

# **Multifitting**

**v.2.0.0**

**User's manual**

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This manual is intended for users of the Multifitting program. It tells about the purpose of the program, how to start using it, as well as comprehensive information about the available functionality and user interface. This document will be updated with program updates to always reflect the latest state. The program interface is presented only in English, and this manual is in two languages: Russian and English. If you find a mistake or you don't understand something, please email me at [svechnikovmv@gmail.com](mailto:svechnikovmv@gmail.com).

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# 1 Introduction

The Multifitting program is intended for numerical simulation of the reflection and transmission of short-wavelength radiation by a planar multilayer structure, as well as the calculation of the distribution of radiation intensity in the structure, the calculation of the intensity of radiation scattered by interlayer roughness and intralayer deviations of the permittivity (embedded particles or density fluctuations). Such calculations are required for diagnosing structures by X-ray methods, evaluating the performance of reflective coatings and transmissive absorption filters, and also for developing coatings with maximum integral reflection. A multilayer structure may include a substrate, individual layers, periodic sections of arbitrary nesting, aperiodic sections. Each layer of the structure is characterized by material, density, thickness, interface at the upper boundary of the layer, roughness, parameters of intralayer inhomogeneities. The calculation takes into account a some of hardware effects that affect the observed value, such as the final angular and energy resolution, polarization, finite dimensions of the probing beam and sample, detector size, and others. Multifitting uses the base of optical constants of the IMD program [1] with minor extensions. Materials can be specified by file name (usually a chemical formula) with the right substance in the database, or they can be composed of individual chemical elements with specific stoichiometric ratios.

Similar programs for numerical simulation of the optical properties of layered structures are created regularly, both free and commercial. Some can be seen here <http://gisaxs.com/index.php/Software> and here <https://www.reflectometry.org/information/software>. One of the most well-known and widely used programs for the development and diagnostics of X-ray optical coatings and free-standing structures is IMD. [1]. For more than 20 years, it has become a de facto standard tool in X-ray optics. It was its interface and functionality that I took as a reference and adapted for a number of tasks.

Multifitting has a graphical interface specifically designed to quickly change the structure parameters and instantly display the results of the calculation. This is especially important when diagnosing samples, when the structure model or measurement parameters are not known exactly, and many options need to be *manually* considered. With frequent solutions to such tasks, the ergonomics of the interface become especially important, so Multifitting will be useful to everyone who is engaged in X-ray diagnostics of thin films, and especially to those who do it regularly.

Basic information about Multifitting is published in the Journal of Applied Crystallography [2]: M. Svechnikov, "Multifitting: software for the reflectometric reconstruction of multilayer nanofilms," J. Appl. Crystallogr. **53**(1), 244–252 (2020). When posting your results from Multifitting, please include a link to this article.

## 2 Installation and launch

Multifitting is available for Windows (starting with Windows 7) and Linux. You can download it from the GitHub repository <https://github.com/svech/Multifitting/releases> and from the website of the Laboratory of X-ray Optics of the Institute of Physics of Microstructures of the Russian Academy of Sciences. The page in Russian: <http://xray-optics.ru/products/software-multifitting> and in English: <http://xray-optics.org/products/software-multifitting>. The program is free for all users.

### 2.1 Windows

Installation is not required, just download the archive, corresponding to the operating system bitness (x64 or x86), unpack it and run the executable file "`Multifitting_X.Y.Z/bin/multifitting.exe`", where "X.Y.Z" is the version number. I recommend running Multifitting from the command line, because if an error occurs and the program crashes, it will be possible to read the error code in order to report it later.

If you receive the following message when starting the program:

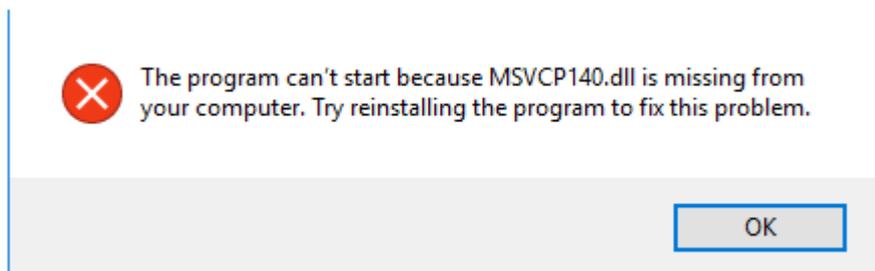


Figure 1. Message from Windows

then it means the absence of "standard" system libraries in the system. You can fix this by downloading the installation package "Microsoft Visual C++ Redistributable" (<https://learn.microsoft.com/en-us/cpp/windows/latest-supported-vc-redist?view=msvc-170>) and installing it in accordance with the bitness of your operating system: [x86](#) or [x64](#).

### 2.2 Linux

The redistributable archive contains all the necessary libraries and the executable file: "`Multifitting_X.Y.Z/bin/multifitting`". Version 2.0.0 has two archives, labeled "`linux-old`" and "`linux-new`", compatible with various distributions. "`linux-old`" has been checked for Debian 11 and Ubuntu 20.04. "`linux-new`" has been checked for Debian 12 (testing), Ubuntu 22.04, Fedora 37, OpenSUSE Leap 15.4, Arch Linux, Manjaro.

## 3 Quick start guide

A good way to get acquainted with the program and evaluate its capabilities is to start working with it immediately. Here is a step-by-step instruction on creating a model structure in Multifitting, on the basics of working with it, comparing the structure of external "experimental" data and solving the diagnostic problem – finding the parameters of the structure from the reflection curve. If you have any problems following this mini-guide, or some transitions raise questions, please let me know and the instruction will be supplemented.

### 3.1 Structure creation

Run the program.

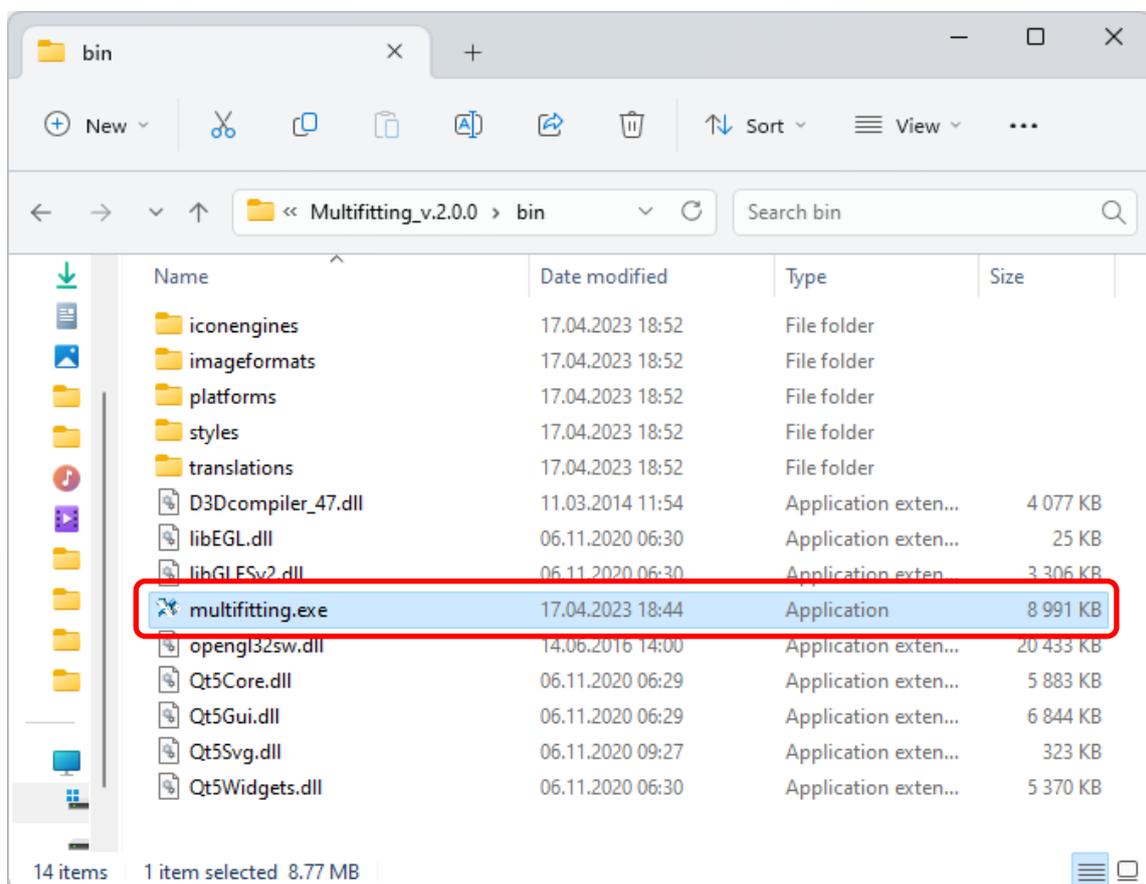


Figure 2. Executable file

The [main](#) Multifitting window and the [console window](#) will open. The console is used by the program to display textual information in the course of work. The main window allows you to set a layered structure and gives access to all other visualization, calculation and parameter modification tools. The main window interface is familiar to IMD users – it is largely reproduced.

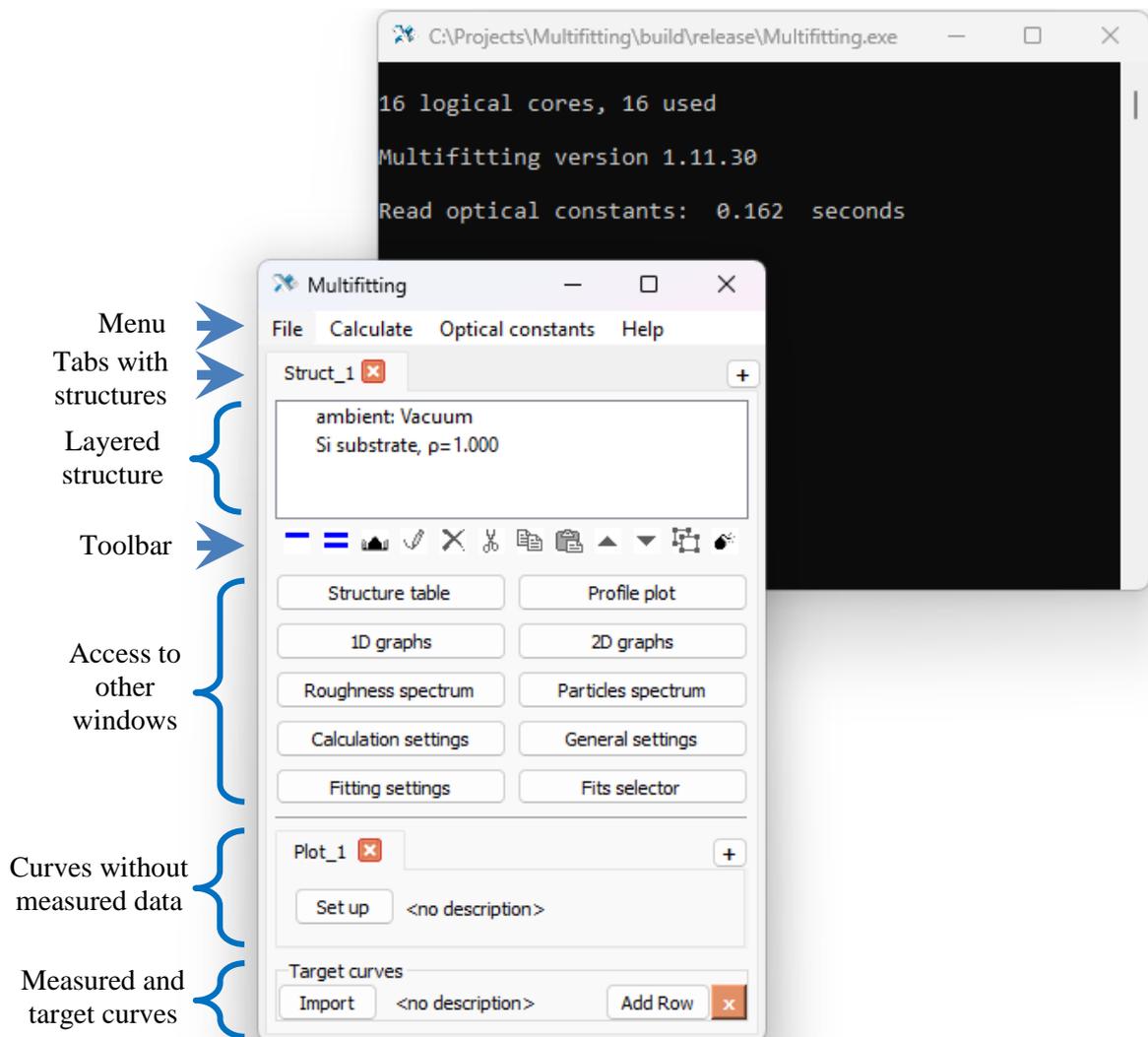


Figure 3. Main window and console

Initially, there is a minimal structure of two half-spaces: the medium and the substrate. Let's add a periodic Mo/Be mirror to the Si substrate. To do this, click the "Add multilayer" button  on the [toolbar](#).

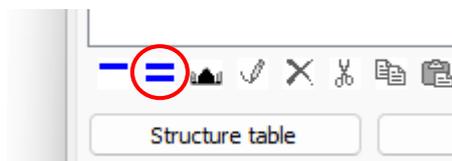


Figure 4. "Add multilayer" button

Now the structure looks like this:

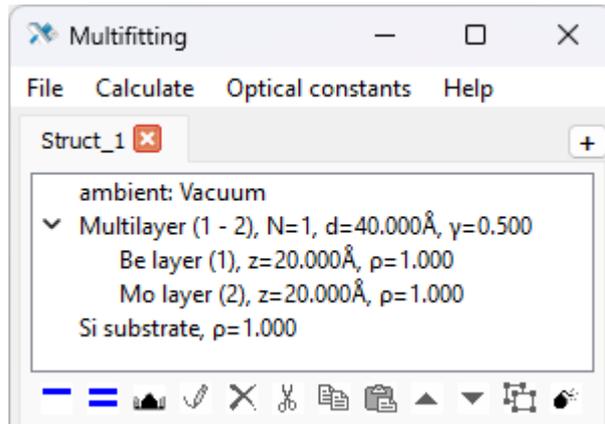


Figure 5. Periodic Mo/Be structure

The structure is represented as [a tree list](#) with basic information about each element. By default, the stack contains one period with two breaks in the cell. Layers also have a material, density, thickness, and top interface with default values. Default values can be changed in the configuration file. You can change the current parameters the [structure element](#) by double-clicking it or by selecting the element and clicking the "Edit"  icon.

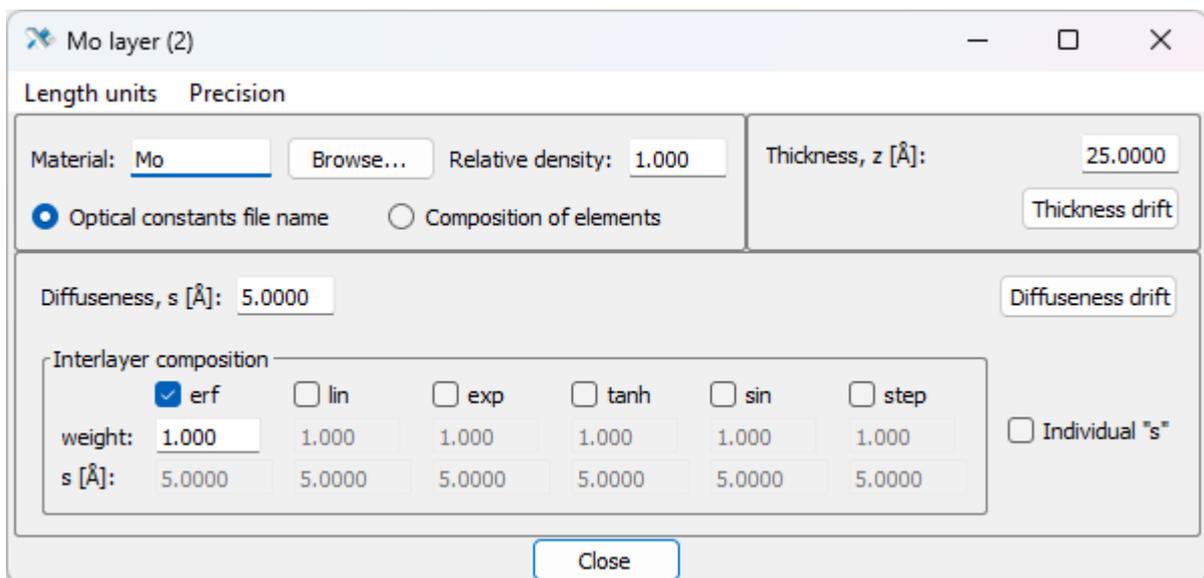


Figure 6. Layer properties window

The window that opens allows you to set various layer parameters. Let's set the following: the first layer: "Material" – Be, "Thickness" – 35 Å, "Diffuseness" – 5 Å. The second layer: "Material" – Mo, "Thickness" – 25 Å, "Diffuseness" – 5 Å. Similarly, the properties of the substrate are edited. Leave the substrate material to Si, and set the "Diffuseness" interface to 3 Å.

Again, similarly, a double click or button opens the stack options window. 

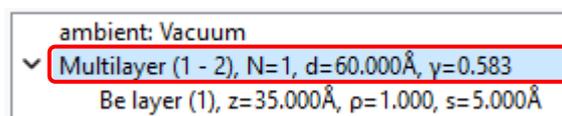


Figure 7. Доступ к свойствам стека

Let's set the number of periods to 110. The value of the period "d" and the thickness ratio "γ" (the ratio of the thickness of the first (upper) layer to the period in two-component mirrors) have already been calculated in accordance with the specified thicknesses of the layers.

