Software users manual

Mykola Biednov

General features

Opal is the software for the simulation of the optical properties of multilayer thin film structures. Current version allows to calculate reflectivity and elipsommetric parameters of any isotropic film sequence as a function of wavelength or angle of incidence. Opal software includes a database of complex refraction indices of different materials and allows user to create or import own ones. For people, interested in the Surface Plasmon Resonance applications, option to simulate coupling of light through a prism is included. Opal software offers easy way to vary selected parameter of the coating and see changes of the optical response on the go. Besides, Opal is fully multithreaded application, that utilizes all available threads and ensures the smoothest possible performance even when working with huge amounts of data.

- **Window overview.** Main window consists out of two main areas: plot area in the center, where result of the calculation is displayed, and info area, which shows overview of the multilayer stack structure and other parameters that will be used for calculation, when user presses *Run*.

- **Simulation.** Parameters of the simulation are controlled through the *Simulation* menu or corresponding buttons on the menu bar. *Simulation-General* allows to define all general features of the simulation, like type of the calculated parameter (Reflectivity or ellipsommetry data), type of the calculation (spectral or angular), etc. *Simulation-Multilayer System* is used to specify the number of layers, their optical properties and thickness. User can either type in values for the complex refraction index of each layer directly, or use materials, defined in the materials database. In the second case, refraction index for each layer will be extracted automatically via line fit. Light propagation direction is from Medium, through all layers down to the Substrate. Simulation is started by pressing *Run*. If custom values for the refraction index are used, layers are considered to have no dispersion.

  - **Prsim menu.** *Prism* menu can be used to simulate coupling of the light through a triangular or cylindrical prism. Resulting geometries are depicted on pic. By default, refraction index of the prism is the same, as for *Medium*. In this case, selection of *Cylindrical prism* results in no changes, because there is no refraction at Prism/Medium interface. Its also possible to select material for a prism from a database.

- **Materials.** Opal software has an inbuilt database of materials, which can be used to automatically extract the refraction index of a certain material at a desired calculation wavelength. Data for each material is stored in the separate .xml file, as a wavelength in nanometers and real and imaginary parts of complex refraction index at that wavelength. *Materials-Show Existing* allows to see dispersion curves for all available materials. New materials are added through *Materials-Add new*. There are two options to add a new material. First option is to type in wavelength, n and k values into the table manually. Second option is to import data from a text file, that contains three columns with wavelength in nanometers, n and k. Text in the file will be ignored. Editing of the materials is done through a *Materials-Modify Existing* menu.

- **Quick modification.** Clicking on one of the parameters of the layer stack in *Info Panel* calls a window that allows to apply quick changes to the value of the parameter by dragging the slider. Spectrum is recalculated when slider position is changed.

