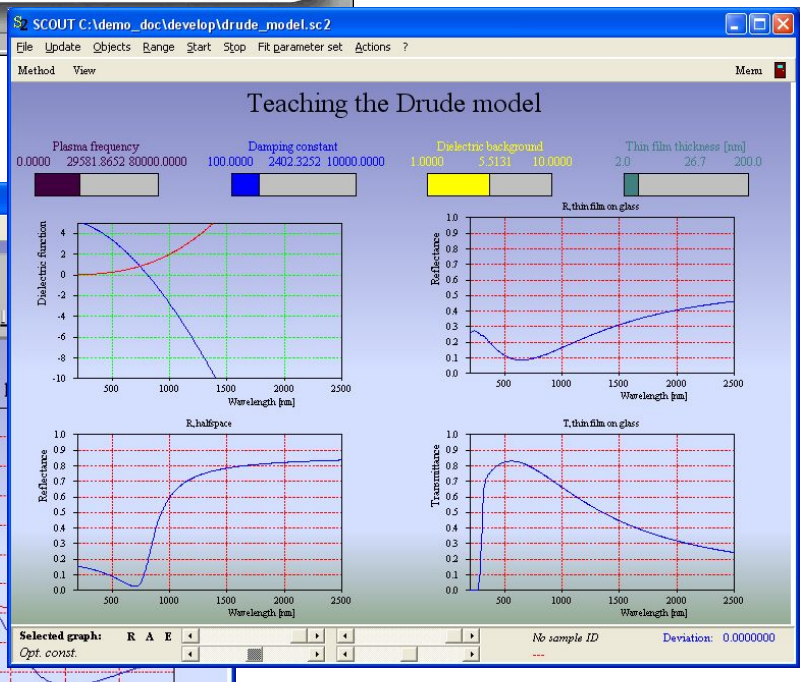
Various effective medium concepts for inhomogeneous materials (Maxwell Garnett, Bruggeman, Looyenga, Bergman representation)

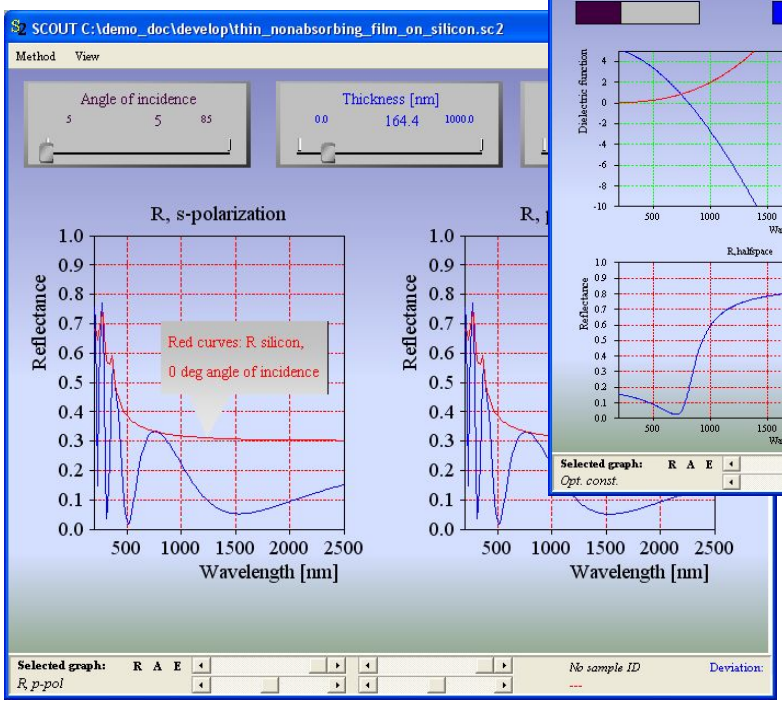
Wave propagation in layer stacks including coherent or incoherent superposition of partial waves, easy definition of superlattices, corrections for scattering losses at rough interfaces. Efficient averaging algorithm for lateral layer thickness inhomogeneities. Gradually changing optical properties. Anisotropic layers. Angle of incidence averaging.

- Flexible manual, 'visual' or automatic fitting of model parameters like film thicknesses or gap energies to adjust simulated to measured spectra
- Simultaneous fits of several spectra like reflectance and transmittance
- Fit several layer stacks with almost unlimited number of layers simultaneously
- Definition of sophisticated fit strategies using fit parameter sets combined with time and deviation thresholds
- Integrated batch operation of large series of input spectra
- Graphics output to Windows printers, metafiles or Windows clipboard
- Data output to clipboard, text files, worksheets in Excel format
- Complete remote control of SCOUT by OLE automation. Create automated reports and fit routines from MS Word, MS Excel, LabVIEW, Windows Scripting Host or any other OLE automation controller.
- Integrated spectrometer modules for complete hardware/software solutions
- User-defined views for easy creation of simple user-interfaces

SCOUT screen shots:





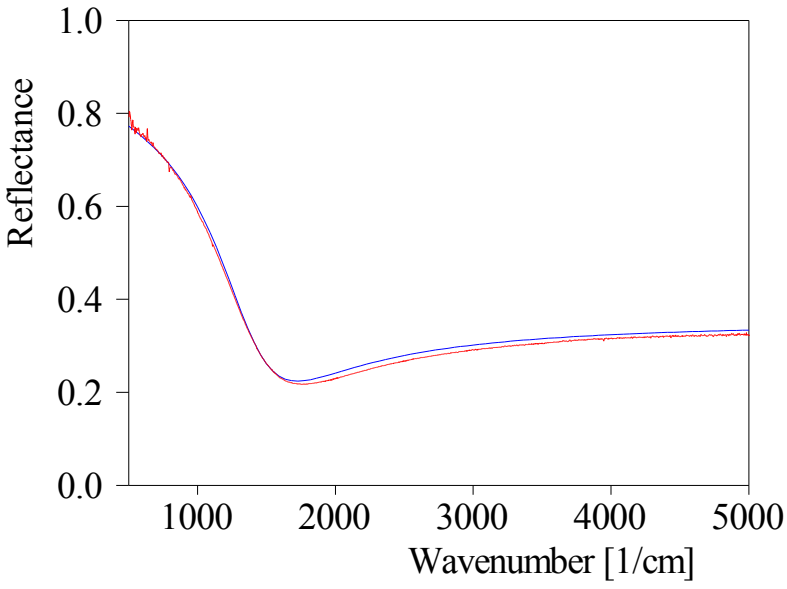


SCOUT application examples

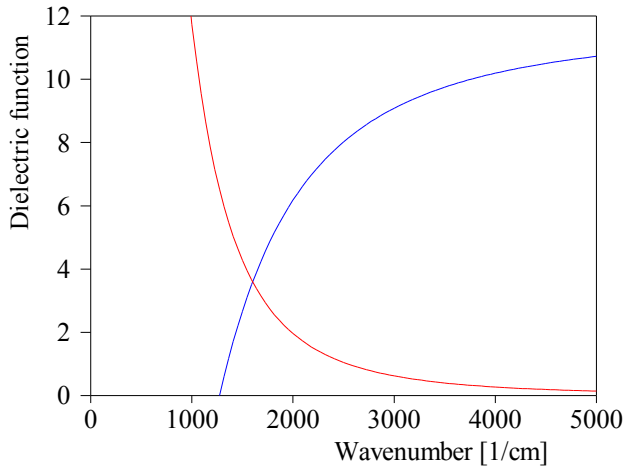
The goal of optical spectroscopy is - in most cases - the determination of microscopic quantities such as resonance frequencies of oscillating atoms, impurity concentrations or thin film thicknesses from macroscopic experiments. This is possible if the microscopic phenomena are coupled to the electric fields of the probing radiation. The key property of a material representing this connection is the dielectric function or its square root, the complex refractive index.
In the case of layered systems a very powerful technique to interpret optical spectra is given by a simulation of the experiment and adjustment of the model parameters to fit the measured data. Fortunately, rather simple models of dielectric functions lead to a realistic simulation of optical spectra. This enables quick parameter fits from which the wanted information can be obtained.
The interpretation of optical spectra is the central task of SCOUT - here some typical application examples are given. All simulated spectra are shown in blue whereas the experimental ones are displayed in red.

Charge carriers in semiconductors

A classical example of optical product control is the determination of carrier concentrations in doped semiconductors. In case of high doping levels the wafers to be inspected can be considered as optically thick (halfspace model). In this case the infrared reflectivity depends on the concentration and damping of the charge carriers only. A simple Drude model with two parameters (plasma freqency and damping constant) to adjust will do an excellent job in most cases. The picture to the right shows the simulation in blue and the measured data for a doped silicon wafer in red.

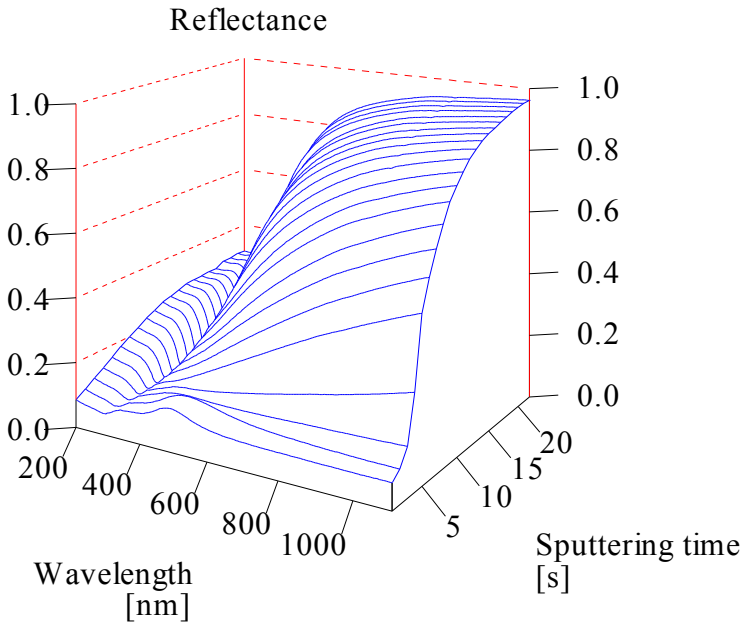


The dielectric function obtained from the parameter fit is shown to the right (real part, imaginary part).
From the Drude model parameters plasma frequency and damping constant that are obtained by the fit one can calculate the carrier concentration and the resistivity. The values for the given example are $1.06 \cdot 10^{20}$ cm^{-3} and 1.74 mΩcm, respectively.

