The Virtual Coating Company

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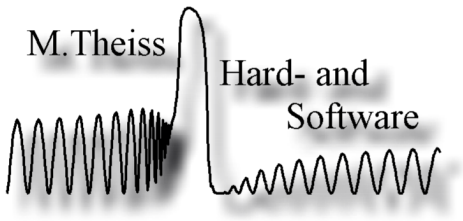

VirCoC

The Virtual Coating Company

by Wolfgang Theiss

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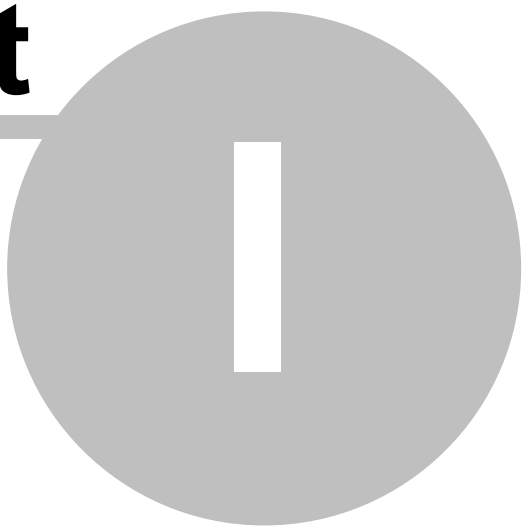

1 Overview

1.1 About this document

The Virtual Coating Company

written by W.Theiss

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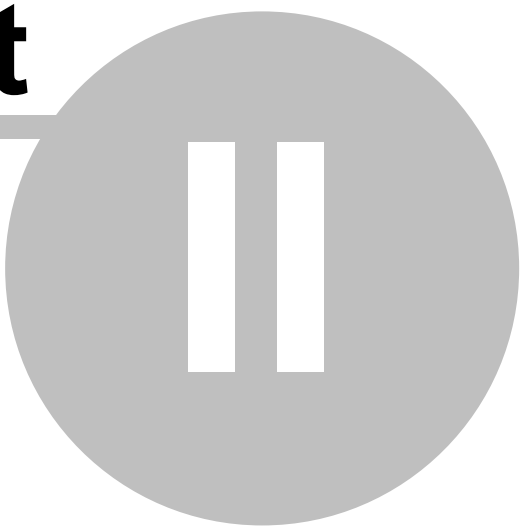
June 2004

VirCoC was established in June 2004 in order to demonstrate the application of our thin film analysis and design tools. Like in a real thin film company, there are (or will be) materials, deposition devices, spectrometers, thin film products and a lot of problems to be solved. In contrast to the real world, money is not very important and financial aspects are almost

completely ignored.
Since we are selling software for optical spectroscopy and design, the focus will be on optical problems and techniques. All other things required to run ***VirCoC*** (like deposition devices, for example) are not discussed in detail.

You can follow the development of the company in the section called The story. Other sections like materials or spectrometer hardware summarize the present status of certain sections of the company. We try to keep everything consistent - before we record spectra of substrates, we buy the substrates and a spectrometer. So we hope that this document contains enough information to understand the ***VirCoC*** problem solving. However, you may have to consult (from time to time) the manuals of the software products for details.

Part



2 The story

2.1 Overview

This section is written like a log file, showing how things have been developed one after the other. The overview you are reading now guides you through the various phases of the company history.

June 2004

Starting the company
Setting up the VirCoC database
Computation of the substrate absorption, an example of simple data juggling with the Data Factory tool
Thick substrates: Optical constant determination, saving substrate definitions to the database
Thin film analysis: Ag layers on glass
Optical constant determination of oxide layers
Automatic coating design with GenetiCode: First steps

2.2 June 2004: Part 1

1/6/2004
VirCoC is established!
Up to now there is nothing except the will to build up a successful thin film coating company and to fill this document with useful examples the solution of optical thin film problems.

2/6/2004
Today we receive our first spectrometer. Since we are going to produce glass coatings for architectural applications, we have to be able to record reflectance and transmittance spectra from the UV to the infrared, i.e. at least from 300 to 2500 nm. We bought a machine that covers the range 200 ... 2500 nm.

In order to analyze the measured spectra and to predict optical properties of our thin film products we bought the CODE software from M.Theiss Hard- and Software. The program is installed today.

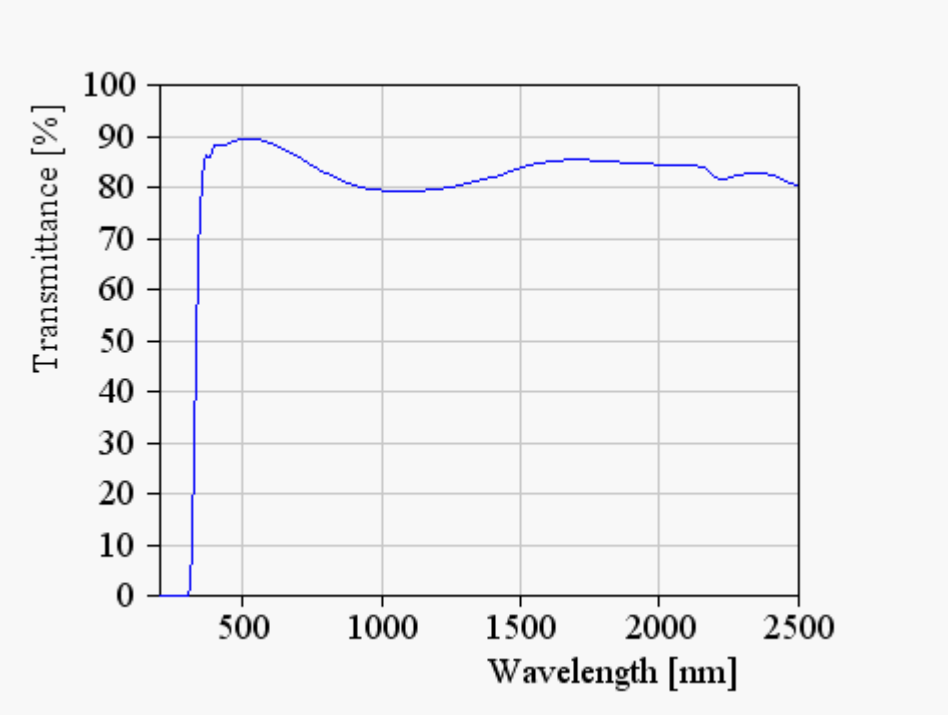
Our first substrate arrives: FLOAT A is a float glass that we can buy from a supplier in thicknesses of 4, 5, 6, 8 and 10 mm. The test sample we receive has a nominal thickness of 5 mm. We instantly record a reflectance and a transmittance spectrum with our new spectrometer S1. The measured spectra will be of interest for some people in the company, so it would be good to make them public somehow. The best way to do this is to implement a shared database.

Starting the ***VirCoC*** database
In order to synchronize our work we decided to build up the ***VirCoC*** database. It will be used to store data and documents of common interest. The database is simply realized as a folder structure available to all interested users in our company network. Since the CODE software comes with a database using a certain folder structure we just follow and extend the CODE system.
The CODE setup routine installs a database in the program folder. The database folder is called 'database' and it has the subfolders 'materials', 'substrates' and 'coatings'. 'Materials' contains a lot of optical constant objects, most of them fixed data tables from literature, but also a few optical constant models. The folders 'substrates' and 'coatings' offer some pre-defined layer stacks that you can use as blocks to build up your own stack definition.
Besides the folder 'database' the CODE setup installs a folder system called 'My database'. This is almost empty and is meant to be used as a template for your own database. In order to start with the ***VirCoC*** database we copied the 'My database' folders to the network path that is going to hold the database of our company.
At this moment, our database has the folders 'materials', 'substrates' and 'coatings'.
In order to collect important measured spectra we manually add the subfolder 'spectra'. Since at the moment we want to publish the measured reflectance and transmittance of the FLOAT A

substrate in the database, a subfolder 'float glass' and therein the subfolder 'Float A' is created. Within this folder the reflectance spectrum is stored in the file r_5mm_s1.spc. The corresponding transmittance spectrum is saved in the file t_5mm_s1.spc. See graphs of these spectra in the Float A database section.

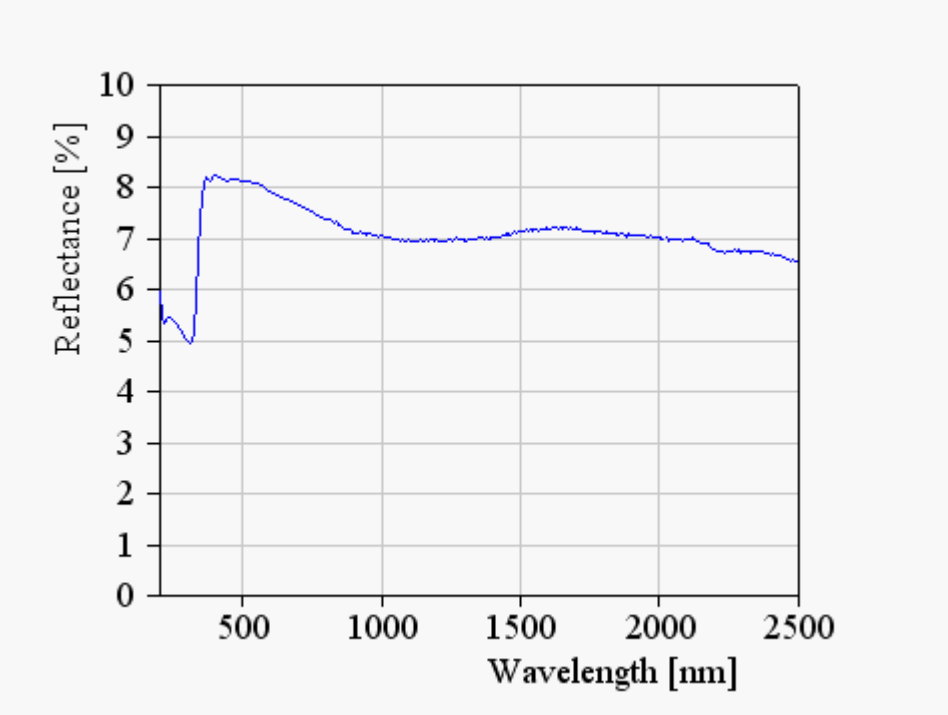
Computation of the substrate absorption

Having measured the reflectance R and the transmittance T of the 5 mm sample of Float A, it is useful to compute the absorption 1-R-T. The small program 'Data Factory' (delivered with CODE) is the right tool to do this. In Data Factory you can load spectra in data fields, and then use the spectral values as numbers in user-defined functions in order to compute new spectra.
First the measured transmittance spectrum is loaded into the data field C1 using the **Import** command. With proper graphics settings the spectrum looks like this:

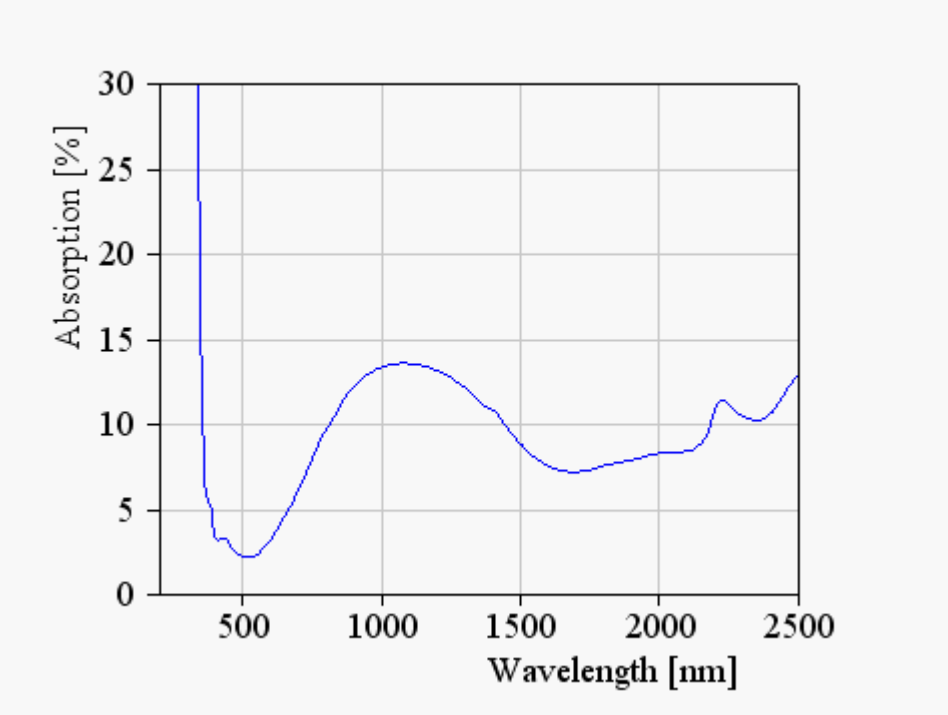


By the way: Once we have typed in suitable graphics parameters to display a certain type of spectrum we store them in the database for future use. In order to do so, a new folder named 'plot parameters' has been created.

The reflectance spectrum is loaded into data field C2:



Now, in the main window of Data Factory, we compute the absorption by typing in the formula '100-C1-C2' and selecting a **Range** from 200 to 2500 nm with 200 data points. The button **Apply formula** does the calculation leading to the following result:



The computed absorption spectrum is then stored to the database folder 'spectra/Float glass/Float A' using the filename a_5mm_s1.spc.

Since we think we will do absorption computations more often, we store the Data Factory configuration to the database. A new folder 'Software configurations' with the subfolder 'Data Factory' is created. Here we store the complete Data Factory configuration (use the

File|SaveAs command) in the file s1_absorption.dtf.

2.3 June 2004: Part 2

3/6/2004

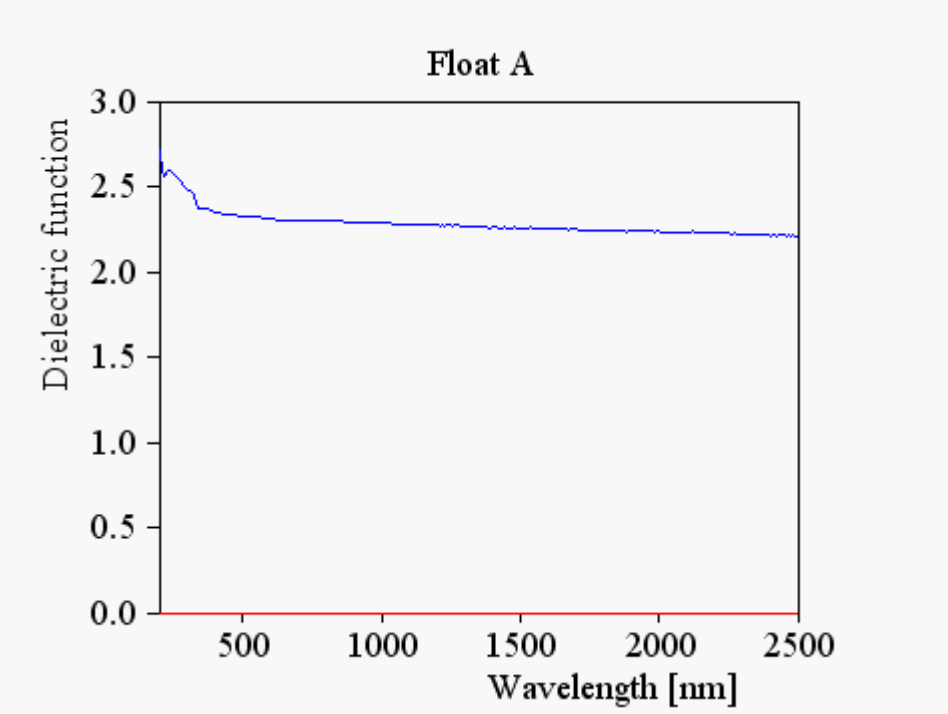
Thick substrates: Optical constant determination

Now, since we have R and T of our first substrate, we would like to determine the optical constants n and k of Float A and make them available in the database. We will need the optical constants of all substrates in order to analyze deposited thin films and to design the optical properties of coating products on these substrates.

There are two methods to determine optical constants from R and T spectra of thick glass plates: We could setup an appropriate model for the optical constants in the CODE software and fit the relevant parameters of this model, or we can use the DirectDF tool delivered with CODE. DirectDF can be applied in the case of thick, homogeneous plates only. Knowing the thickness of the plate, the optical constants can be determined directly from R and T, if the transmission is significantly different from zero. Using DirectDFis much faster than fitting an optical constant model, so in this case we will use DirectDF.

The DirectDF manual gives a detailed description of all required actions, and we just follow the sequence. A little problem arises at the point where we have to type in the thickness of the plate: Although the supplier specified a thickness of 5 mm, our mechanical measurement gives a value of 4.8 mm. Very likely the reason for this mismatch is a glass production at the lower limit of the thickness tolerance. Nevertheless, we decide to work with 5 mm thickness in DirectDF. This will lead to absorption coefficients being slightly too low, but if we consistently use 5 mm thickness in all computations later on, the calculated absorption of the glass plate will be correct. Using the nominal 5 mm thickness instead of the true 4.8 mm will avoid a lot of confusion within the company.

We compute the optical constants in DirectDF in the range 200 ... 2500 nm using 1000 points. The program computes the so-called dielectric function which is the square of the complex refractice index n + i k. The result is the following:

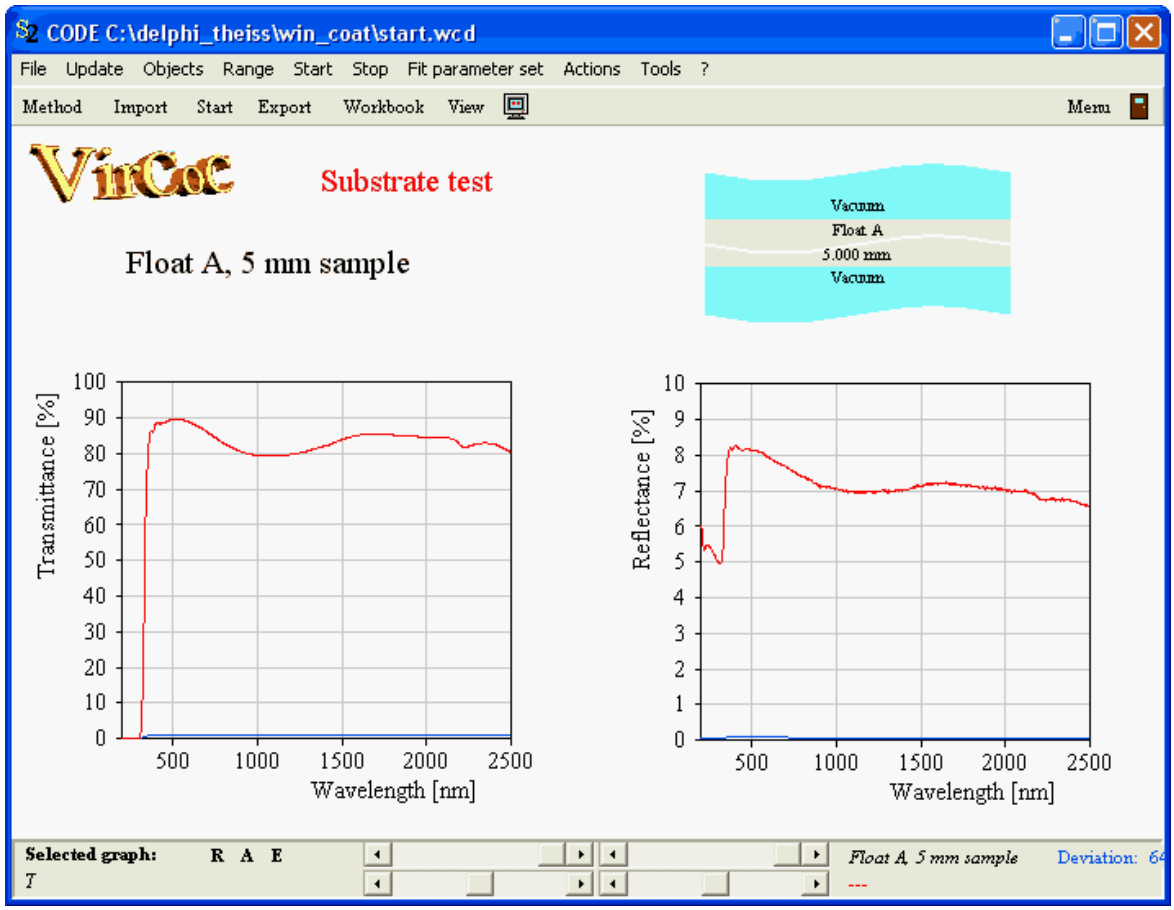


The new optical constants are stored to the database with the database connection of DirectDF.

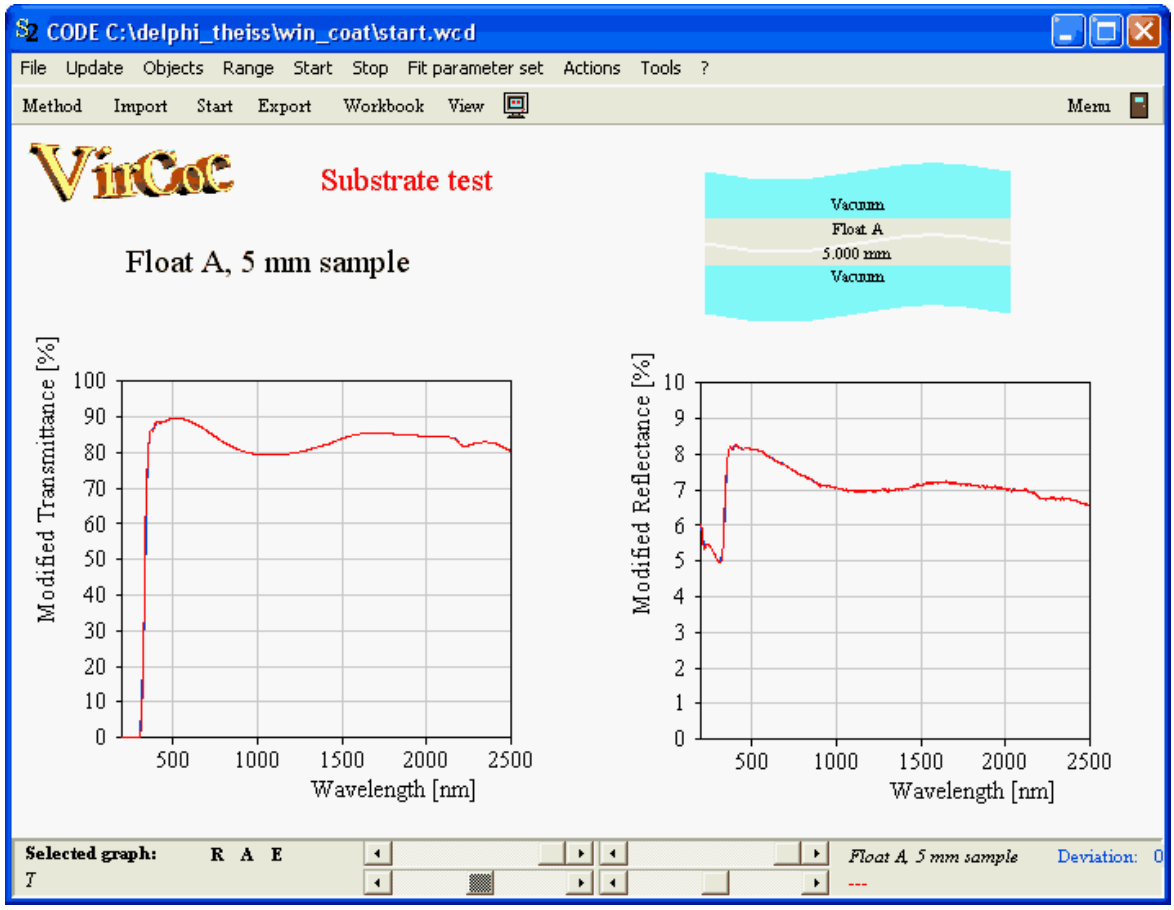
After the computation of the optical constants of Float A, we save the configuration of DirectDF to the database (database/software configurations/directdf/float_a.ddf).