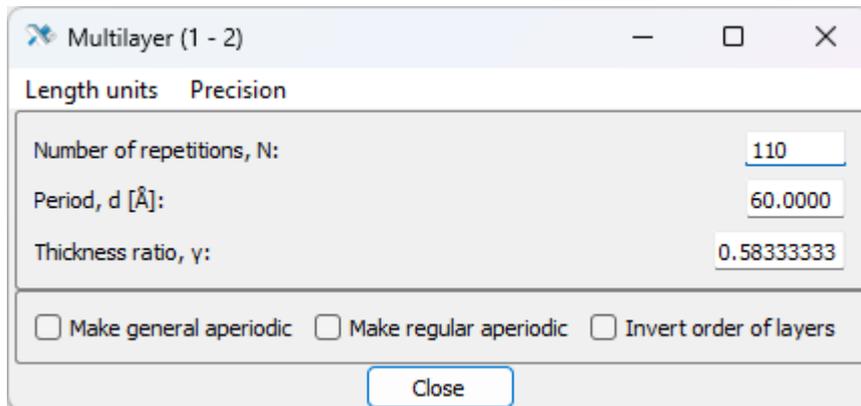


Figure 8. Stack options

That's it, the structure of the periodic Mo/Be mirror is set!

### 3.2 Saving and loading

Multifitting saves data in a binary format, the files have the extension ".fit". You can save the project by selecting an item in the "File" menu or by pressing the appropriate keyboard shortcut. "Save" (= "Ctrl+S") saves to the last open file. If the project is new, that is, there was no previous opening, then a dialog box will appear, as for the option "Save as".

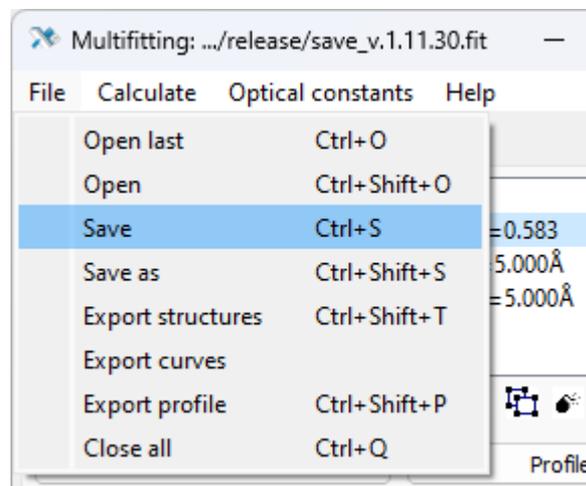


Figure 9. Menu "File"

"Open last" (= "Ctrl+O"), as the name implies, opens the last file that was worked on. If there is none, then a dialog box will appear, as for the option "Open". You can also open a file by simply dragging and dropping it into the main Multifitting window.

Save the project and continue.

### 3.3 Calculation of the reflectivity curve

Now let's calculate the X-ray reflection curve from this mirror. To do this, you need to specify what value should be calculated (reflection/transmission/absorption) and set the properties of the probing beam, the type and range of values of the argument.

In the block of "[independent](#)" curves (i.e. without experimental data), you need to add a new curve. There is already a tab for it, but the inscription "<no description>" indicates that the parameters are not set.

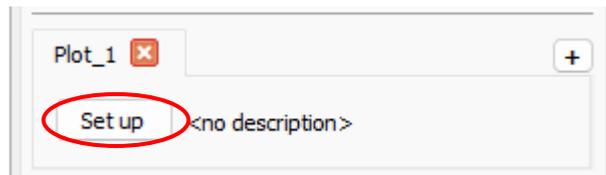


Figure 10. Stack parameters

Click the "**Set up**" button and select the "**Specular scan**" curve type.

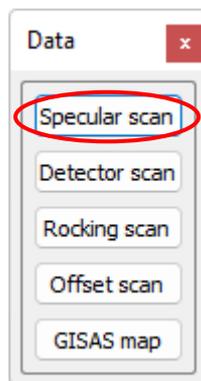


Figure 11. Choosing scan geometry

After setting the type of curve, the corresponding [settings window](#) will open. The default values correspond to an angular scan of 1000 points from 0 to 7 degrees at the wavelength of  $\text{CuK}\alpha$ . Increase the number of points in the scan to 5000. Now the curve settings window can be closed.

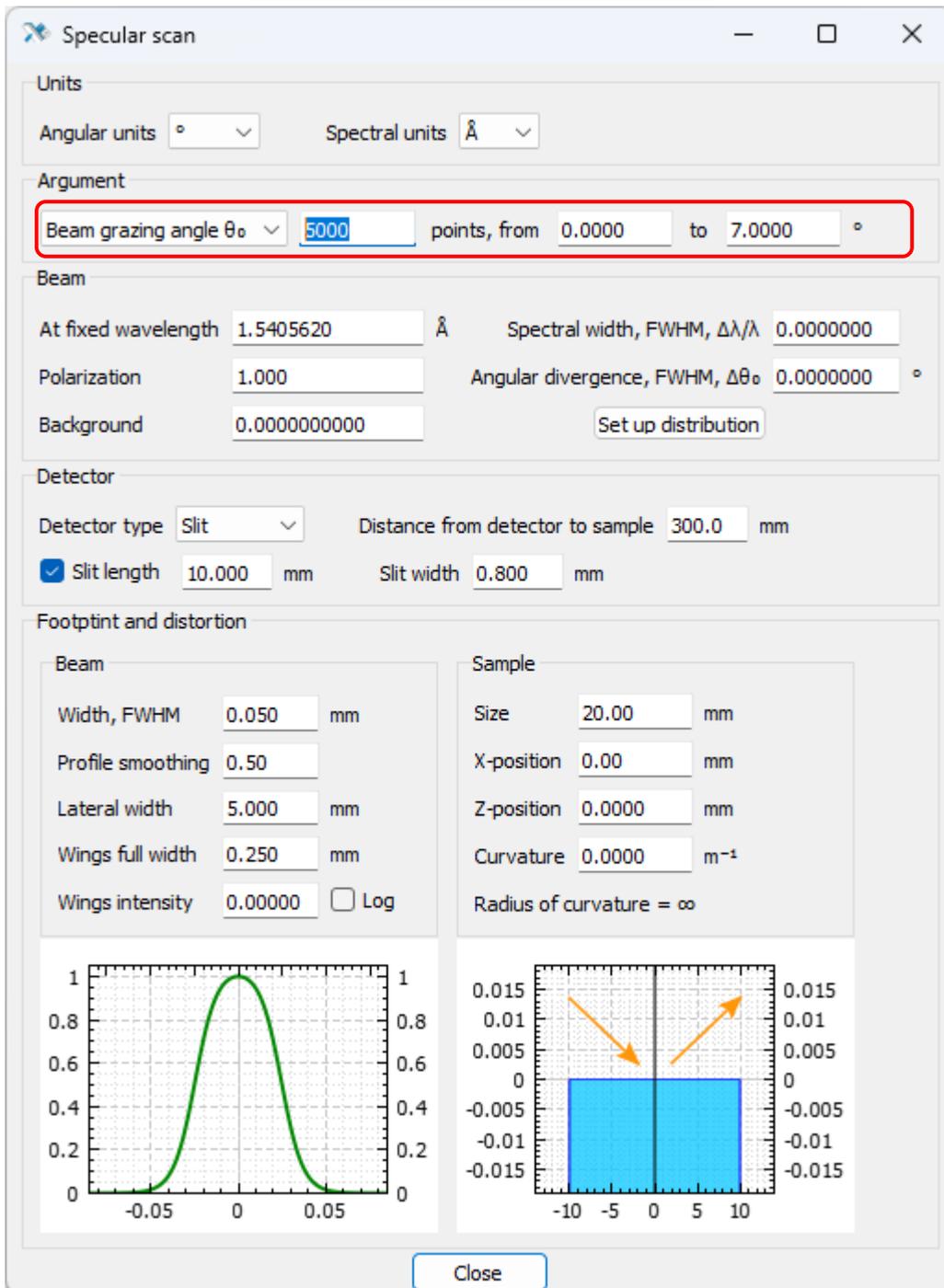


Figure 12. Reflectometric curve settings

Next, you need to run the calculation. To do this, you can press "Ctrl+Shift+C" or select the "**Calculate curves**" item in the "**Calculate**" menu of the main window.

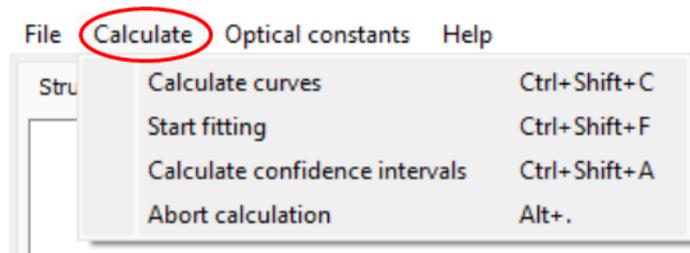


Figure 13. Main menu "Calculate"

Curve calculated! The time spent on the calculation is printed to the console.

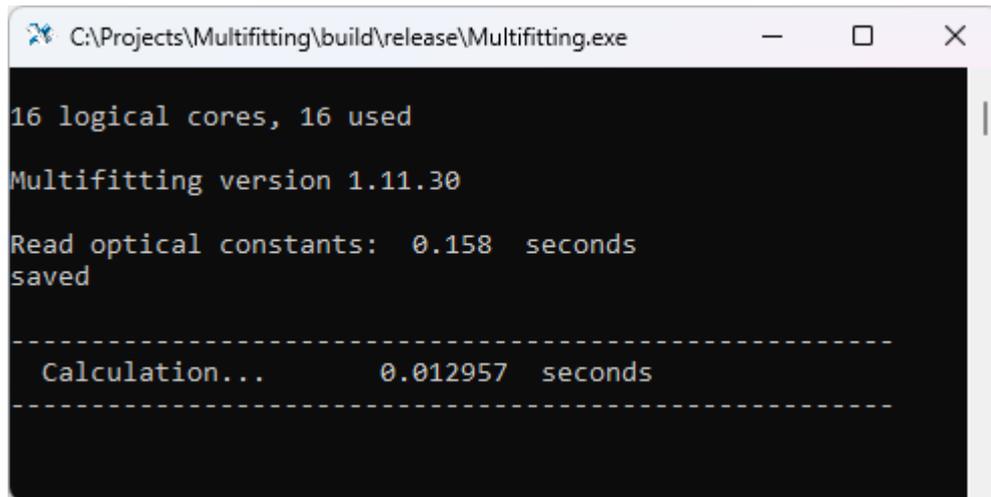


Figure 14. Information in the console

to see the graph you need to open a [window](#) with graphs of one-dimensional curves. the button to open it is located in the main window:

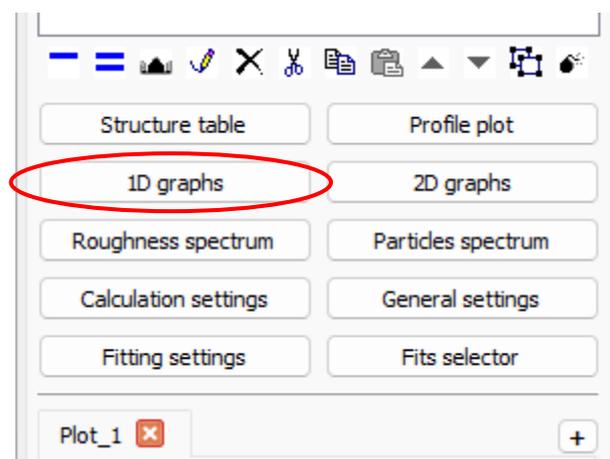


Figure 15. "1D graphs" window button

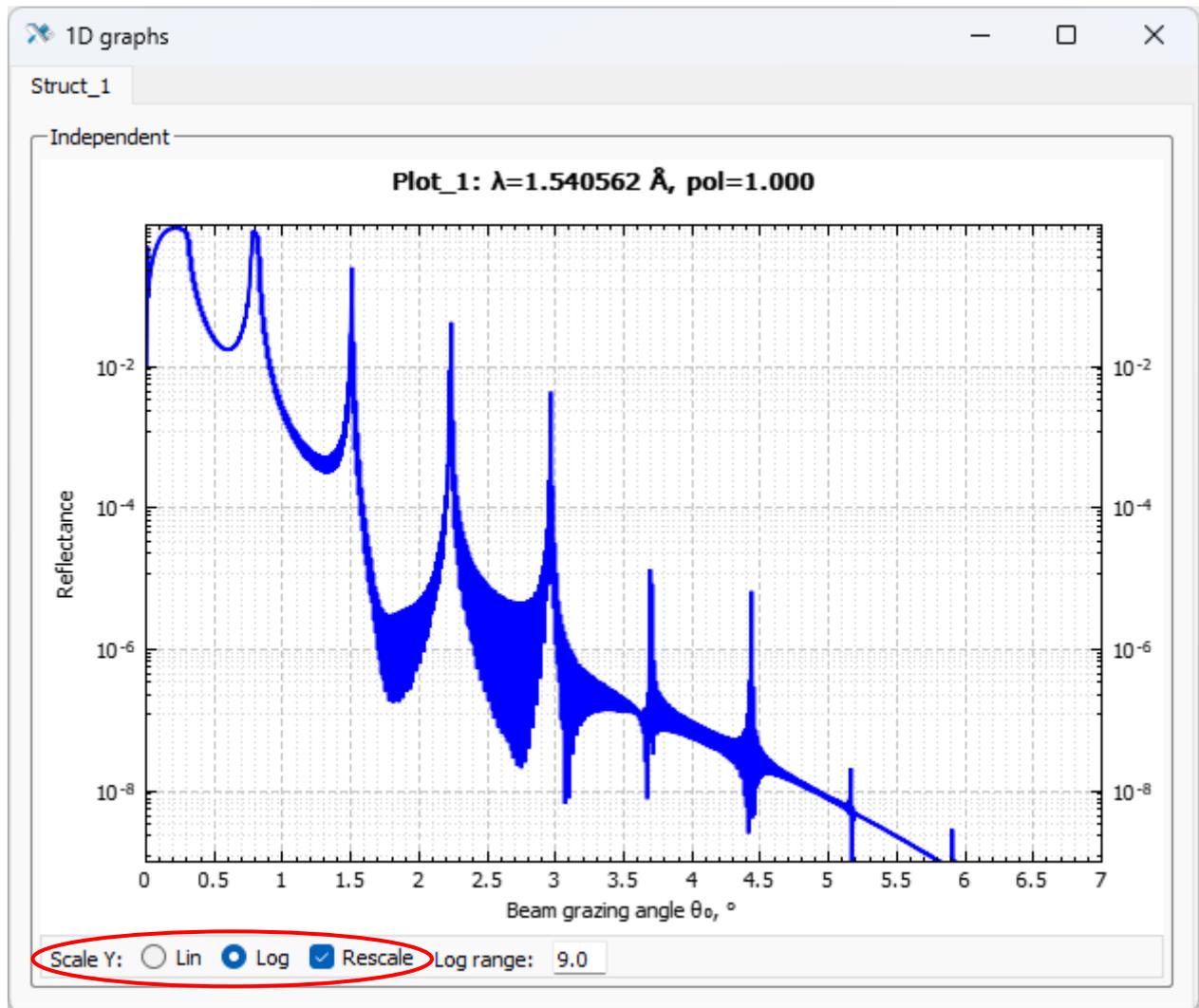


Figure 16. "1D graphs" window

This window can be kept open, then when changing and recalculating the structure, the graph will also be updated. Graphs can be displayed in linear and logarithmic scale; by default the scale is logarithmic. Using the mouse wheel, you can zoom in or out, separately on each axis. To return to the original scale, in which the entire curve is visible at the same time, press the scale switch again. This works when the "Rescale" option is enabled, also with this option the scale returns to the original at each structure recalculation. When the "Rescale" option is disabled, the scale does not automatically change during recalculation and remains user-defined all the time. The name of each graph indicates the name of the curve and the main parameters of the scan.

### 3.4 Working with the structure table

You can change the structure parameters by clicking on individual layers and setting the desired values in the window that opens. But this is inconvenient and inefficient if you need to repeat the procedure at least several times. A more correct way is [to use a common table](#), which shows all the numerical parameters that describe the structure. You can open it with the "Structure table" button:

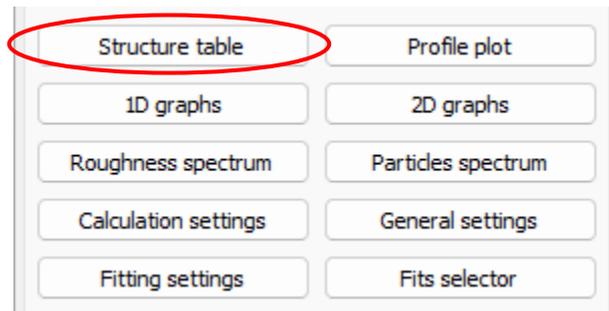


Figure 17. "Structure table" window button

The table contains many fields, so it takes up a lot of screen space. Its upper part contains a color legend for the parameters and options that allow you to change the parameter values in a more convenient way.