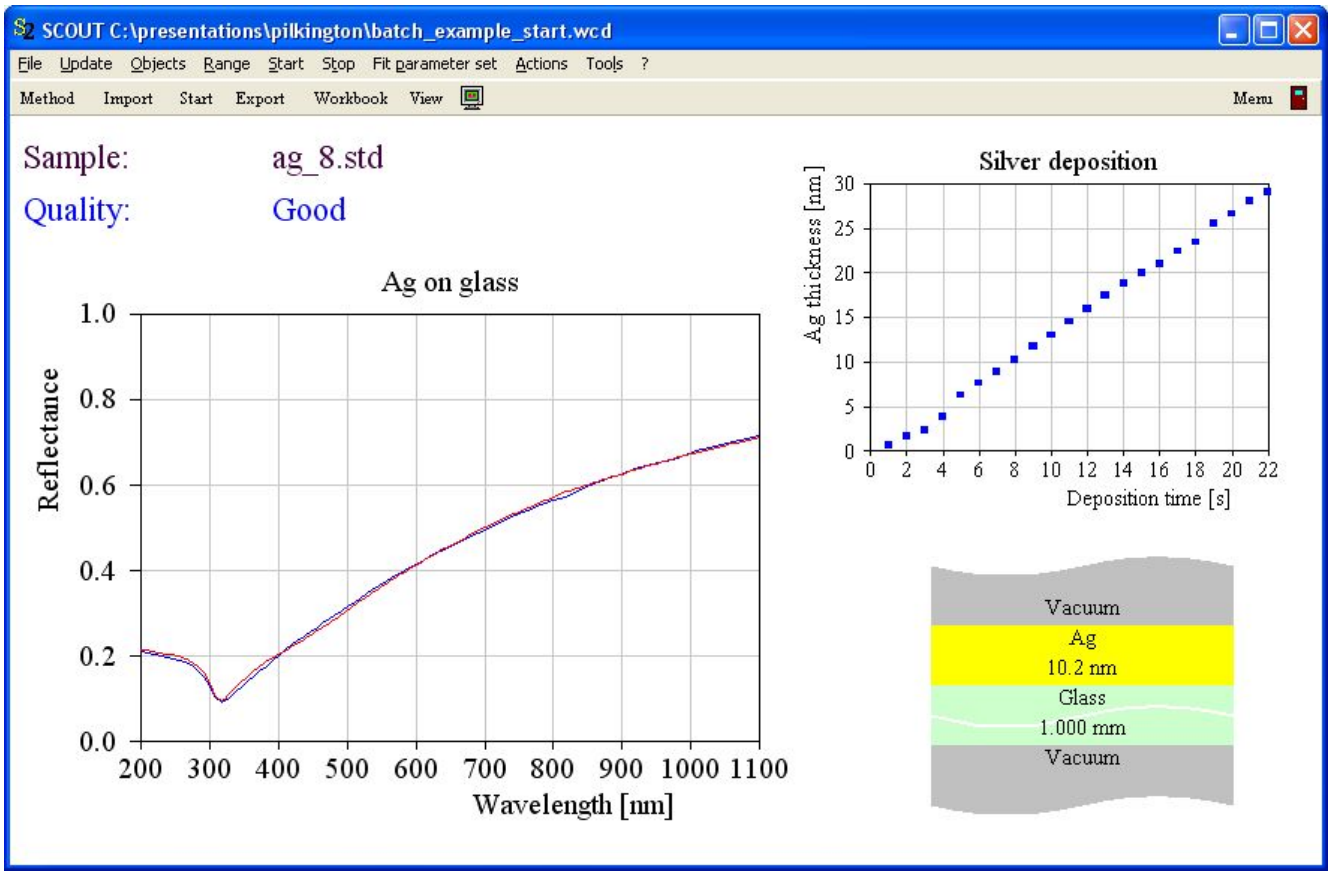


A simple batch processing example

To demonstrate the batch processing of a series of input spectra the set of reflectance spectra shown to the right of thin silver films deposited on microscope slides are investigated. The samples were prepared by sputtering with varying deposition time.
The spectra were recorded by a Perkin-Elmer grating spectrometer in the range 200 ... 1100 nm wavelength making use of an acquisition program also developed by our company.

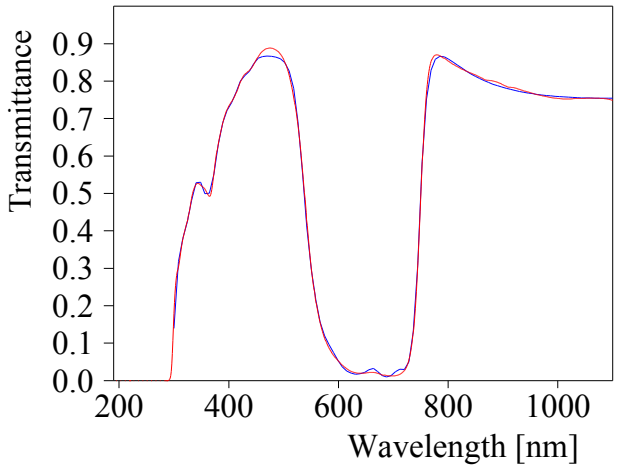


For deposition times less than 5 s an inhomogeneous island film grows, for larger times a compact layer develops building up the high metallic reflectivity in the visible and infrare spectral range (400 ... 1100 nm).
To determine the sputtering rate the simple model of a homogeneous Ag film on glass has been used, taking literature data for silver from the optical constant database. Although the quality of the sputtered silver may differ from that used to obtain the literature data the individual simulations have a satisfying quality like the one shown below. Only the spectra of the island films are not reproduced well. This is no surprise since the optical properties of inhomogeneous metal films are very different from those of homogeneous ones.
The results for the Ag thickness (which has been the only fitting parameter) show a nice linear relation to the sputtering time from which the sputtering rate of roughly 1.3 nm/s is easily obtained.



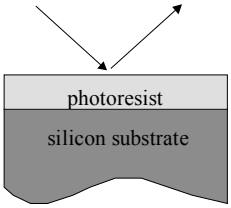
Description of CD-R coatings

This example has been selected to demonstrate thin film spectroscopy involving organics, namely the optical analysis of dye coatings on recordable CD's (CD-R's).
The spectrum is a transmission spectrum of a dye layer on a polycarbon carrier. The gold layer required for the final CD-R has not yet been deposited. From the fit one can obtain the dye thickness and the optical constants of the dye which are important quantities for quality control during CD-R production.

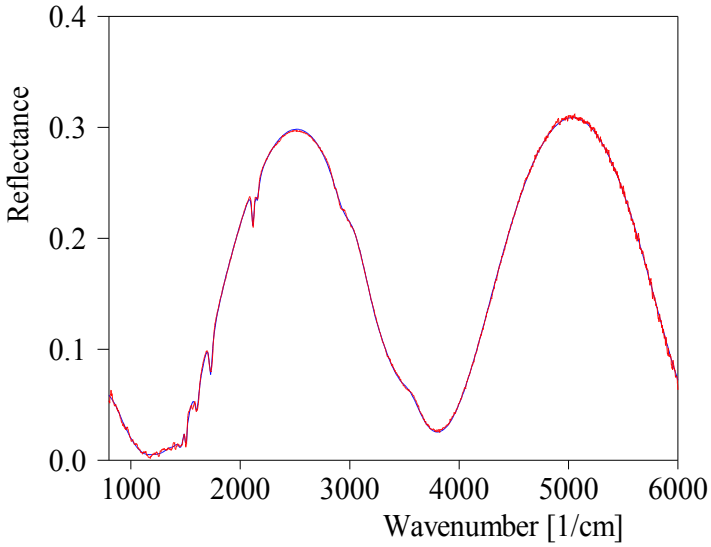


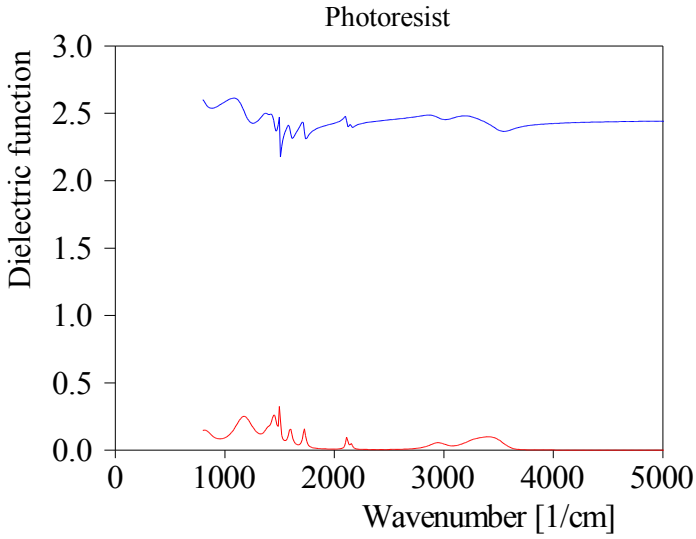
IR absorption bands and interference fringes

The analysis of infrared absorption bands in thin films which are mixed with interference patterns nicely demonstrates the advantage of using the simulation approach. All the experimentally observed structures are easily reproduced by the model – without any baseline

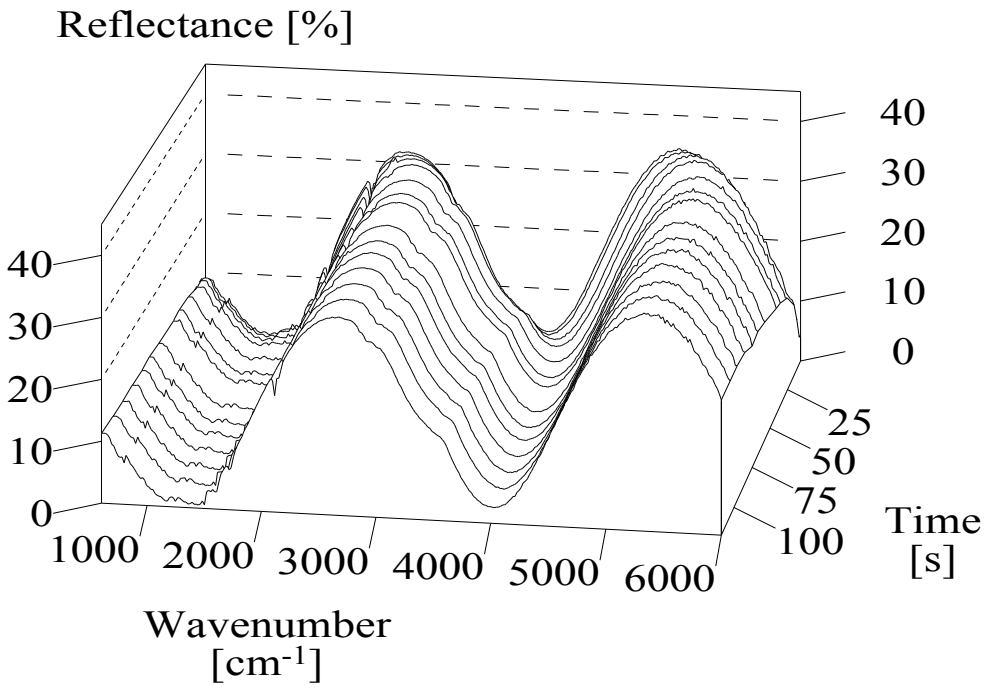


correction or other manipulation of the measured data.
Note that one gets from a quantitative fit like the one shown to the right the thickness as well as the refractive index simultaneously. This is because not only the periodicity but also the amplitude of the interference patterns are used.
The thickness of the photoresist layer in this case is 1.29 µm. The obtained complex dielectric function featuring the vibrational modes of the photoresist is shown to the left.