The new material in the ***VirCoC*** database is tested using an appropriate CODE configuration. R and T are computed based on the database data and compared to the measured spectra. A first

comparison is rather disappointing:

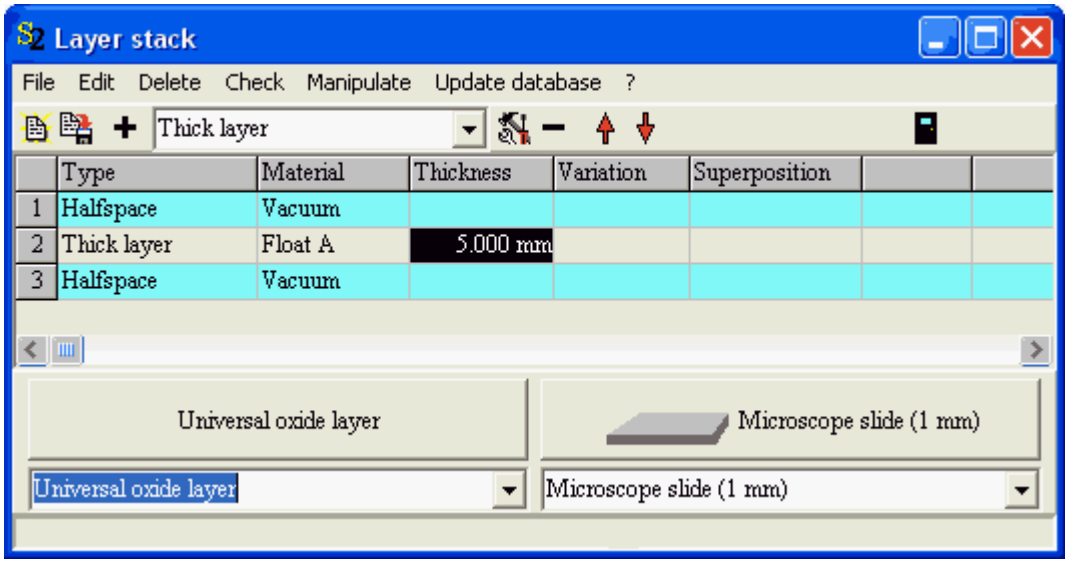


The blue computed spectra do not match the experimental ones. A closer inspection gives the reason: Whereas the measured data are stored in % units, the simulated spectra are reflection and transmission coefficients ranging from 0 to 1.0 . The easiest way to avoid this mismatch is to multiply the simulated data by a factor of 100 which can be done using the user-defined formula for the manipulation of simulated spectra. Just enter the formula 'Y*100' in both the R and T simulations. Now the agreement is perfect:



Adding substrate layer stack definitions to the database

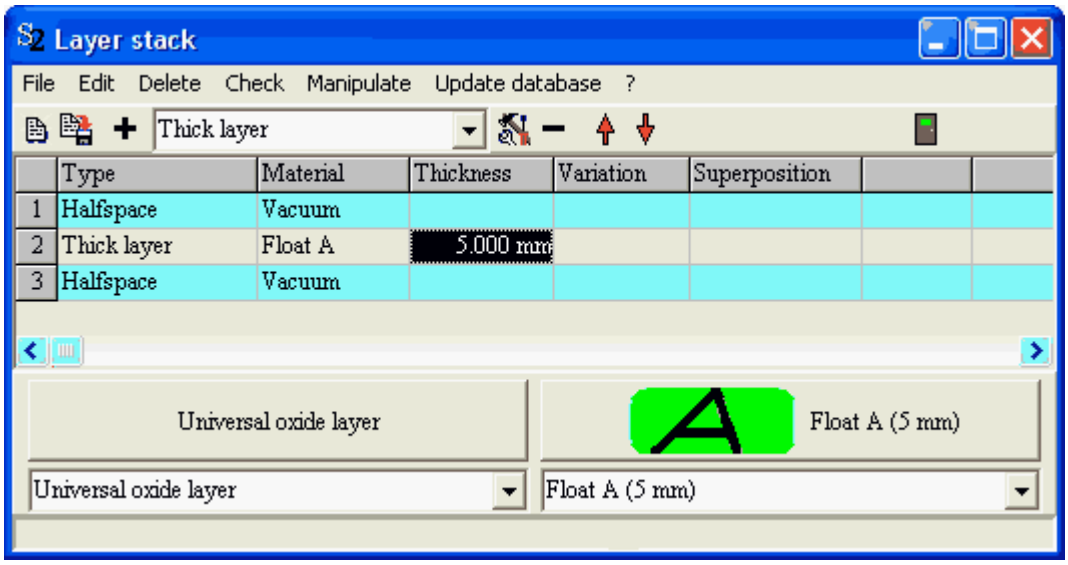
After the successful comparison with the measured spectra, the substrate layer stack definition (a thick layer of the material 'Float A' with a thickness of 5 mm) is stored in the database folder 'substrates'. We open the layer stack definition window



and use the command **File|Save layer stack definition**. The layer stack is saved in the file 'Float A (5 mm)' in the subfolder 'substrates'. The **Update database** command is used to reload the substrate definitions from the database. From now on the 'Float A (5 mm)' substrate can easily be dragged into any layer stack definition.

In order to clearly indicate the type of float glass we place a kind of logo for 'Float A' in the

'substrate' database folder. The bitmap 'Float A (5 mm).bmp)' is displayed in the layer stack definition window when the stack 'Float A (5 mm)' is selected:



Based on the optical constants of 'Float A' we can vary the thickness of the glass and store other substrate definitions to the database as well. As soon as we will receive samples of these additional thicknesses we will check if the computed spectra match the measured ones. Thicknesses of 4, 6, 8 and 10 mm have been added. Corresponding bitmap files named 'Float A (4 mm).bmp', 'Float A (6 mm).bmp', 'Float A (8 mm).bmp' and 'Float A (10 mm).bmp' are created as well.

2.4 June 2004: Part 3

7/6/2004

A first deposition device

For our first deposition experiments we have bought a small scale sputtering machine called DD1. It is installed today. The device comes with targets for metal layers and can be operated with reactive gas inlets in order to produce oxides and nitrides.

A fast spectrometer system

In order to be prepared for the large number of samples we are going to produce with DD1, we decided to buy the fast array spectrometer system S2. This machine can simultaneously record reflectance and transmittance spectra. With all samples of a deposition experiment lined up on a scanning table, S2 can automatically process a whole sample series within a few minutes.

8/6/2004

Ag on glass: Our first deposition experiment

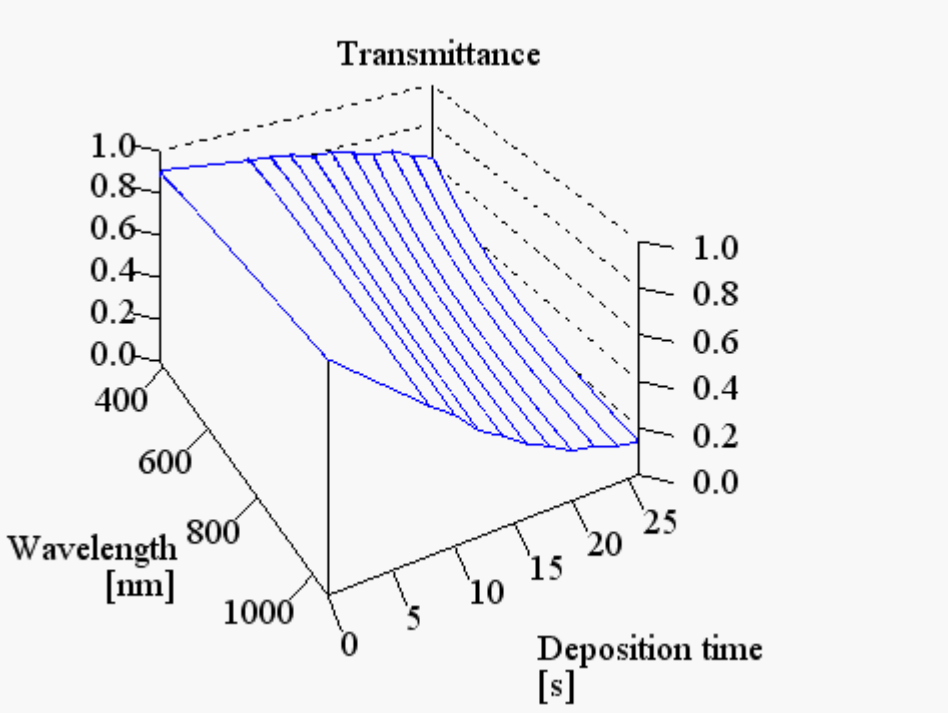
Using the new DD1 sputtering device we deposit Ag on microscope slides. 10 samples were prepared: With constant electric power we varied the deposition time:

Sample	Ag sputtering time [s]
dd1_ag_ms_08_06_2004_0	0
dd1_ag_ms_08_06_2004_1	8
dd1_ag_ms_08_06_2004_2	10
dd1_ag_ms_08_06_2004_3	12
dd1_ag_ms_08_06_2004_4	14
dd1_ag_ms_08_06_2004_5	16
dd1_ag_ms_08_06_2004_6	18
dd1_ag_ms_08_06_2004_7	20
dd1_ag_ms_08_06_2004_8	22
dd1_ag_ms_08_06_2004_9	24

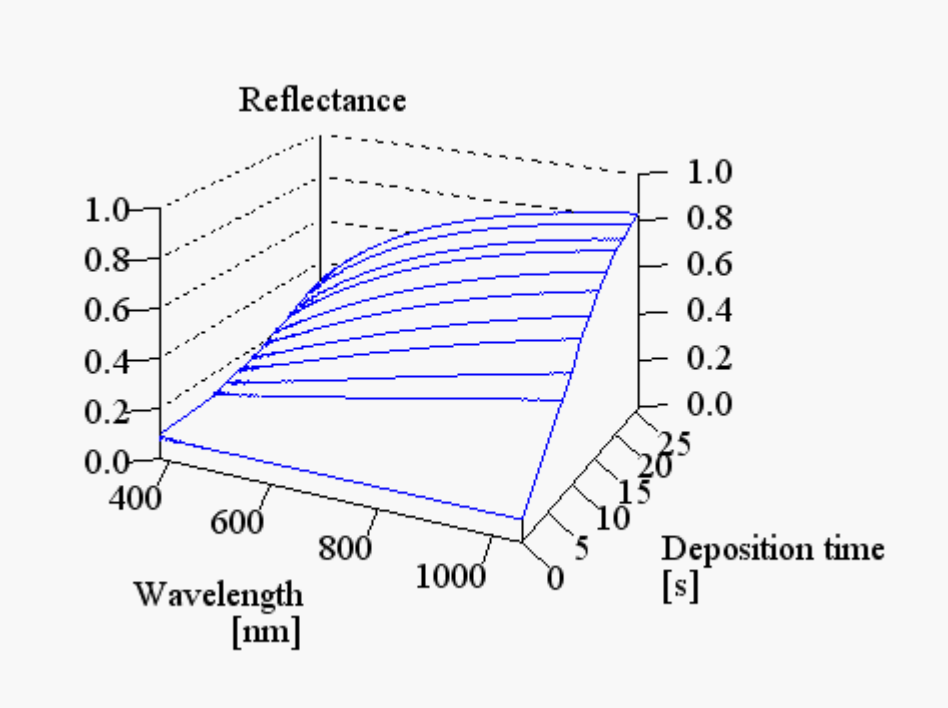
dd1_ag_ms_08_06_2004_10 26

The reflectance and transmittance spectra of these samples have been measured with the S2 spectrometer system and stored to the database.

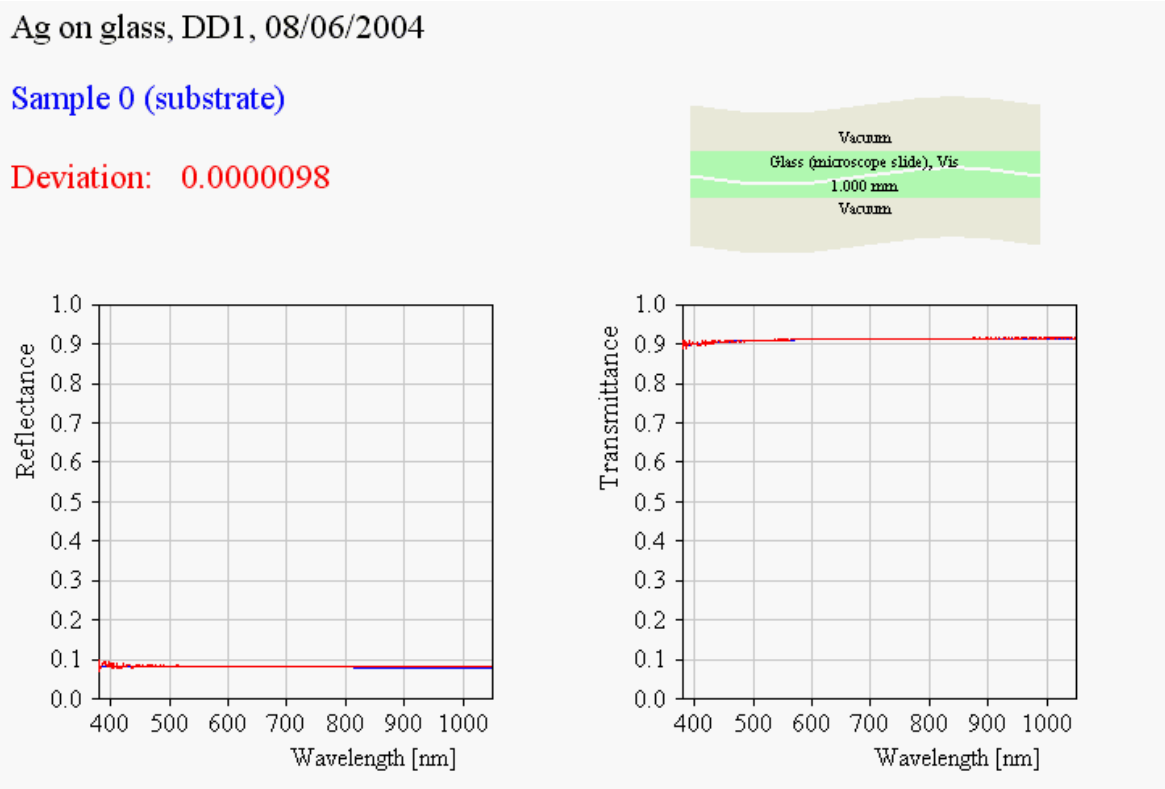
To get an overview, the measured spectra are displayed using the Collect tool which is delivered with CODE. Here are the transmission data



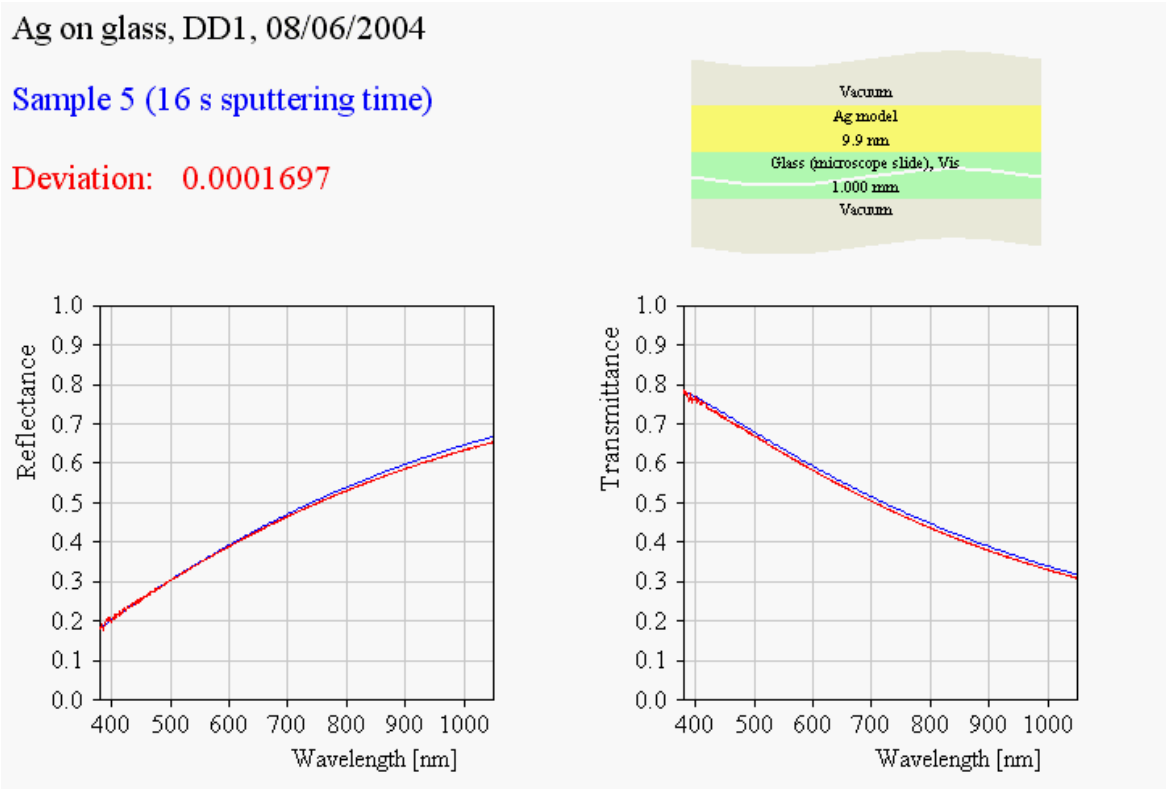
and here the reflectance spectra:



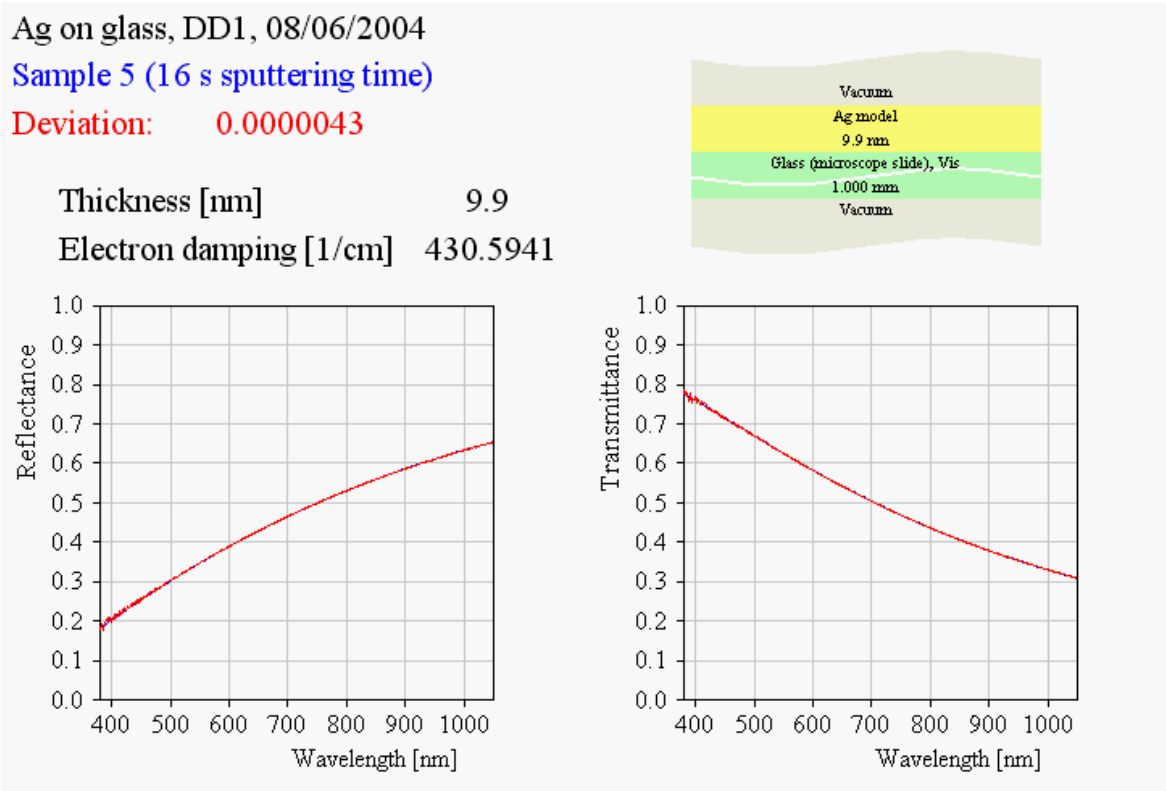
We analyze the spectra with a CODE configuration that computes R and T in the spectral range of the S2 spectrometer. First of all we check if the substrate spectra are consistent with the expectations based on the optical constants of microscope slide glass from our database. That is the case as the following comparison shows:



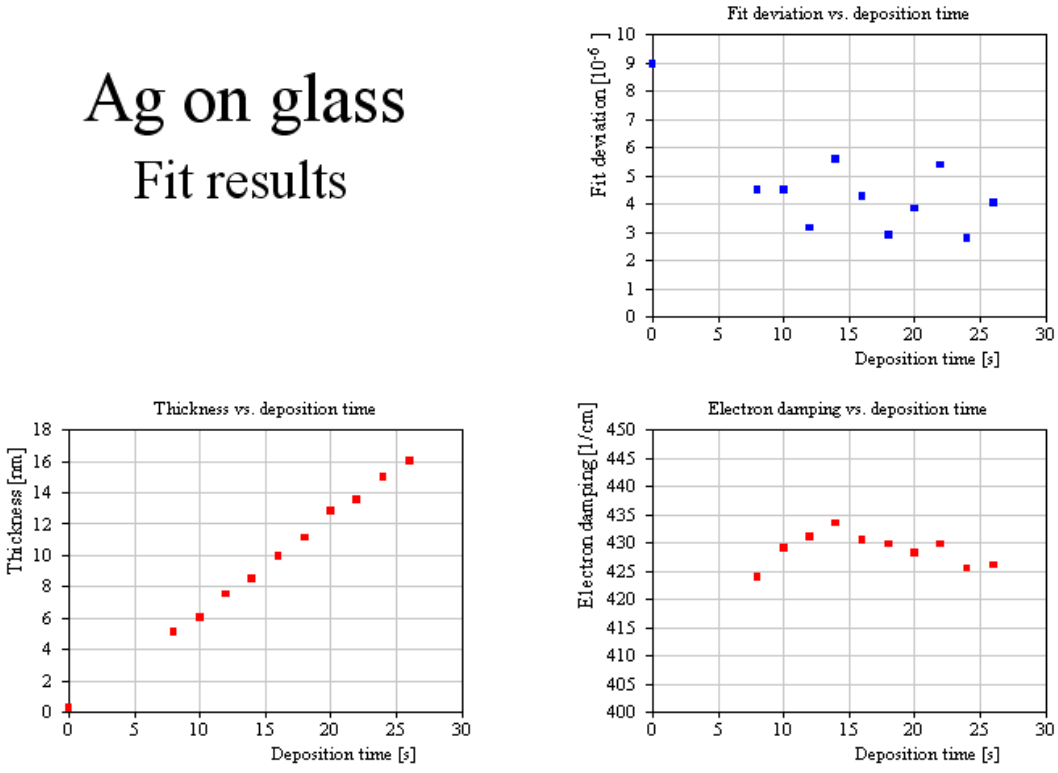
We now load the spectra of sample #5. For the optical constants of Ag we have nothing in our database yet. We start with data taken from the original CODE database. There are several versions - we take the object called 'Ag model' because this will allow us to change the model later on if necessary. Fitting the thickness of the Ag layer in the model the following best fit is achieved:



The agreement is not bad although there is a significant difference between model and measurement. There can be several reasons for this: The measurements could be wrong, the layer could have a surface roughness, there could be a depth gradient in the Ag properties within the layer, or the Ag sputtered with our device is different from the one that was used to determine the optical constants found in literature. Most likely is the last reason: Ag obtained by sputtering may have more internal damage (grain boundaries, impurities) than material evaporated under very clean conditions. Grain boundaries or impurities will increase the scattering of the electrons, i.e. reduce the conductivity of the metal. In the framework of the simple Drude model (that is used in our Ag model) this means that the damping constant should be higher. Introducing the damping constant as additional fit parameter, we give CODE the chance to take into account different Ag qualities. The agreement of model and measurement is almost perfect now:



Being satisfied with the current model we try if we can fit all measured spectra using the method. We process all samples making use of CODE's batch operation feature. Because there are only two fit parameters the analysis of all sample spectra takes a few seconds only.
A second view is created which summarizes the results from the batch control window:



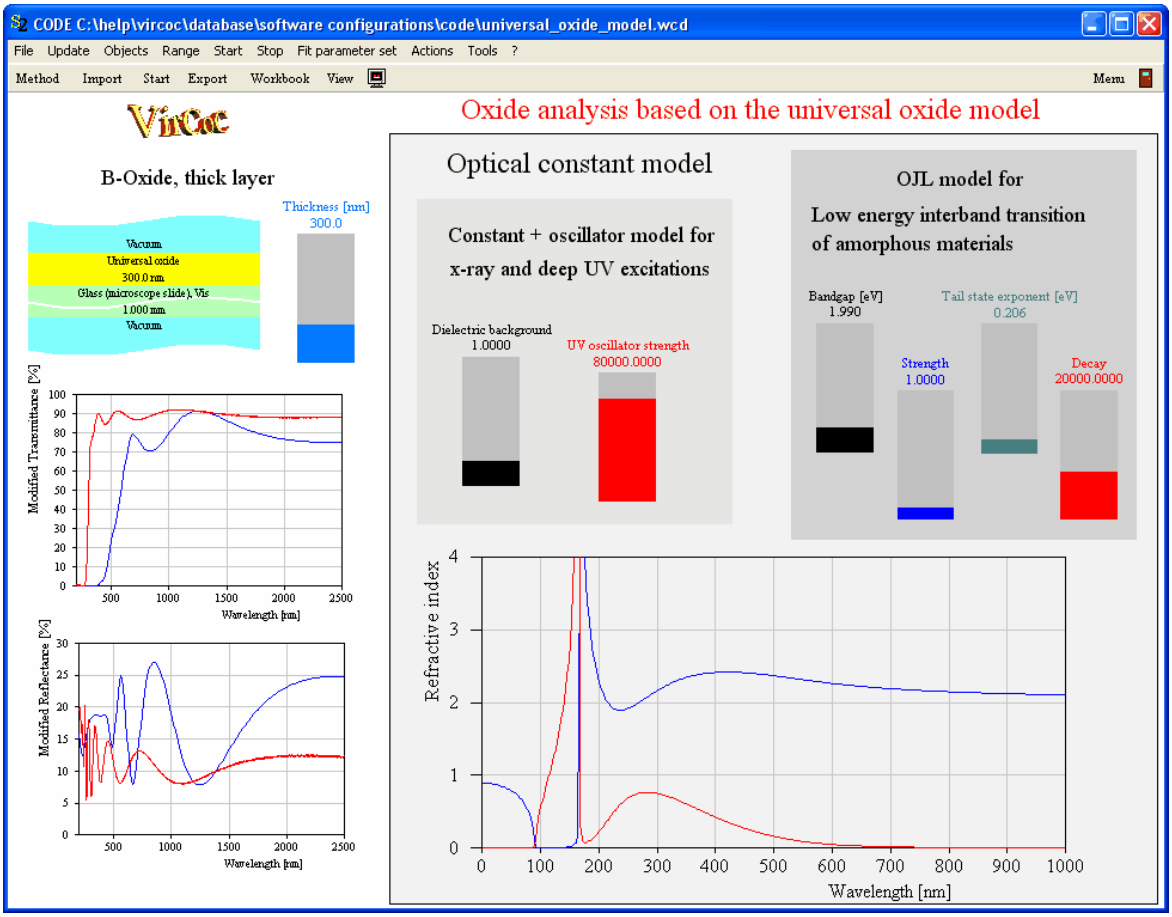
The fits are all very good (the fit deviation is below 0.00001). The thickness shows a nice linear

relation to the deposition time. The deposition rate is about 0.6 nm/s. In all cases the electron damping is close to 430 1/cm. This value is significantly higher than the 145 1/cm from the 'literature model'.
We can conclude that we should store our own Ag version (with a damping constant of 430 1/cm) to the ***VirCoC*** database. We name it 'Ag model (DD1)' to indicate the machine which is used to produce this kind of Ag.

2.5 June 2004: Part 4

8/6/2004
Oxide layers
Using DD1 we produce three types of oxide. With metallic targets and the highest possible oxygen flow, we try to produce stochiometric A-oxide, B-oxide and C-oxide layers. According to literature, these oxides should have different refractive index values that we will need for our coating products. In this first test, for each oxide type we produce a thin and a thick layer (on microscope slides).
Transmittance and reflectance spectra are recorded with the S1 spectrometer and stored to the database. Before we record the oxide layer spectra, we take spectra of a bare substrate in order to check if everything is Ok with the measurements. The substrate spectra are stored in the database directory of A-oxide.

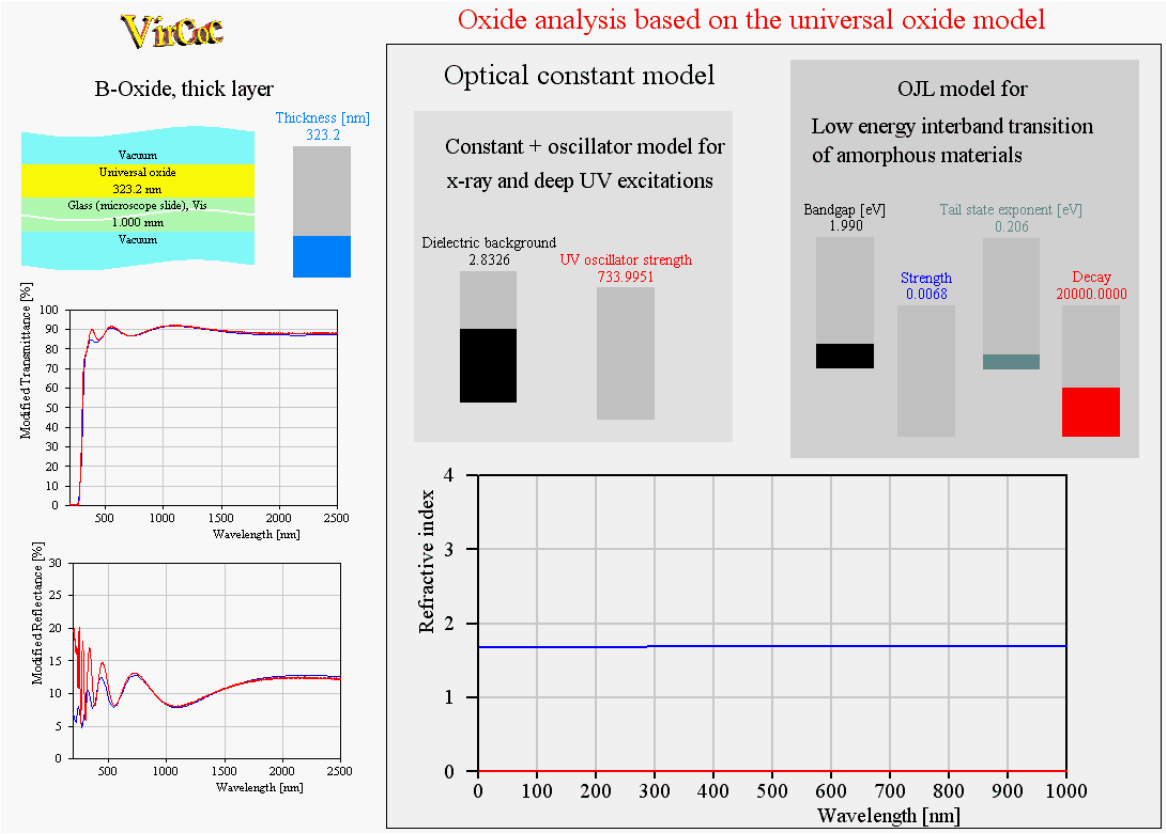
13/6/2004
Optical constants of the oxides
Today we try to determine the optical constants of the produced oxides. A visual inspection of the measured spectra shows that in the case of A-oxide the spectra are not very different from the substrate spectra. This looks a little difficult, so we decide to start with B-oxide. Clearly the spectra of the thick layer exhibit more structures (we think we see an interference pattern) and we decide to start the analysis with the thick layer.
M.Theiss Hard- and Software (the supplier of the CODE software) sent us a CODE configuration that they recommend for oxide analysis. They customized a general solution based on the so-called 'Universal oxide' model. The configuration looks like this:



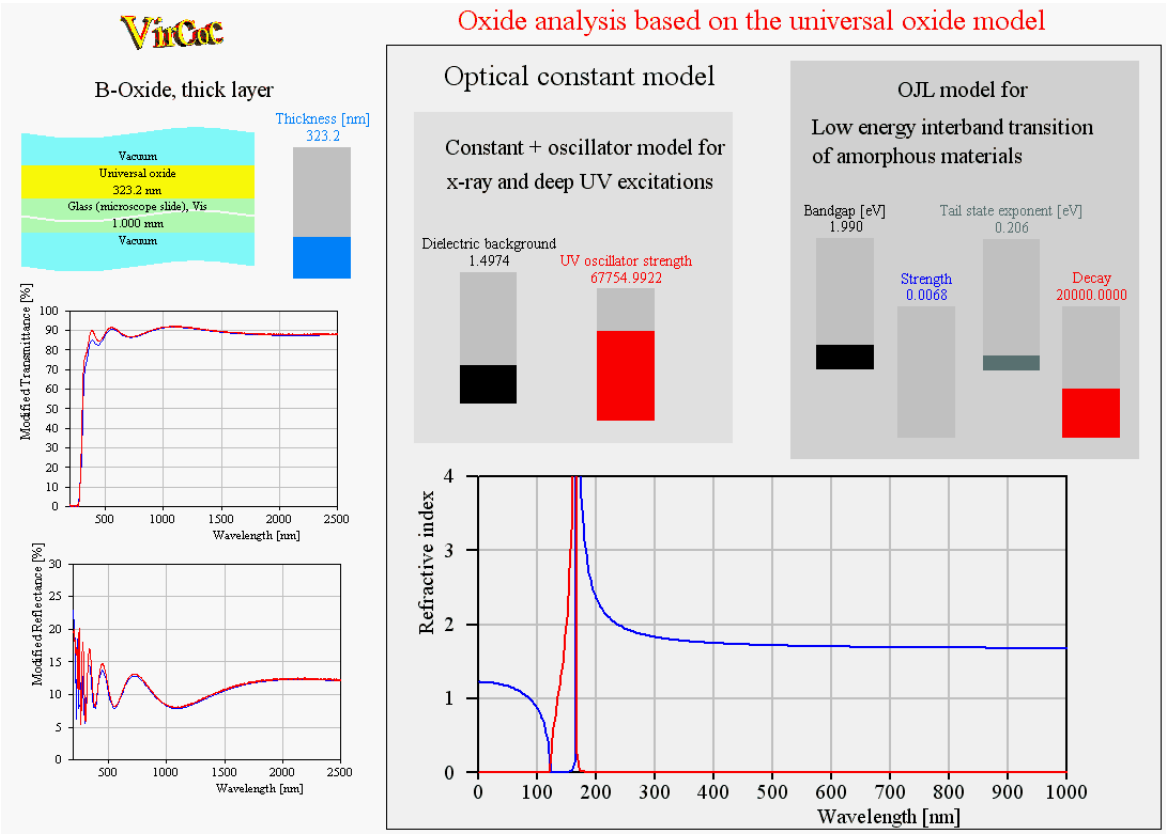
The optical constant model consists of three susceptibility contributions:

1. A constant (called 'Dielectric background') describes the response of electronic excitations in the x-ray and deep UV region, far away from the spectral range of interest in this case. This contribution does not lead to any absorption or dispersion.
2. Interband transitions in the far UV are represented by a single harmonic oscillator model. The model has three parameters: the resonance frequency, the oscillator strength and the damping constant (see SCOUT technical manual). We use this oscillator to 'summarize' interband transitions outside the investigated spectral range - it need not describe any details of these transitions. The resonance frequency is fixed at 60000 1/cm (167 nm wavelength). The low and fixed damping of the oscillator (100 1/cm) ensures that no absorption is caused by this term in visible spectral range. However, this contribution causes dispersion in the spectral range we are interested in.
3. For the interband transition with the lowest energy we use the OJL model which has turned out to be excellent for amorphous materials. This model will be able to introduce both tail state absorption and absorption by electronic transitions from the valence to the conduction band. (both assumed to be parabolic). The corresponding dispersion of the real part of the complex refractive index is included as well.

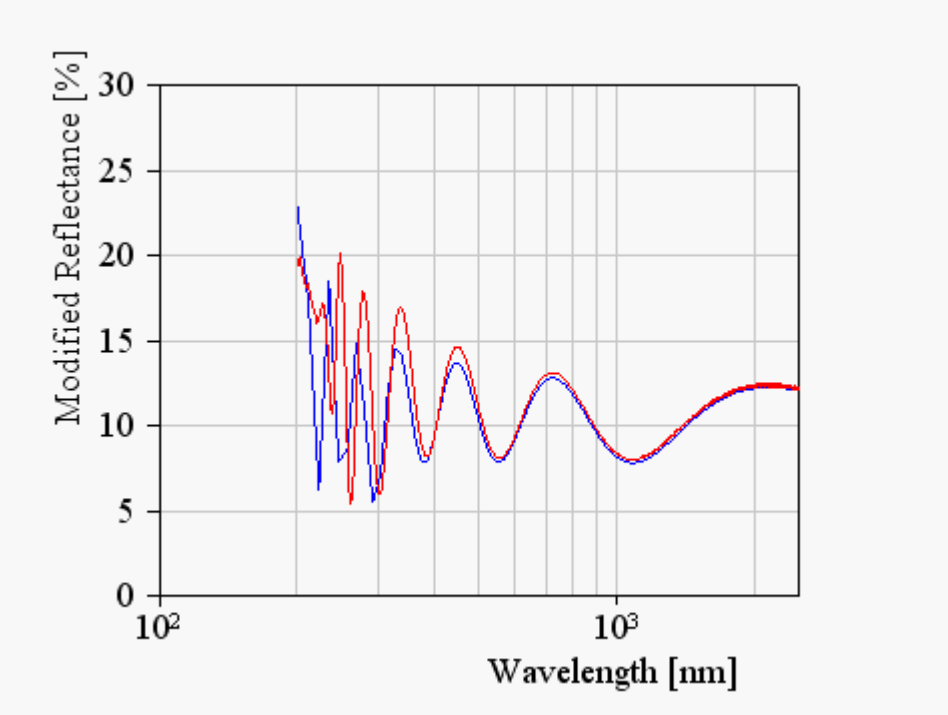
Using the sliders in the CODE configuration we play with different strengths of the individual contributions to the optical constants and inspect the consequences for the optical properties of the material. First we switch off the 2nd and 3rd term and work with a constant refractive index only. With a proper layer thickness we find good agreement of model and measurements in the infrared:



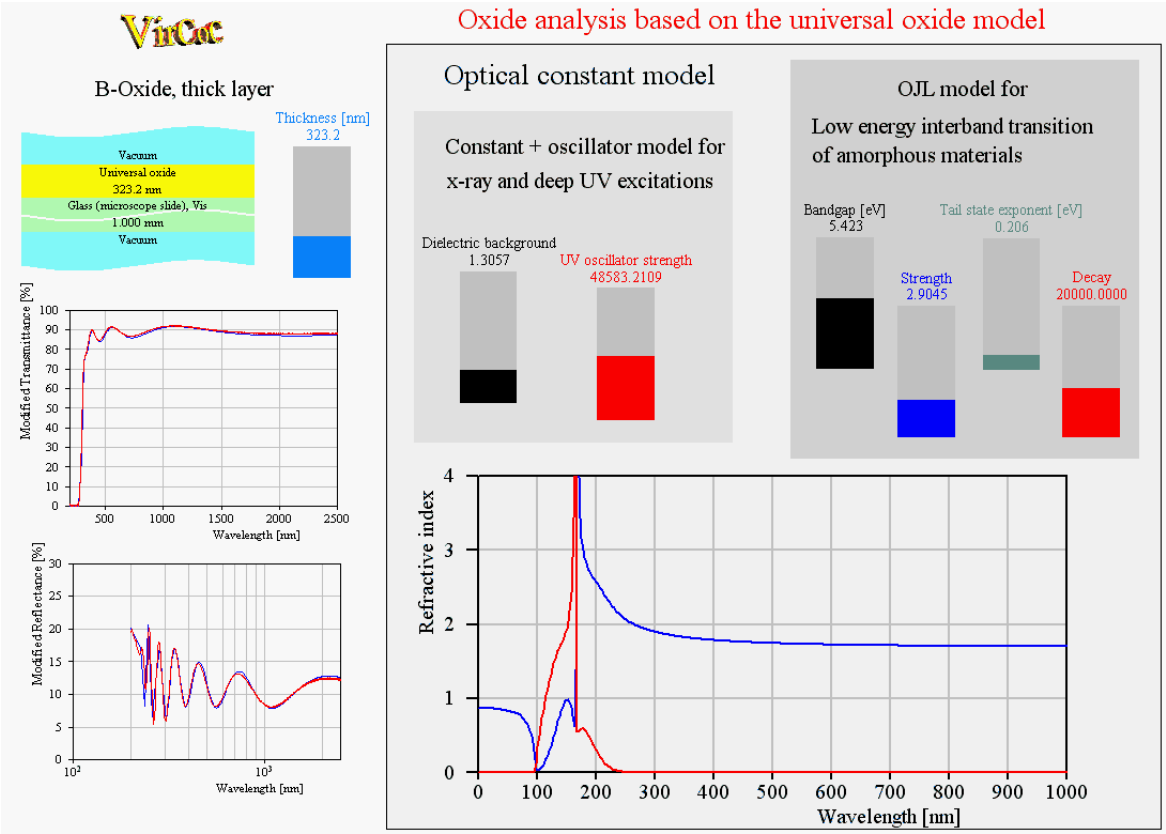
However, above 500 nm a higher refractive index is needed, keeping the infrared level of the refractive index the same. This dispersion can be achieved by increasing the 'UV oscillator strength' and decreasing the 'Dielectic background':