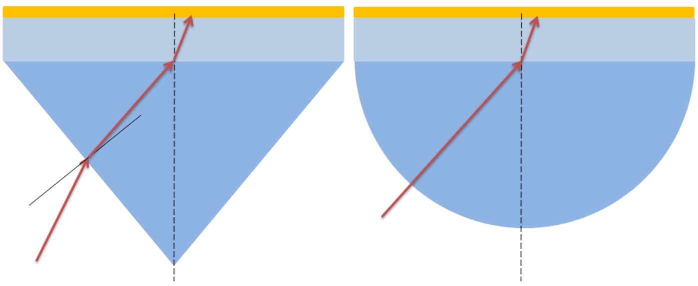


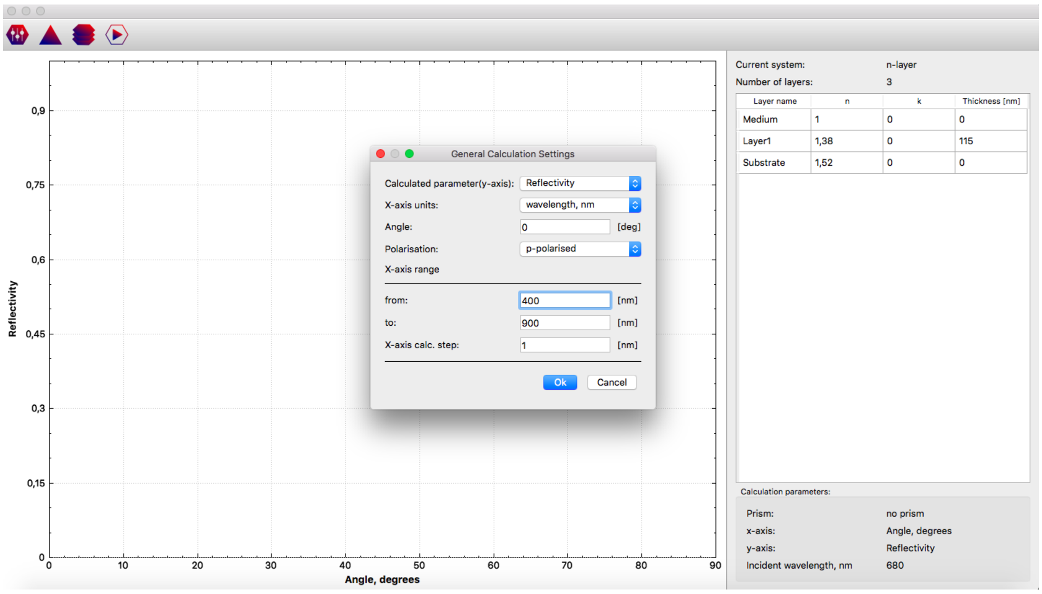
Figure 1: Representation of ray tracing through available prism geometries. Triangular prism (left) and cylindrical prism (right). In both cases beam goes from *Air* into prism, than it is incident on the Prism/*Medium* interface and then hits first thin film layer.

Examples

Lets now go through examples of some common multilayer systems.

Anti-reflection coating

Lets assume that we want to model antireflfection coating for a glass substrate, formed out of quarter-wavelength layers, for center wavelength of 650nm. First of all, we open *Simulation-General*, change units of x *axis* to nanometers, and angle of incidence to 0 degrees. *Polarization* at this AOI

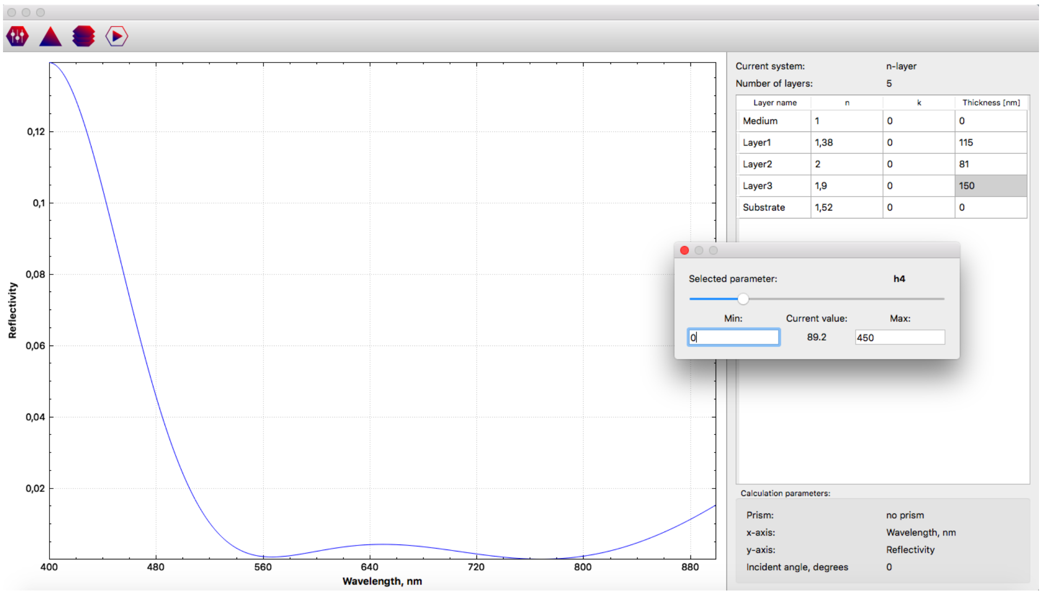


doesnt matter, so we leave it unchanged. As our center wavelength is 650nm, lets change range of x *axis* for calculation from 400 to 900 nm.
At the next step we go to *Simulation-Multilayer* system and change refraction indices of the layers to values in the following table.