Structure table

File Calculate Length units Other units Precision

Struct\_1

pure slave	confidence interval	active fit	$\rho$	$z/d$	$s$		
master/slave	master/confidence	use particles	Reset	Reset	Reset		
pure master	free parameter	not parameter	-10.0%	$\pm 10.0\%$	$\pm 10.0\%$		

Parameter change steps

<input checked="" type="checkbox"/> Mouse wheel	<input checked="" type="checkbox"/> Change dependent		$\rho$	$z/d$ [Å]	$s$ [Å]	$\gamma$	interl
<input checked="" type="checkbox"/> Recalculate	Set model		0.100	0.1000	0.100	0.0100000	0.100

Struct\_1

<input checked="" type="checkbox"/> Multilayer (1 - 2)			N	$d$ [Å]		$\gamma$	
			110	60.0000		0.5833333	
			<input type="checkbox"/> fit	<input type="checkbox"/> fit		<input type="checkbox"/> fit	
			1	20.0000		0.0000000	
			100	60.0000		1.0000000	

		Be	$\rho$ [r.u.]	$z$ [Å]	<input checked="" type="checkbox"/> $s$ [Å]	<input checked="" type="checkbox"/> erf	
		Browse	1.000	35.0000	5.000		1.000
<input checked="" type="checkbox"/> Be layer (1)			<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit		<input type="checkbox"/> fit
			0.700	10.0000	1.000		s erf
			1.000	30.0000	20.000		5.000

		Mo	$\rho$ [r.u.]	$z$ [Å]	<input checked="" type="checkbox"/> $s$ [Å]	<input checked="" type="checkbox"/> erf	
		Browse	1.000	25.0000	5.000		1.000
<input checked="" type="checkbox"/> Mo layer (2)			<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit		<input type="checkbox"/> fit
			0.700	10.0000	1.000		s erf
			1.000	30.0000	20.000		5.000

		Si	$\rho$ [r.u.]		<input checked="" type="checkbox"/> $s$ [Å]	<input checked="" type="checkbox"/> erf	
		Browse	1.000		3.000		1.000
			<input type="checkbox"/> fit		<input type="checkbox"/> fit		<input type="checkbox"/> fit
			0.700		1.000		s erf
			1.000		20.000		3.000

Si substrate

Figure 18. Structure table

The "Recalculate" modifier  Recalculate is enabled by default, which means that every time you change any parameter, the curves are automatically recalculated. This can be seen if the chart window is open and in front of your eyes. You can change the values both by typing from the keyboard and by "scrolling" the values using the mouse wheel or the keyboard arrows  $\uparrow$  and  $\downarrow$ . The step of changing the parameter is set in the "[Parameter change steps](#)" section.

### 3.5 Inverse problem

Now let's try to solve the inverse problem: to find the parameters of the structure according to the measured reflection curve from the Mo/Be mirror. The file with the curve is called "Sample\_D364\_Mo\_Be\_angular\_0.154nm. txt", it is attached to the program. To load it into Multifitting and compare it to the model structure, you need to click on the "Import" button at the bottom of the main window in the "[Target curves](#)" section. The inscription "<no description>" means that no curve has been loaded at the moment.

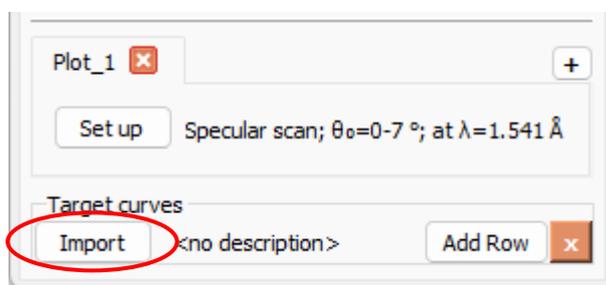


Figure 19. Loading an experimental curve

As for an independent curve, you need to specify the type of scan. Select "Specular scan".

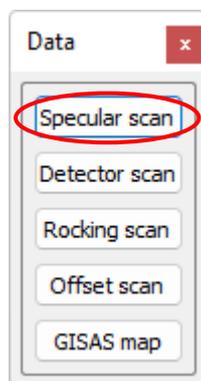


Figure 20. Choosing scan geometry

The opened [window](#) serves to import data and setting the measurement parameters, such as the measured value, argument, units of measurement, normalization, polarization, background, parameters of hardware function. To load data, just drag and drop a text file with data into this window. An alternative is to select a file by clicking the "Browse" button, or enter the path to the file and click "Read data".

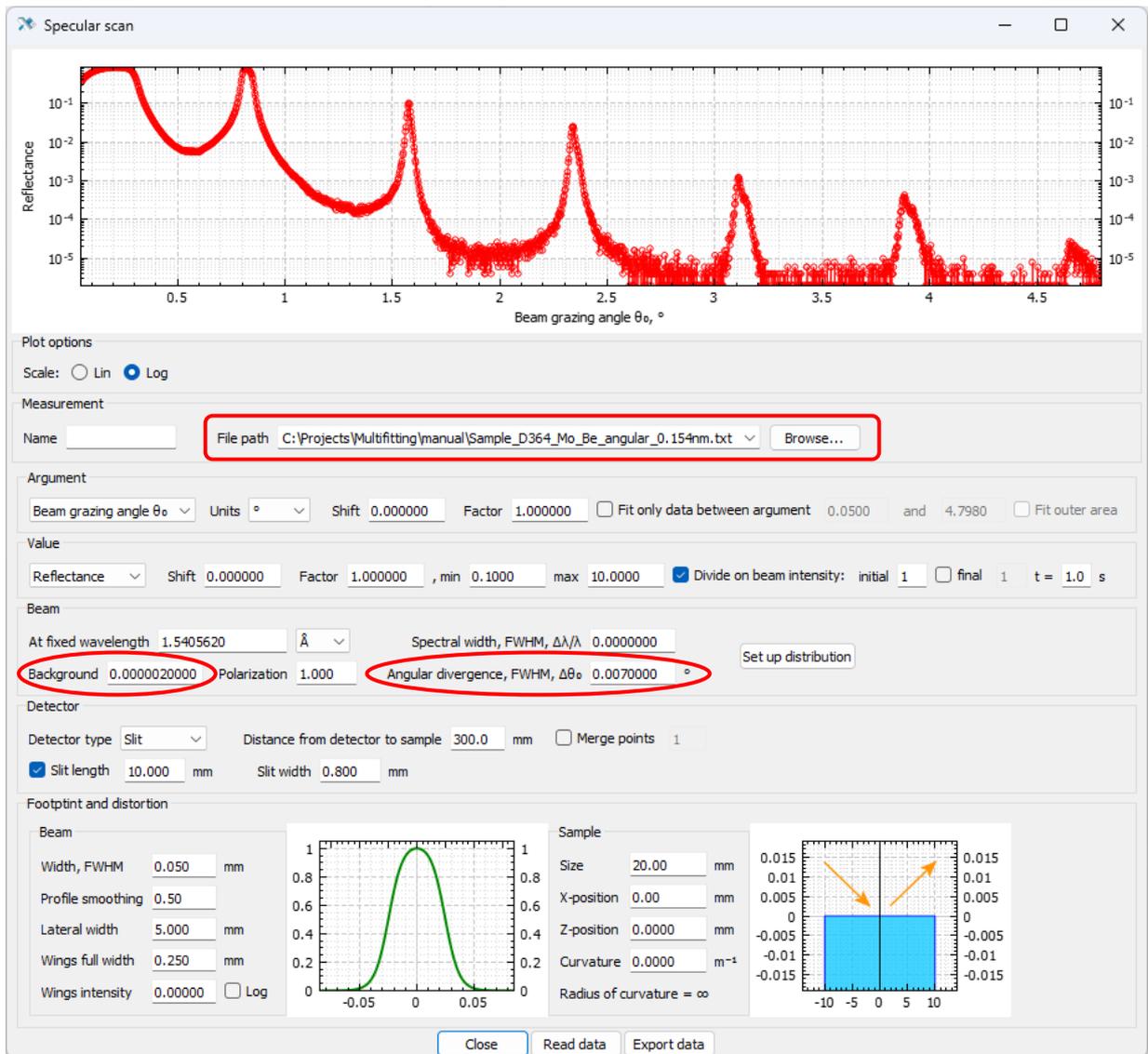


Figure 21. Experimental curve settings

Set the value "**Background**" to  $2 \times 10^{-6}$ . The background is added to the calculated reflection coefficient. The background will not affect the fit process, but will allow the charts to look more aesthetic. The angular divergence of the beam is set at  $0.007^\circ$ . Leave the other parameters values default and close the window. Now brief information about the loaded curve is displayed in the main window in the "**Target curve**" area.

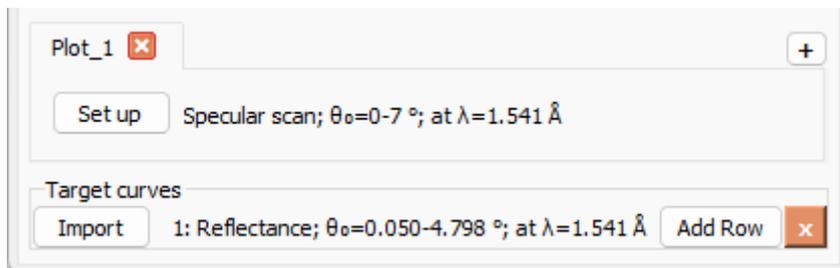


Figure 22. Brief description of curves

If you now open the graphs window again, then a loaded curve will appear in the "**Measured**" section. When clicking "**Ctrl+Shift+C**", a calculated curve imposed on experimental.

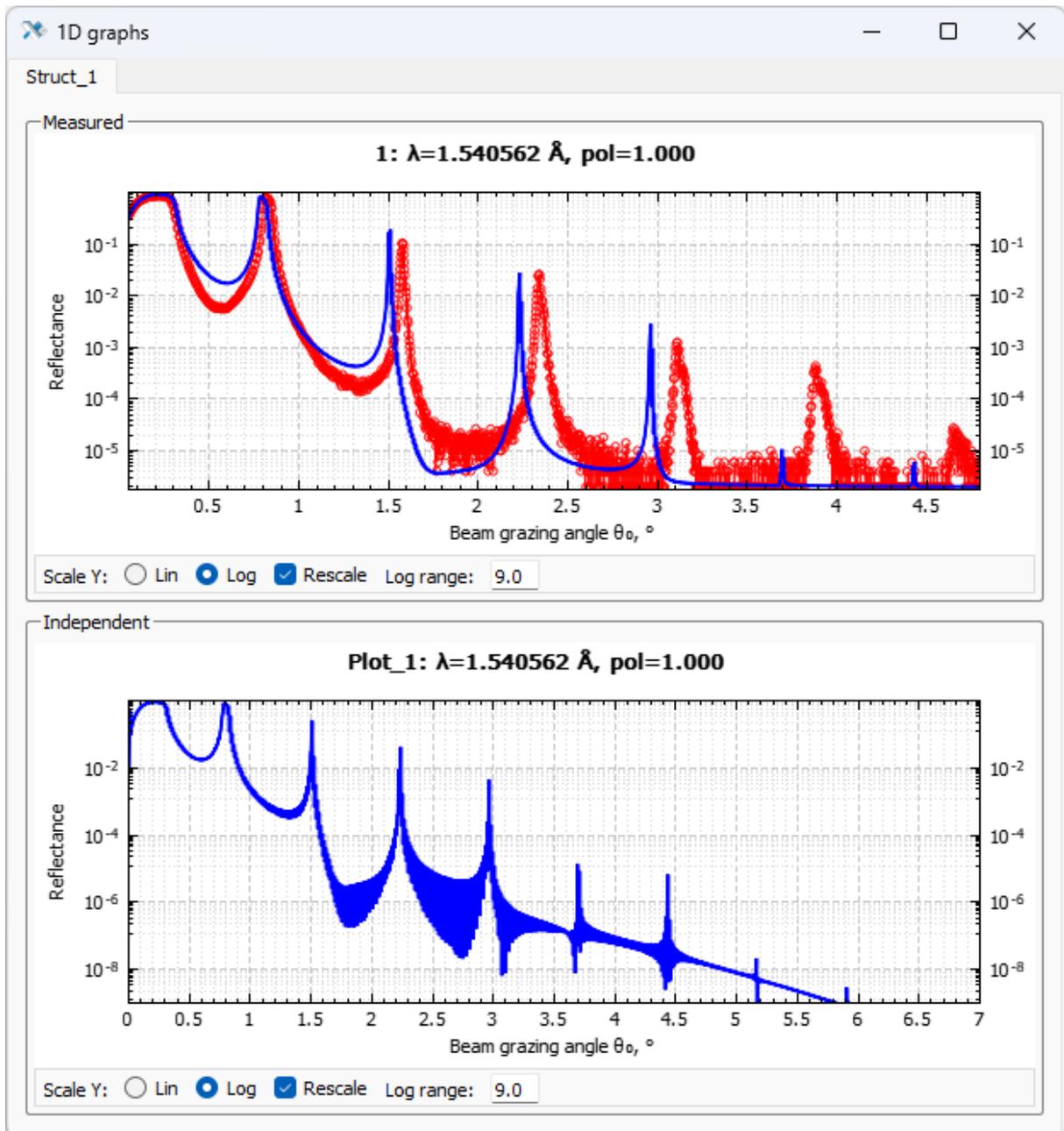


Figure 23. The graphs of all curves

At the same time, the curve in the "Independent" section won't go away. But we don't need it anymore, so you can delete or disable it to make the calculation go faster. You can delete it by clicking on the cross on the tab:

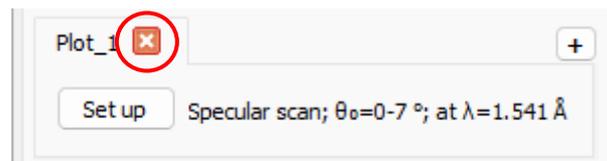


Figure 24. Deleting an independent curve

You can disable the curve in the "[Calculation settings](#)" window.

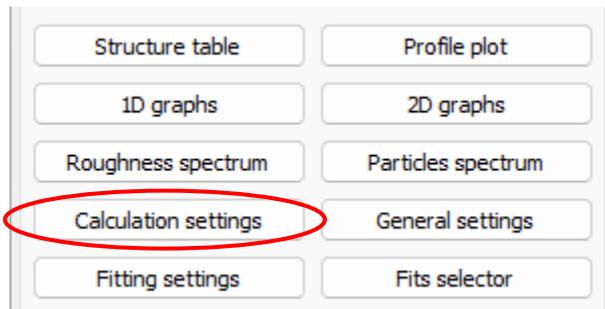


Figure 25. "Calculation settings" window button

From here you can manage all curves calculated by "experimental" and "independent" grids. Uncheck the whole "Independent" section or a specific curve.

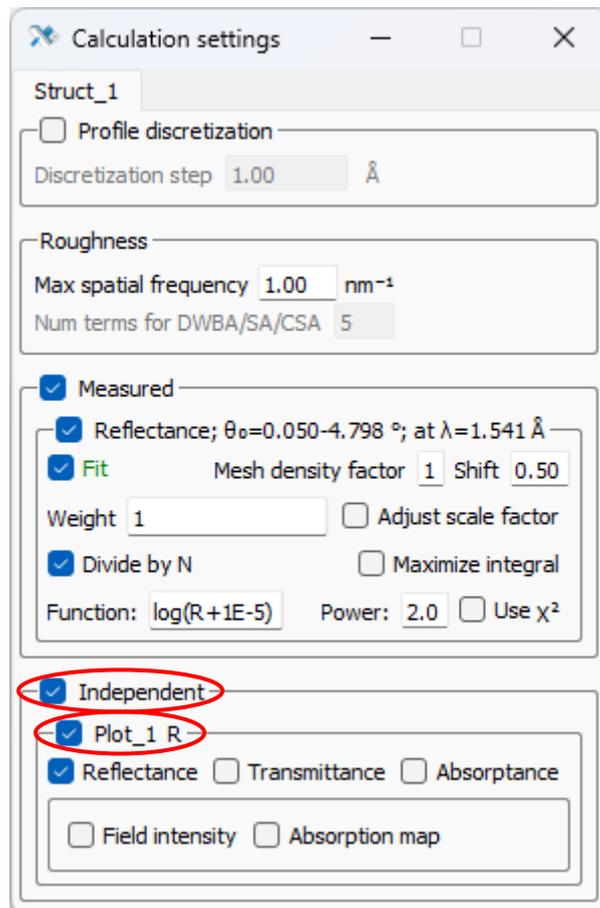


Figure 26. "Calculation settings" window

Then we work only with an experimentally given grid and compare two curves – model and measured. Having an open table and graphs in front of your eyes, you can start changing the parameters of the model. The goal is to find physically reasonable values to make reflectivity curves as similar as possible. You can start the parameter selection by manually changing in the table (scrolling with a suitable step) the values of the period, "Y", the thicknesses of the layers and a diffuse interface. But we can see that even with a good visual coincidence of the position and height of the peaks, we will get the difference in the form and width of the peaks. In the picture below, an example of such a "coincidence" obtained manually.