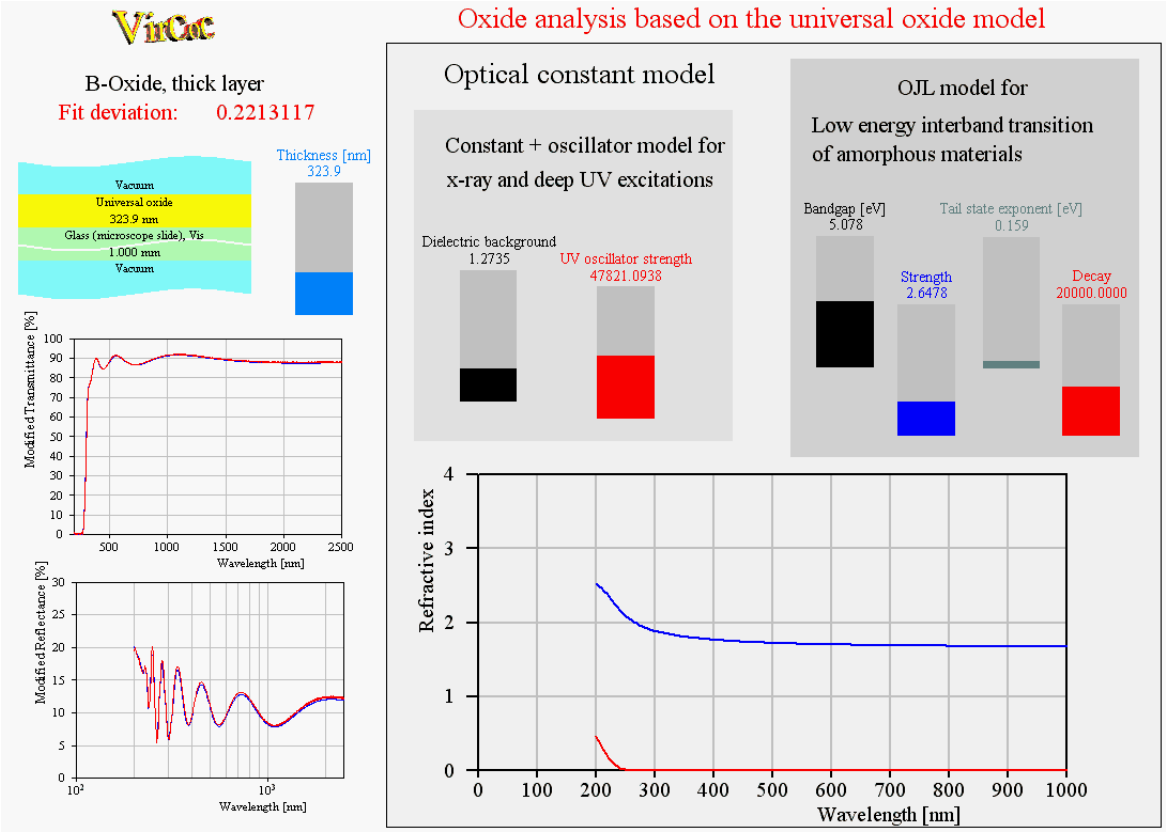
To inspect the remaining problems of the model in the UV reflectance we switch to a logarithmic scaling of the wavelength axis for reflectance:



In order to improve the fit in this range the OJL model has to be applied. Increasing its strength (while decreasing the dielectric background and the oscillator strength) and adjusting manually the bandgap a rather good approach is found:

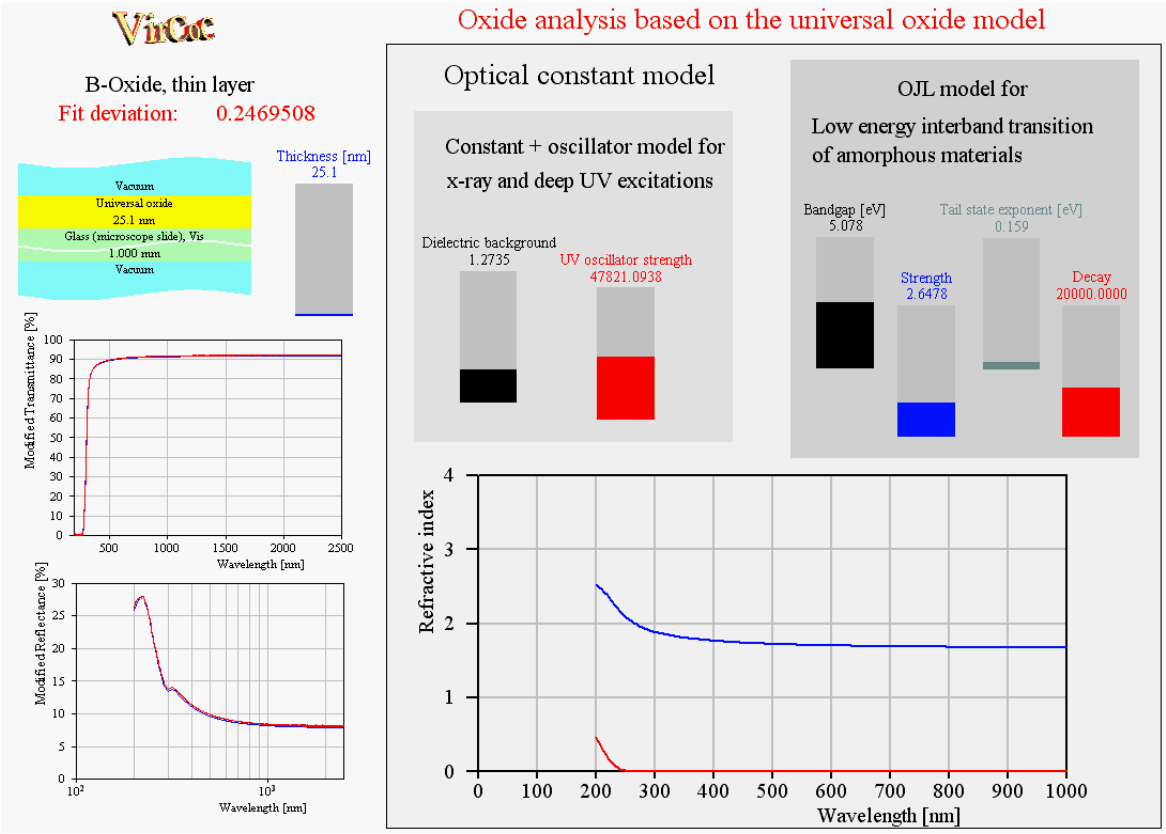


The model is now ready for an automatic parameter fit. We select the layer thickness, the dielectric background, the UV oscillator strength and the strength, the bandgap and the tail state exponent of the OJL model as fit parameters. Important: The tail state exponent must not be smaller than 0.01 (otherwise you risc a nasty crash of CODE) - so we set a lower and an upper limit for the tail state exponent in the list of fit parameters.
In addition, it turns out to be useful to increase the number of data points (use the global **Range** command in the main window) from 200 to 500 in order describe the sharp interference structures in the reflectance between 200 and 300 nm. The final fit looks rather good:



This configuration is saved in the database folder 'software configurations/code' using the filename B_oxide_fit_thick_layer.wcd.

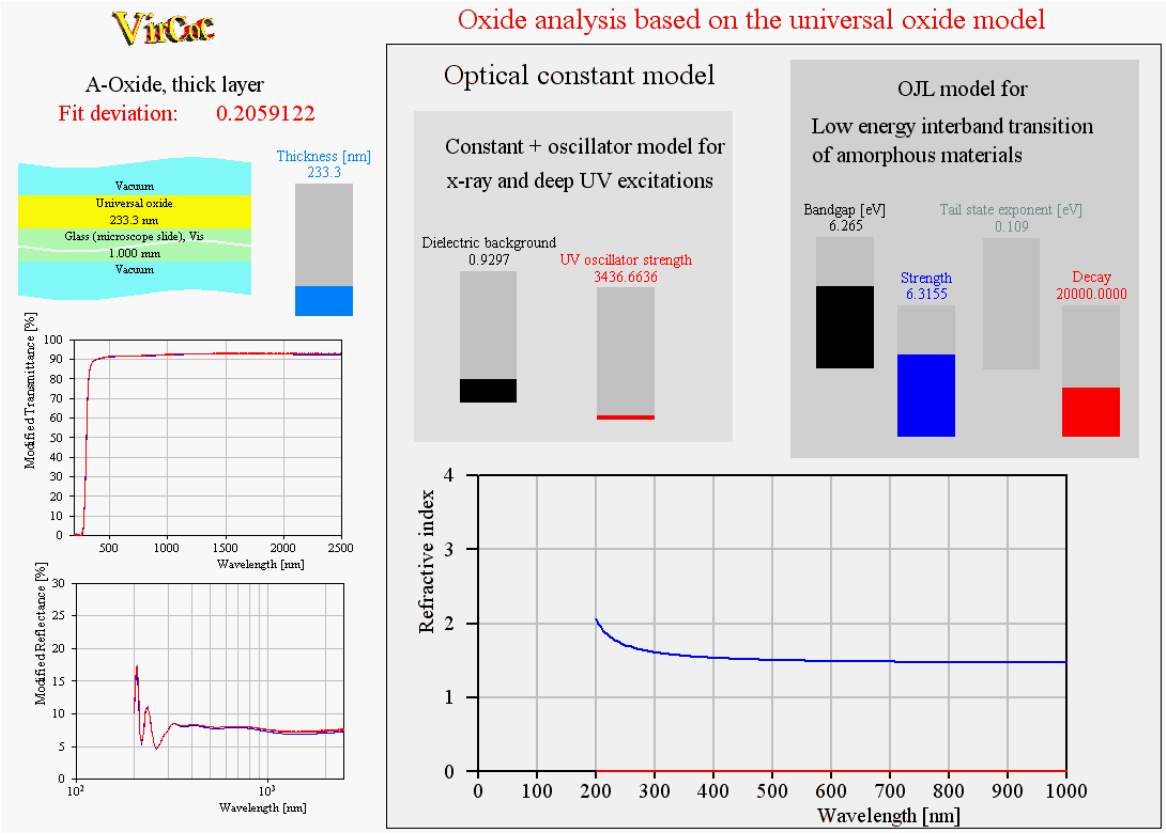
Before we save the optical constants for B-oxide to the database we check if the thin film sample can be described as well with the current model. Using the **Import** command in the main window we load the thin film spectra of B-oxide. After freezing all optical constant parameters in the fit we select the grid fit option for the layer thickness (see SCOUT technical manual, boundaries for the thickness: 0 ... 500 nm, grid with 100 points). Immediately CODE finds good agreement with a thickness of 25.1 nm:



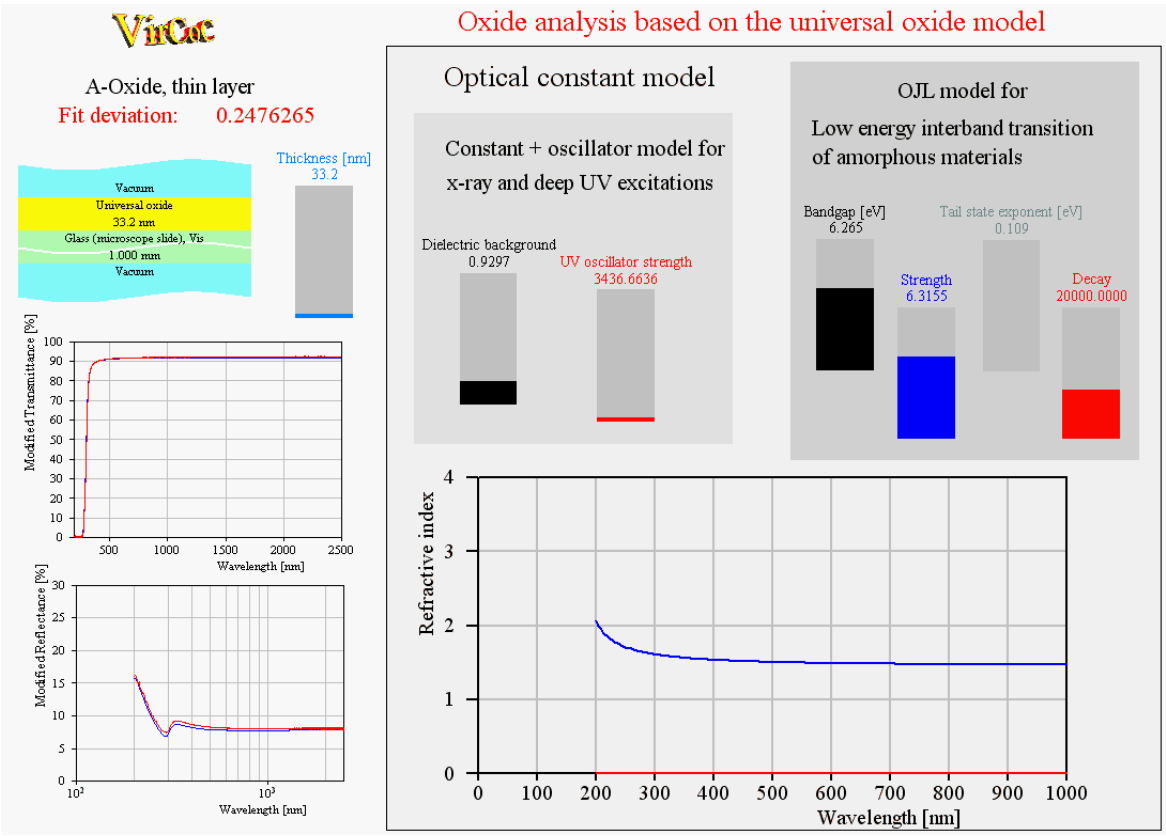
This is convincing! Both the thin and thick layer of B-oxide can be described with the same optical constant model. We save the model to the database with an appropriate comment. Let's hope that we can have similar success for the A- and C-oxides as well.

14/6/2004
After yesterday's success, today we hope to get good results for the other oxides as well.

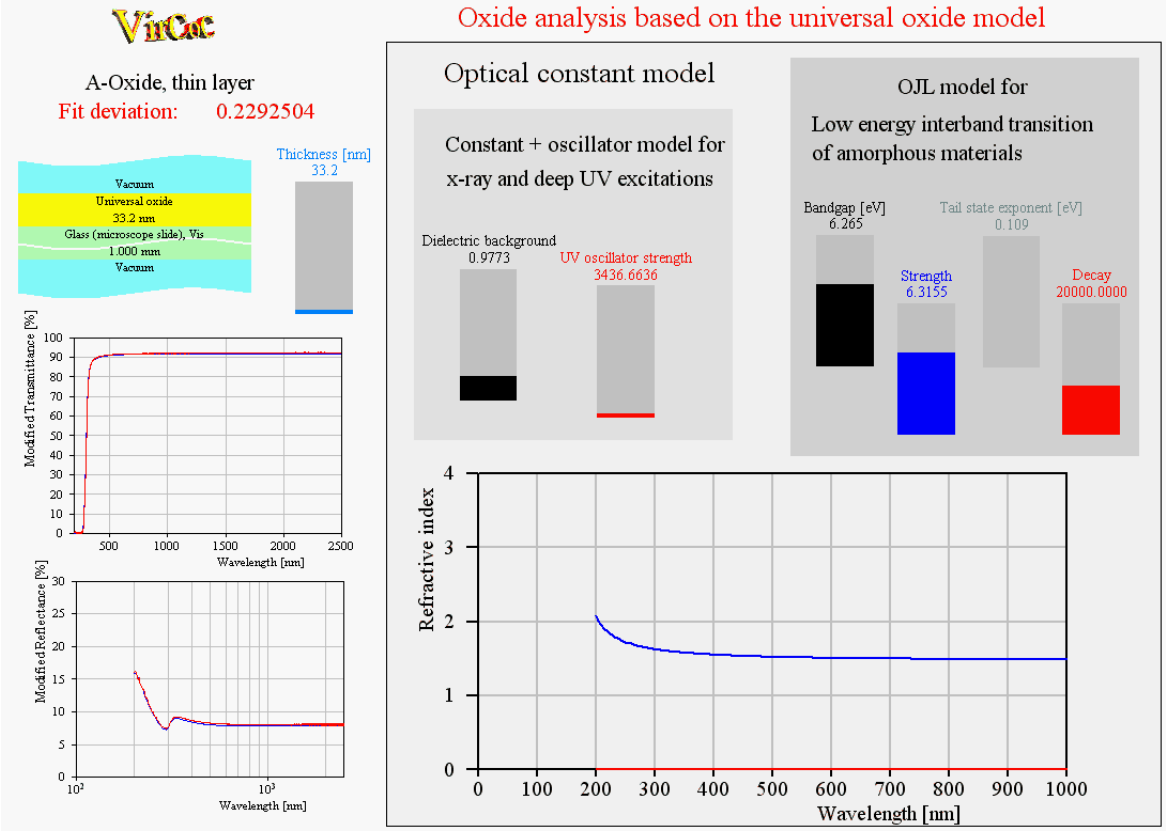
A-oxide
In the case of A-oxide, we already noticed that the spectra are similar to the substrate spectra. Therefore, very likely A-oxide has optical constants similar to those of glass. After some manual slider adjustments the fit goes well for the thick layer:



The corresponding thin film fit without further modifications of the optical constant model is satisfying but there is a small disagreement in the reflectance:



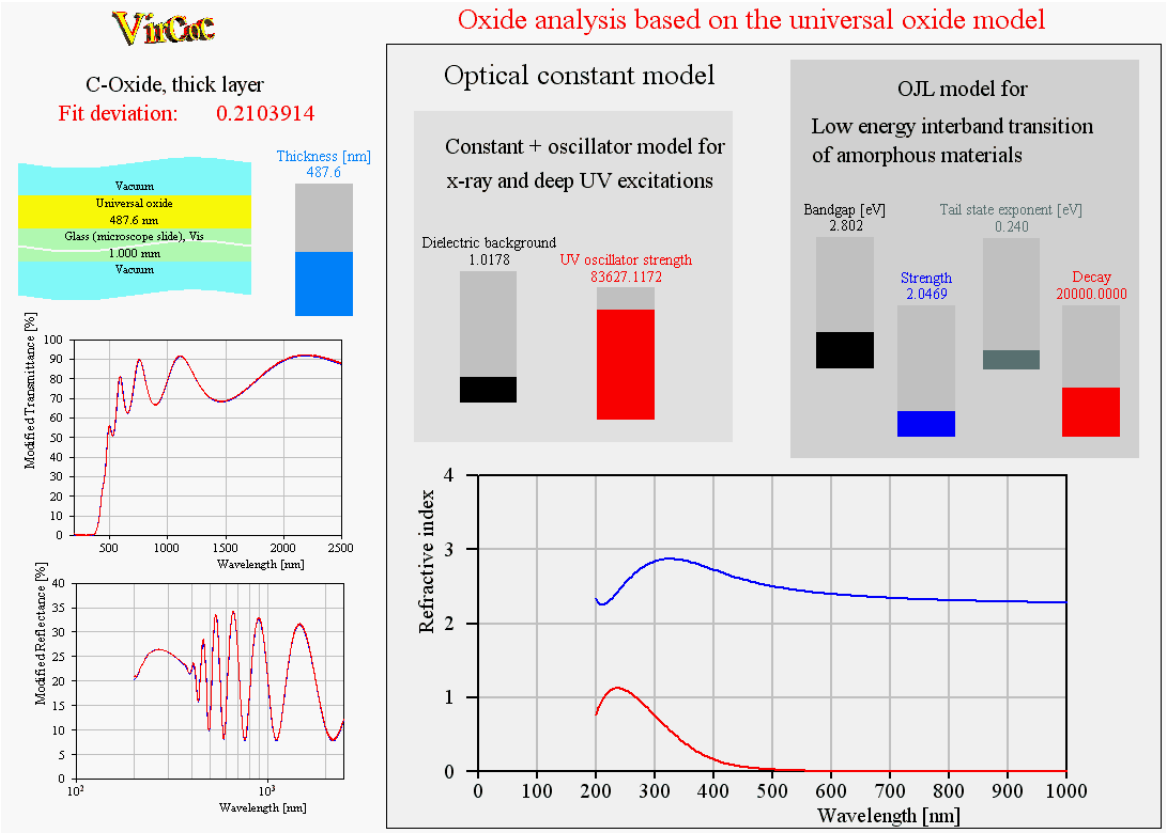
A slightly higher refractive index would improve the fit a little. The easiest way to achieve this is to 'unfreeze' the dielectric background and fit it together with the thickness. The result is the following:



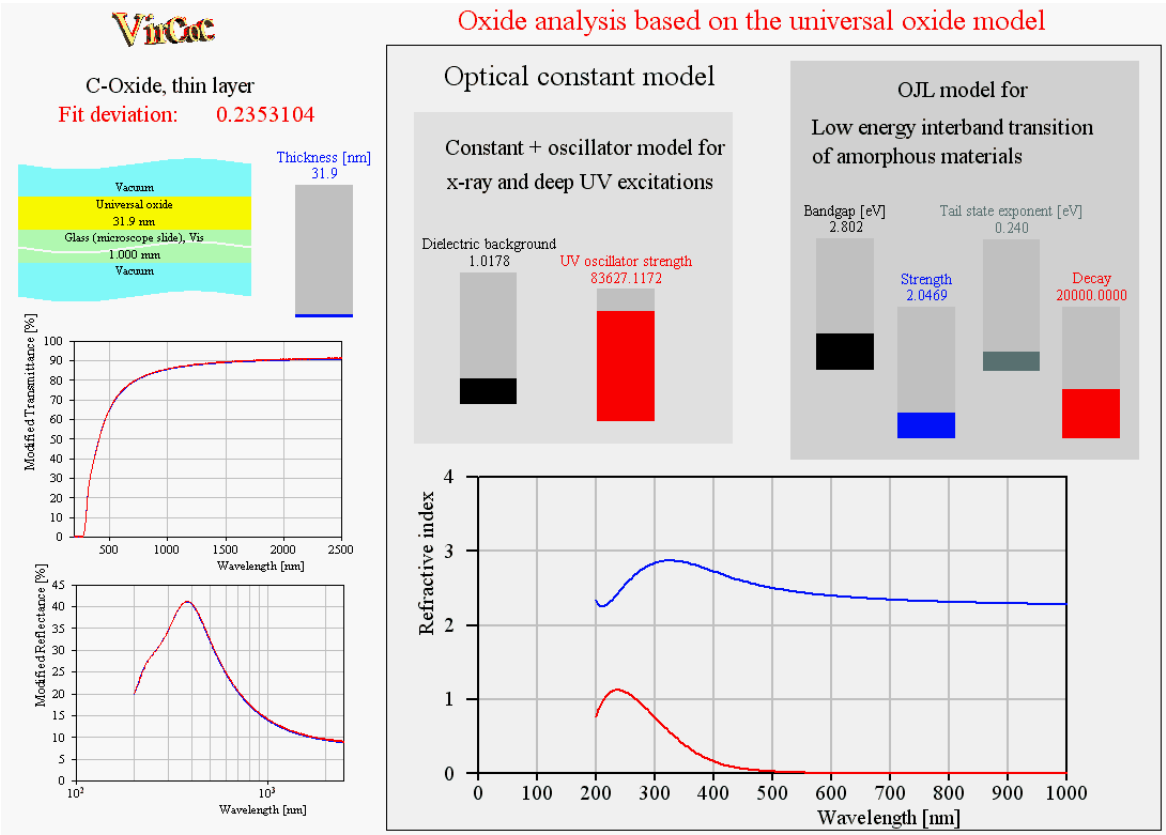
The slightly increased refractive index could mean that the thin layer is - on the average - a little more compact than the thick layer. In any case, we store both optical constant versions of A-oxide to the database.