Layer name	n	k	Thickness[nm]
Medium	1	0	0
Layer1	1.38	0	117
Layer2	2	0	81
Substrate	1.52	0	0

After pressing *Ok*, our multilayer stack appears in the right part of the main window. Now we press *Simulation-Run* and see result of the simulation. Reflection curve has one minimum at 650nm, as we wanted.
Now, lets assume that we want to broaden region of low reflectance. In order

to do this, we have to add, for example, extra quarter-wavelength layer to our stack. We do this in *Simulation-Multilayer system* by increasing *Number of layers* to 5. Lets set RI of the new layer to 1.9 and thickness to approximately 150nm and press *Ok*. Clicking on the thickness of the newly added layer in *Info panel*, triggers recalculation of the spectrum and creates a window which allows to continuously adjust value of the selected parameter. We can now



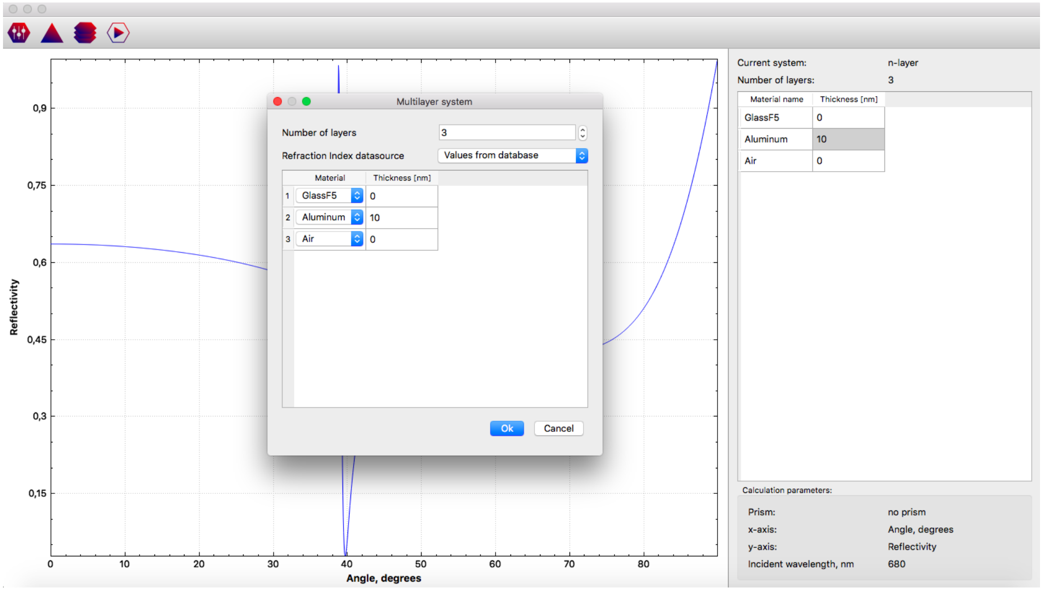
drag the slider left and right to find thickness that gives lowest possible reflection in the area around 650nm. This is achieved at thickness of 90nm.

Surface Plasmon resonance sensor

Lets now model coupling of light to metal-dielectric interface. It requires presence of total internal reflection and evanescent light field. We start modelling again by changing *Simulation-General.* Units of *x-axis* are degrees again, incident *wavelength* is 632 nm. Light has to be p-polarized. Lets now open *Simulation-Multilayer system* and build our sensor. As total internal reflection is needed, *'Medium'* layer has to have higher refraction index then *'Substrate'.* For example Glass and Air interface.

Let's use some of the predefined materials. We change *Refraction index Datasource* to *Values from database*, and set number of layers to 3. As discussed before, for first layer we select Glass, for second Aluminum, for third Air. Thickness of Aluminum has to be 10nm. Pressing *Run* triggers the calculation.

If we want to see, how coupling of light through a triangular prism will



change the situation, we have to go to *Simulation-Prism*, and select there *Triangular prism*. By default, material of the prism is suggested to be the same, as first layer in multilayer system, but it can be changed to any material from database. If material with non-zero absorption is selected, imaginary part of refraction index will be ignored. Lets type in 60 degress for prism angle and recalculate the spectrum. We see, that resonance angle shifted to lower values.

Lets now deposit some Alumina on top of Aluminum and see, what happens. In *Multilayer system* we increase *Number of layers* to 4 and select for a new layer material Al_2O_3, with thickness of 50nm. Now we click on thickness of this layer in *Info panel*, as we did when modeled AR coating, and see, that with increase in oxide thickness Surface plasmon resonance dip broadens, shifts to higher angle values and finally disappears. With further increase in thickness new minima are formed, they are due to waveguide coupling of light into oxide. In the same fashion we could model immobilization of the target molecules on top of our biosensor to estimate its sensitivity and see how resonance curve would shift.