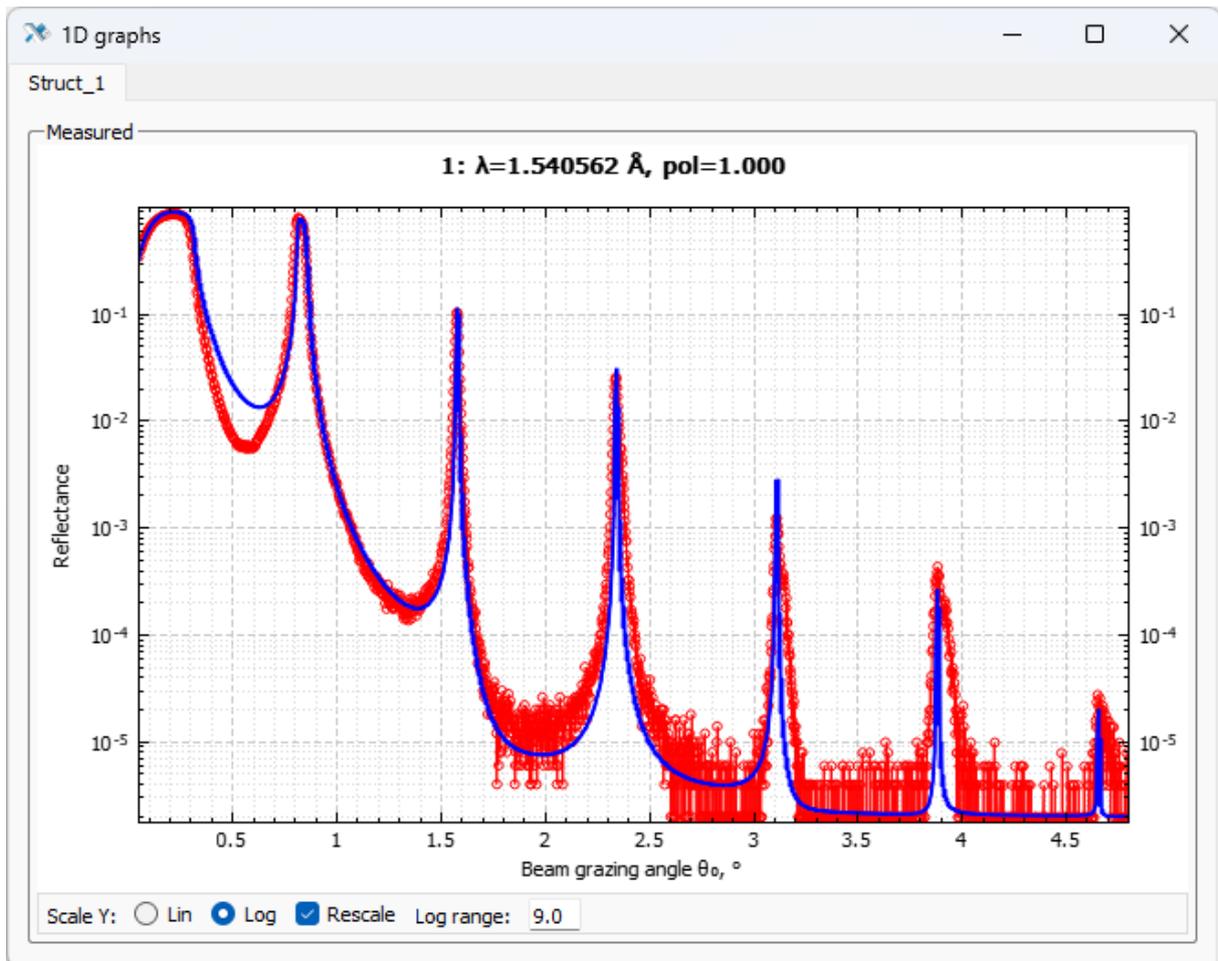


Figure 27. Preliminary manual fitting of curves

The parameters of the model structure presented on the graph are as follows:

```

ambient: Vacuum
  Multilayer (1 - 2), N=110, d=57.100Å, γ=0.550
    Be layer (1), z=31.405Å, ρ=1.000, s=7.100Å
    Mo layer (2), z=25.695Å, ρ=0.951, s=3.900Å
    Si substrate, ρ=1.000, s=3.000Å
  
```

Figure 28. Preliminary fit parameters

What kind of mismatch between the curves are we observing? The first is the difference in the area between the critical angle and the first Bragg peak. The simplification of our model is affected here: the reflection in this area of the angles is largely determined by the surface layer of the structure, which is oxidized in the air and covered with an adhesive layer of water, hydrocarbons, etc. First of all, the thickness of the surface layer, and not the exact chemical composition, affects the reflection curve at the wavelength of 0.154 nm. To account for these effects, at least to a first approximation, you should add a BeO layer on top of the Be layer. To do this, close the structural table, select the topmost element of the structure with the mouse (this is the external environment) and click the "Add layer" icon  on the toolbar. Layers are always added below the selected item, but above the watermark. You can reposition an existing selected structure layer using the "Move up"  and "Move down"  buttons  on the toolbar.

With an open table, the toolbar is inactive! This is done to simplify the synchronization of the structure in the main window and in the table. Therefore, if you cannot add a layer, check if the table is closed.

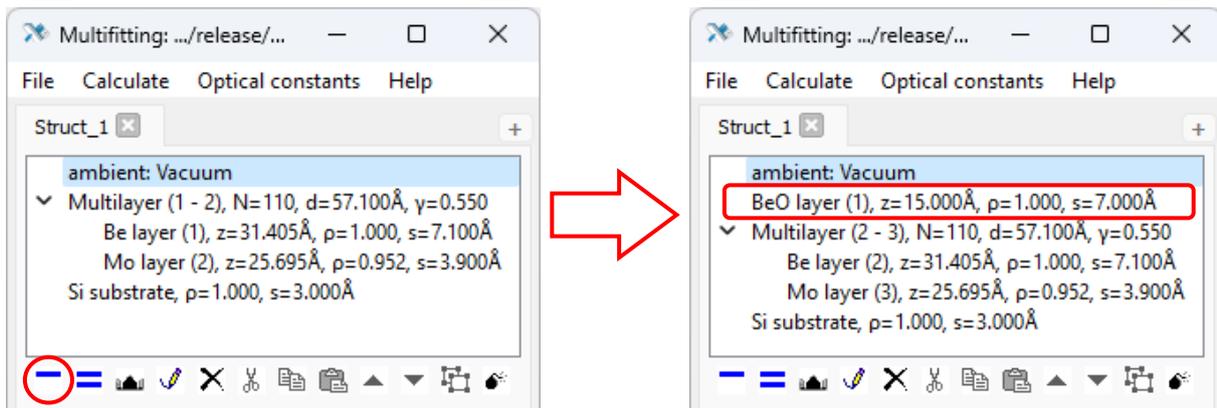


Figure 29. Adding a surface layer

Bragg peaks are also different. The first peak is shifted in angle, and the model 4,5,6 peaks are much narrower than the measured ones. Resonances are determined by the periodic part of the structure, and therefore they must be adequately described by the presented model. What have we not taken into account? That the real structure is not perfectly periodic. In the process of magnetron sputtering, the pressure of gases changes, the target erosion occurs, and with it the growth rate of the films changes. The easiest to detect is the effect of a monotonous increase or decrease in the thickness of the period throughout the depth of the structure. The magnitude of this effect depends on the amount of drift, the number of periods, and the ordinal number of the Bragg peak. Multifitting allows you to set such deviations from the strict periodicity, so let's add them to the stack.

Open the table again. By default, the table contains some minimal set of parameters, and to introduce additional ones, you need to perform a couple of actions. First, you need to open the [window for selecting imperfections of the model](#) by clicking the "Set model" button under the color legend:

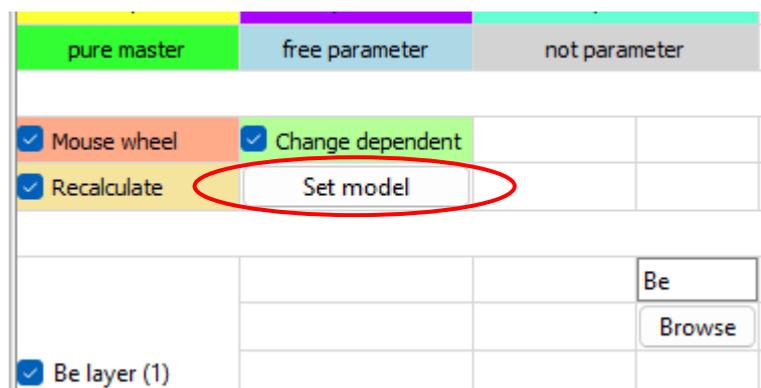


Figure 30. Structure imperfections model settings button

In the window that opens, we turn on the additional profile of the transition layer and linear drift of thickness. Now these parameters will appear in the table, so the window can be closed.

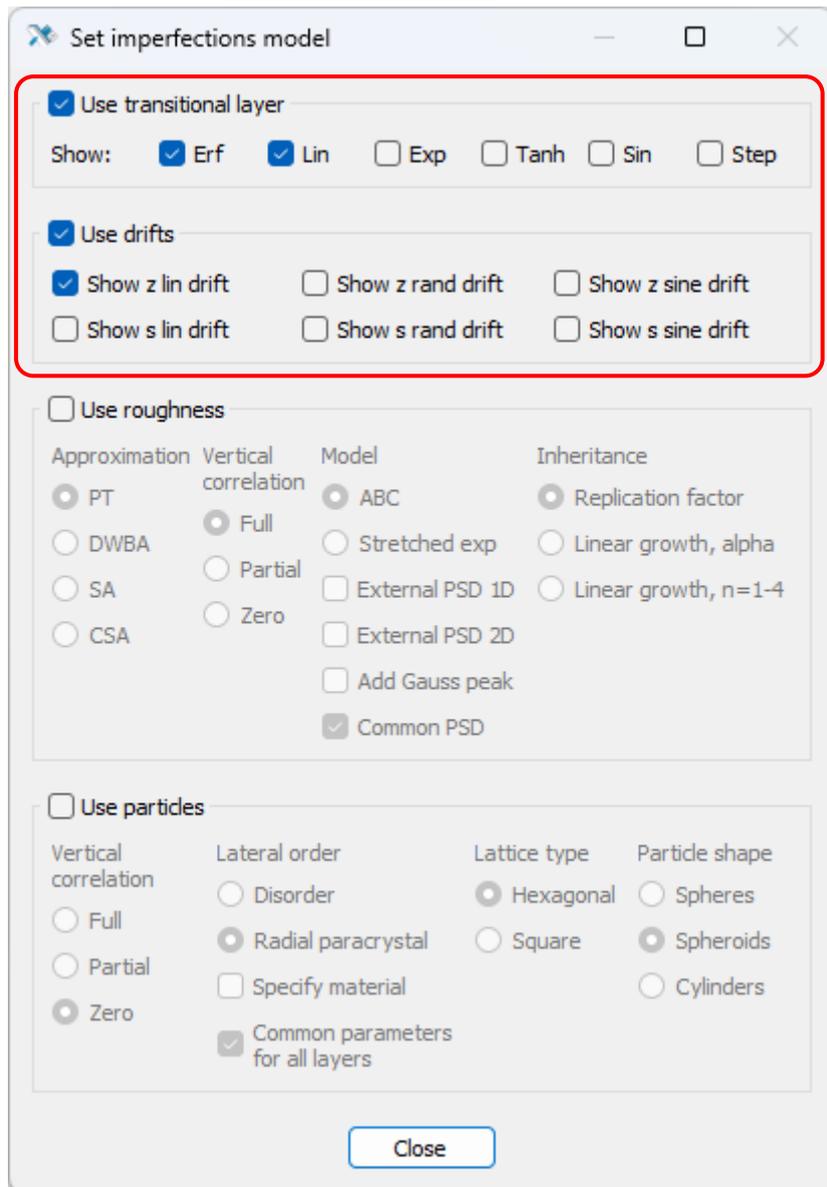


Figure 31. Choosing additional structure parameters

Linear drift means a linear change in the thickness of the layer with an increase in the period number. The unit is percent of the nominal thickness of the layer. The average thickness is preserved. The drift can be both positive and negative, i.e. the layers can become thicker or thinner into the deep of the stack. In our case, as it follows from the shape of experimental peaks, the layers near the substrate are thinner than layers near the surface.

The interface profile between layers is another factor that affects the heights of peaks and their ratio between each other. By default, the laterally averaged dielectric permittivity profile is described by the error function "erf" (see the checkboxes in the table in each of the layers), but in reality the shape may differ. You can change the profile, including other functions (erf, lin, exp, tanh, sin, step). The weight of each function is given under its name. Only the ratios of these values between different functions are important; the absolute value is not important. If the weight is zero, it is equivalent to disabling this profile function.

We turn on the new parameters by clicking on their headers.

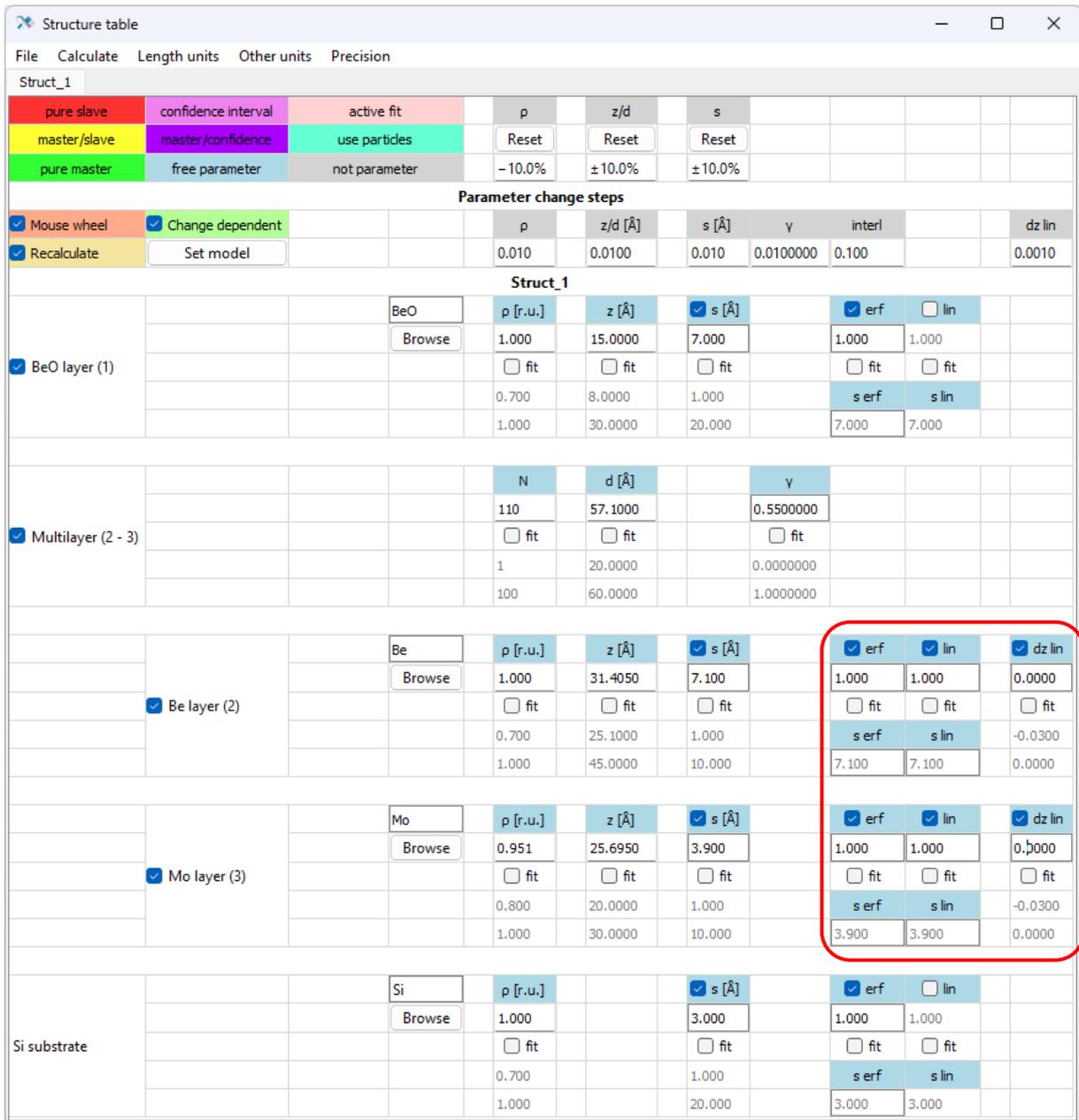


Figure 32. Structure table with new parameters

So, now the model structure has become much more complex and multi-parametric. You can still change the parameters manually and look at the result in real time (and this is always useful to do, at any stage of reflectometric reconstruction), but the chances of finding the desired area of parameters are very small. At this stage, automated fitting becomes necessary. Before moving on to automatic fitting, you should pay attention to the following circumstance. Although the optimally selected residual function to some extent "equalizes" the contribution of the parts of curve with different intensity, but it does not completely eliminate the imbalance. A great difference in the intensity of different parts of the reflection curve leads to the fact that the algorithm often tries to reduce the mismatch in total external reflection area (angles 0–0.3°), often to the detriment of the important features of the reflection curve, such as the Bragg peaks of high orders. To prevent such a conflict, it should be taken in advance that the area of total external reflection, which depends more on the geometry of measurements than on the features of the structure itself, does not have too much mismatch and, even better, did not participate in the fitting at all. You can improve the coincidence of the calculated and measured curves by setting the size of the

sample, the width and shape of the probing beam, the displacement of the sample relative to the center of the beam. An example is given on the picture below.

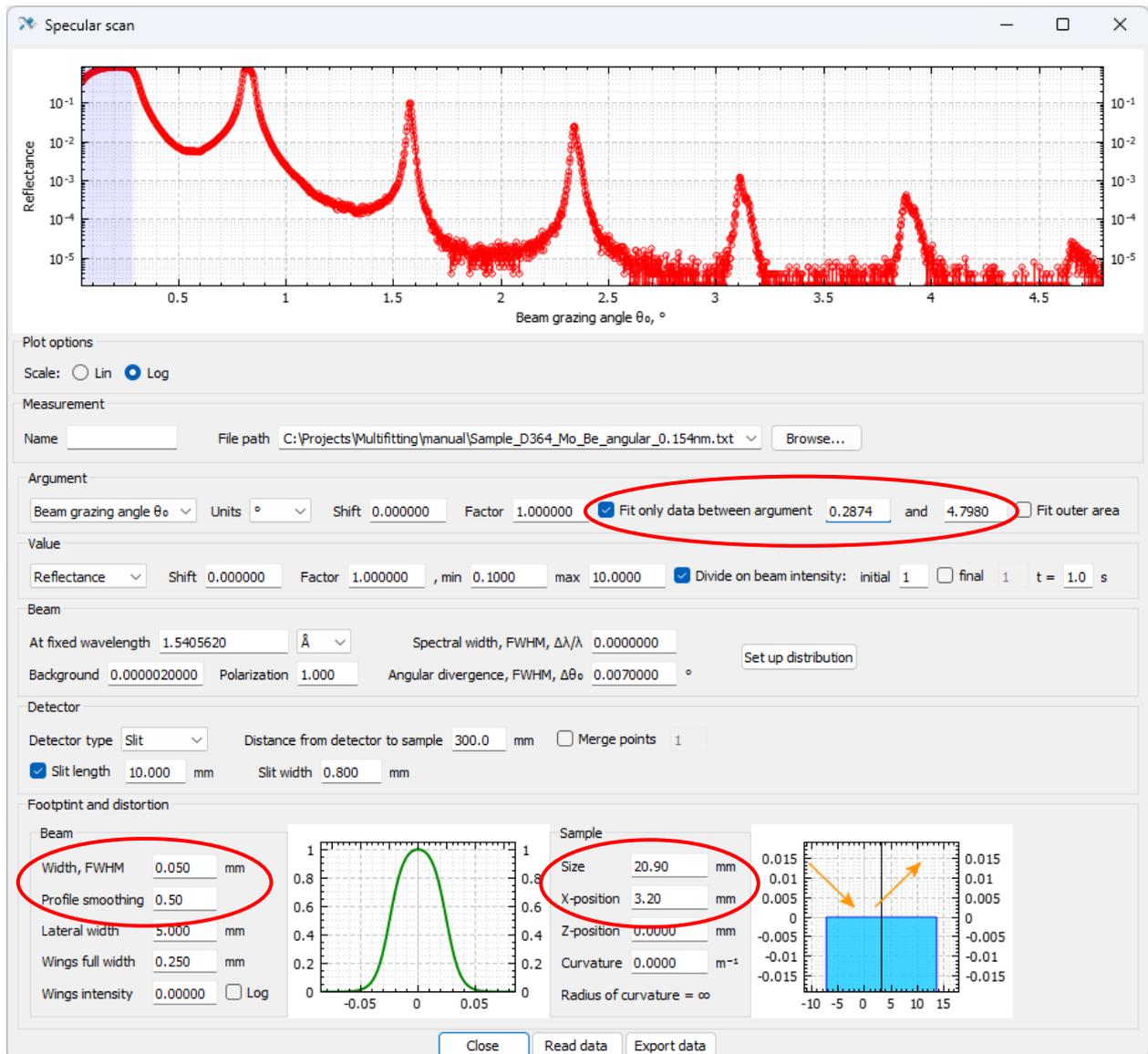


Figure 33. Parameters specifying the footprint effect and the argument range for fitting

To find the appropriate values, you need to keep the window with graphs open and recalculate the curve on parameters change. To ensure that the scale of the curves does not change to the original, you need to disable the "Rescale" option in the graph window.