C-oxide

The fit for the thick C-oxide layer is easy after some manual adjustments (reducing the bandgap, for example):



The agreement of the thin film spectra is satisfying. No further modification is required in this case:



2.6 June 2004: Part 5

23/6/2004

Low-e coatings: First designs with GenetiCode

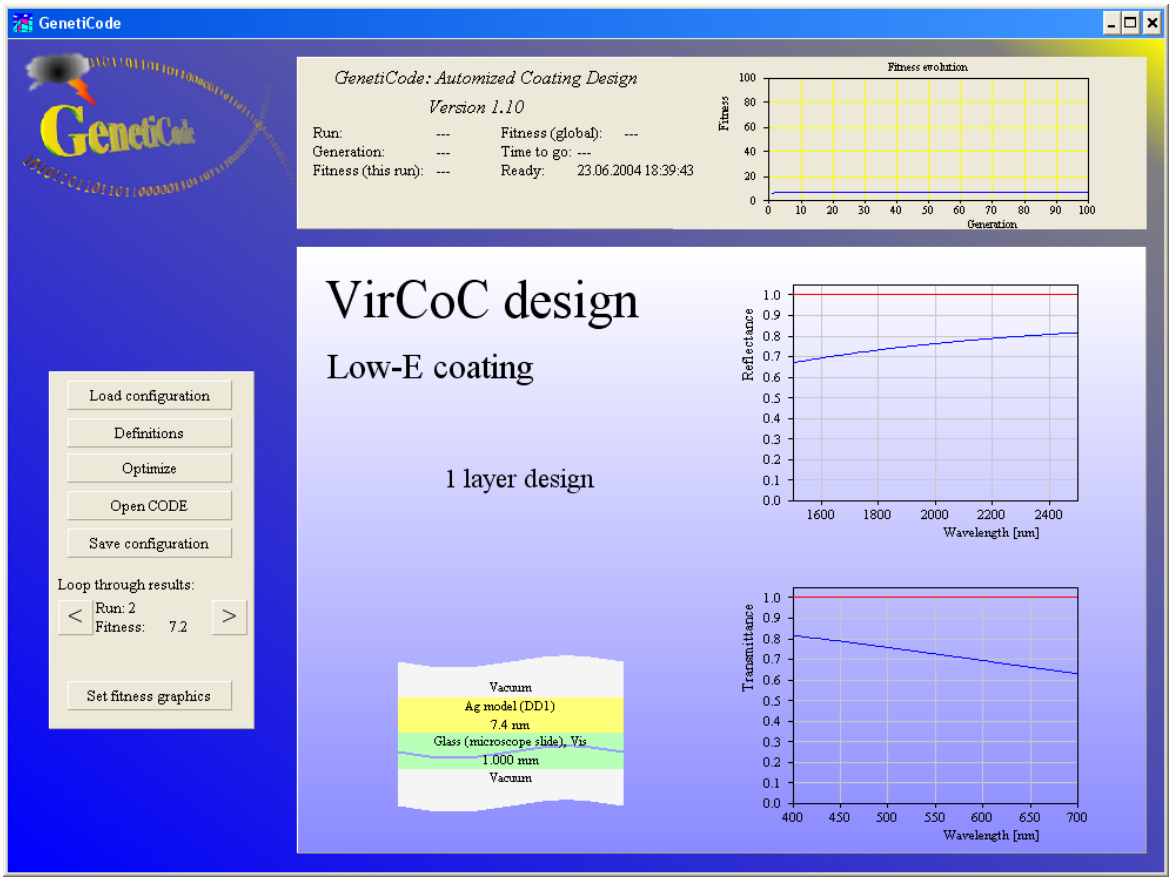
We can now produce layers of silver and 3 oxides. Although we plan to have a larger variety of materials, we are keen to try if we could produce reasonable thin film products with these materials already.
Soon we will get some large area coating equipment with targets like the ones used in our small DD1 device. We could then produce low-e and solar control coatings for architectural glass, for example. Although we know already how these kind of coatings are designed in principle, we will use a new approach of automatic coating design. Our favourite software developer *M.Theiss Hard- and Software* has just released a new design tool based on a genetic algorithm. The software is called ***GenetiCode*** and promises completely automatic thin film design. Since we do not have too much experience with coating design we will just try how it works and what we can get.

From M.Theiss Hard- and Software we received a starting configuration which computes a reflectance spectrum in the infrared (1500 ... 2500 nm wavelength) and a transmittance spectrum in the visible (400 ... 700 nm). In both spectral ranges the target spectrum is set to 1: CODE (which is working inside GenetiCode) will have a low fit deviation if both the IR reflectance of the coating and the transmittance in the visible are high. The coating is placed on top of a 1 mm microscope slide.
GenetiCode optimizes materials and thicknesses. You have to tell the program how many deposition steps you have in your equipment, and what materials are available in each deposition step. Every deposition step is assigned to a layer in a CODE layer stack. We start our design attempts with a single layer, and then we try to improve the design by adding layer by layer. For each layer we allow all our 4 materials to occur, i.e. it can be a silver layer or a layer of oxide A, B or C.

1-layer design
Using just one layer, we do not expect good results, but we start with this simplest choice to practise a little bit and to appreciate the more powerful multilayer solutions that are to follow. The possible materials in the only deposition step are the following:

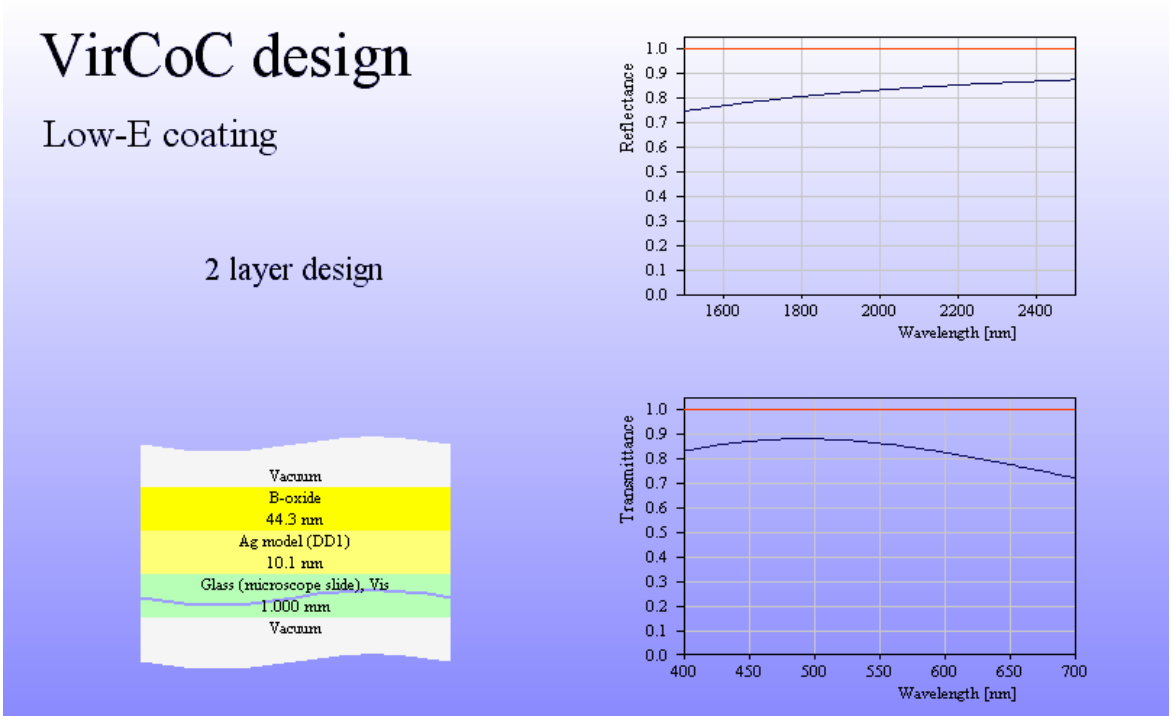
A-oxide (thickness range: 3 ... 100 nm)
B-oxide (thickness range: 3 ... 100 nm)
C-oxide (thickness range: 3 ... 50 nm)
Ag (thickness range: 3 ... 20 nm)

The genetic algorithm of GenetiCode requires that you let it run several times. In every run, a certain number of designs (i.e. choices of materials and thicknesses) is randomly generated. Then this population develops from generation to generation creating child designs with inherited properties (in most cases), but also new features created by mutation. Good designs have a higher chance to inherite to the next generation, and the quality of the best design increases in many cases from generation to generation. The evolution is followed for a pre-defined number of generations, and finally the best design is taken as the result of the method.
In this 1 layer case the result in all runs is the same, and it is achieved in a very short time. The program suggests to use a silver layer of 7.4 nm thickness:



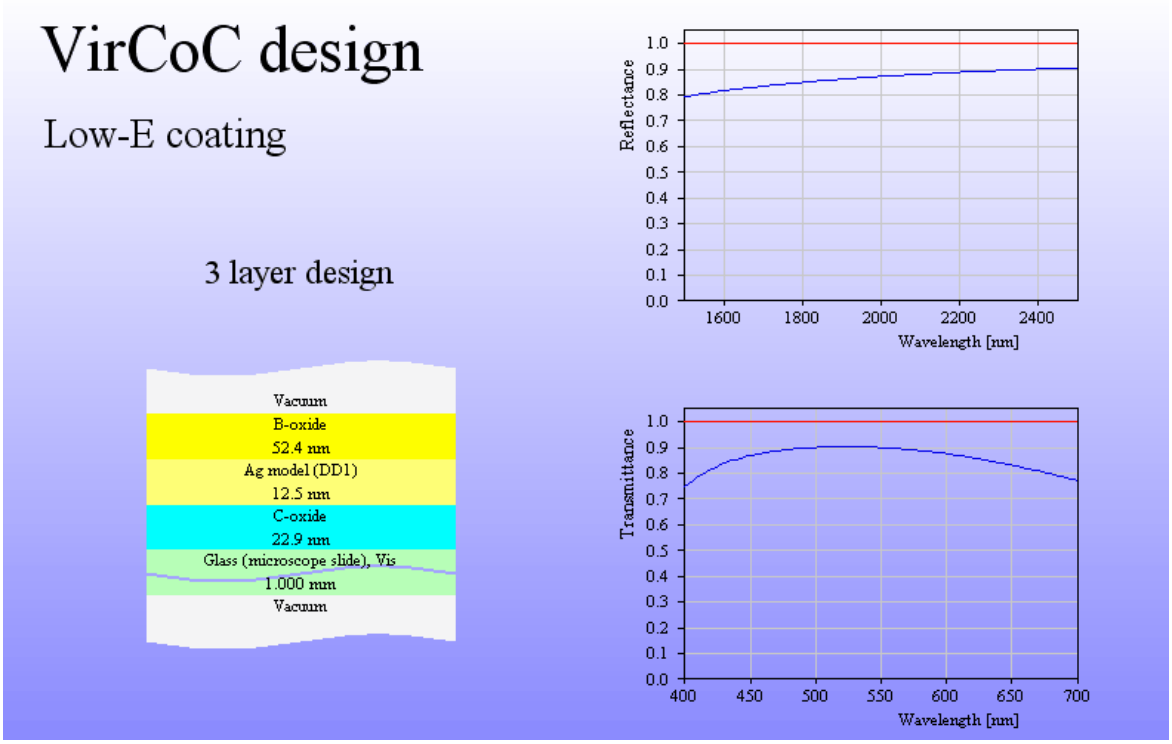
The quality of the design is expressed in the quantity **fitness** which is 1/(0.0001 + deviation) where deviation is the CODE fit deviation. If the fit deviation is 0 the fitness is 10000, if the deviation is large the fitness is close to 0.
This poor single layer design has a fitness of 7.2 which will be improved by adding more layers (i.e. do more deposition steps).

2-layer design
Let's invest in a second deposition step to improve the coating. Also here only a few generations are needed to get the final result which the program cannot improve any more:



As we hoped, the fitness is increased to 16.1: Clearly both the IR reflectance and the transmittance in the visible are higher compared to the first 'design' above.

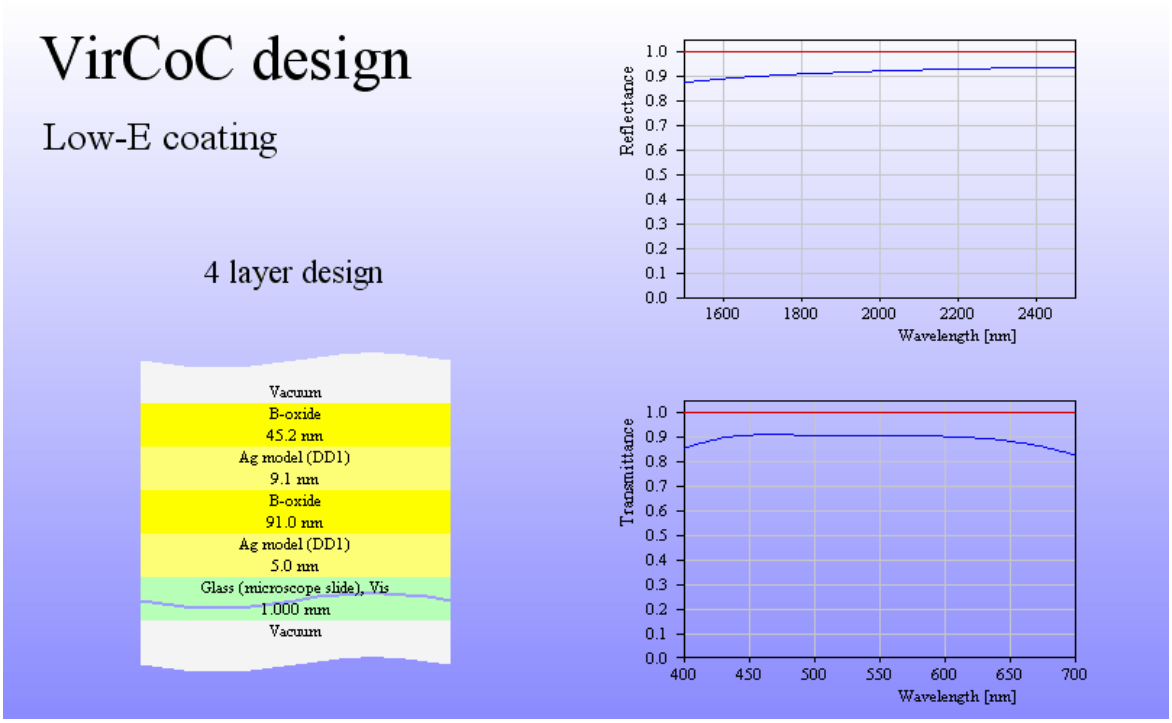
3-layer design
We continue and add another deposition step. This time the achieved fitness is 24.4, and GenetiCode has invented the 'standard' low-e layer stack oxide/metal/oxide:



Due to the oxide layers enclosing the silver a high transmittance in the visible is achieved. Compared to the 2-layer case the Ag thickness is significantly higher which results in a higher IR

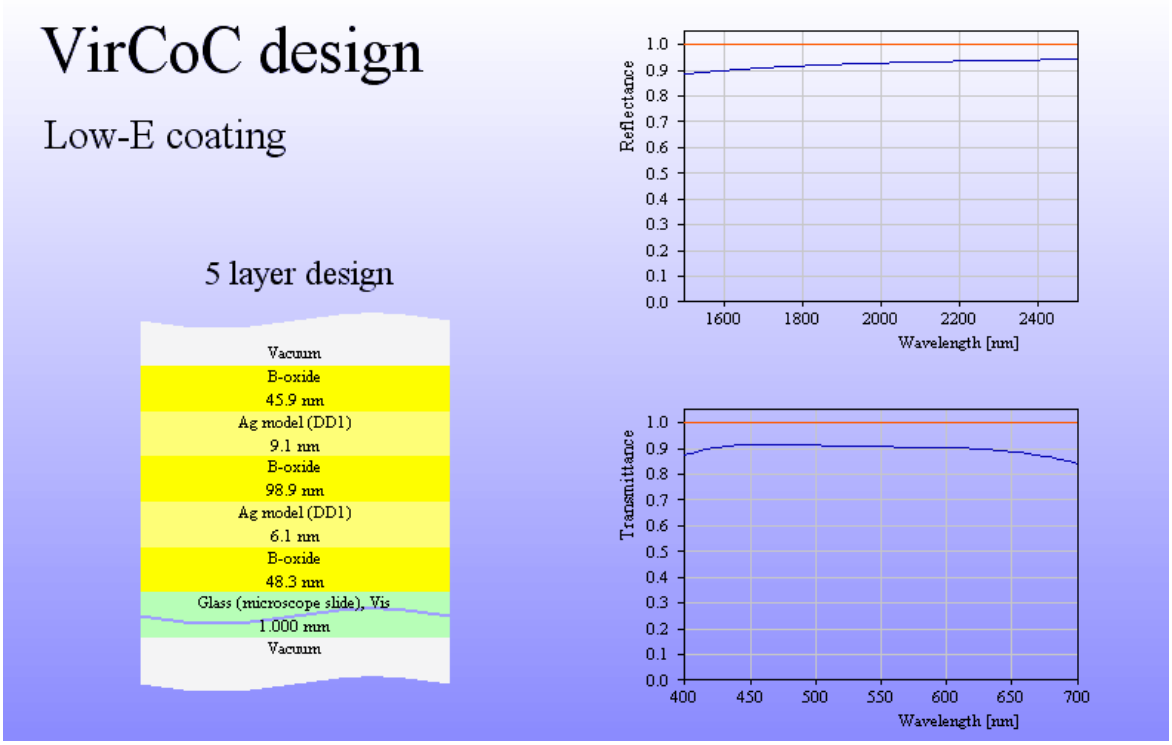
reflectance. Note that C-oxide (our oxide with the highest refractive index) was selected to be the oxide between substrate and silver layer.

4-layer design
Adding another layer gives GenetiCode the freedom to develop a new concept: The high IR reflectance is made by two Ag layers with an oxide spacer layer in between. The fitness is significantly increased to 52.3:



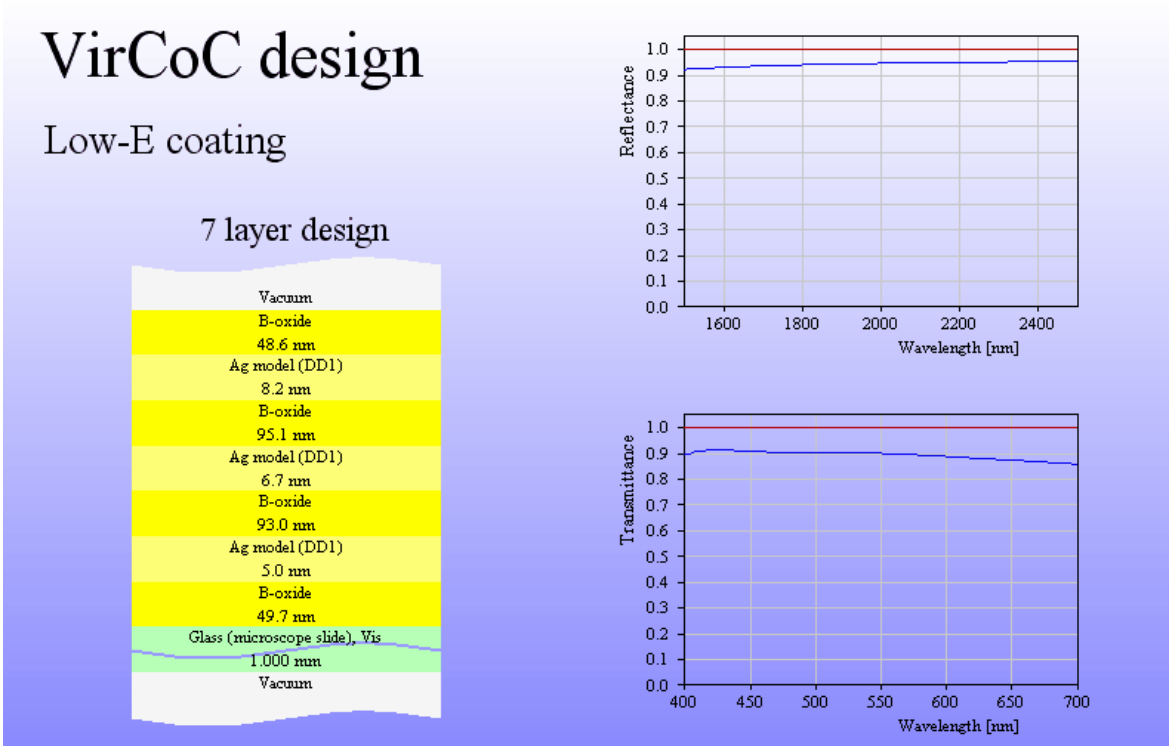
The total Ag thickness is now more than 14 nm, and the transmittance is above 0.8 in the whole visible spectral range. This kind of double silver layer is used in several commercial coating products at present, and we are happy and satisfied that the ***GenetiCode*** software can find such a solution so easily.

5-layer design
The silver double layer coating is re-fined a little more using a fifth layer. The largest fitness that we find with 5 layers is 60.1:



The total silver thickness is again increased (to 15.2 nm) without any loss of transmittance. The best layer stack is not found in all ***GenetiCode*** runs - with a finite number of runs there is no guarantee that the program finds the best solution.

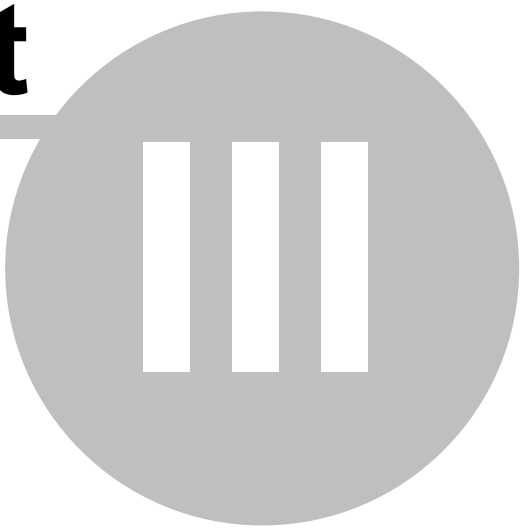
7-layer design
Finally we try a 7-layer stack - just to see if ***GenetiCode*** gets another good idea. The best solution with a fitness of 67.0 is obtained by further splitting of the silver layer, now into three layers:



Note the very high IR reflectance which is due to the 19.9 nm silver in the coating!