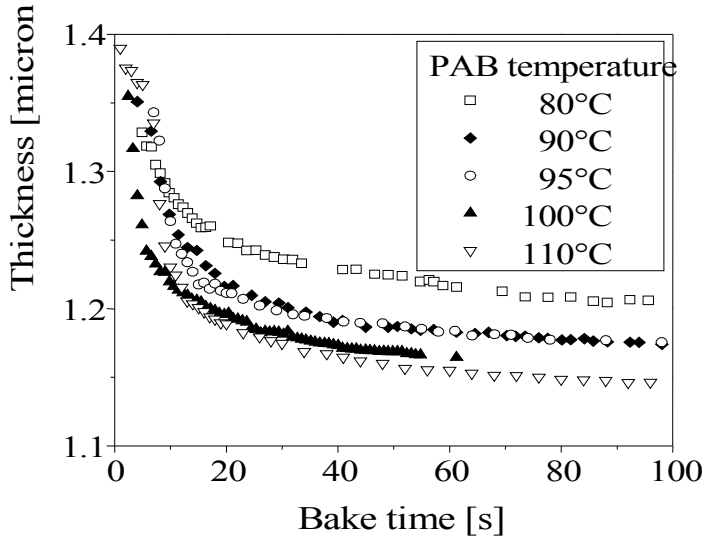




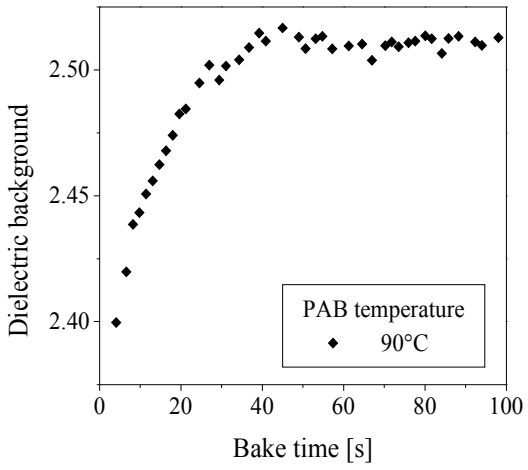
Now some detailed results are given that have been obtained in annealing experiments. The time dependence of the infrared reflectance spectra has been analyzed in an automated batch fit routine. A typical series is shown in the graph below.

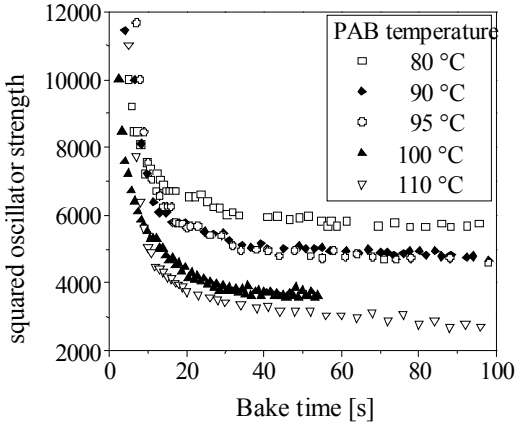


For various postbake temperatures the shrinkage of the photoresist nicely is demonstrated by its thickness evolution shown in the graph below.



The layers obviously become more compact during the postbake which is also reflected by an increase of the real part of the dielectric function (the square root of which is roughly the refractive index, in this case with small imaginary part).
The analysis of the vibrational modes leads to an understanding of what happens chemically during the postbake step. As an example the evolution of the squared oscillator strength (which is a fit parameter of the photoresist dielectric function model) of one of the modes is shown to the right below. This quantity is proportional to the concentration of the oscillators which clearly are diminished during the process.

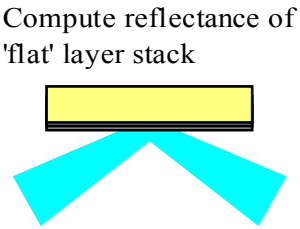


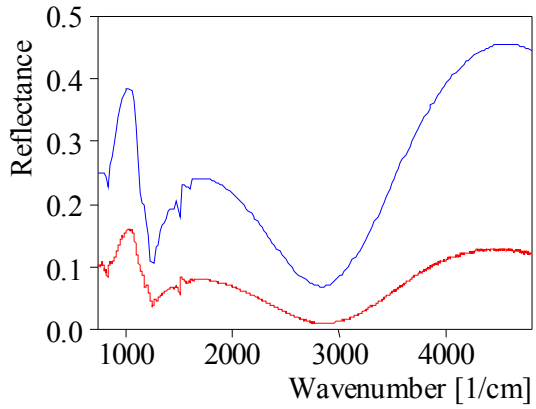


An example of advanced multilayer analysis

Here we show the analysis of a SiO_x double layer deposited by reactive sputtering on a microscopically rough and macroscopically curved polymer substrate. The goal of the investigation is to determine the oxygen concentration in each of the two layers as well as the two layer thicknesses.

Computed spectra for the flat layer stack are much too large as shown here:





Obviously the roughness and the curvature ask for some corrections which can be done in SCOUT quite easily. After some thinking, experimental tests and trying it turns out that two corrections lead to the wanted result.
We have to scale down the spectrum by a constant factor independent of frequency which accounts for the sample curvature. This can be done in SCOUT because each spectrum of a flat layer stack can be modified after the computation by an almost arbitrary, user-defined function. This gives the following improvement:

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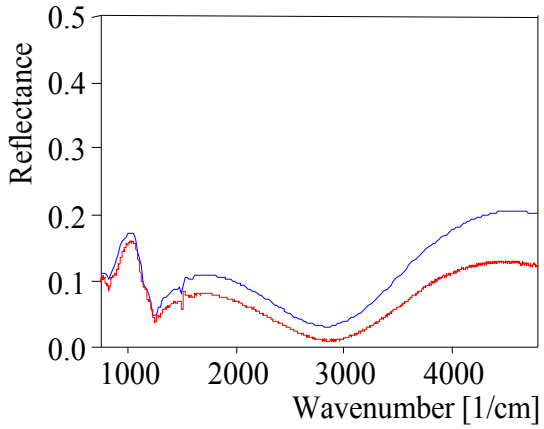
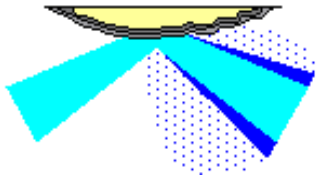
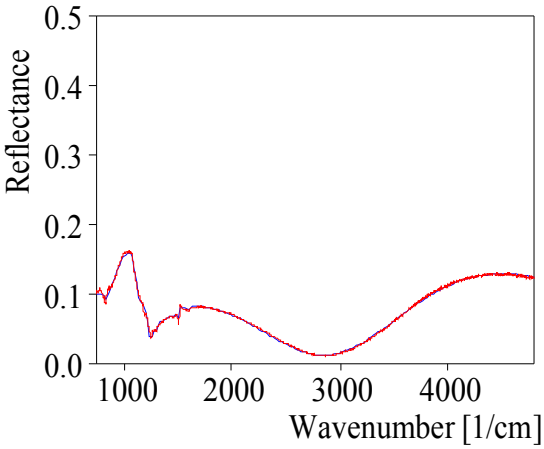
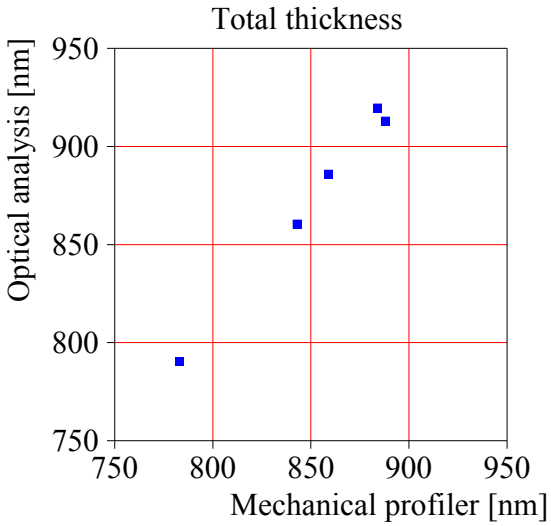


In addition, we need a frequency dependent light scattering correction to describe the scattering losses due to the substrate roughness. At each interface an 'interface roughness' object is entered into the layer stack which modifies the amplitude reflection and transmission coefficients of the light waves by user-defined formulas. With a reasonable choice (the same function is used for all interfaces) the following fit is achieved:

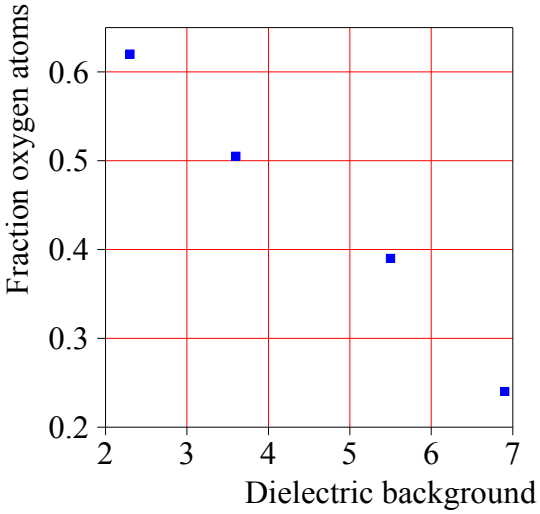


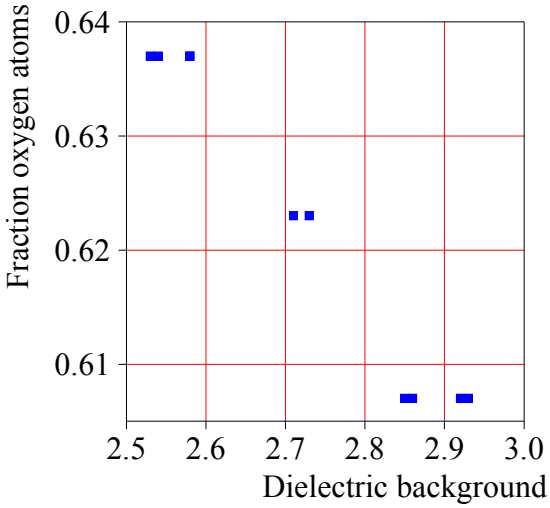


Many samples have been analyzed and quite satisfying results have been obtained. The total thickness of the double layer as determined from the optical analysis compares nicely to mechanical profiler measurements:



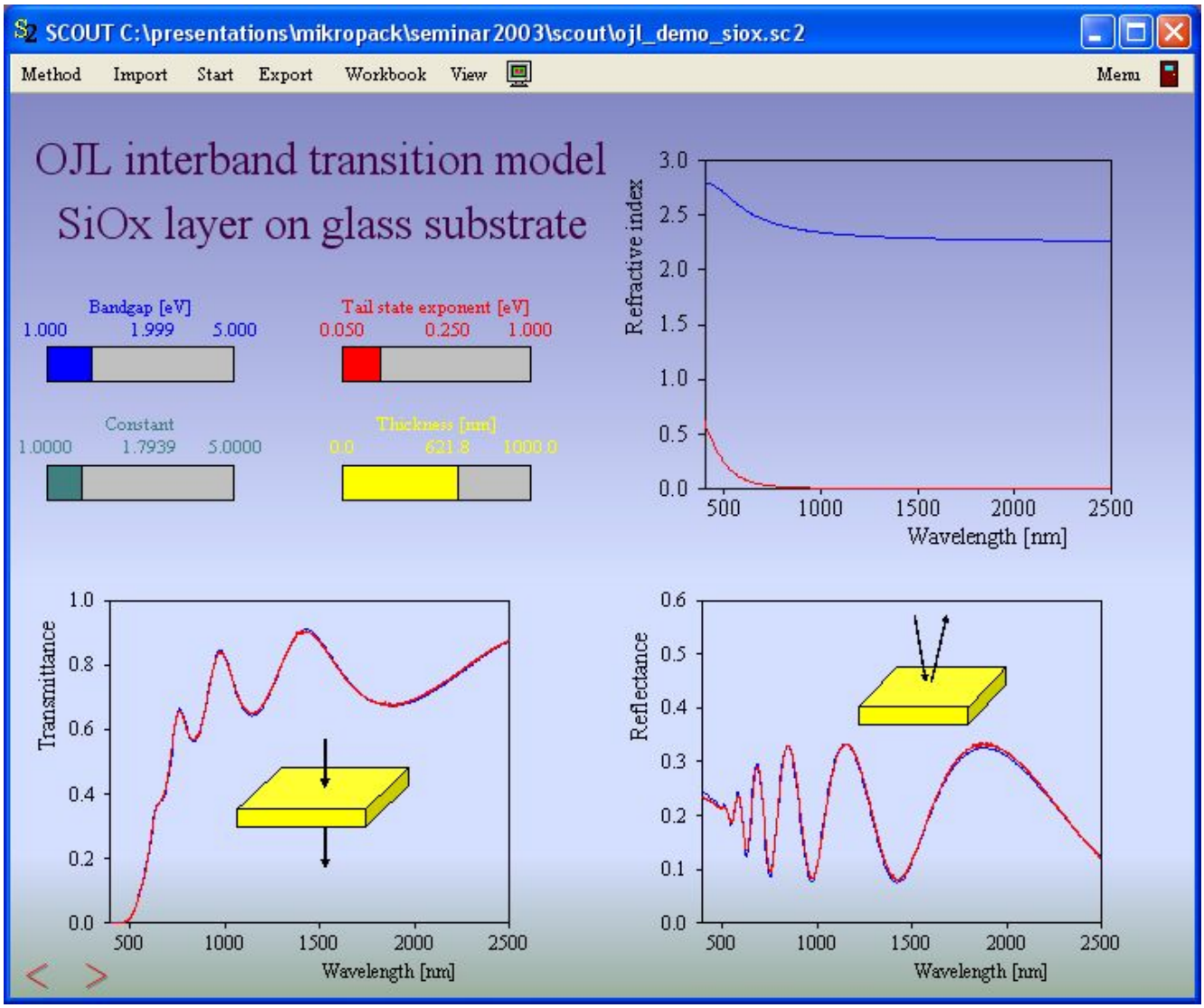
The dielectric background (i.e. the real part of the dielectric function at large wavenumbers) turned out to be related to the oxygen content of the layers almost linearly. Even rather small differences in the oxygen content could be detected:



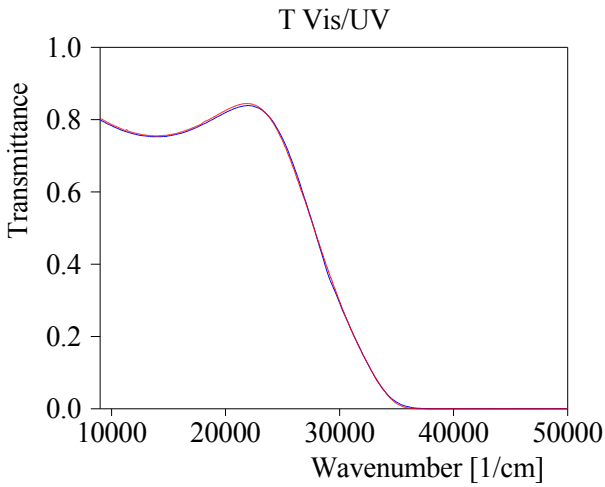


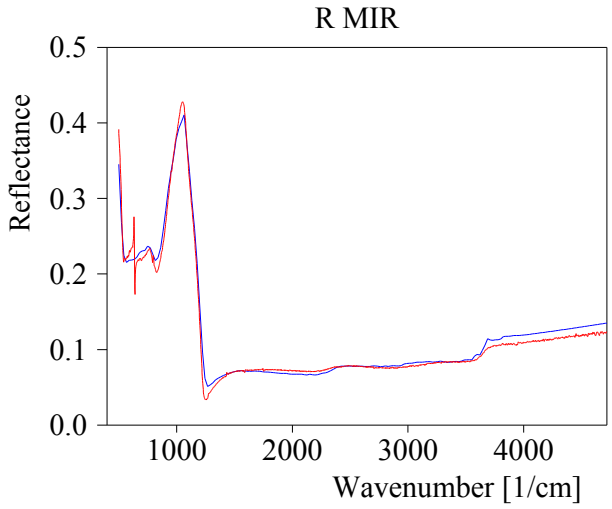
Interband transitions in amorphous materials

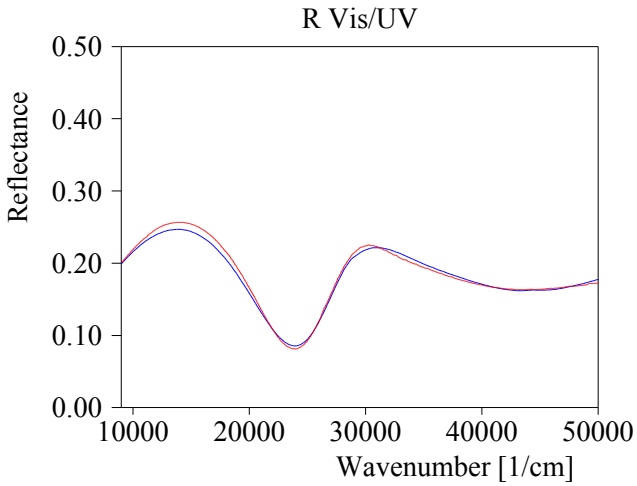
SCOUT contains some useful dielectric function models for interband transitions, namely the Campi-Coriasso, Tauc-Lorentz and OJL model. The latter, in particular, is very suitable to describe amorphous materials with significant tail state absorption.
The examples given below show the application of the OJL model to model the optical constants of oxides the composition of which may depend on the deposition conditions, in particular on the oxygen flow during sputtering.
For a single silicon oxide film on glass the reflectance and transmittance in the visible spectral range are reproduced quite well. Besides the layer thickness only four fit parameters have been adjusted, the most important ones being the gap energy and the exponential of the tail state decay:

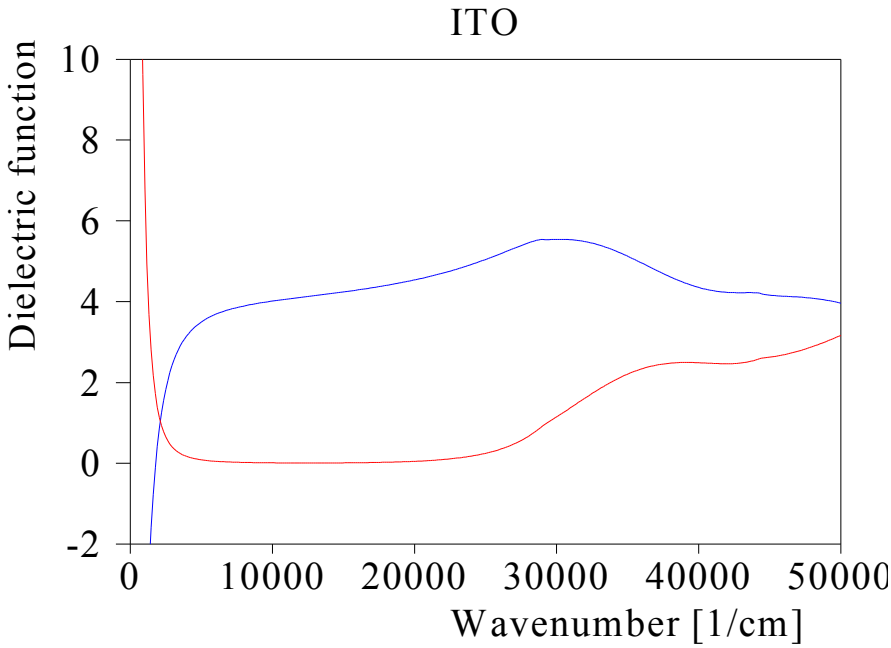


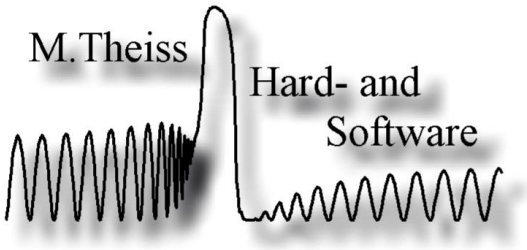
A similar model with two interband transitions was used to describe ITO on glass.
In this case an infrared reflectance spectrum had been measured as well. To fit all three spectra with a unique optical constant model a Drude model for the free carriers of the conducting ITO had to be added.











Coating Designer

CODE is the up-to-date solution for realistic design of optical coatings. Based on our powerful SCOUT thin film analysis software we have developed the right tool for you if you

- Design thin films on glass for architectural applications
- Develop car glass coatings
- Produce thin films for displays
- Design properties of optical filters
- Optimize coatings for solar energy conversion

CODE predicts optical spectra for almost arbitrary layer stacks, angles of incidence and polarizations. Several quantities characterizing coating products are computed and can be optimized:

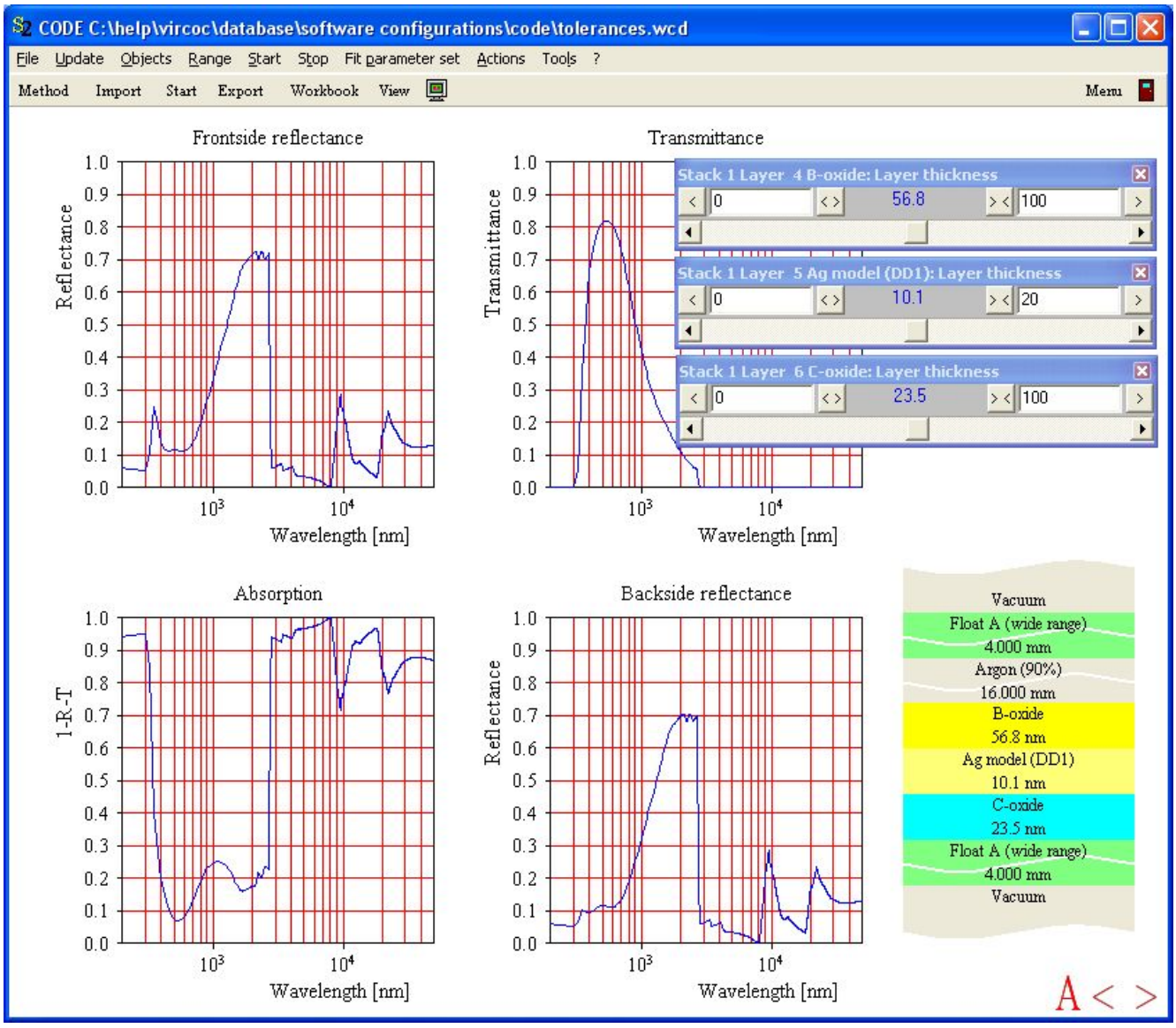
- Color coordinates (L*, a*, b*, X, Y, Z, x, y, z, L, a, b for light sources A, D65, C and observation angles of 2° and 10°), color visualization
- Light transmittance for light sources A, D65, C
- Light reflectance for light sources A, D65, C
- Solar transmittance (DIN 67507, EN 410, P.Moon)
- Solar reflectance (DIN 67507, EN 410, P.Moon)
- g (DIN 67507, EN 410)
- Color rendering index R_a
- Emissivity (normal and effective)
- U (15° and 10° temperature difference)
- Dominant wavelength, Purity
- Front pane absorption

With automatic spectrum multiplication and integration you can easily compute and optimize efficiencies of absorbers or reflectors.
Achieve highest flexibility making use of OLE automation technology.

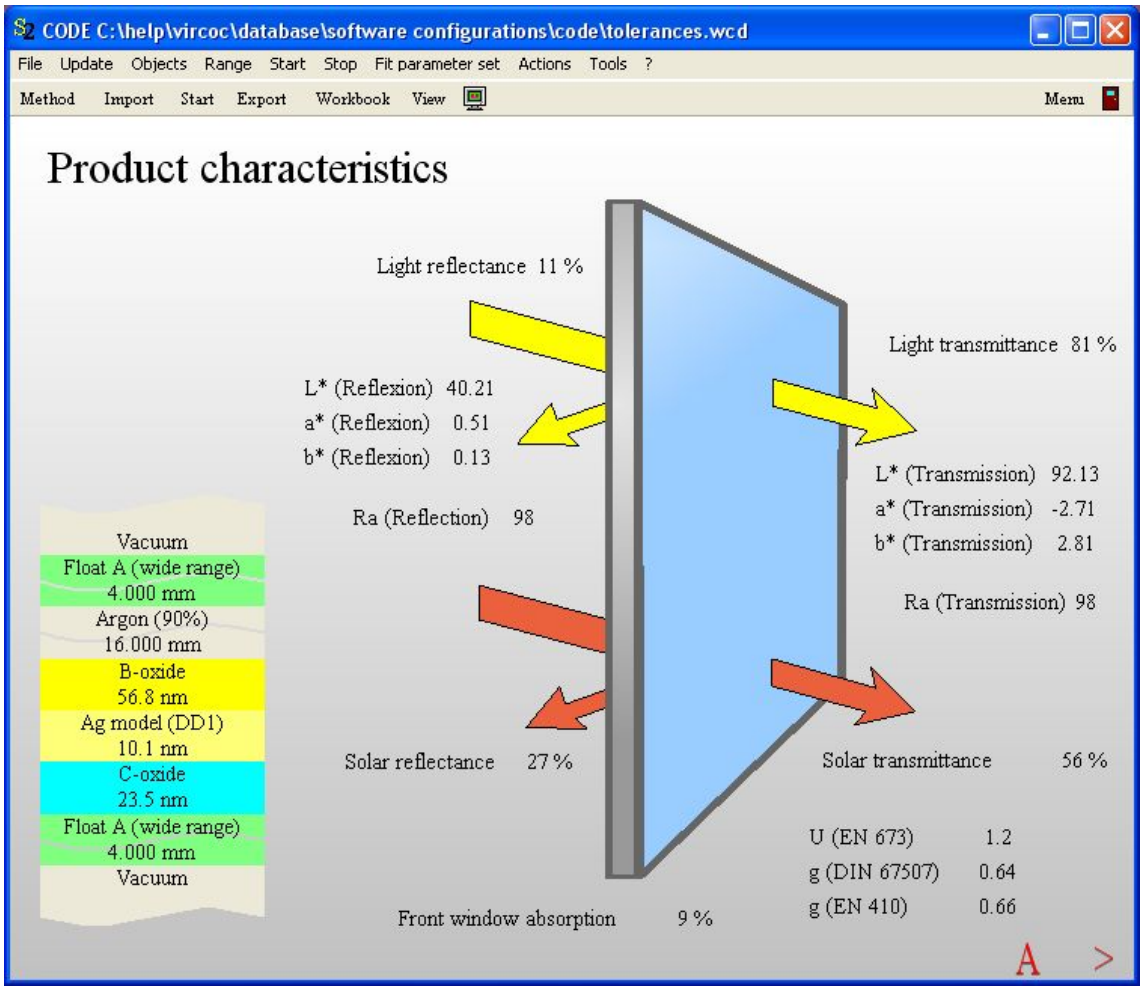
Graphically varying thicknesses or optical constant parameters you can easily inspect and optimize coating properties. Investigate systematically the consequences of parameter variations and fluctuations (due to production tolerances) and create corresponding charts.

Application example: Optical properties of a three-layer system (Low-E coating) between two glass panes

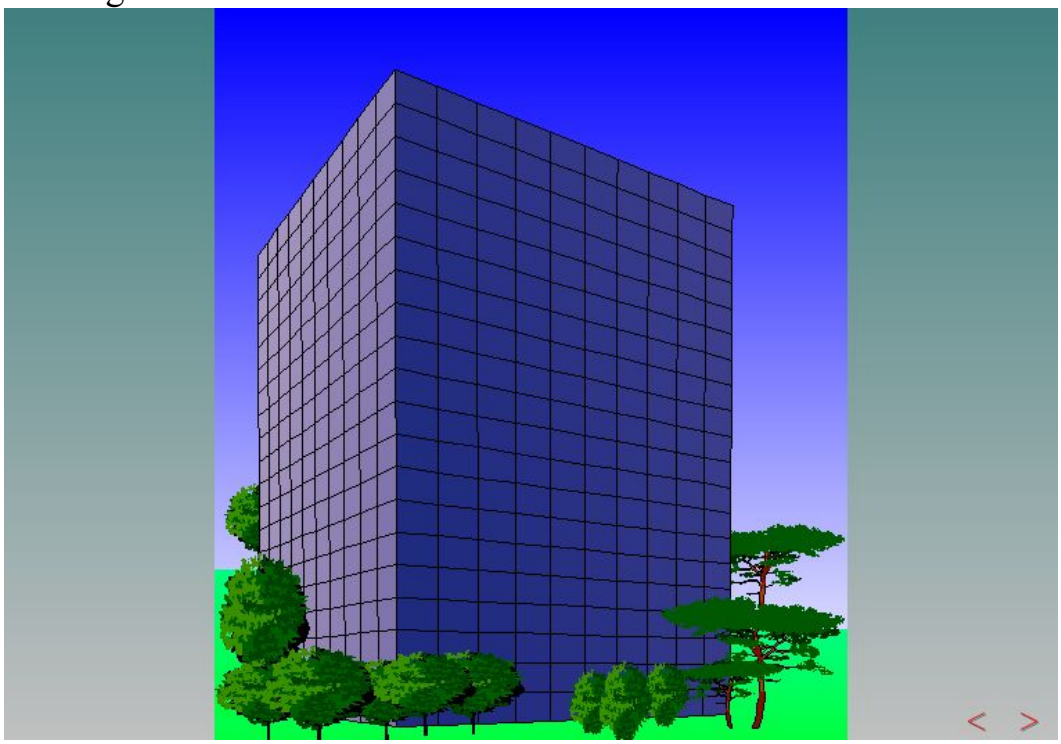
CODE computes optical spectra from the far infrared to the UV. Moving the three 'thickness' sliders on the right you can intuitively investigate the 'response' of the spectra to thickness changes:

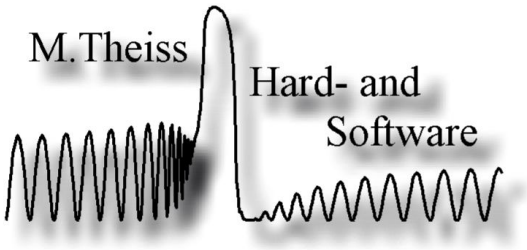


Based on the computed spectra several technical data like color coordinates, integral transmittance and reflectance values as well as energy related numbers such as emissivity, U and g are computed:



CODE visualizes the appearance of a virtual office tower equipped with newly designed coatings:

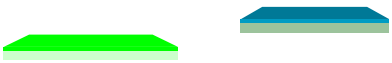




Coating Designer

One tool for research, design and production:

Research



Analyse single layers of all your deposition materials. Investigate how their optical constants depend on the deposition conditions (such as gas flows or temperatures) making use of the very flexible models of the program.
Store the obtained optical constants in the built-in database.

Design

Use the research results and predict the properties of complex layer stacks.
Optimize thicknesses or optical constants for your thin film products.

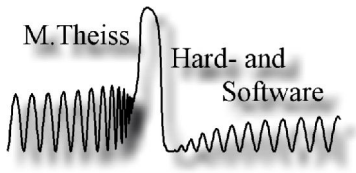
Production

Analyze your thin film products by optical spectroscopy and compare thicknesses and optical constants of the deposited layers with the design.