To fit not along the entire axis, you need to enable the "Fit only data between argument" option in the curve settings and set the minimum argument not far from the critical angle.

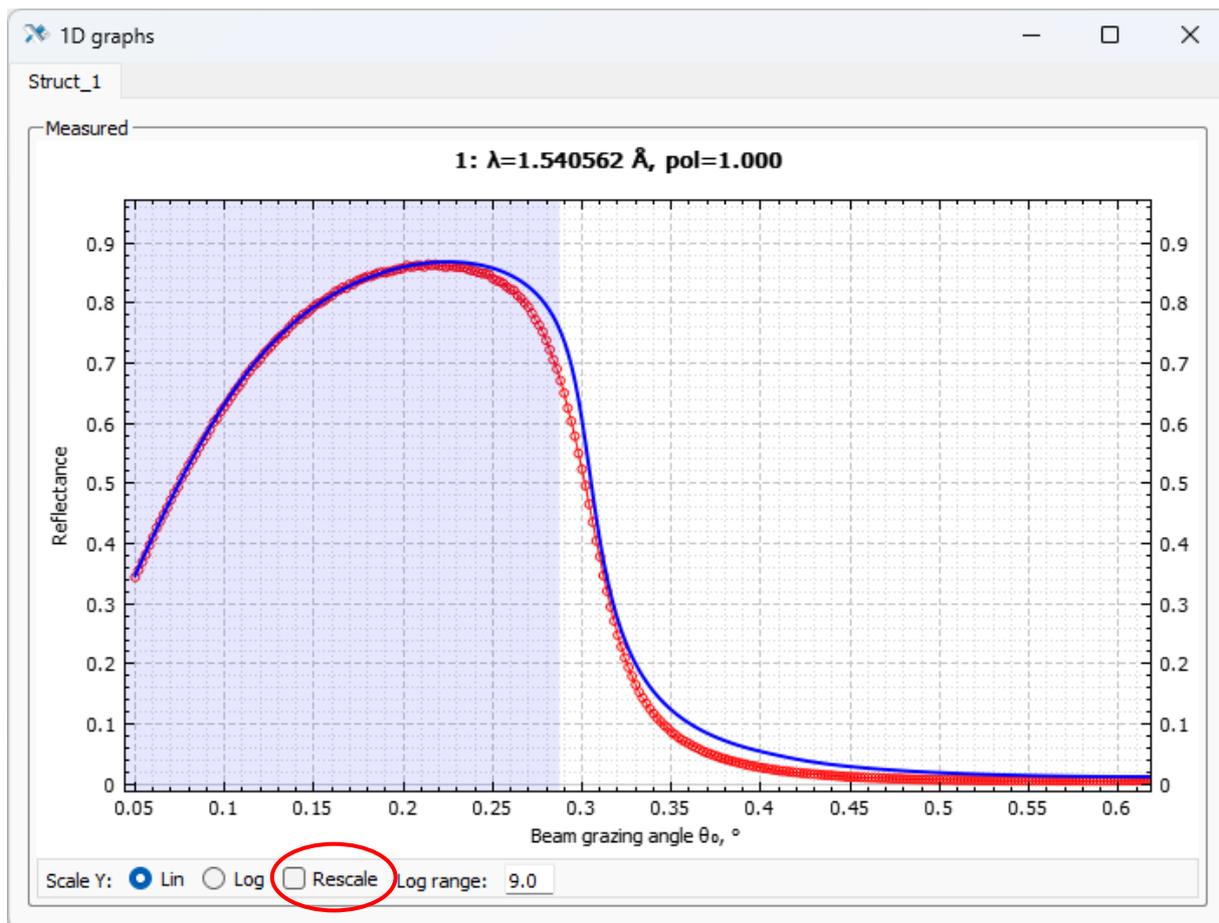


Figure 34. Shaded area excluded from fitting

Now let's prepare the structure for fitting. First of all, this will require you to mark in the table the parameters that will be varied. For these parameters, you need to enable the "fit" option  fit and set the lower and upper limits of the values.

	$z \text{ [Å]}$
current value	32.5470
fitting on/off	<input checked="" type="checkbox"/> fit
min	25.1000
max	45.0000

Figure 35. Preparing a parameter for fitting

It is reasonable to assume that the thicknesses of Mo and Be drifts are the same during the deposition process, so we will reduce the number of degrees of freedom of the model and couple the drift parameters of the Mo and Be layers. To do this, right-click on the parameter header "**dz lin**" calling the context menu:



Figure 36. Parameter context menu

The only context menu action opens the "[Coupling editor](#)" window for Be layer drift. To add a dependent parameter, you need to put the cursor in one of the "Slaves" fields and then also right-click on the target parameter, i.e. the Mo drift of the layer. The name of the added parameter will be visible to the left of the editable field.

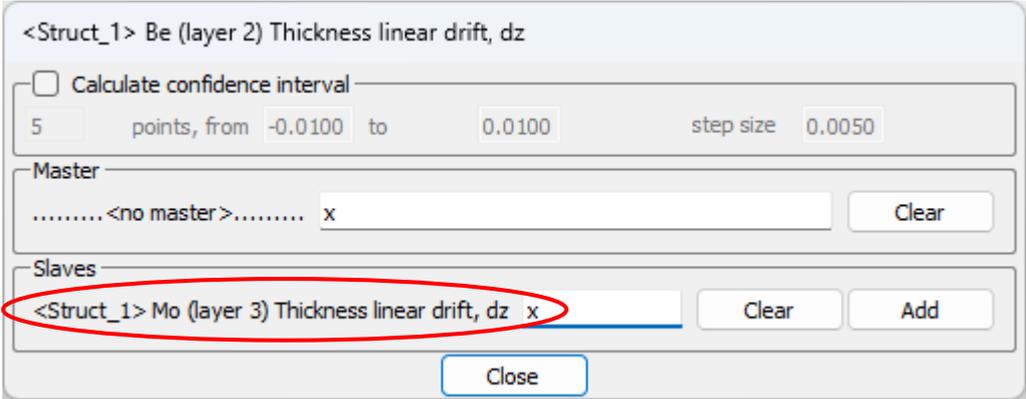
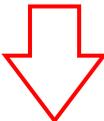
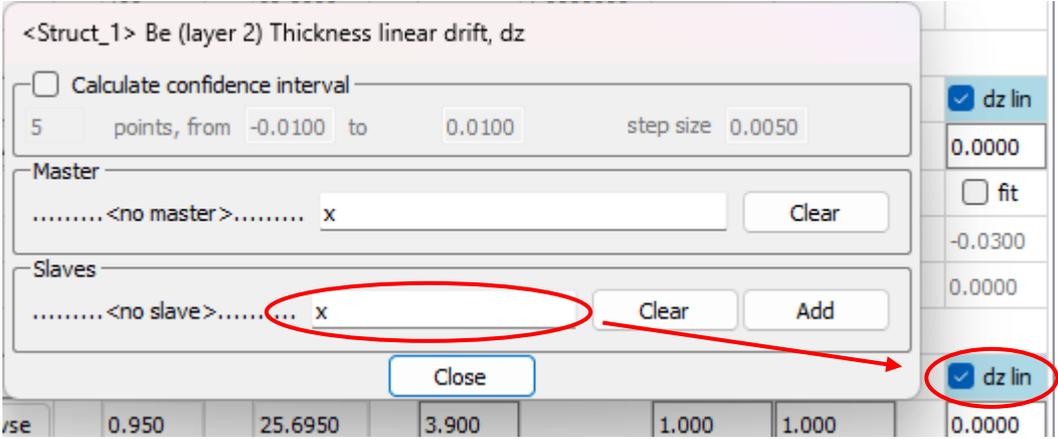


Figure 37. Adding a dependent parameter

"[Coupling editor](#)" can be closed now. The table with all the variables and their initial values now looks like in the following figure. During the first runs, you don't have to enable a surface layer in the model. Layers with all their parameters can be quickly turned on and off in the table.

Structure table									
File Calculate Length units Other units Precision									
Struct_1									
pure slave	confidence interval	active fit		p	z/d	s			
master/slave	master/confidence	use particles		Reset	Reset	Reset			
pure master	free parameter	not parameter		-10.0%	±10.0%	±10.0%			
Parameter change steps									
<input checked="" type="checkbox"/> Mouse wheel	<input checked="" type="checkbox"/> Change dependent			p	z/d [Å]	s [Å]	γ	interl	dz lin
<input checked="" type="checkbox"/> Recalculate	Set model			0.010	0.0100	0.010	0.0100000	0.100	0.0010
Struct_1									
		BeO		p [r.u.]	z [Å]	<input checked="" type="checkbox"/> s [Å]	<input checked="" type="checkbox"/> erf	<input type="checkbox"/> lin	
		Browse		1.000	15.0000	7.000	1.000	1.000	
<input type="checkbox"/> BeO layer (1)				<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	
				0.300	5.0000	1.000	s erf	s lin	
				1.000	30.0000	20.000	7.000	7.000	
				N	d [Å]		γ		
<input checked="" type="checkbox"/> Multilayer (2 - 3)				110	57.1000		0.5500000		
				<input type="checkbox"/> fit	<input type="checkbox"/> fit		<input type="checkbox"/> fit		
				1	20.0000		0.0000000		
				100	60.0000		1.0000000		
		Be		p [r.u.]	z [Å]	<input checked="" type="checkbox"/> s [Å]	<input checked="" type="checkbox"/> erf	<input checked="" type="checkbox"/> lin	<input checked="" type="checkbox"/> dz lin
		Browse		1.000	31.4050	7.100	1.000	1.000	-0.0230
<input checked="" type="checkbox"/> Be layer (2)				<input type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit
				0.700	25.1000	1.000	s erf	s lin	-0.0320
				1.000	40.0000	20.000	7.100	7.100	-0.0150
		Mo		p [r.u.]	z [Å]	<input checked="" type="checkbox"/> s [Å]	<input checked="" type="checkbox"/> erf	<input checked="" type="checkbox"/> lin	<input checked="" type="checkbox"/> dz lin
		Browse		0.950	25.6950	3.900	1.000	1.000	-0.0230
<input checked="" type="checkbox"/> Mo layer (3)				<input type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input type="checkbox"/> fit
				0.800	20.0000	1.000	s erf	s lin	-0.0300
				1.000	30.0000	20.000	3.900	3.900	0.0000
		Si		p [r.u.]		<input checked="" type="checkbox"/> s [Å]	<input checked="" type="checkbox"/> erf	<input type="checkbox"/> lin	
		Browse		1.000		3.000	1.000	1.000	
Si substrate				<input type="checkbox"/> fit		<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	
				0.700		1.000	s erf	s lin	
				1.000		20.000	3.000	3.000	

Figure 38. Fitting parameters in the table

Before starting, you need to set the residual function. This can be done in "Calculation settings" window. You can leave the default values; they correspond to a logarithmic residual, in which values less than 1E-5 do not make a noticeable contribution. The "fit" checkbox for the curve must be enabled.

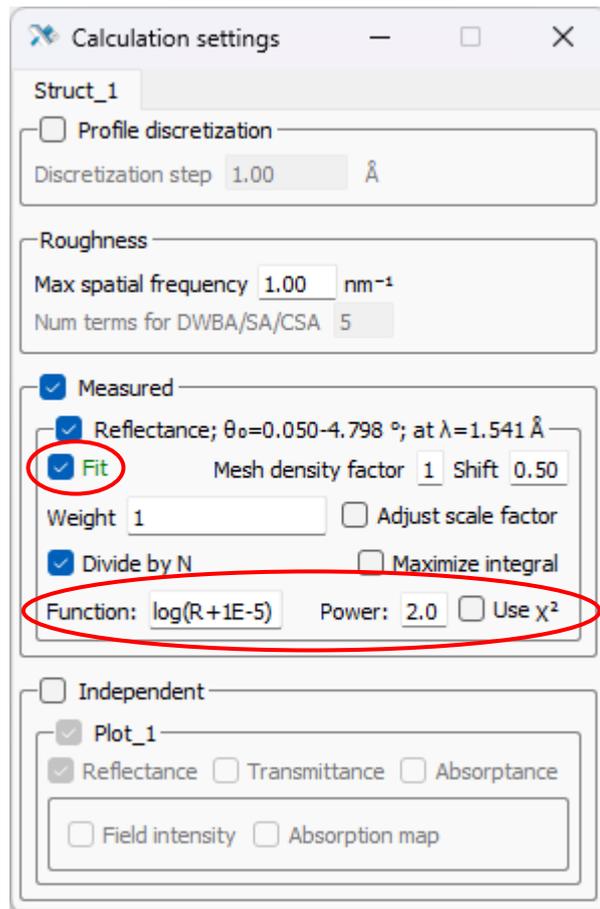


Figure 39. Curve fitting tumbler switch and the residual function

The minimization algorithm is selected and configured in the special "[Fitting settings](#)" window, which is also opened from the main window panel.

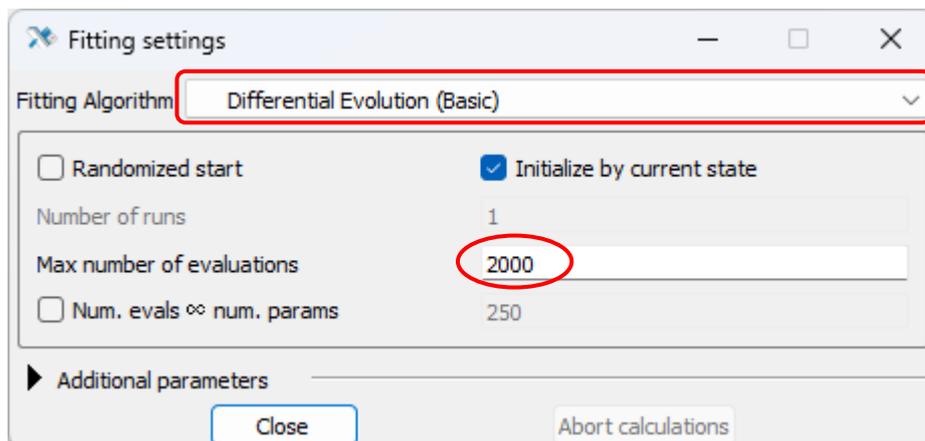


Figure 40. "Fitting settings" window

Here we select "**Differential Evolution (Basic)**" as an algorithm. We leave the number of residual calculations 2000, which is usually enough to cause convergence.

The preparation is over. Now you need to start the fitting by pressing "**Ctrl+Shift+F**" or by selecting "**Start fitting**" from the "**Calculate**" menu of the main window. The calculation process that is displayed

in the console will go. In the console you will see the iteration number, the current values of the variable parameters, and the current residual values.

```

-----
fitting...
-----
S0 "Differential Evolution (Basic)" optimization
iter 0 :1.000000 1.000000 7.100000 31.405000 -0.023000 1.000000 1.000000 3.900000 25.695000 |f|=0.867284
iter 10 :0.871107 0.681943 2.946312 36.696790 -0.031074 0.322832 0.228453 3.197965 28.871324 |f|=7.21889
iter 20 :0.046393 0.014560 19.606953 31.940839 -0.024119 0.928064 0.897122 4.792234 29.285861 |f|=4.04328
iter 30 :0.085437 0.696682 15.545184 28.840906 -0.031507 0.153010 0.635433 19.852061 21.744063 |f|=6.03919
iter 40 :0.526316 0.712750 12.087520 26.097306 -0.016643 0.703102 0.651316 2.562803 22.054125 |f|=6.4954
iter 50 :0.051623 0.169845 12.468597 26.988939 -0.021557 0.759320 0.345747 10.132880 26.880967 |f|=4.43336
iter 60 :0.153446 0.881131 2.704411 27.399153 -0.030452 0.611591 0.081611 9.508235 25.370719 |f|=4.79994
iter 70 :0.667955 0.656753 2.156626 34.935030 -0.021308 0.400616 0.984948 7.741173 29.130881 |f|=6.5955

```

Figure 41. Displaying the fitting process in the console

At the end, a comparison of the initial and final residuals will be displayed in the console. The user will be prompted to accept the result or return to the original state. Clicking "Yes" will update the structure in the table. If not, the structure will revert to the state before fitting.