After these design exercises we are convinced that ***GenetiCode*** will be a useful tool for our work. The future will show if we can really produce some of the developed coatings. As far as we know we will have to protect the silver layers in the stack by additional thin films which will change the design conditions a little.

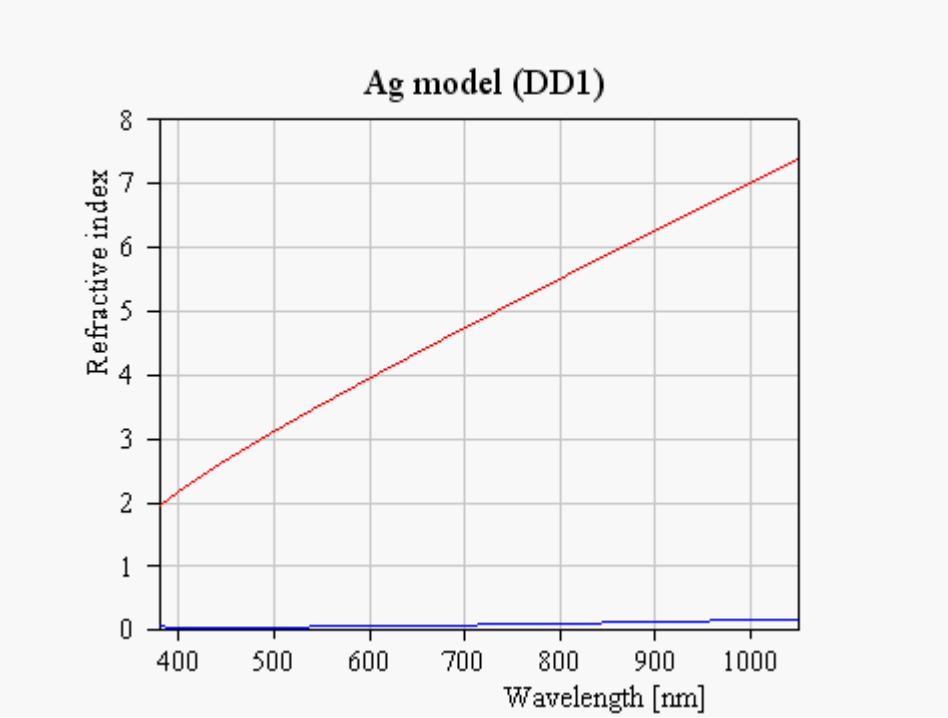
Part



3 Materials

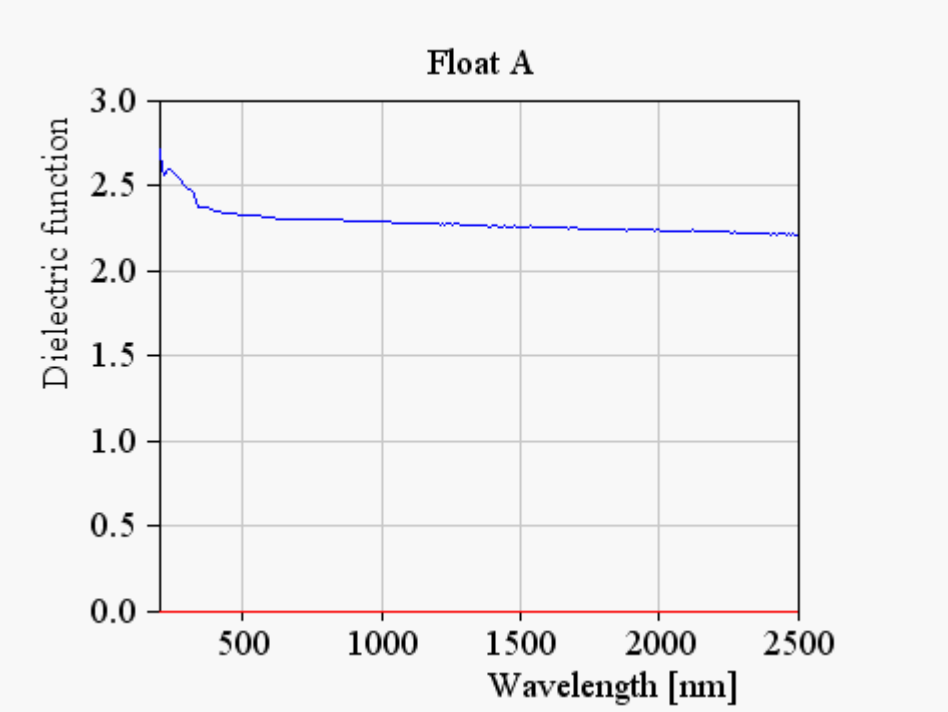
3.1 Ag model (DD1)

These optical constants have been determined analyzing a series of samples prepared by DD1. Optical reflectance and transmittance spectra were collected with S2. The data analysis is described above. The damping constant of the electrons in this type of silver is 430 1/cm. The complex refractive index of this model is the following:

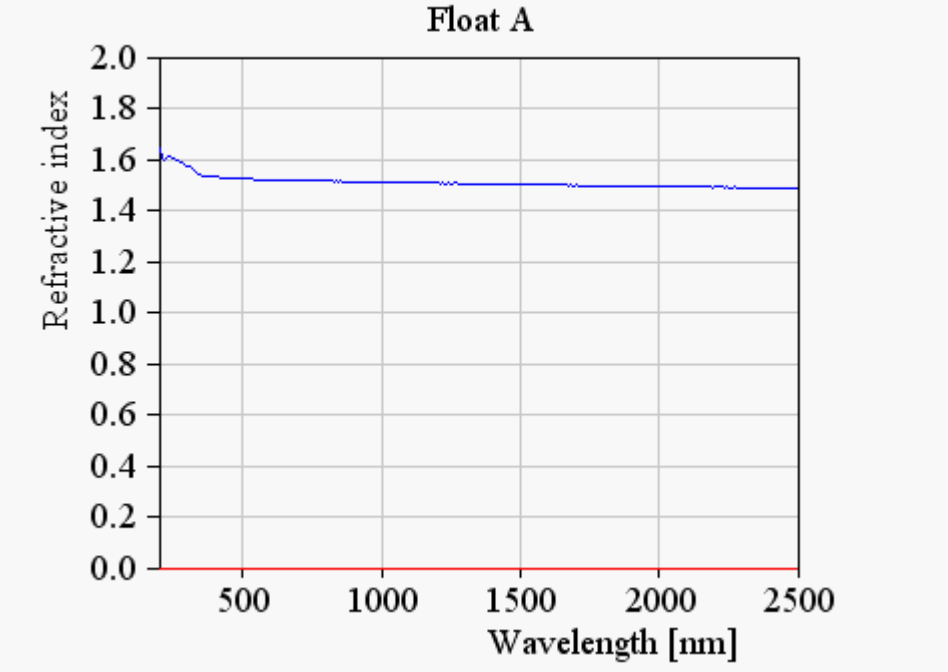


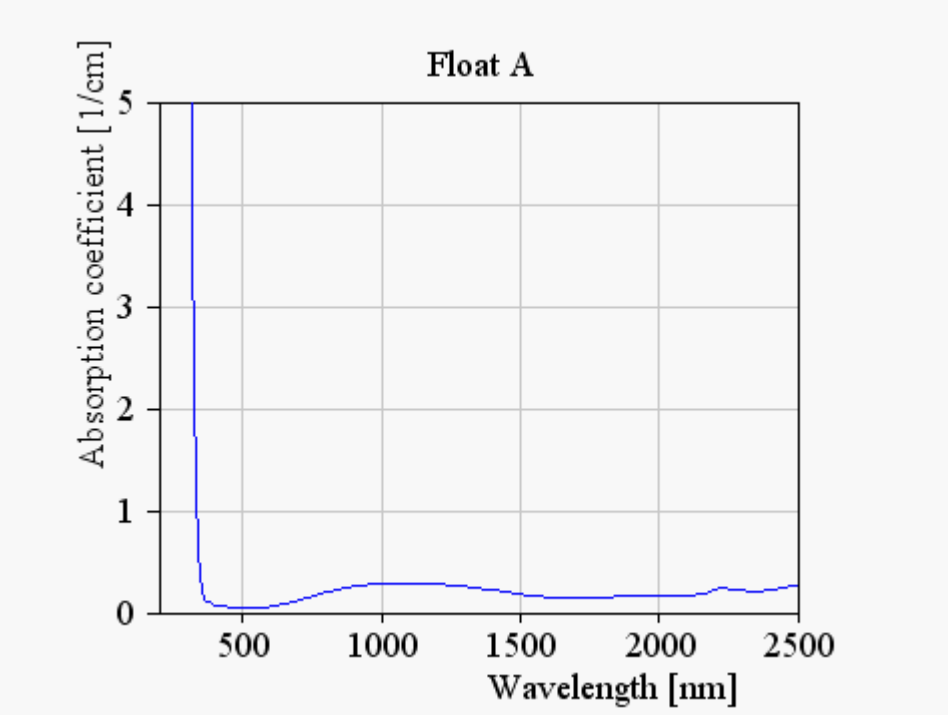
3.2 Float A

An important substrate material is 'Float A'. The optical constants of 'Float A' have been determined from R and T measurements using spectrometer S1. The DirectDF tool has been used. The dielectric function is this:



The following graphs show the refractive index and the absorption coefficients of this material:





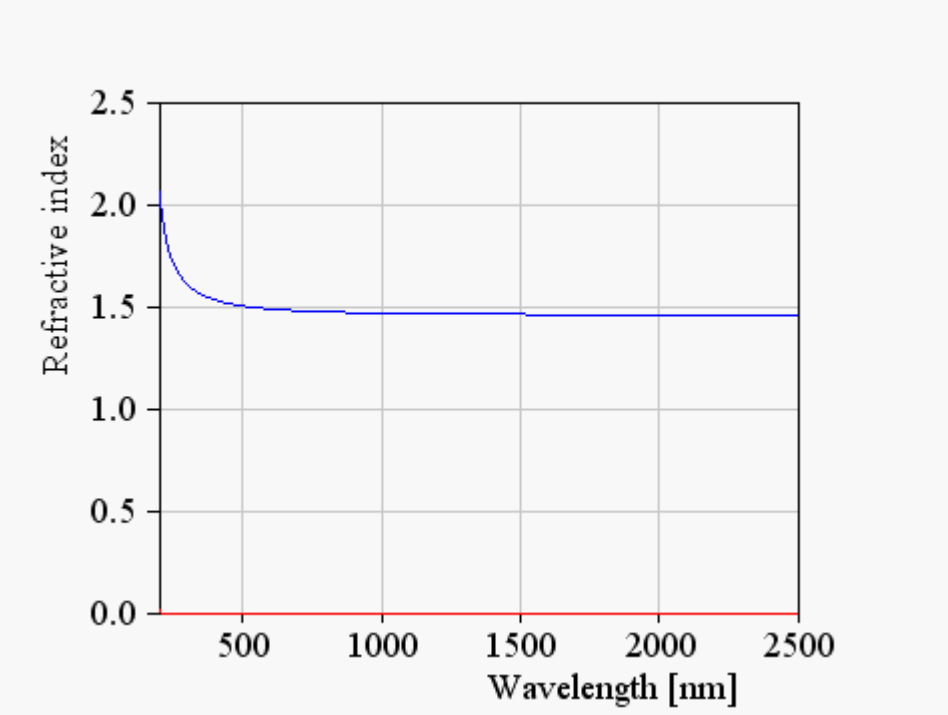
3.3 A-oxide

For A-oxide we have two versions of optical constants: A set obtained from a universal oxide fit of R and T spectra of a thick layer, and another set for a thin film.

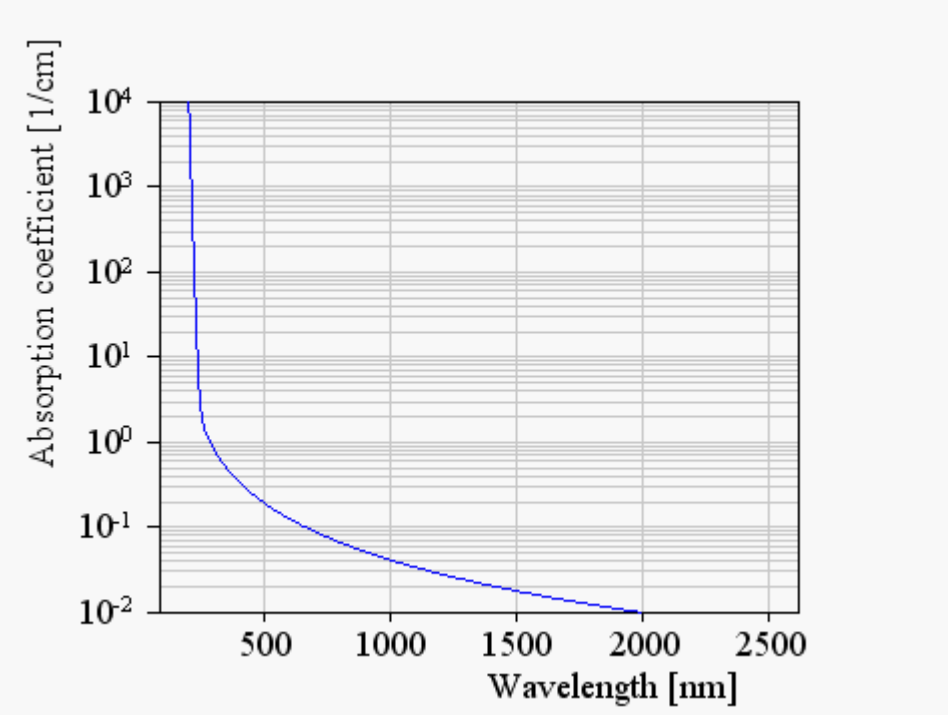
Thick layer (233 nm):
Spectra: DD1_A-Oxide_MS_thick_S1_r.spc and DD1_A-Oxide_MS_thick_S1_t.spc

Bandgap (OJL model):	6.265 eV
Tail state exponent (OJL model) :	0.109 eV
Dielectric background:	0.930

Refractive index:



Absorption coefficient:



Thin layer (33 nm):
Spectra: DD1_A-Oxide_MS_thin_S1_r.spc and DD1_A-Oxide_MS_thin_S1_t.spc

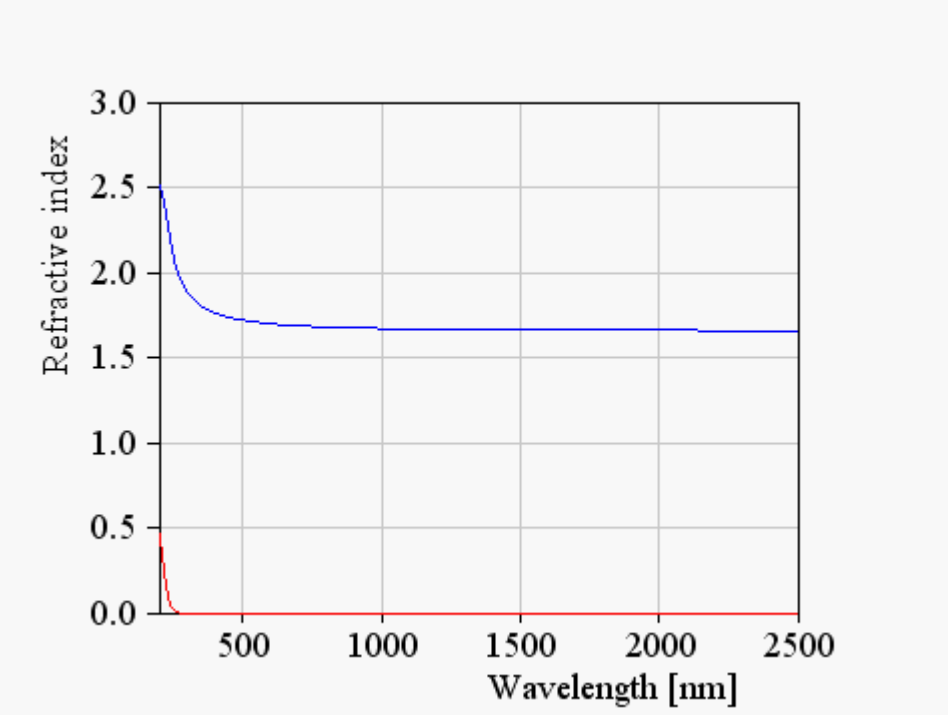
Dielectric background: 0.977
All other parameters like above (thick layer)

3.4 B-oxide

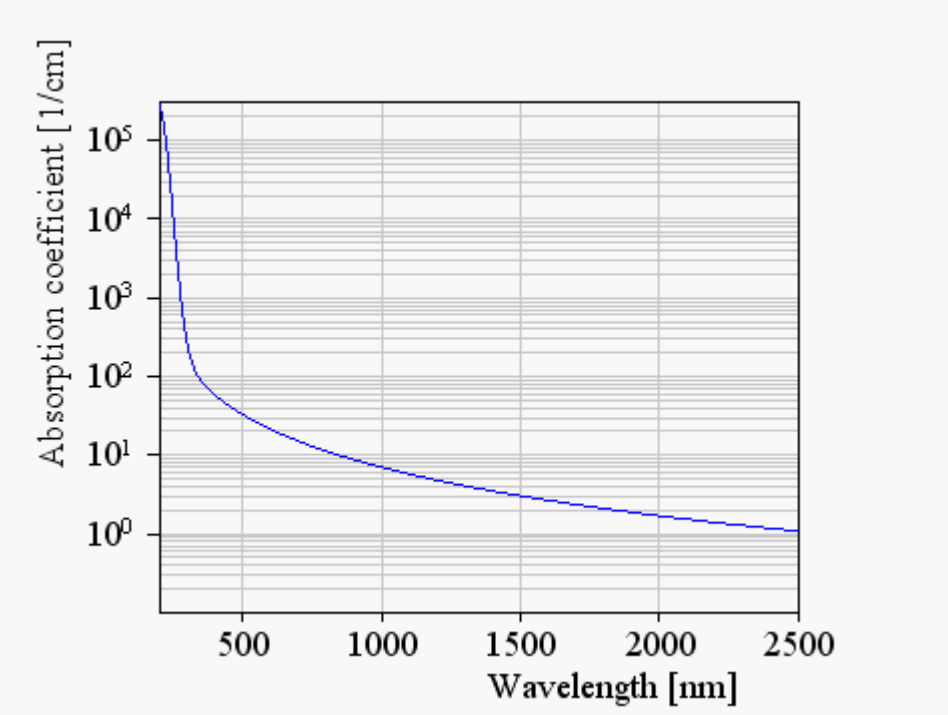
Result of our first OJL model fit.
Spectra: DD1_B-Oxide_MS_thick_S1_r.spc and DD1_B-Oxide_MS_thick_S1_t.spc

Bandgap (OJL model): 5.078 eV
Tail state exponent (OJL model) : 0.159 eV

Refractive index:



Absorption coefficient:

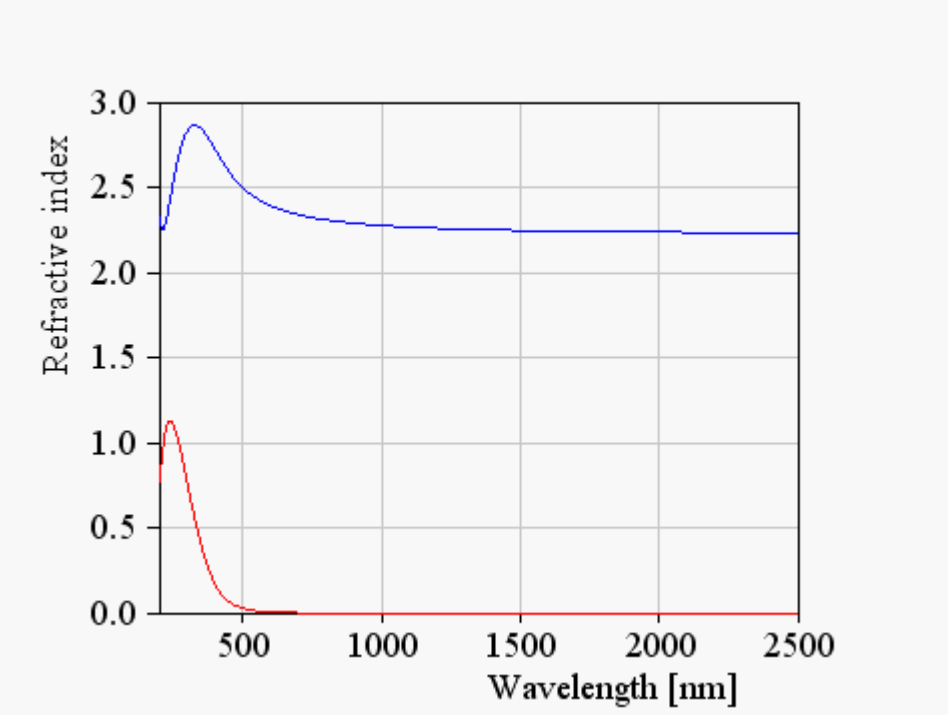


3.5 C-Oxide

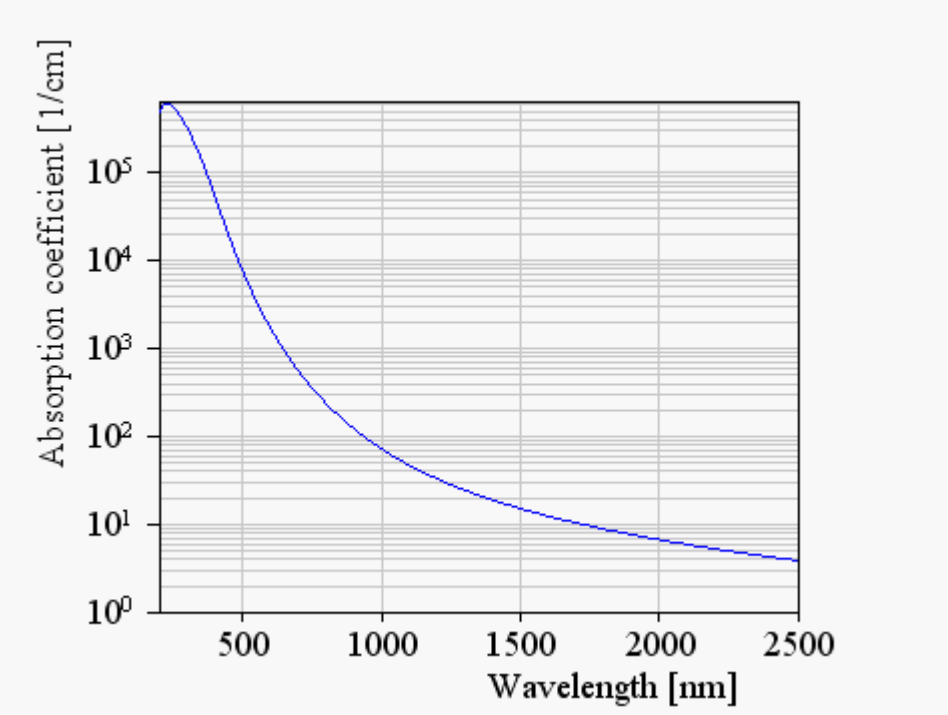
Result of a universal oxide fit.
Spectra: DD1_C-Oxide_MS_thick_S1_r.spc and DD1_C-Oxide_MS_thick_S1_t.spc

Bandgap (OJL model): 2.802 eV
Tail state exponent (OJL model) : 0.240 eV

Refractive index:



Absorption coefficient:



Part IV

4 Substrates

4.1 Float glass

The following types of float glass are available as substrates for thin film deposition:

Float A
This float type comes in thicknesses of 4, 5, 6, 8 and 10 mm.
The following substrate definitions of 'Float A' are in the database:

Float A (4 mm).ls
Float A (5 mm).ls
Float A (6 mm).ls
Float A (8 mm).ls
Float A (10 mm).ls

The bitmap files with the corresponding logos are all the same:

4.2 Microscope slide

For some of our lab experiments we use microsope slide substrates. The optical constants of the glass are taken from the original CODE database without modification.