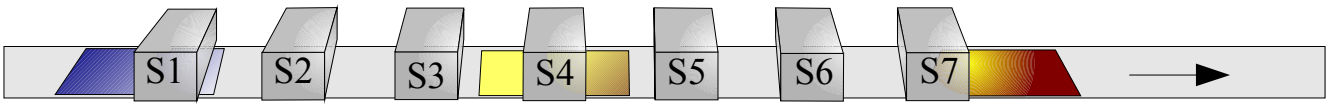

SCORE
Compute the properties of window products combining panes, gases and coatings from your CODE database. SCORE computes technical data, spectra and building views, and generates your product catalog.
Building views
SCORE
Factory
Performance
Welcome
Refresh
Views
Technical data
Setup
Word report
Copy view
Copy product
VirCoc
Window products
Float A (4 mm)
Argon (90%) (16 mm)
Low-e_blue_prototype_1
Panes
Gases
Coatings
Absorption
Reflectance (backside)
Wavelength [nm]
1-R-T
Reflectance

GenetiCode

Automatic coating design



Optimize material selection and thickness for each deposition step



GenetiCode assists your design of optical coatings with automized material selection and thickness optimization. You will have more free time to concentrate on the real issues to improve your thin film products, e.g. the increase of your deposition capabilities in quantity and quality.
Automatic coating design with **GenetiCode** works like this:

Goal: Define the target of the optimization

The goal of the coating optimization is defined like in our CODE software (which is the basis of GenetiCode): You can specify target values for integral data like light transmittance, color coordinates, IR emissivity, U and g, or you can import target spectra that your design should reproduce.

Materials: Define available materials and their thickness ranges

In a second preparational step, you tell GenetiCode which materials you can produce (you must have the optical constants of these materials, of course) and what thickness ranges you can achieve in a single deposition step.

Deposition: List possible materials for each deposition step

Now you specify the size and structure of your deposition equipment: Tell GenetiCode how many single deposition steps you have (7 in the sputtering example below), and list for every step the available materials (i.e. possible targets in the case of sputtering). The number of deposition steps and the freedom to select materials will determine the performance of the coating!

Optimization: Start, relax and let GenetiCode invent

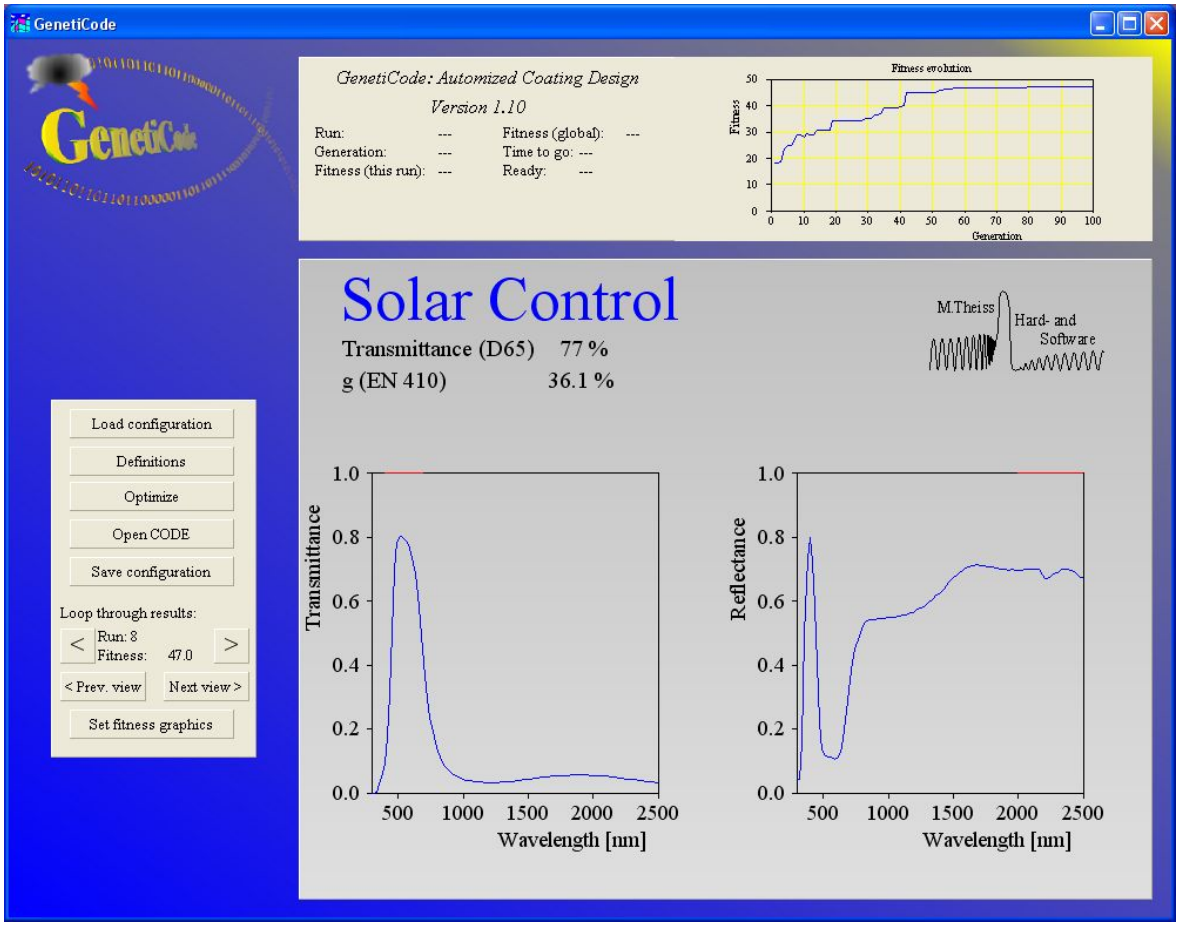
Finally you set a few parameters to control the optimization (which is a genetic algoritm) and start the automized coating design. Easy cases give you the opportunity to have a cup of coffee, complicated ones may require overnight work (of your computer!). While it runs, GenetiCode tells you when the computations will be finished.

Results: Pickup and inspect the best and alternative designs

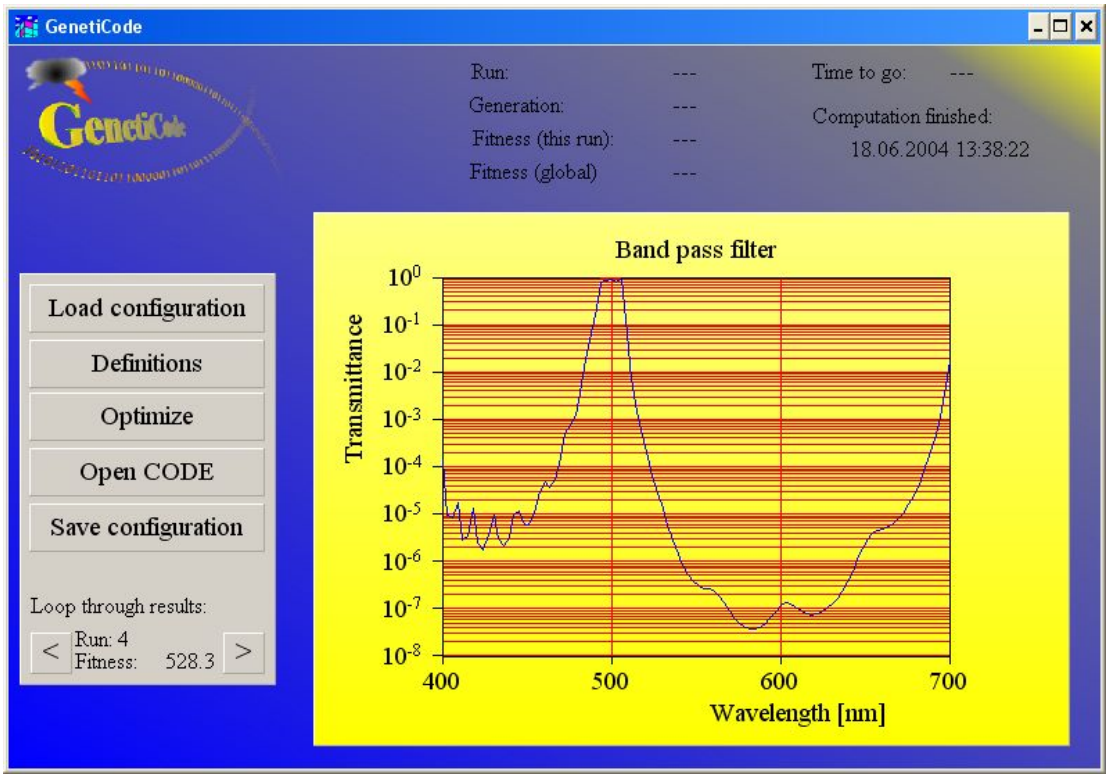
GenetiCode creates a table of the best designs, i.e. the materials and the thicknesses for each deposition step.

GenetiCode design examples

GenetiCode easily invents 'Low-e' or solar control coatings with one or two silver layers between oxide layers:



Construction of a band pass filter on glass for 500 nm radiation:



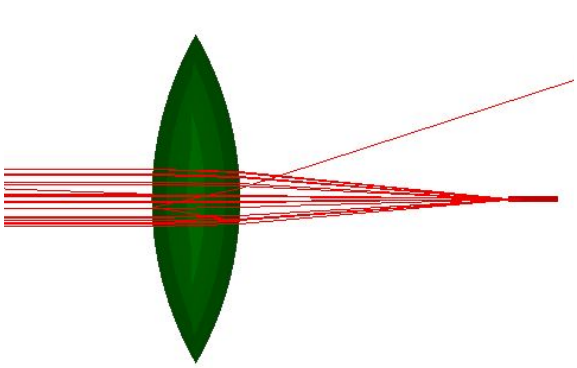
SPRAY

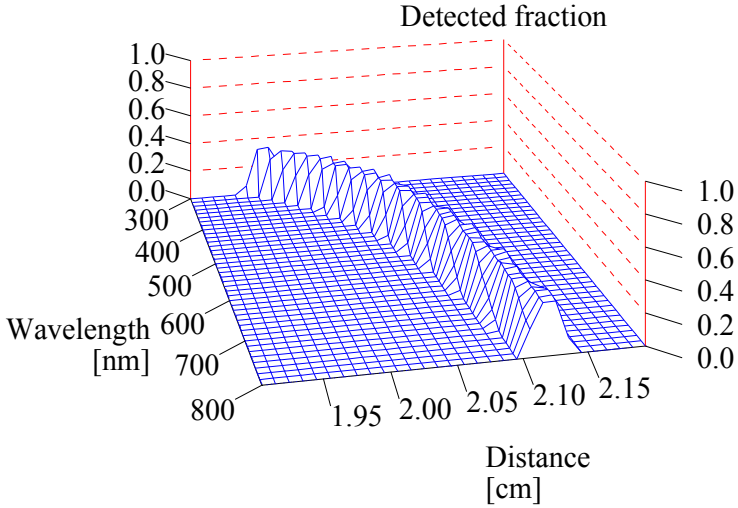
M.Theiss Hard- and Software

SPRAY simulates the performance of optical setups by **frequency resolved ray-tracing**. Various types of light sources emit 'photons'. SPRAY tracks their path through the 3-dimensional arrangement of objects until they escape to infinity or finally are absorbed.