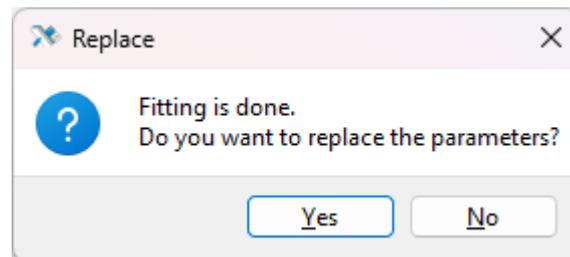


Figure 42. End of fit

It is not always necessary to fit all parameters at the same time, because if the dimension of the parametric space is too high, it is more difficult to find the appropriate range of parameters and the algorithm will converge worse. Therefore, you should turn off and on groups of parameters in successive fittings, combining automatic fitting with manual parameter changes, residual correction, turning auxiliary layers on and off, etc. From one run, it is possible to obtain an acceptable curve fit only for very simple structures with a minimum of parameters. In the general case, fitting is an iterative process that requires manual intervention. As a result of the combined search, you can get something like the following picture:

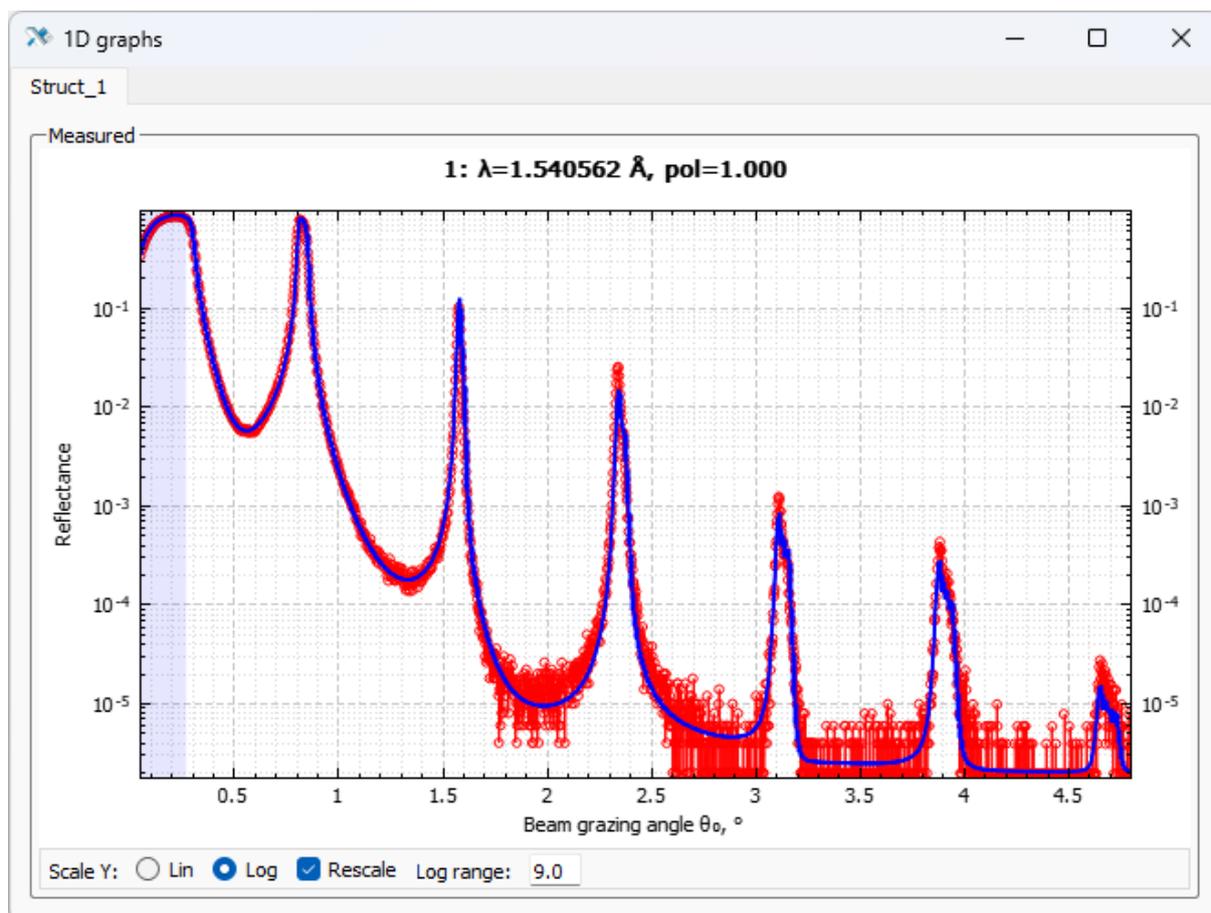


Figure 43. Resulting fit

The found structure corresponding to the picture above has the following parameters:

```

ambient: Vacuum
BeO layer (1), z=16.750Å, ρ=0.999, s=12.548Å
▼ Multilayer (2 - 3), N=110, d=56.658Å, γ=0.586
  Be layer (2), z=33.181Å, ρ=1.000, s=5.522Å
  ---> dz = {line, -0.0245%}
  Mo layer (3), z=23.477Å, ρ=0.951, s=3.170Å
  ---> dz = {line, -0.0245%}
Si substrate, ρ=1.000, s=3.000Å

```

Figure 44. Structure parameters

An important question: does the coincidence of the reflection curves mean the truth of the found parameters? No, it does not mean, but it is a weighty argument for operating with the found values in further work. Assessing the reliability of certain data requires some experience of such "reconstruction" work and experience with real structures; it is also highly desirable to draw on the results of additional sample studies.

### 3.6 Additional experimental curves

Good agreement between calculated and measured curves in one spectral range does not mean agreement in another. Therefore, it is important to use for modeling not just single curves, but data sets.

Let us add for the considered Mo/Be mirror the spectral reflection curve obtained at near-normal angle. To do this, at the bottom of the main Multifitting window on the existing experimental curve, click the "Add row" button. Another line will appear in which you can load the experimental curve in the same way as it was done the first time:

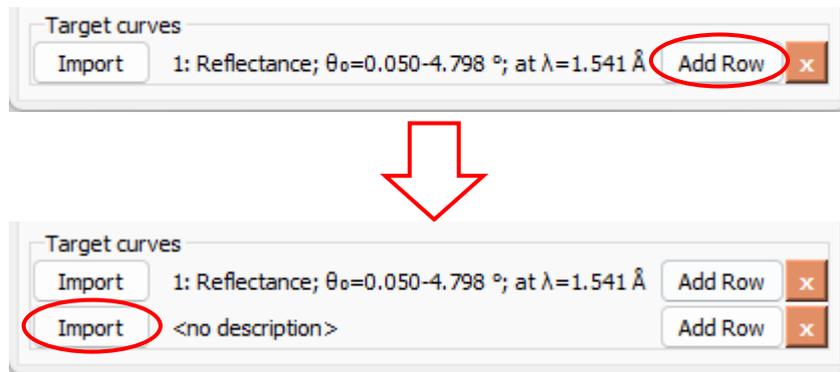


Figure 45. Adding a second curve

After clicking on the "Import" button, select the type of curve "Specular scan". The corresponding window opens, in which you should drag-and-drop the file with the second curve, "Sample\_D364\_Mo\_Be\_spectral\_88deg.txt".

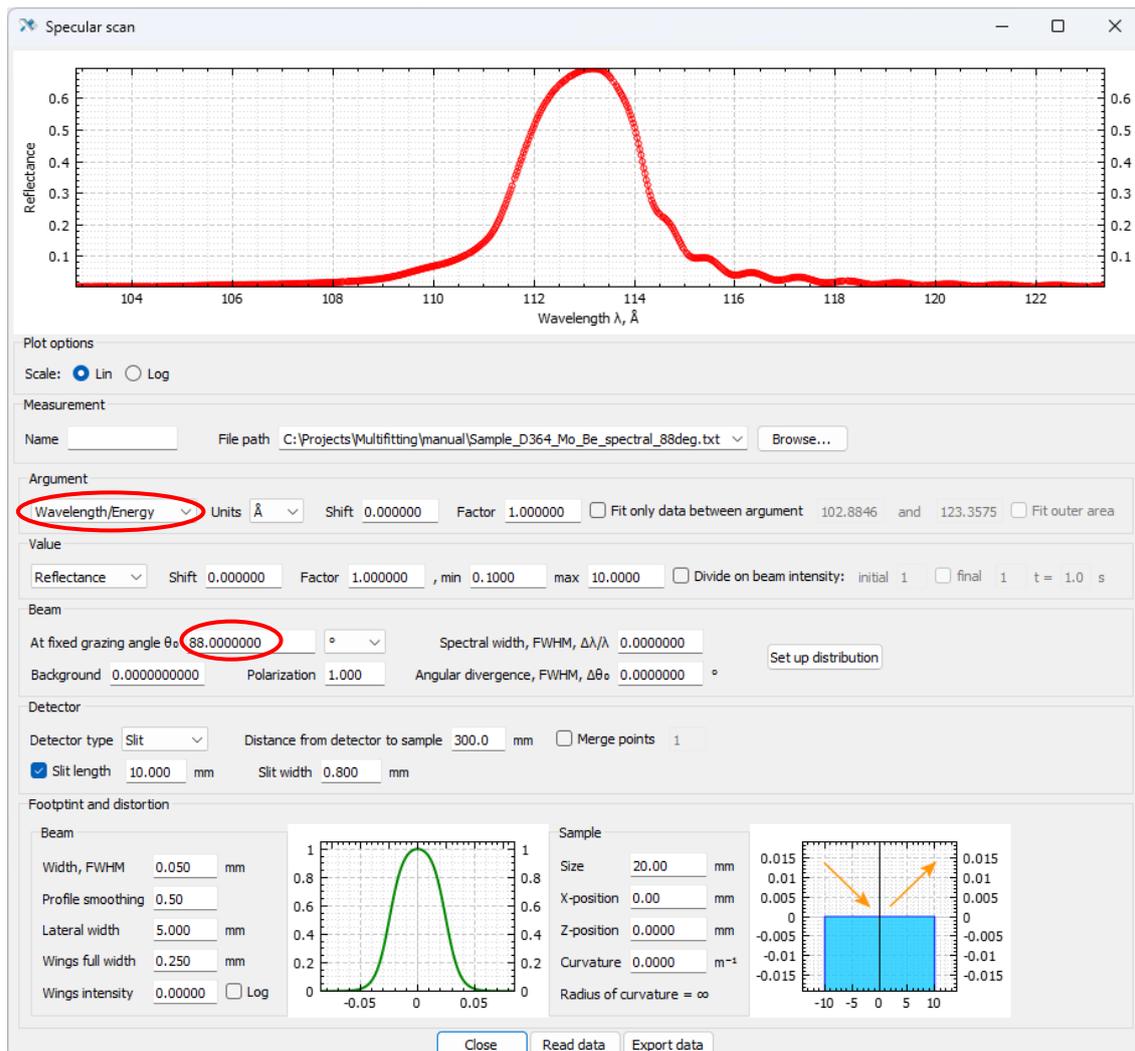


Figure 46. Spectral curve

Compared to the default parameters, you should change the argument type to "**Wavelength/Energy**", make sure that the argument units are "**Å**", since in this file the wavelengths are given in angstroms, set the grazing angle to 88°. Now you can close the import window.

There are now two curves in the "**1D graphs**" window. Options for both curves are now available in the "**Calculation settings**" window. It is possible to fit two curves at the same time, if both of them have the "**Fit**" checkboxes enabled. The total residual is the root-mean-square sum of the residuals of each curve with the corresponding weight, which can also be set in the "**Weight**" field. Let's adjust the parameters to increase the contribution of the spectral curve, and run the fitting again by pressing "**Ctrl+Shift+F**".

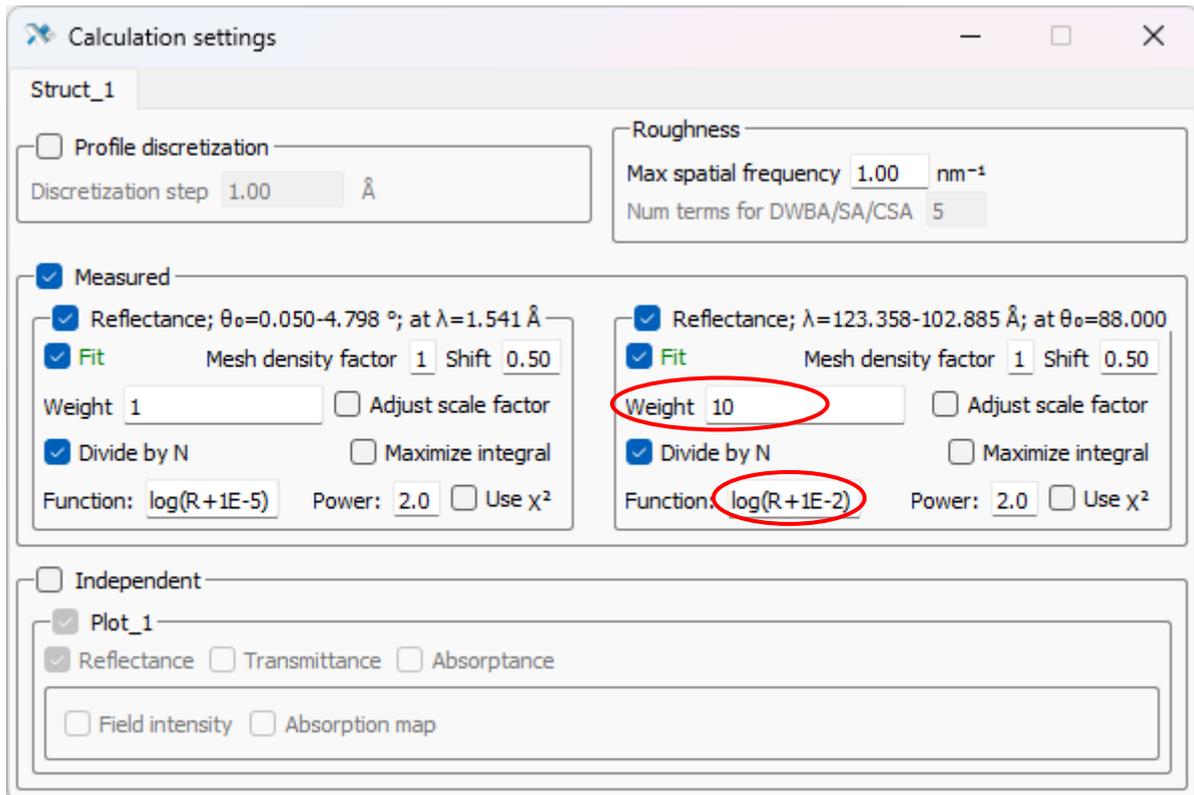


Figure 47. Setting the ratio between curve contributions

By changing the relative weight, adjusting the residual function and the fit interval you can move focus between the curves and areas inside curves.

Our final result:

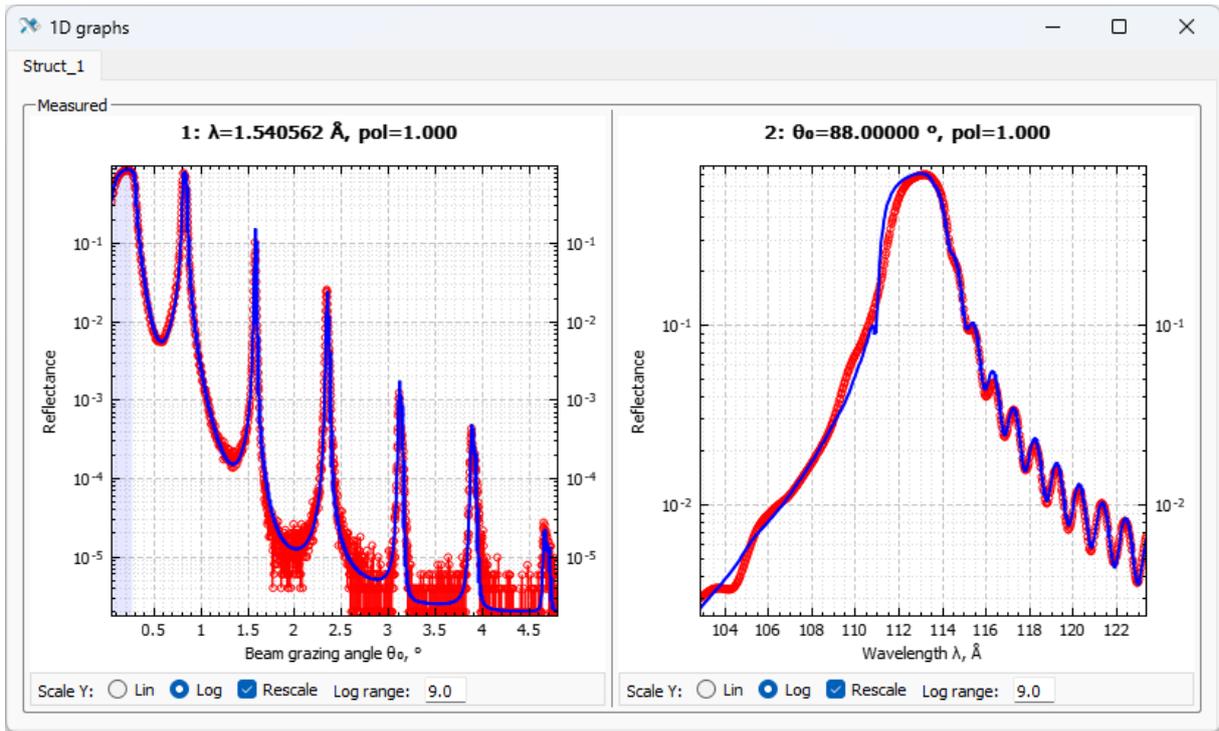


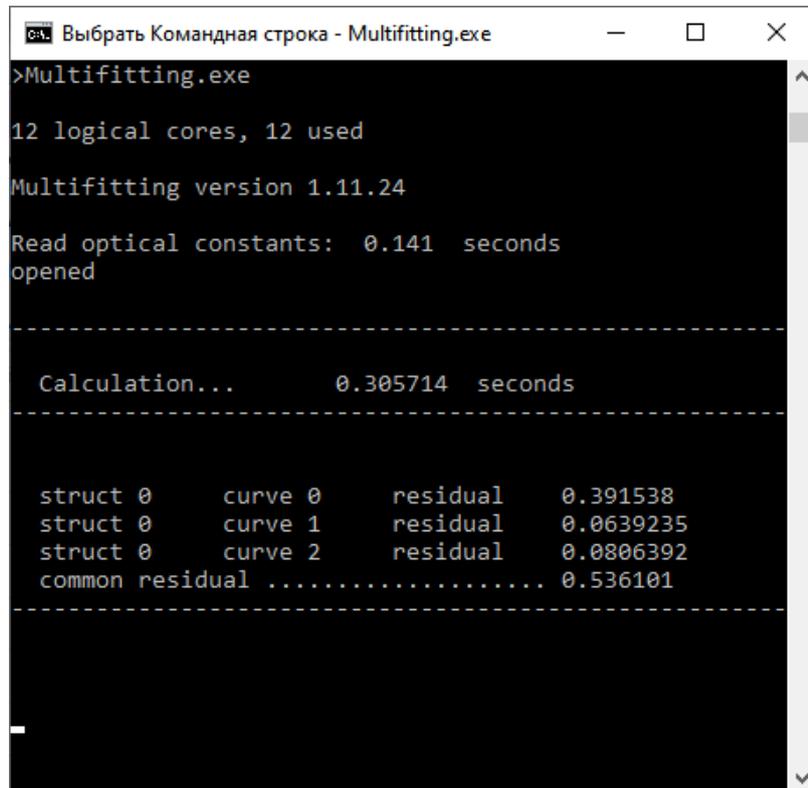
Figure 48. The result of fitting on two curves at the same time

## 4 User interface

Multifitting has a multi-window interface, which makes it possible to see a large number of currently required parameters. Multi-window allows one to use the program more conveniently when working with multiple monitors. The position and size of windows is saved automatically: the next time you open the program, the windows will open in the same positions as the previous time. The window geometry is saved during normal completion, i.e. when the main window is closed, but does not occur during an abnormal, i.e. during crashes as a result of an error, closing the command line from which the program was launched, or when forced closing by means of the operating system.