Part V

5 Deposition devices

5.1 DD1, a small sputtering device

DD1 is a small sputtering device that can deposit thin films on small substrates such as microscope slides. Looking at the geometry of the machine, we do not expect the films to be very homogeneous. But we can do a lot of rather cheap deposition experiments with the following materials:

Metals
- Au
- Ag
- Cr

Oxides
- A-oxide
- B-oxide
- C-oxide

Nitrides
- Si3N4

DD1 has a rotating wheel with 20 positions for microscope slides. Each sample can be placed over various sputtering targets. A system of programmable shutters enables us to vary the deposition time for each target and each individual sample.

Part

6 Spectrometer hardware

6.1 Overview

The spectrometer hardware is the following:

- Grating spectrometer (200 ... 2500 nm)
- Array spectrometer system (380 ... 1050 nm)

6.2 S1, grating spectrometer (200 ... 2500 nm)

This instrument records reflectance or transmittance spectra in the spectral range 200 ... 2500 nm. It is an accurate, but slow scanning instrument with a rotating grid. The acquisition of a spectrum takes a few minutes. In order to switch from reflectance measurements to transmittance measurements, one has to exchange the sample holder which takes a few minutes as well.
The acquired spectra can be saved in several formats: A simple text format with two columns for the wavelengths and the corresponding reflectance or transmittance value (default file extension *.xy), or the binary SpectraCalc fomat with the default extension *.spc. The spectral values are stored in %, i.e. the reflectance or transmittance values are between 0 and 100.

6.3 S2, array spectrometer system (380 ... 1050 nm)

This spectrometer system records simultaneously reflectance and transmittance spectra of the same sample spot. It uses a halogen light source and two array spectrometers which record spectra in the spectral range 380 ... 1050 nm. Typical Acquisition times are 1 s or less. Light source and spectrometers are connected to the probeheads by fiber optics.
The size of the illuminated sample spot can be varied from 1 mm to 1 cm. The angle of incidence is about 5 degrees.

A scanning table (10 cm by 60 cm) can be moved along its long dimension, and automatical measurements of R and T at pre-defined positions are performed. The software driving the spectrometer and the scanning table can transfer the measured spectra to CODE for analysis and pick up the results. Alternatively, all spectra can be saved and be processed offline in a CODE batch operation.

The acquired spectra are saved in several a simple text format with two columns for the wavelengths and the corresponding reflectance or transmittance value (default file extension *.xy). The spectral values are absolute reflectance or transmittance values (range: 0.0 to 1.0).

Part VII

7 Software

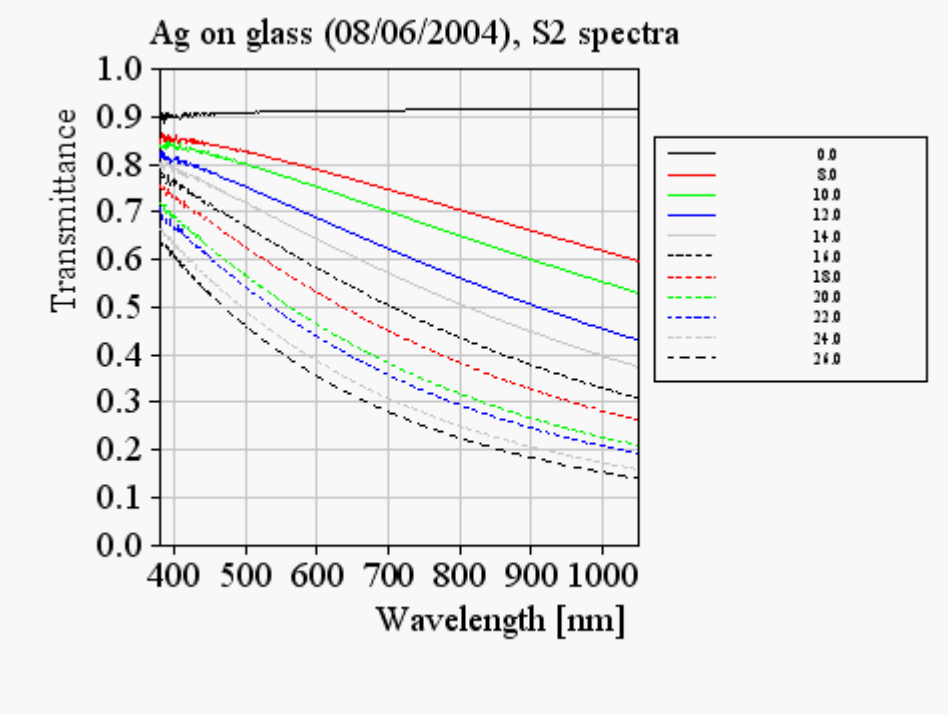
7.1 CODE

Coating Designer software, developed by M.Theiss Hard- and Software (www.mtheiss.com)

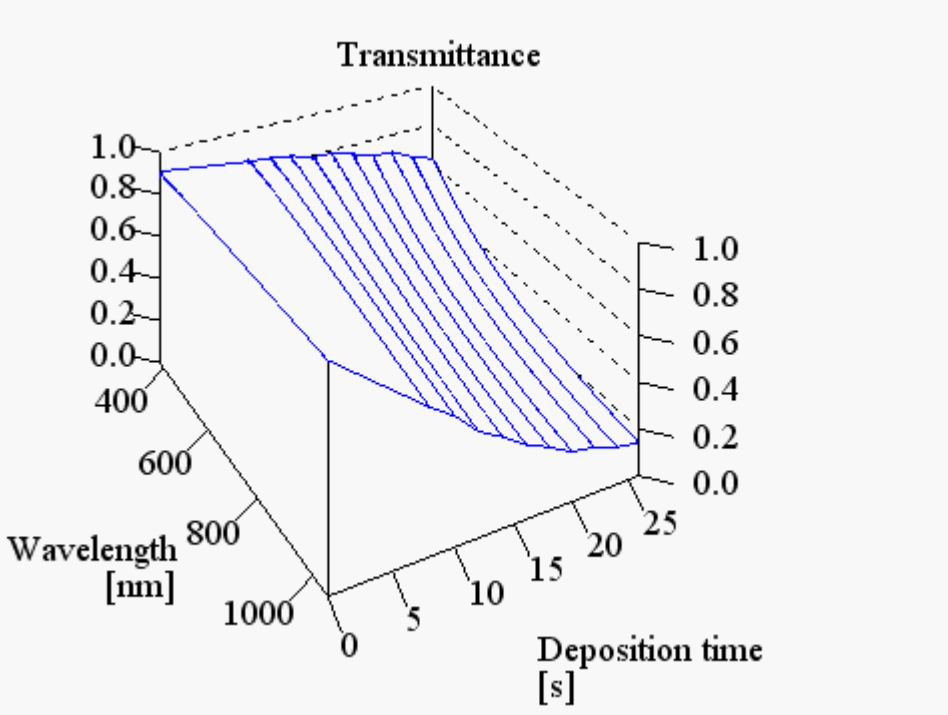
This program is used to analyze optical spectra of thin film stacks and to design the optical (and thermal) properties of coatings. A description is given in www.mtheiss.com/wcd.htm.

7.2 Collect

Use this tool to display many spectra in one graph. Here is an example:

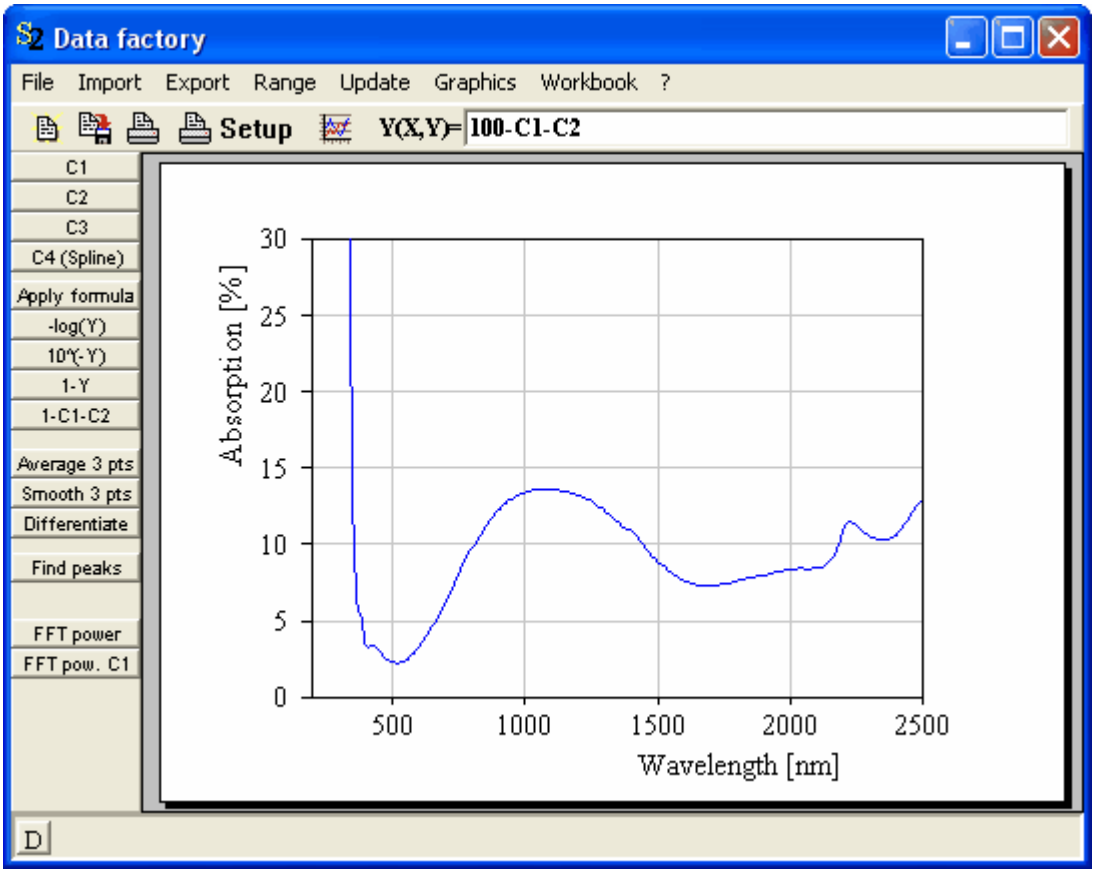


You can also display 3D graphs if the spectra are sorted by a parameter:



7.3 Data Factory

This tool is used for simple spectrum manipulations. It is delivered with all major software packages made by M.Theiss Hard- and Software.
The following screen shot shows how an absorption spectrum is computed from a measured transmittance spectrum (contained in subwindow C1) and the measured reflectance (contained in subwindow C2):



Here is a link to the online version of the Data Factory manual.

7.4 DirectDF

This tool (delivered with CODE) is used to determine the optical constants of thick substrates. You must know the thickness, and both the reflectance R and the transmittance T must be different from zero. No interference fringes must be contained in R and T.

Here is a link to the online version of the DirectDF manual.

7.5 GenetiCode

GenetiCode assists the design of optical coatings with automized material selection and thickness optimization.
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!

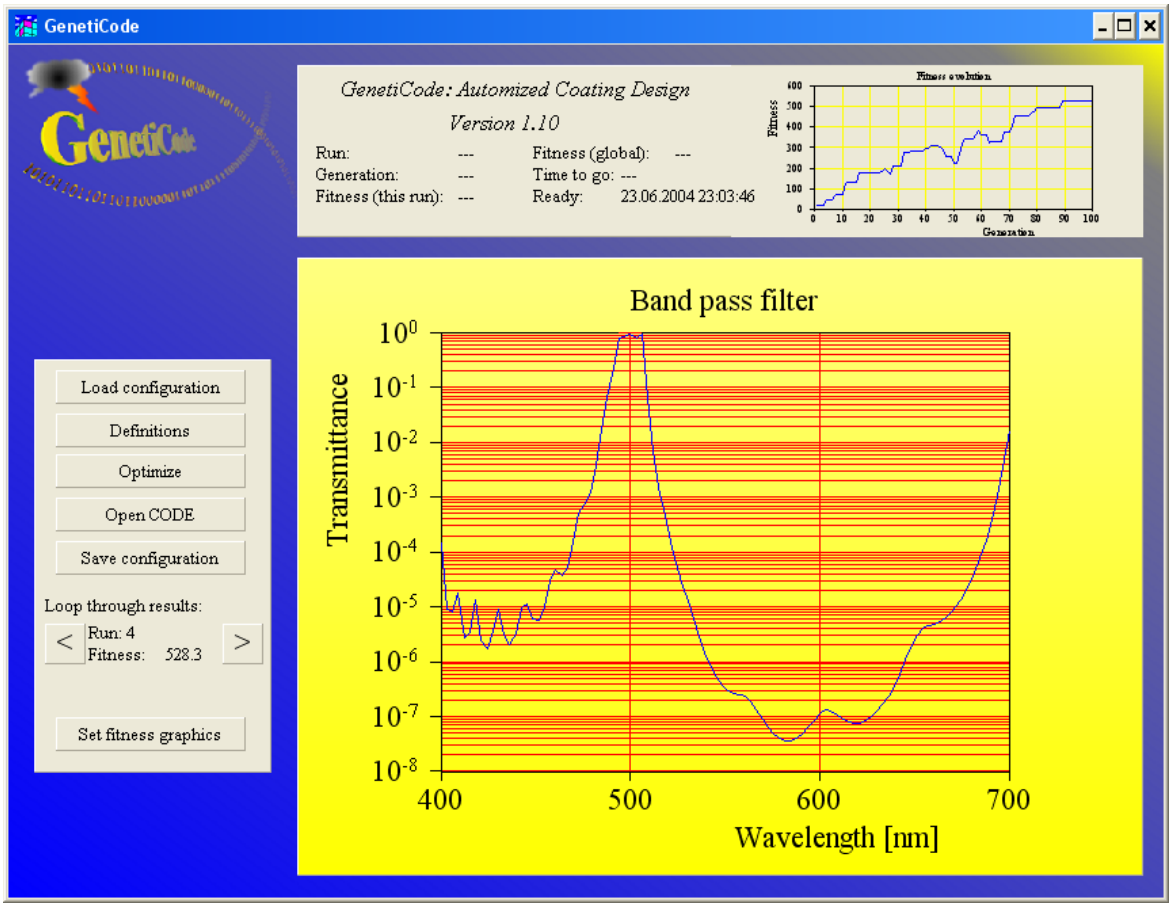
Optimization: Start, relax and let GenetiCode invent

Finally you set a few parameters to control the optimization (which is a genetic algorithm) 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.

Here is a ***GenetiCode*** screenshot (optical band pass design):



Part VIII

8 The VirCoC database

8.1 Overview

The ***VirCoC*** database contains all documentation, measured spectra and optical models mentioned in this text.

The database structure is the following:

- Materials: This folder is used by CODE to store optical constants
- Coatings: This folder is used by CODE to store layer stack definitions
- Substrates: This folder is used by CODE to store layer stack definitions of typical substrates
- Spectra: This subfolder is used to store measured spectra.
- Software configurations: Collection of useful program configurations
- Plot parameters: Here some useful plot parameter sets are stored.

8.2 Materials

Ag model (DD1)	Ag as deposited by sputtering device DD1
Float A	Float glass, based on ***VirCoC*** R and T measurements
Glass (microscope slide), Vis	This item has been copied from the CODE database
B-oxide	B-oxide deposited by DD1, thick (320 nm) and thin (25 nm) film
A-oxide	A-oxide deposited by DD1, thin (33 nm) film
A-oxide (thick layer)	A-oxide deposited by DD1, thick (233 nm) layer
Universal oxide	This item has been copied from the CODE database

8.3 Substrates

Current substrates:

Float A (4 mm).ls	4 mm of 'Float A'
Float A (5 mm).ls	5 mm of 'Float A'
Float A (6 mm).ls	6 mm of 'Float A'
Float A (8 mm).ls	8 mm of 'Float A'
Float A (10 mm).ls	10 mm of 'Float A'
Microscope slide (1 mm).ls	1 mm microscope slide glass (CODE database)

8.4 Coatings

There are no coatings yet.

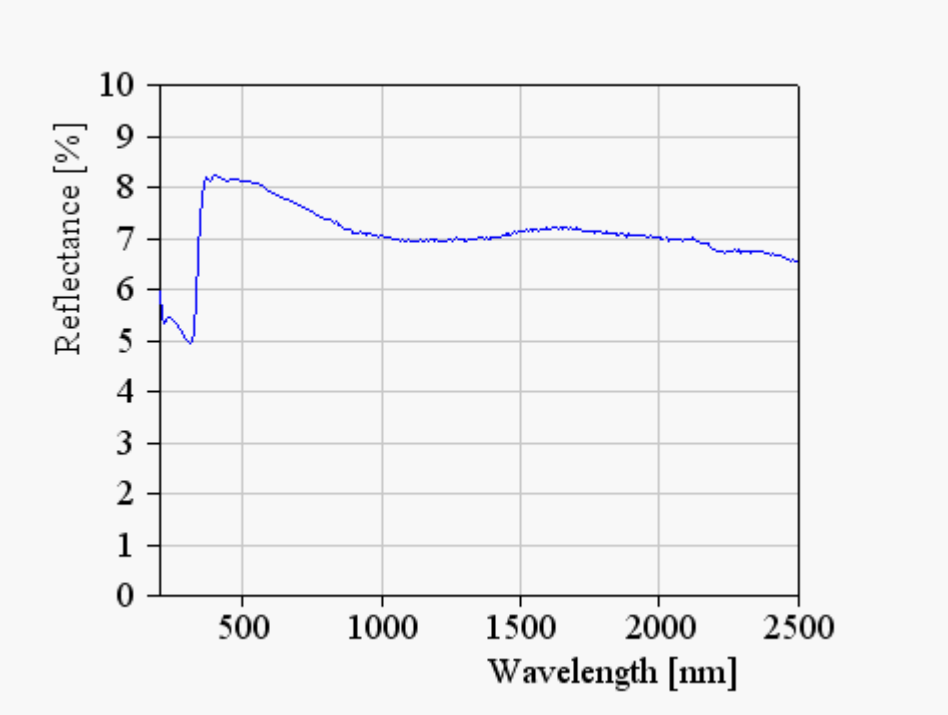
8.5 Spectra

8.5.1 Float glass

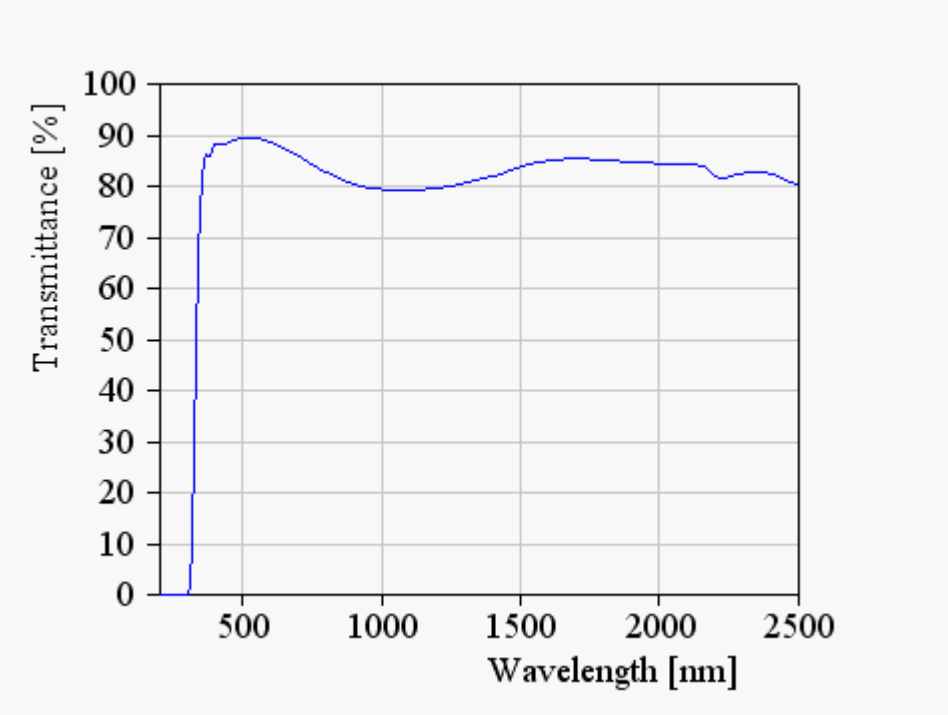
8.5.1.1 Float A

Available files:

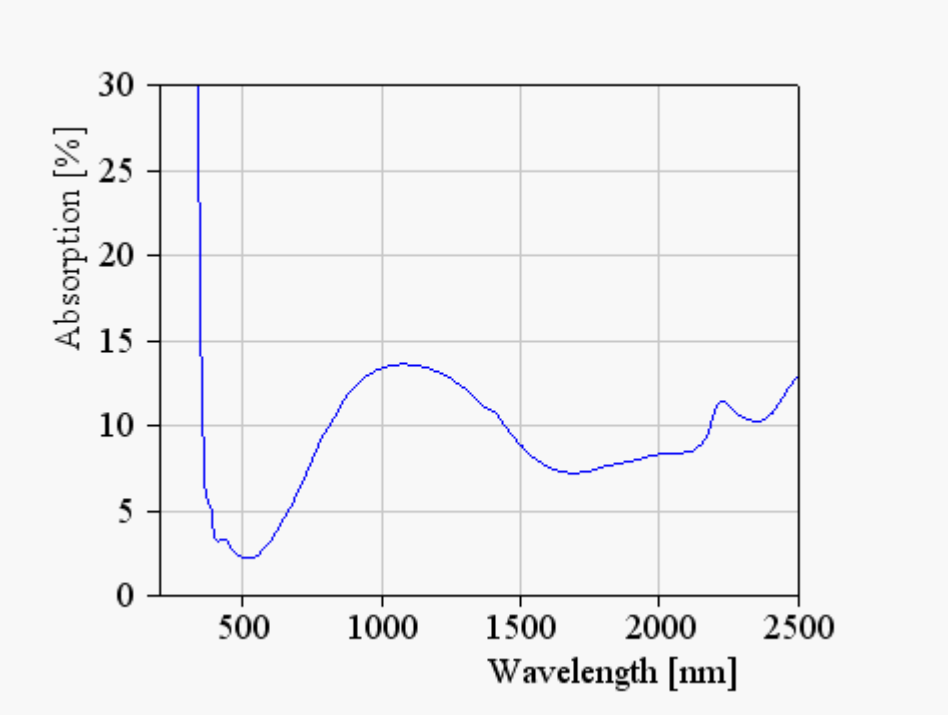
2/6/2004:
r_5mm_s1.spc: reflectance of a 5 mm thick sample measured by spectrometer S1



t_5mm_s1.spc: transmittance of a 5 mm thick sample measured by spectrometer S1



a_5mm_s1.spc: absorption spectrum computed as 100-R-T



8.5.2 Metal layers

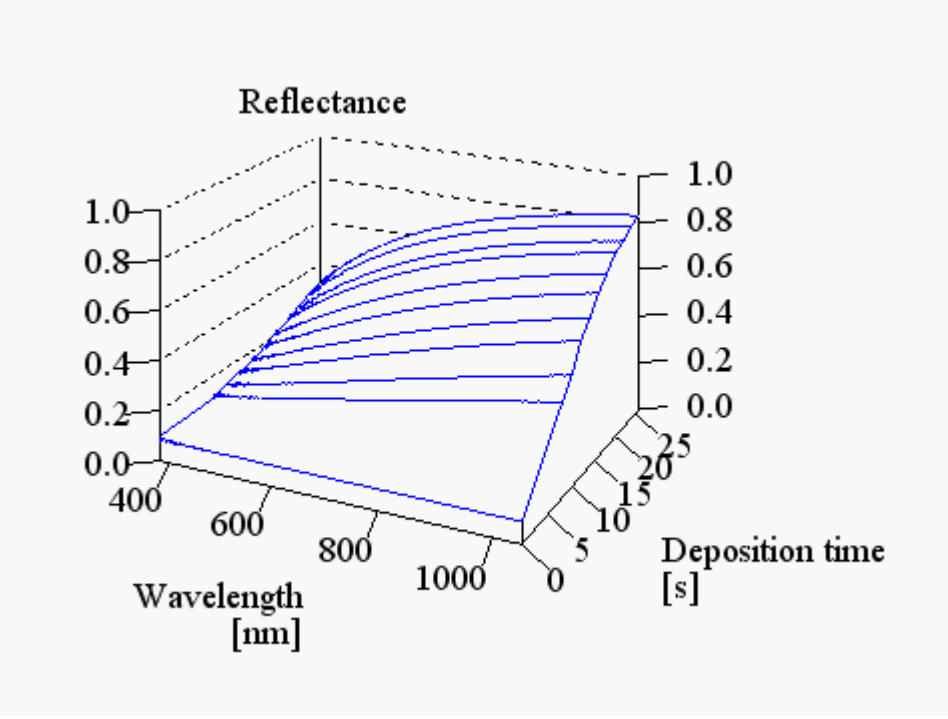
8.5.2.1 Ag on glass

Deposition experiment, 08/06/2004

Ag layers on glass, deposited by DD1, variation of deposition time

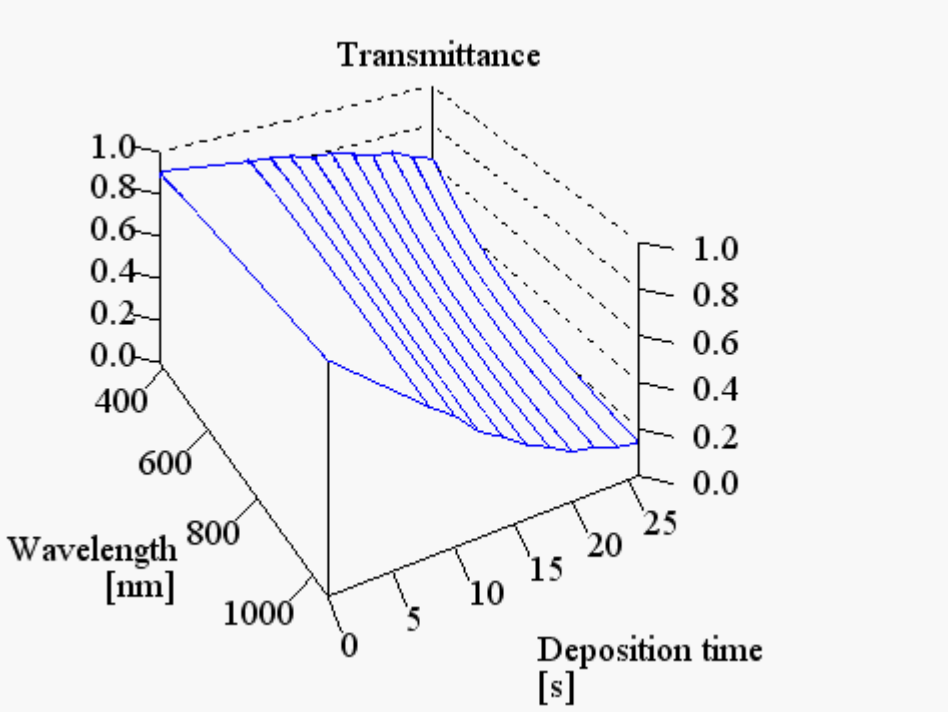
Sample	Ag sputtering time [s]
dd1_ag_ms_08_06_2004_0	0
dd1_ag_ms_08_06_2004_1	8
dd1_ag_ms_08_06_2004_2	10
dd1_ag_ms_08_06_2004_3	12
dd1_ag_ms_08_06_2004_4	14
dd1_ag_ms_08_06_2004_5	16
dd1_ag_ms_08_06_2004_6	18
dd1_ag_ms_08_06_2004_7	20
dd1_ag_ms_08_06_2004_8	22
dd1_ag_ms_08_06_2004_9	24
dd1_ag_ms_08_06_2004_10	26

Corresponding R spectra, recorded by S2:
dd1_ag_ms_08_06_2004_0_s2_r.xy
dd1_ag_ms_08_06_2004_1_s2_r.xy
dd1_ag_ms_08_06_2004_2_s2_r.xy
dd1_ag_ms_08_06_2004_3_s2_r.xy
dd1_ag_ms_08_06_2004_4_s2_r.xy
dd1_ag_ms_08_06_2004_5_s2_r.xy
dd1_ag_ms_08_06_2004_6_s2_r.xy
dd1_ag_ms_08_06_2004_7_s2_r.xy
dd1_ag_ms_08_06_2004_8_s2_r.xy
dd1_ag_ms_08_06_2004_9_s2_r.xy
dd1_ag_ms_08_06_2004_10_s2_r.xy



Corresponding T spectra, recorded by S2:

dd1_ag_ms_08_06_2004_0_s2_t.xy
dd1_ag_ms_08_06_2004_1_s2_t.xy
dd1_ag_ms_08_06_2004_2_s2_t.xy
dd1_ag_ms_08_06_2004_3_s2_t.xy
dd1_ag_ms_08_06_2004_4_s2_t.xy
dd1_ag_ms_08_06_2004_5_s2_t.xy
dd1_ag_ms_08_06_2004_6_s2_t.xy
dd1_ag_ms_08_06_2004_7_s2_t.xy
dd1_ag_ms_08_06_2004_8_s2_t.xy
dd1_ag_ms_08_06_2004_9_s2_t.xy
dd1_ag_ms_08_06_2004_10_s2_t.xy



8.5.3 Oxides

8.5.3.1 A-Oxide

Deposition experiment, 08/06/2004

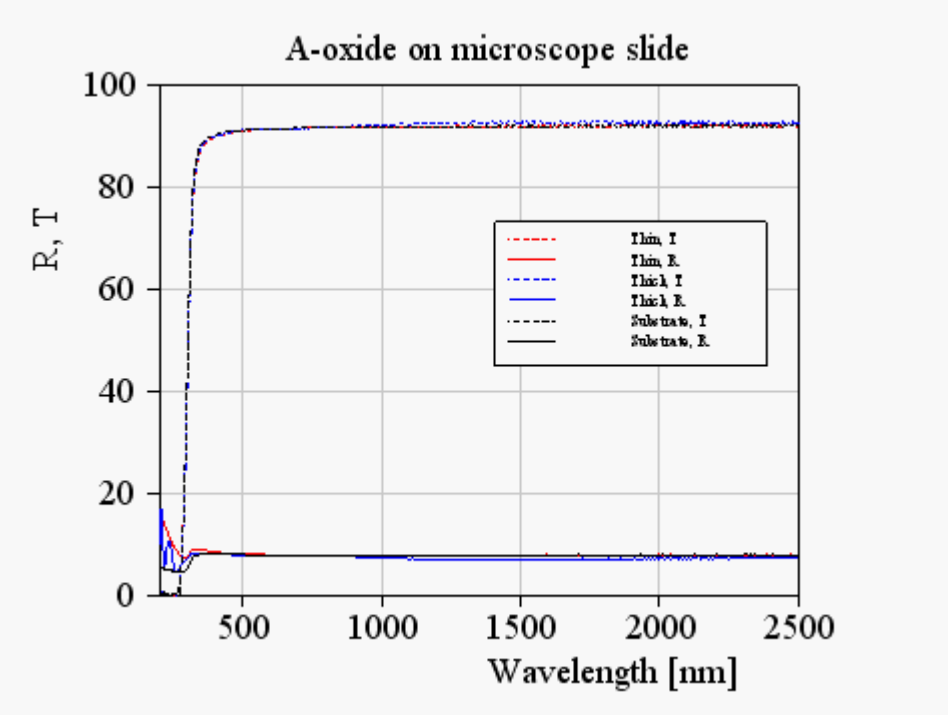
A-oxide layers on microscope slide, deposited by DD1

Substrate spectra:
DD1_A-Oxide_MS_substrate_S1_r.spc
DD1_A-Oxide_MS_substrate_S1_t.spc

A-oxide spectra:

Thin layer:
DD1_A-Oxide_MS_thin_S1_r.spc
DD1_A-Oxide_MS_thin_S1_t.spc

Thick layer:
DD1_A-Oxide_MS_thick_S1_r.spc
DD1_A-Oxide_MS_thick_S1_t.spc



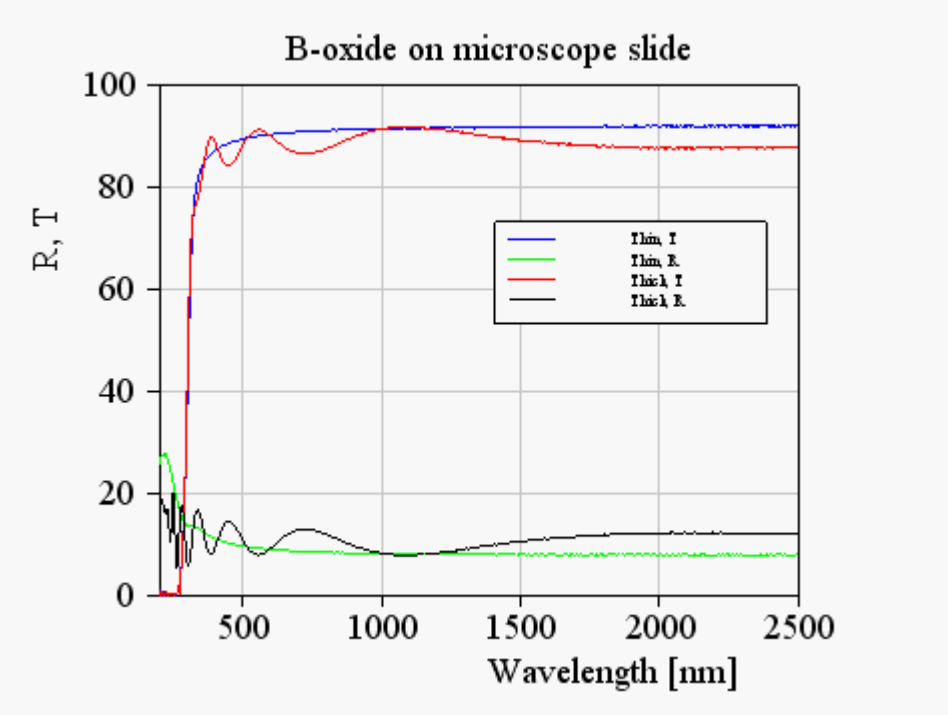
8.5.3.2 B-Oxide

Deposition experiment, 08/06/2004

B-oxide layers on microscope slide, deposited by DD1

Thin layer:
DD1_B-Oxide_MS_thin_S1_r.spc
DD1_B-Oxide_MS_thin_S1_t.spc

Thick layer:
DD1_B-Oxide_MS_thick_S1_r.spc
DD1_B-Oxide_MS_thick_S1_t.spc



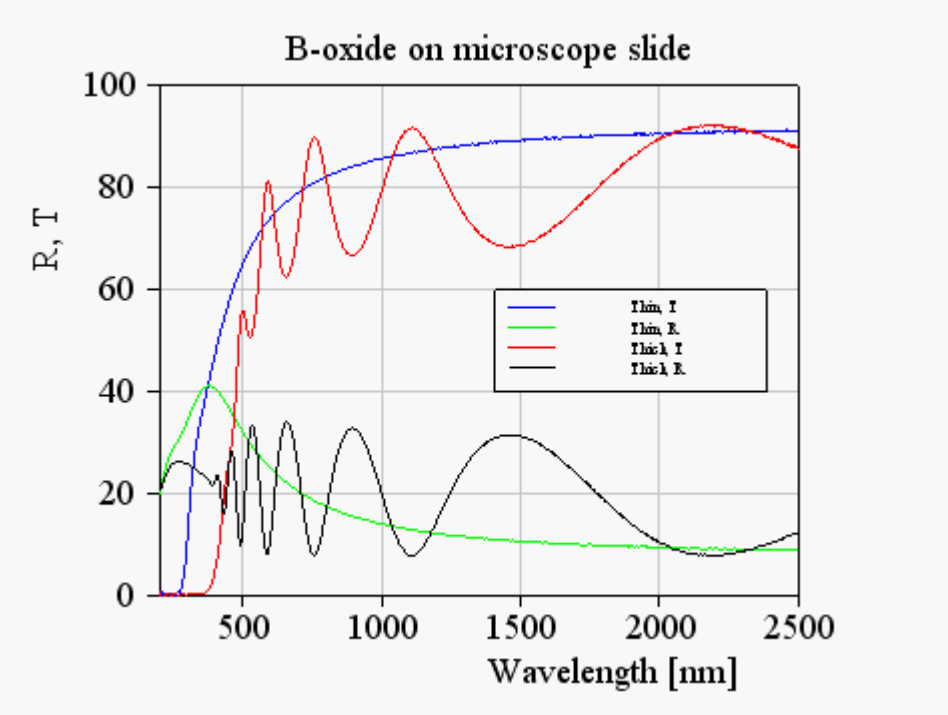
8.5.3.3 C-Oxide

Deposition experiment, 08/06/2004

C-oxide layers on microscope slide, deposited by DD1

Thin layer:
DD1_C-Oxide_MS_thin_S1_r.spc
DD1_C-Oxide_MS_thin_S1_t.spc

Thick layer:
DD1_C-Oxide_MS_thick_S1_r.spc
DD1_C-Oxide_MS_thick_S1_t.spc



8.6 Software configurations

8.6.1 CODE

Up to now the following configurations have been added to the database:

substrate test.wcd (Configuration to test optical constants of substrates in the database)

ag_on_glass_DD1_08_06_2004.wcd (Analysis of single Ag layers on microscope slide)
ag_on_glass_DD1_08_06_2004_batch.wcd (Batch analysis of single Ag layers on microscope slide)

universal_oxide_model.wcd (Starting configuration for the exploration of optical constant models for oxides)

A_oxide_fit_thick_layer.wcd (Fitting R and T of the thick A-oxide layer on microscope slide)
A_oxide_fit_thin_layer_variable_db.wcd (Fitting R and T of the thin A-oxide layer on microscope slide)
B_oxide_fit_thick_layer.wcd (Fitting R and T of the thick B-oxide layer on microscope slide)
C_oxide_fit_thick_layer.wcd (Fitting R and T of the thick C-oxide layer on microscope slide)

8.6.2 Collect

The following configurations are available up to now:

- ag_on_glass.col (R and T spectra of the dd1_ag_ms_08_06_2004_xx samples)
- ag_on_glass_r_only.col (R spectra of the dd1_ag_ms_08_06_2004_xx samples)
- ag_on_glass_t_only.col (T spectra of the dd1_ag_ms_08_06_2004_xx samples)

8.6.3 Data Factory

In this folder useful configurations of the Data Factory program are collected. Up to now we have

- s1_absorption.dtf (computation of the absorption spectrum of substrates from R and T spectra recorded with the S1 spectrometer)

8.6.4 DirectDF

float_a.ddf Configuration to determine the optical constants of 'Float A'.

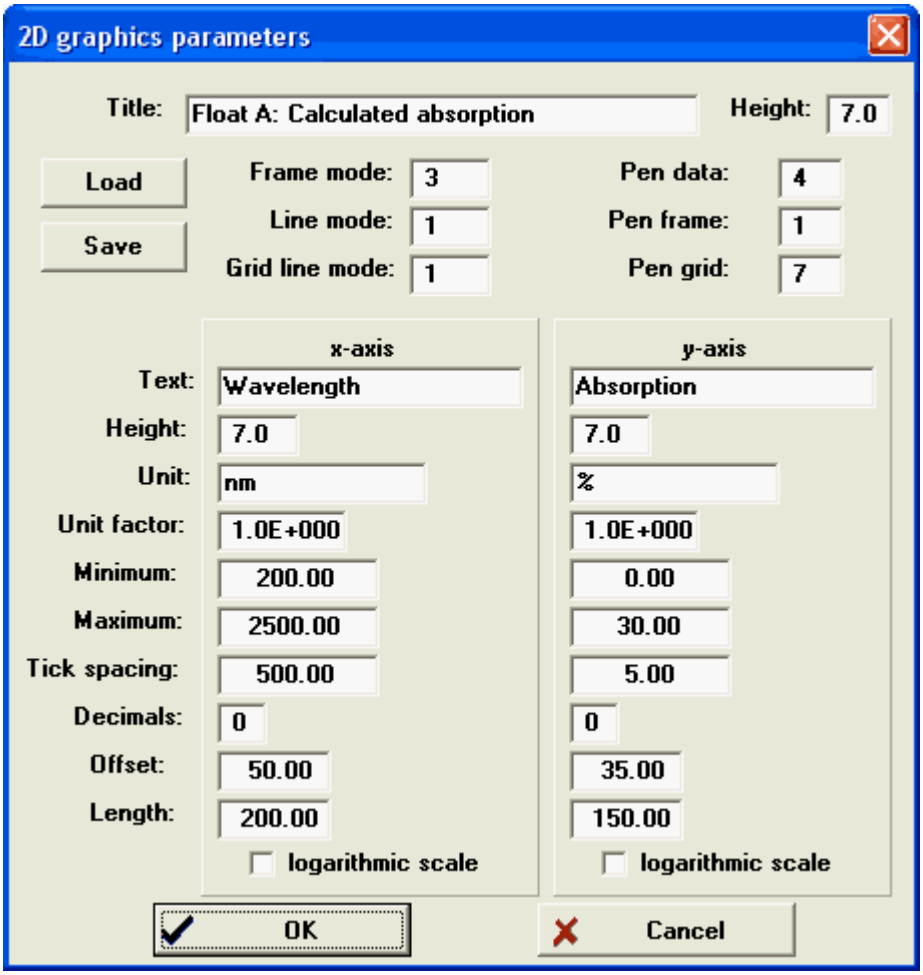
8.6.5 GenetiCode

Here are the ***GenetiCode*** configurations of the ***VirCoC*** database:

low_e_1layers.gcd (first attempt to design a low-e coating with a single layer)
low_e_2layers.gcd (first attempt to design a low-e coating with a double layer)
low_e_3layers.gcd (first attempt to design a low-e coating with 3 layers)
low_e_4layers.gcd (first attempt to design a low-e coating with 4 layers)
low_e_5layers.gcd (first attempt to design a low-e coating with 5 layers)
low_e_7layers.gcd (first attempt to design a low-e coating with 7 layers)

8.7 Plot parameters

Some plot parameter sets have been stored in the database subfolder 'plot parameters'. Use the **Load** and **Save** buttons in the dialog for the graphics parameters in order to load or save plot parameter sets:



The following sets have been stored up to now:

- s1_transmittance.2d (display transmittance spectra, spectrometer S, range 0 ... 100 %)
- s1_reflectance.2d (display reflectance spectra, spectrometer S1, range 0 ... 100 %)
- s1_absorption.2d (display absorption spectra, spectrometer S1, range 0 ... 100 %)
- s2_reflectance.2d (display reflectance spectra, spectrometer S2, range 0 ... 1)
- s2_transmittance.2d (display transmittance spectra, spectrometer S2, range 0 ... 1)
- ag_on_glass_results_deviation.2d (display results of the Ag on glass experiment from 8/6/2004)
- ag_on_glass_results_thickness.2d (display results of the Ag on glass experiment from 8/6/2004)

- collect_s2_reflectance_vs_time.3d (Collect tool, 3D display of reflectance spectra, spectrometer S2)
- collect_s2_transmittance_vs_time.3d (Collect tool, 3D display of transmittance spectra, spectrometer S2)
- collect_s1_transmittance__reflectance.3d (Collect tool, 2D display of transmittance and reflectance spectra, spectrometer S1)

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