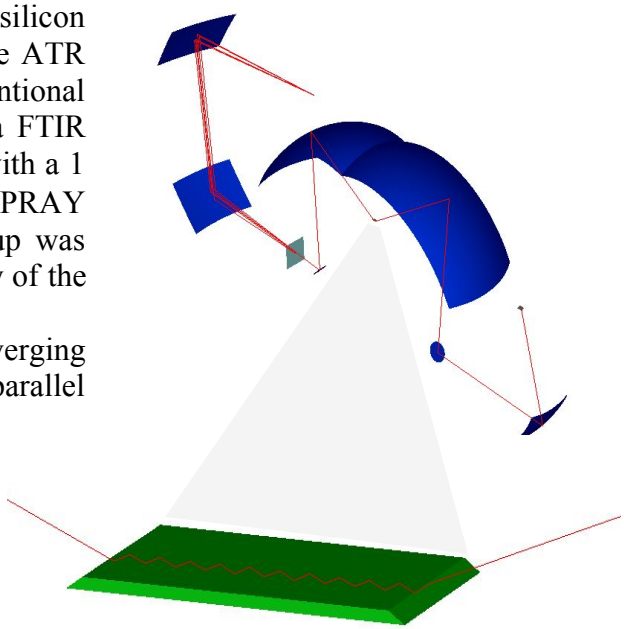
- Full 3-dimensional ray-tracing
- Point light source, rectangular and circular light sources, volume light sources
- Various interfaces (rectangle, triangle, sphere, cylinder, prism, ellipsoid, paraboloid, …). Each interface can be a perfect absorber, a perfect mirror, an almost arbitrary layer stack of thin films or a diffusely reflecting and transmitting surface.
- Various detectors for spectrum recording (including detector arrays), rectangular screens for visualizing spatial radiation distributions
- Powerful optical constant models, large optical constant database
- Absorbing, scattering and fluorescent media
- Integration of Mie computations to calculate the scattering characteristics of uncoated or multiply coated spheres
- Integrated color computation, ideal for the prediction of optical properties of paints and diffuse reflectance spectra
- Ideal tool for teaching optics
- Flexible programming of SPRAY simluations by OLE automation control of all objects

The simple example below demonstrates chromatic errors of a lens. Parallel rays from the left are directed by the lens to a detector array close to the focal point. The position dependent detector signal in the right picture nicely shows how the focal point depends on wavelength:





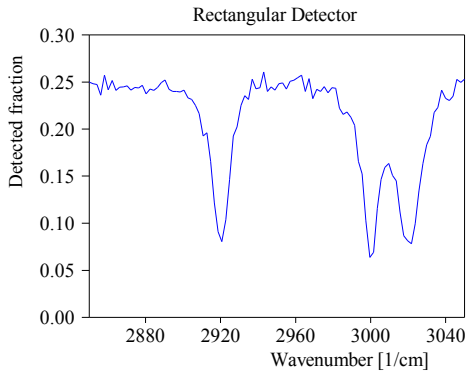
The next pictures show an advanced example. A silicon wafer with 45° inclined edges is used as a multiple ATR (attenuated total reflection) prism in a conventional reflection unit for variable angle of incidence in a FTIR spectrometer. The bottom of the prism is covered with a 1 µm layer of an absorbing organic material. Using SPRAY OLE automation and Excel's VisualBasic the setup was optimized and analyzed with respect to the visibility of the absorption bands of interest.



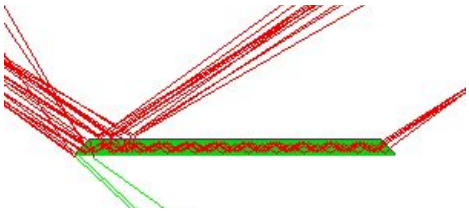
The principle setup is shown to the right. Diverging radiation from the light source at the top is made parallel by a parabolic mirror. A second parabolic mirror creates a focus on a rotatable plane mirror (a polarizer is placed in between) which is in a focus of a large ellipsoidal mirror. The second focus is at the sample stage where the ATR prism (see the enlarged insert) is placed. A second ellipsoidal mirror, followed by a rotatable plane and another (final) ellipsoidal mirror guide the radiation to the detector.

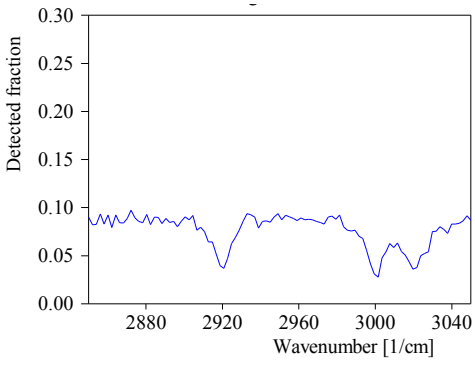
In order to get significant intensity, one has to work with a finite size of the light source. Here we show the answer to the question how the absorption contrast depends on the size of the light source. The pictures below show that changing from an ideal point light source to a more realistic 2 mm radius the contrast of the absorption bands decreases significantly. The graphs also show why: A large fraction of the light is reflected at the top of the ATR element and is not available for absorption by the organic layer:

Ideal point light source

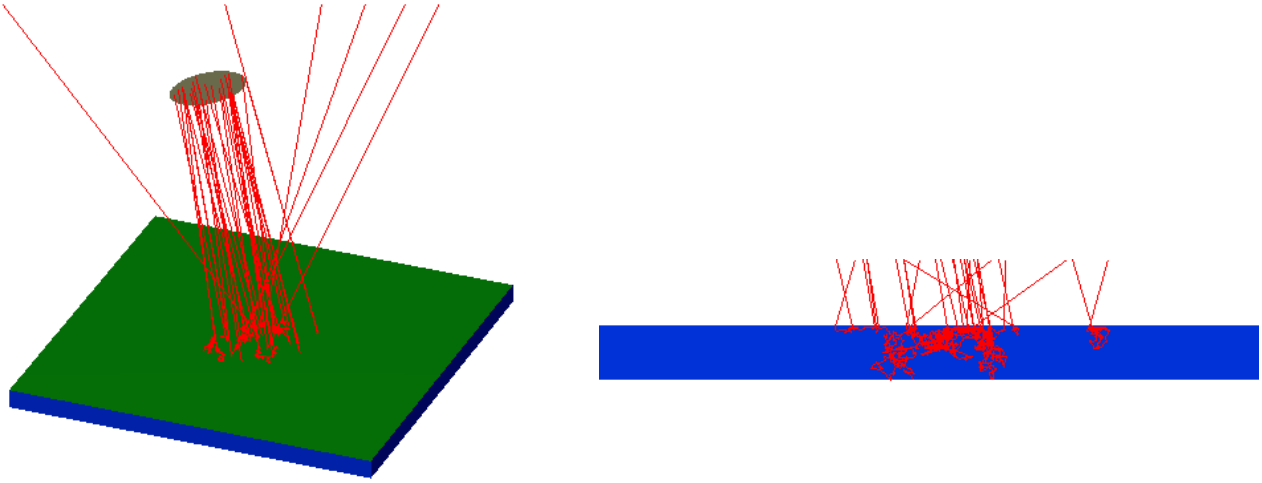


Circular light source with 0.2 cm radius

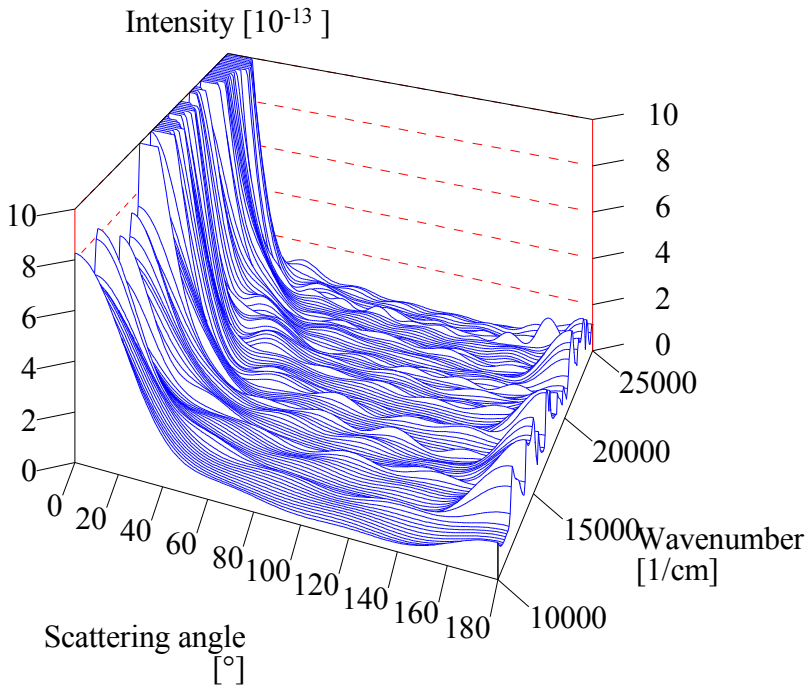




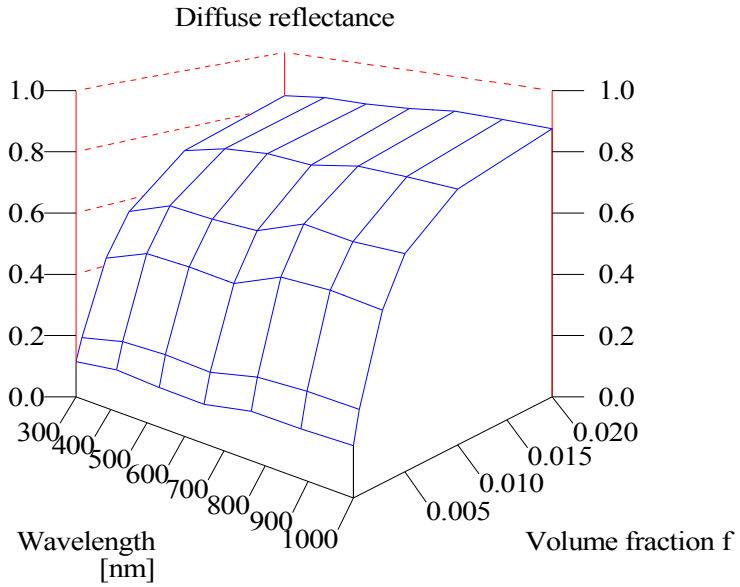
SPRAY is an excellent tool to predict the colors of paints. The next graph shows as a model system a resin layer filled with TiO_2 and CdS particles. This paint is illuminated from the top. A large detector (not shown in the sketches below) records all radiation that is reflected by the paint. The next graphs show an overview and a sideview of the resin layer with a few test rays:



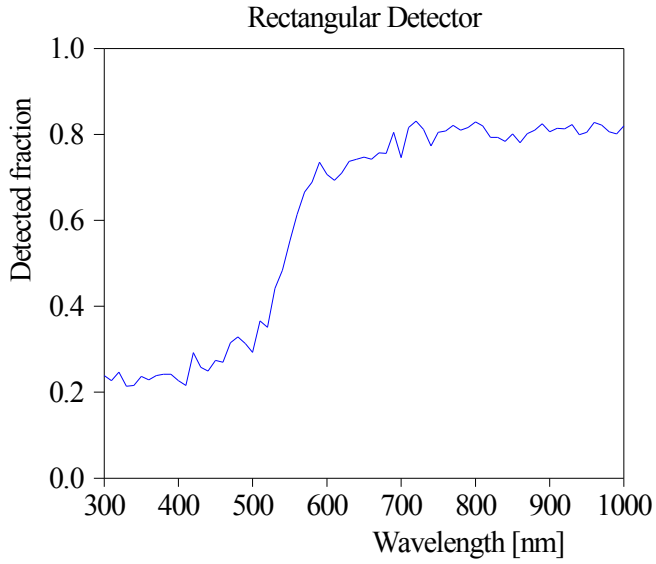
The scattering characteristics of the embedded particles are computed with the integrated Mie program (which can handle spheres with a user-defined size distribution and multiple thin film coatings of the sphere core). Here is the angle distribution of the scattered radiation for TiO_2 particles computed by the Mie module:

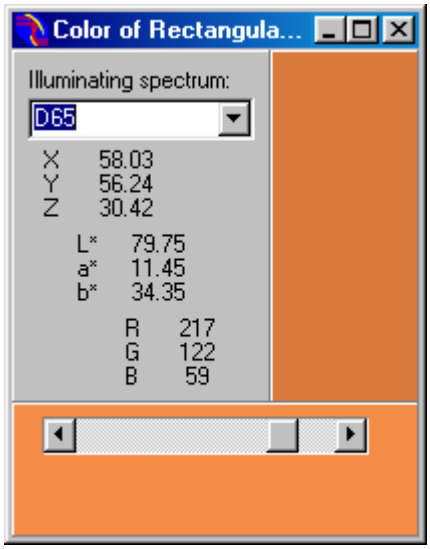


The next graph shows how the diffuse reflectivity of a TiO_2-filled resin layer on a black substrate depends on the volume fraction of the TiO_2 particles. This answers the question how much scatterers are needed to make a white color independent of the substrate:

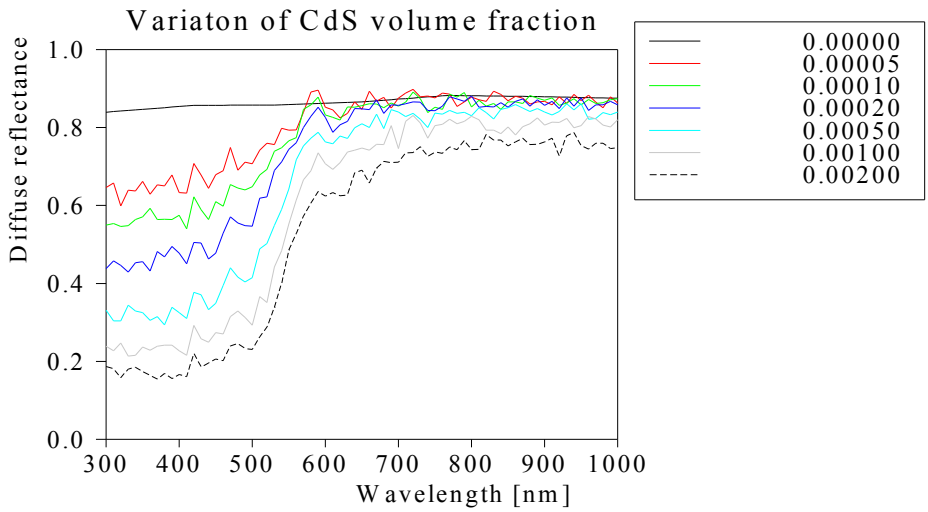


Now let's make a real color and put in some absorbing CdS particles. Mixing a paint with f = 0.02 of the TiO2 particles and f = 0.001 of CdS clusters, the following spectrum and color is obtained:





Here are spectra for a series of CdS volume fractions:



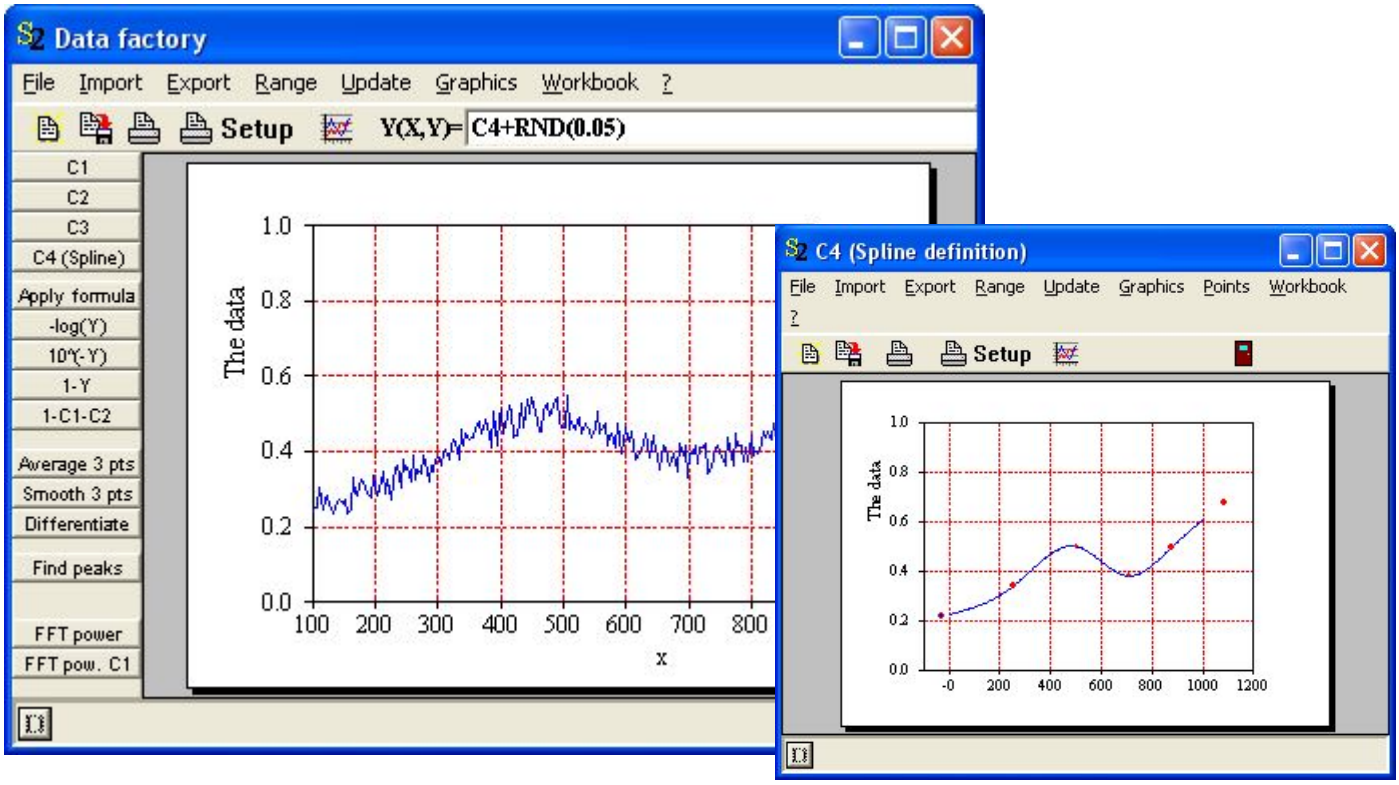
Data Factory

M.Theiss Hard- and Software

Data factory is a utility to create and manipulate data. It was written to support other M.Theiss Hard- and Software products which exchange with *Data factory* data like optical spectra by easy drag&drop operations.

With *Data factory* you can

- Compute new data by applying user-defined formulas
- Create data by 'drawing' (spline interpolation)
- Manipulate existing data by user-defined formulas
- Use up to three input spectra in your formula: Each input spectrum may be part of the formula that determines the output spectrum (Add, multiply, divide, ...)
- Reduce the number of data points by averaging
- Smooth curves
- Fourier transform data



Digit

M.Theiss Hard- and Software

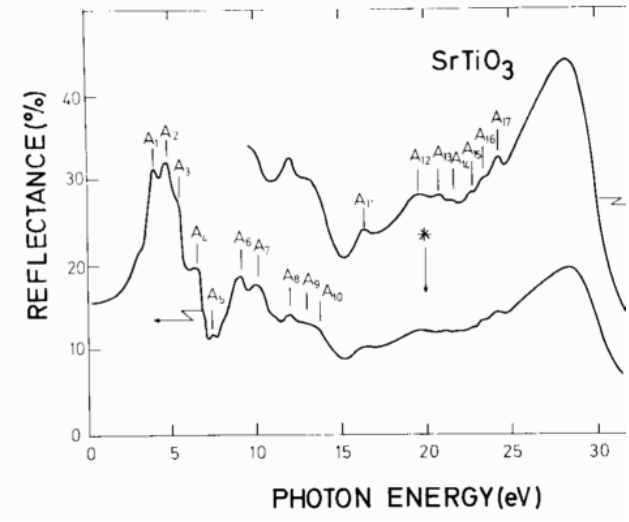
Digit is an easy to use program to get digitized data from scanned pictures containing scientific graphics.

Manual point selection

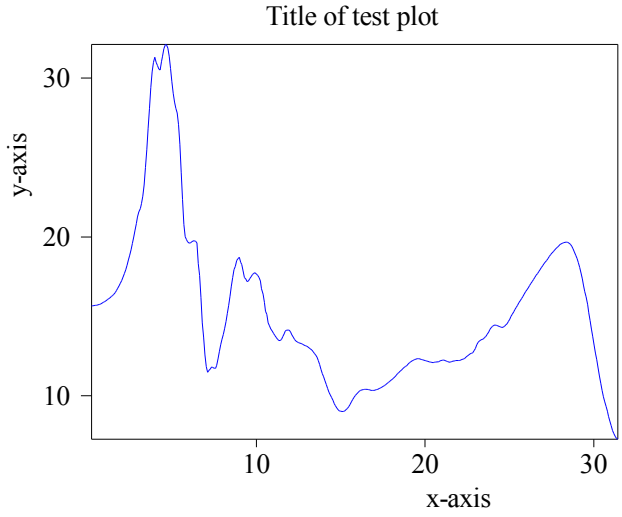
Start with a bitmap like the one shown to the right. After the definition of three scaling points you simply click along the curve that you want to digitize. Every mouse click is recorded and the coordinates of the mouse cursor position are added to the list of data points.

This method is easy to learn and recommended for getting a few points in a quick manner. On the other hand, it is not very accurate and rather tedious if you want to collect many points.

Input picture



Digitized data



Semi-automatic point selection

This method is more accurate than the first one, and certainly much more elegant. On the other hand, you have to learn a little more to use it.

After the definition of three scaling points and the background color you only have to move the cursor roughly along the curve to be digitized. All pixels whose color differs significantly from the background color are identified and recorded. Based on this set of points an equidistant set of output points is constructed by suitable averaging.

After a little training you can generate digitized output data like the one to the left in less than 2 minutes.