### 4.1 Console

The console serves to display both text information about the current state of the program and messages about internal program errors. It will start automatically when you run the Multifitting executable, but I recommend that you first open the console separately, and then run Multifitting in it; thus, if the program crashes, the output will not be lost and the reason for the crash can be determined.



```
>Multifitting.exe
12 logical cores, 12 used
Multifitting version 1.11.24
Read optical constants: 0.141 seconds
opened
-----
Calculation... 0.305714 seconds
-----
struct 0      curve 0      residual    0.391538
struct 0      curve 1      residual    0.0639235
struct 0      curve 2      residual    0.0806392
common residual ..... 0.536101
-----
```

Figure 49. Example information on the console

The console displays information about the facts of opening and saving projects, about the calculation time, about the discrepancy between the measured and calculated curves. While fitting, the iteration number, the value of the total residual and the current values of the varied parameters are displayed in the console, which allows you to monitor the progress of the operation.

## 4.2 Main window

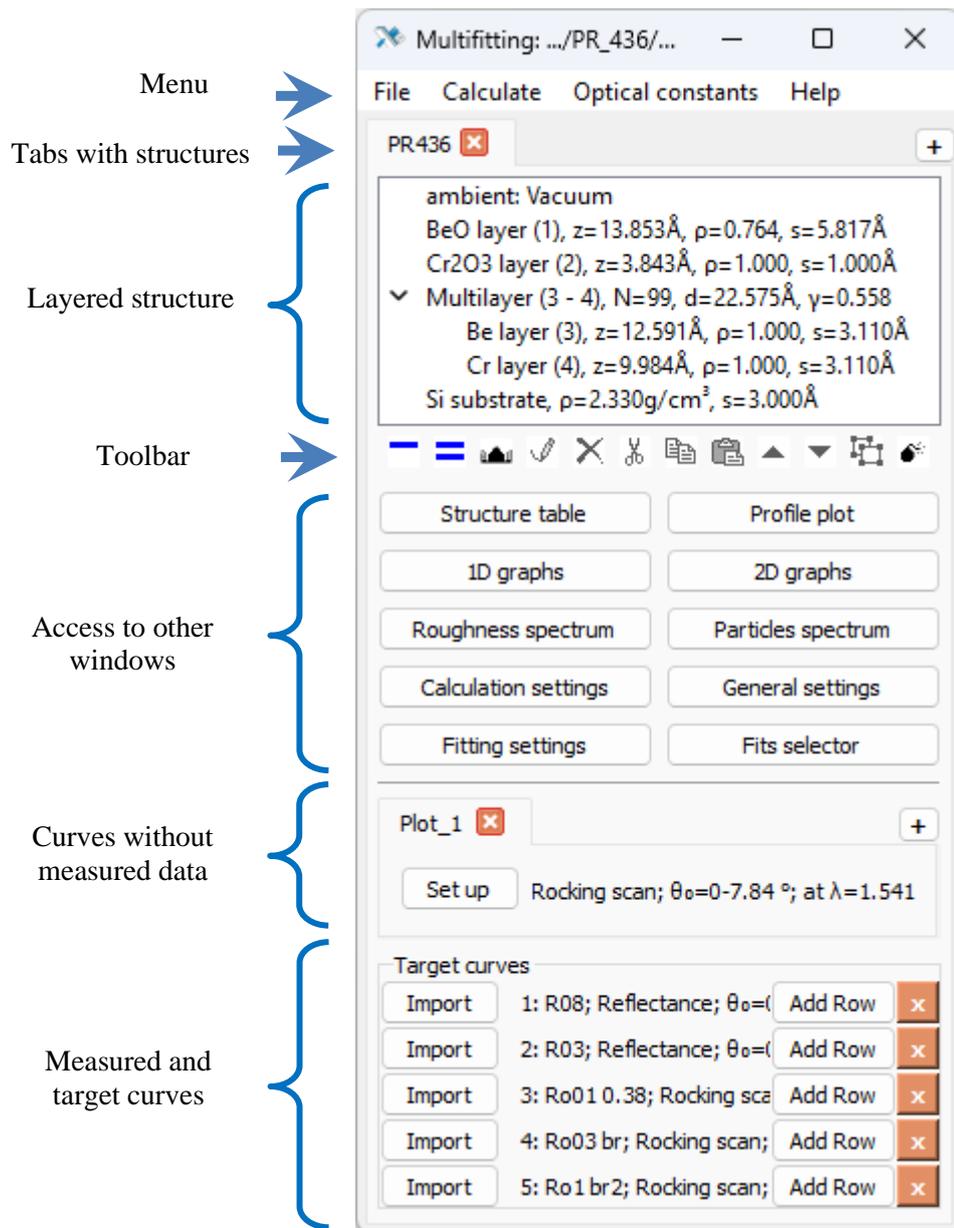


Figure 50. Structure of main window

The main window appears when you start the program and largely repeats the main IMD window. The various zones are arranged vertically in the main window. The first area from the top is the main menu.

### 4.2.1 Menu

#### 4.1.1.1 File

Menu "File" contains mainly actions for loading and saving data. Almost all of them have corresponding keyboard shortcuts. Related settings are also in window "[General settings](#)". Details regarding file names and contents are described in chapter [Importing and exporting data](#).

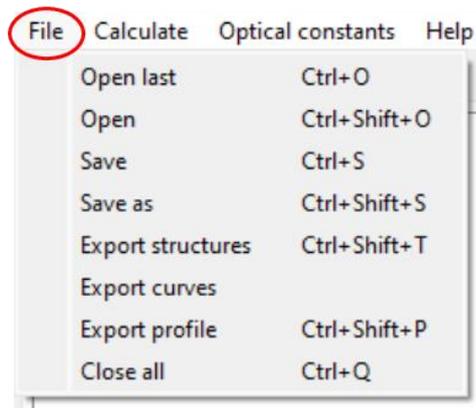


Figure 51. Menu "File"

- **"Open last"** – the exact action depends on the settings. The main point is to start working with the last project immediately after starting the program. If the **"Always open last file"** option is enabled in the **"General settings"** window, the last project will be opened even after fresh start of the program. If this option is disabled, then only the last project in the session will be opened. If such a file does not exist, a corresponding notification will be shown. The working directory is also set in the **"General settings"** window.
- **"Open"** opens a dialog box for selecting a project file.
- **"Save"** saves the current project. If the project is new, the dialog box will appear.
- **"Save as"** opens a dialog for saving the project.
- **"Export structures"** saves information about the layered structure in the text file **"structure\_<struct\_name>.txt"**, where **"<struct\_name>"** – is the name of a specific structure (tab). If there are several tabs, there will also be several files.
- **"Export curves"** calculates and saves all calculated curves in text files named **"<struct\_name>\_target\_<N>\_<curve\_name>.txt"** or **"<struct\_name>\_independent\_<curve\_name>.txt"**. **"target"** or **"independent"** means that the curve is calculated on an independent or experimental grid. **"<N>"** – is the serial number of the experimental curve, counting from one. **"<curve\_name>"** is the editable name of the curve.
- **"Export profile"** exports a layered structure profile to a file. Depending on the settings, the profile describes dielectric permittivity, the relative density of the material, the concentration of chemical elements.

#### 4.1.1.2 Calculate

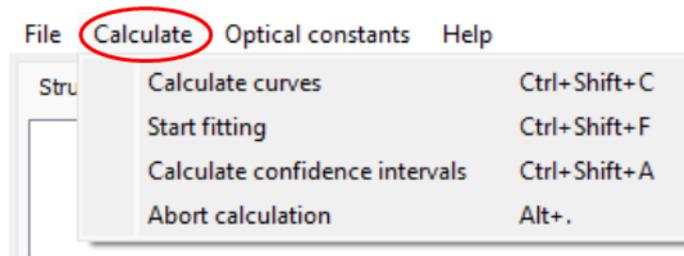


Figure 52. Menu "Calculate"

- "Calculate curves" starts a single calculation. Calculation results can be automatically saved to a text file, depending on the "[General settings](#)".
- "Start fitting" starts automatic fitting.
- "Calculate confidence intervals" runs a series of fits at different values of the estimated parameters to determine confidence intervals. The result is saved in the file "confidence.txt"
- "Abort calculation" stops the current fit.

#### 4.1.1.3 Optical constants

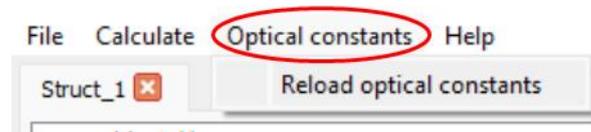


Figure 53. Menu "Optical constants"

- "Reload optical constants" re-reads the database of optical constants from the folders "nk" and "f1f2". This allows you to apply changes made to the database without restarting the program.

#### 4.1.1.4 Help

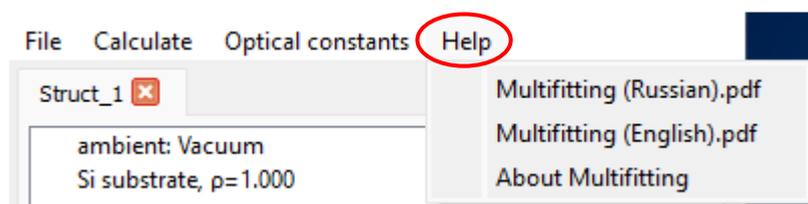


Figure 54. Menu "Help"

- "Multifitting (Russian).pdf" opens the manual in Russian.

- "Multifitting (English).pdf" opens the manual in English.
- "About Multifitting" shows an information window.

## 4.2.2 Structure tabs

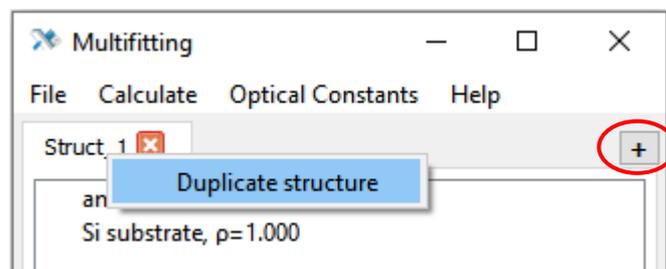


Figure 55. Adding a structure: duplicating an existing one or creating a new one

The main window contains one or more tabs, each dedicated to one structure. You can change the name of a tab by double-clicking on it.

*Note:* It is recommended that you always assign unique names to your modeled structures. If the structure corresponds to a real sample, give the name of this sample. So later you will always be able to see what exactly you are working with. This is especially important if there are several structures in one project.

Also, each tab with all its contents can be duplicated by calling the context menu with the right mouse button. You can destroy the structure by pressing the red button with a cross on the tab. To add a new "blank" tab, click on the "+" button in the upper right corner. By dragging the tabs, you can change their order. If at least one of the windows "Structure table", "Profile plot", "1D graphs", "2D graphs", "Roughness spectrum", "Particles spectrum", "Calculation settings" is open in parallel, then the ability to add, remove and move tabs are blocked. All listed windows contain as many tabs as the main window.

## 4.2.3 Layered structure

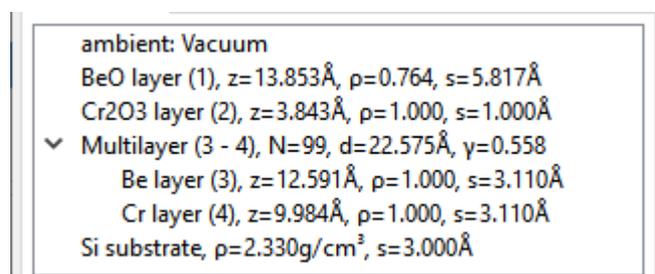


Figure 56. Tree-like list describing the structure

Under the name of the tab there is a window with a tree-like list illustrating the general view of the multilayer structure and showing basic information about its parameters. For layers, this is the material, the thickness "z", the spread of thicknesses (if the layer is part of a "regular" aperiodic), the relative or

absolute density " $\rho$ ", the root-mean-square thickness of the transition region at the upper boundary of the given layer " $s$ ". For a substrate, this is the material, density, and thickness of the transition region. For a periodic multilayer, this is the number of periods " $N$ ", the thickness of the period " $d$ ", the thickness factor " $\gamma$ " is the ratio of the thickness of the upper layer to the thickness of the period (if there are two layers in the period).

#### 4.2.4 Toolbar

Below the structure there is a toolbar that allows you to add, delete, copy, paste, and move the components of the structure.

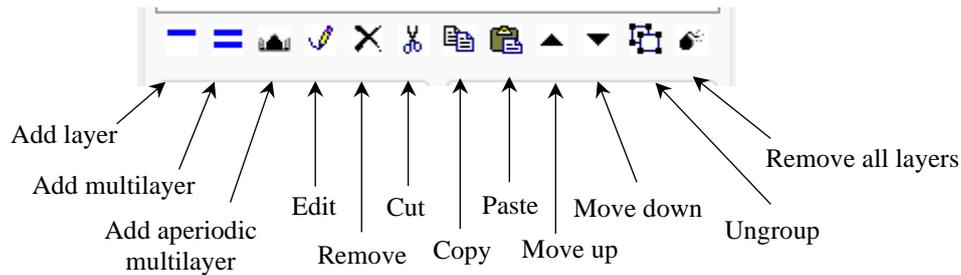


Figure 57. Toolbar

-  "Add layer" inserts a new layer with default settings.
-  "Add multilayer" inserts a periodic structure with two layers per cell and one period by default. You can add new layers to a cell after it has been created.
-  "Add aperiodic multilayer" adds an aperiodic structure read from a text file. See the chapter [Importing and exporting data](#) for details.
-  "Edit" opens a window with the basic properties of the layer/multilayer. An equivalent action is a double click on the corresponding element of the structure. The settings are described in the chapter [Editing a structure element](#).
-  "Remove" removes a structure element. The equivalent is the «Delete» key.
-  "Cut" cuts the structure element and places it on the clipboard. Key combination: "Ctrl+X"
-  "Copy" places the structure element on the clipboard. Key combination: "Ctrl+C"
-  "Paste" pastes a structure element from the clipboard. Key combination: "Ctrl+V"
-  "Move up" moves the element up in the structure.
-  "Move down" moves the element down in the structure.

-  "Ungroup" removes the multilayer and inserts in its place the elements that were in its composition. Reduces the nesting of a structure.
-  "Remove all layers" removes all elements except for the substrate and ambient.

## 4.2.5 Editing a structure element

Double-clicking on a structure element or pressing "Edit" opens a window in which the main characteristics are set. There are several types of elements: layer, substrate, external environment (ambient), periodic multilayer (multilayer), general aperiodic multilayer (general aperiodic), regular aperiodic multilayer (regular aperiodic). You can close the window with the "Close" button, by pressing the "Enter" or "Escape" key.

### 4.2.5.1 Layer

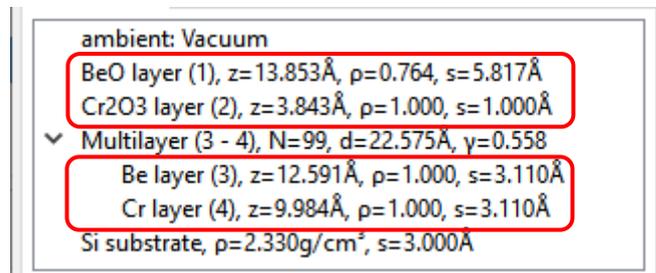


Figure 58. Layers in the structure tree

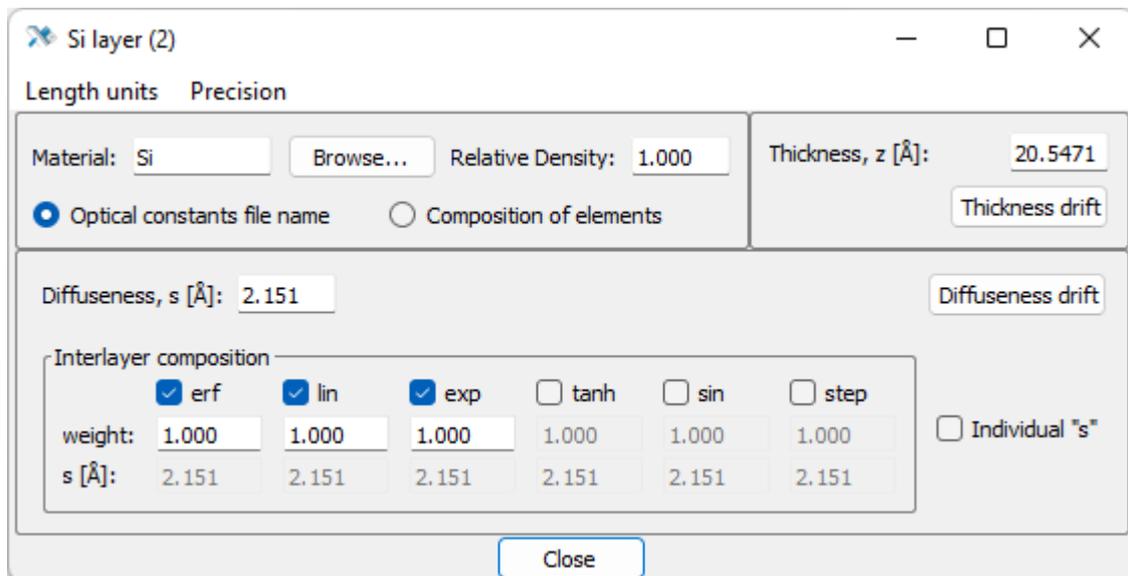


Figure 59. Window "Layer"

Structurally, the window consists of the following parts: title, menu, material setting block, thickness setting block, interlayer interface setting block.

#### 4.2.5.1.1 Title

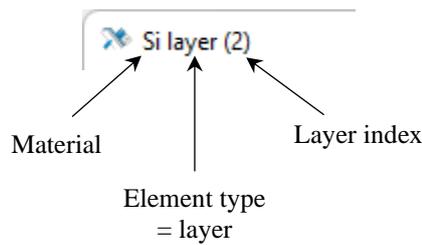


Figure 60. "Layer" window title

The title of the window allows you to uniquely identify which element of the structure you are currently dealing with. Each layer has an index – a unique serial number in the structure, which is indicated in brackets. Only structure layers are indexed. The title also indicates the material of the layer.

#### 4.2.5.1.2 Menu

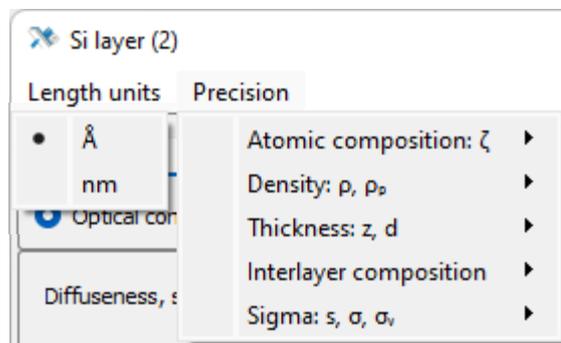


Figure 61. "Layer" window menu

The "Length units" menu allows you to switch the length units for structural parameters. Changes apply to the entire program. In the "Precision" menu, you can change the number of decimals used to represent parameter values.

#### 4.2.5.1.3 Material

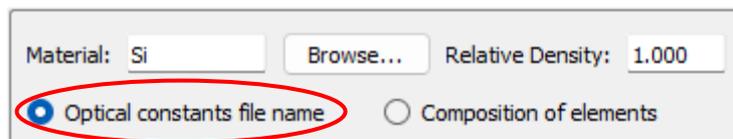


Figure 62. Block "Material" with tabulated material

There are two ways to set a material in Multifitting. The first is to use the refractive index library located in the "nk" folder. To do this, set the switch to the "Optical constants filename" position. In the "Material" field, the name of the text file "\*.nk" is indicated, which also serves as the name of the material. You can also specify a file outside the library by clicking the "Browse..." button. The real density of the material is not necessarily known, as only the refractive index is given. But this density can be changed by setting the "Relative density". This is the factor by which the nominal polarizability of the substance is multiplied.

Another way to define a material is to construct it from chemical elements, specifying stoichiometry and density.

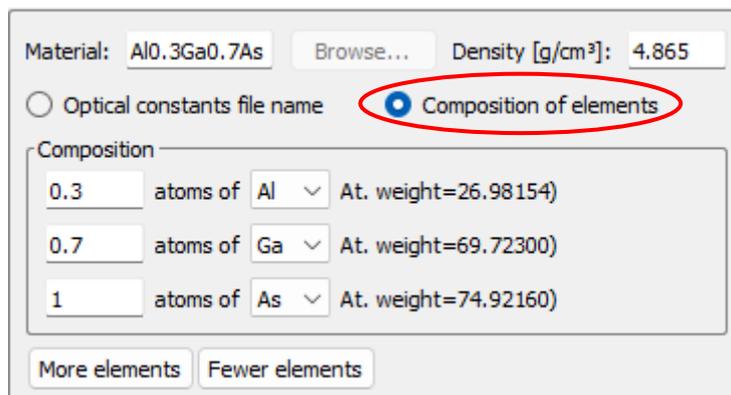


Figure 63. Block "Material" with material composed from chemical elements

To do this, set the radio button to the "Composition of elements" position. The "Material" field will become uneditable. In the "Composition" block, you can add and remove chemical elements using the "More elements" and "Fewer elements" buttons. Each item is selected from a dropdown list. Elements can also be scrolled with the mouse wheel; by pressing a letter on the keyboard, you can jump to an element starting with that letter. If the number of elements is more than one, then you can set the stoichiometric ratio between them. This is precisely the ratio of the number of atoms to each other, i.e. "WSi<sub>2</sub>" is the same as "W<sub>2</sub>Si<sub>4</sub>". The absolute concentration of atoms is given by the absolute density of the material, in g/cm<sup>3</sup>.

#### 4.2.5.1.4 Thickness



Figure 64. Block "Thickness"

Here you can set the thickness of the layer. If a layer is part of a periodic multilayer, then it is duplicated N times during the calculation, where N is the number of periods. In this case, in addition to the base thickness, you can specify the change in the layer thickness from period to period. To do this, there is a button "Thickness drift". If you click on it, a window will open:

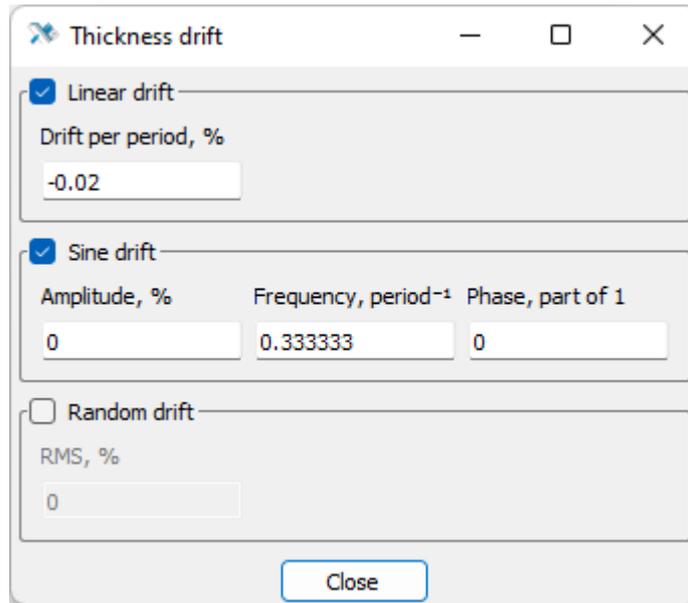


Figure 65. Window "Thickness drift"

"Linear drift" sets the change in the layer thickness along the depth of the structure, proportional to the number of the period. The drift is given as a percentage of the nominal thickness per period. The average layer thickness over all periods is equal to the nominal thickness, i.e. on one part the layers will be thinner, and on the other part thicker.

"Sine drift" sets the periodic change in thickness with depth, described by a sinusoid. The amplitude is set as a percentage of the nominal thickness. The frequency is set in "reverse periods", i.e. a value of 0.3333 means that the layer thickness is repeated every three periods. The phase determines the initial position of the modulating sinusoid, it is set in the range from 0 to 1.

"Random drift" determines the random deviation of the layer thickness from the nominal value. The standard deviation is indicated as a percentage of the nominal thickness. The thicknesses themselves are generated randomly with Gaussian statistics on each curve recalculation.

#### 4.2.5.1.5 Diffuseness

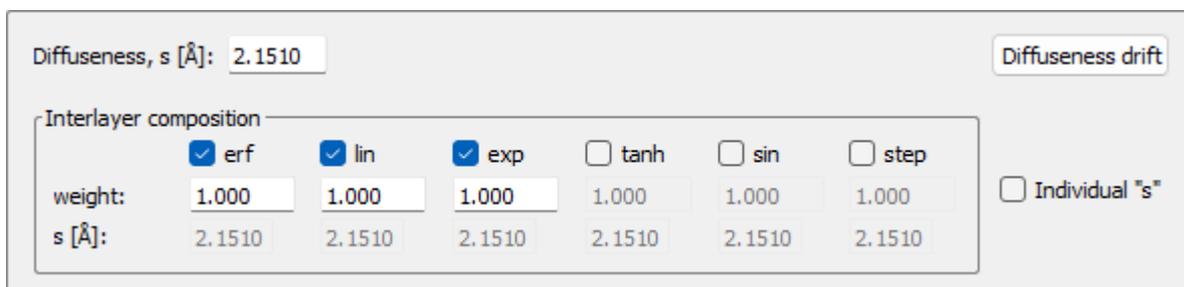


Figure 66. Block "Diffuseness"

"Diffuseness" – is the amount of interpenetration of the materials of the layers into each other, their mixing at the boundary. It can also be understood as a limit of roughness with a lateral correlation tending to zero. The thickness of the transition region is specified in the mean square sense (parameter "s"), and the type of distribution can be selected from several options. The distribution of matter in the transition region is composed of several functions with appropriate weights [3]. By default, the root-

mean-square thickness is the same for all profile functions, but if you enable "Individual "s"", then an individual thickness can be set for each function.

If the layer is part of a periodic multilayer, then, as in the case of the layer thickness, one can also indicate the change in the thickness of the interlayer interface from period to period. To do this, use the "Diffuseness drift" button. The interface drift setting window is [exactly the same](#) as for thickness.

#### 4.2.5.2 Substrate

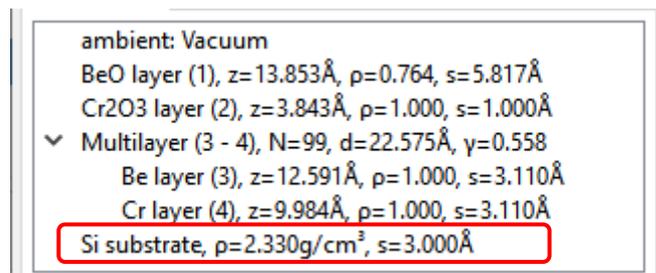


Figure 67. Substrate in the structure tree

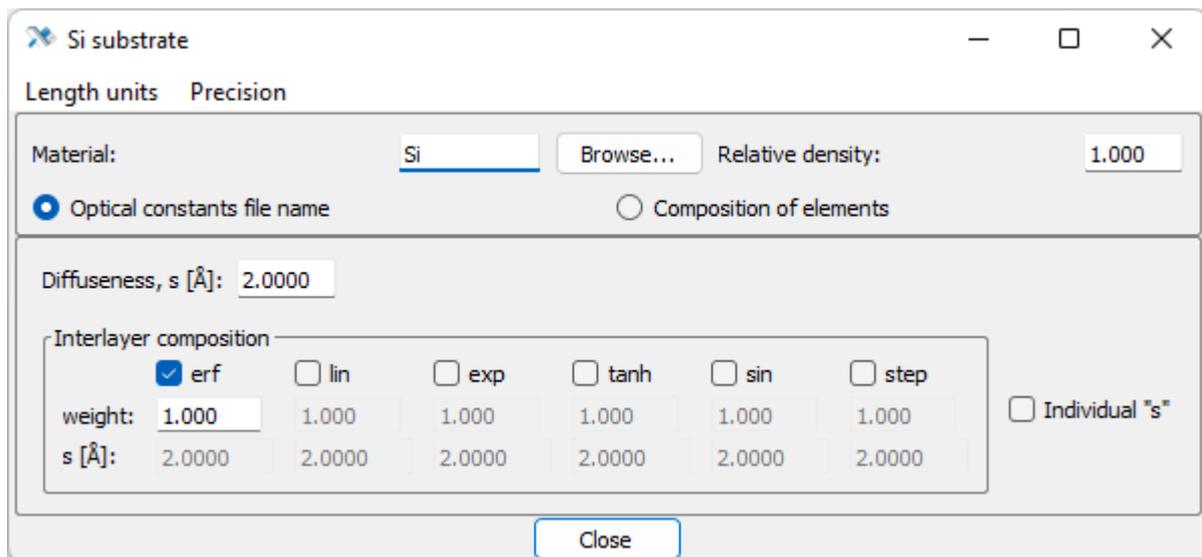


Figure 68. Window "Substrate"

The "Substrate" window is the same as the "Layer", window, but does not contain the thickness. The thickness of the substrate is assumed to be infinite. The title also indicates the material and says that it is a substrate. The [menu](#), [material settings block](#), [interlayer interface settings block](#) are the same as for the layer.

### 4.2.5.3 Ambient

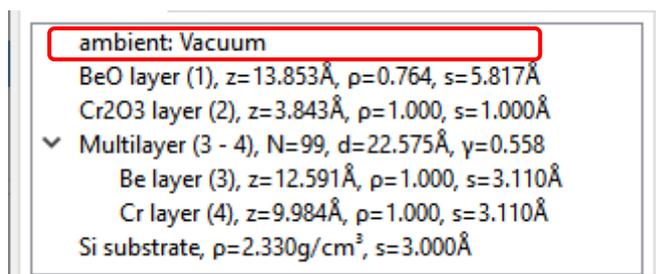


Figure 69. Ambient in the structure tree

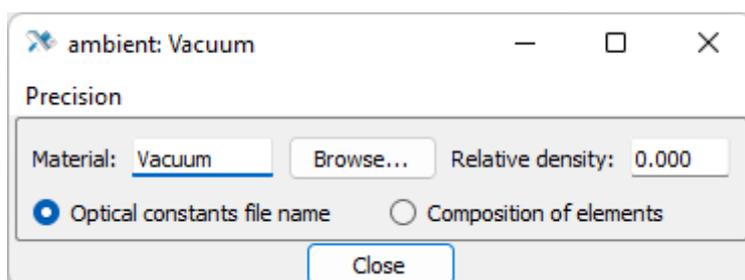


Figure 70. Window "Ambient"

The "Ambient" window is the same as the "Layer", window, but does not contain the thickness and interface. The [menu](#), [material settings block](#), [interlayer interface settings block](#) are the same as for the layer.

### 4.2.5.4 Multilayer

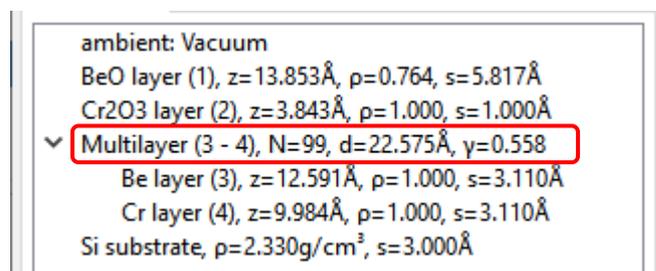


Figure 71. Periodic stack in the structure tree

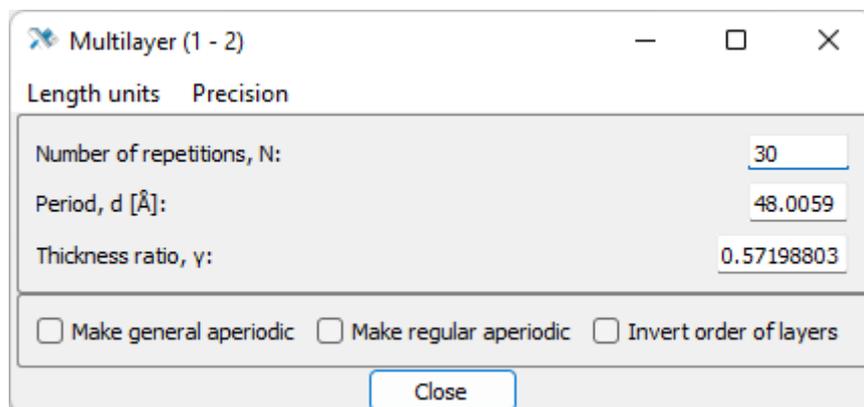


Figure 72. Window "Multilayer"

Structurally, the "Multilayer" window consists of the following parts: title, menu, parameter setting block, structure type control block.

#### 4.2.5.4.1 Title

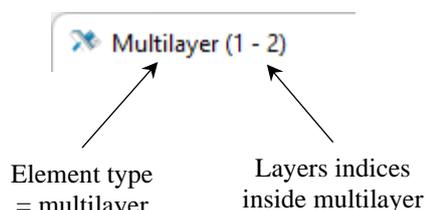


Figure 73. "Multilayer" window title

The window title indicates that you are dealing with a periodic multilayer. The range of indexes of layers inside this structure is indicated in brackets.

#### 4.2.5.4.2 Menu

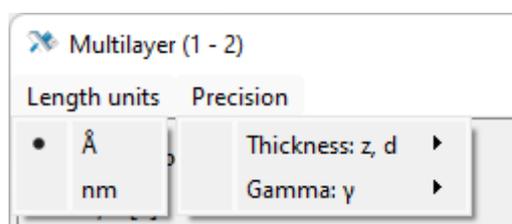


Figure 74. "Multilayer" window menu

The "Length units" menu allows you to switch the length units. In the "Precision" menu, you can change the number of decimal places used to represent parameter values. Changes apply to the entire program.

#### 4.2.5.4.3 Parameters

Number of repetitions, N:	30
Period, d [Å]:	48.0059
Thickness ratio, γ:	0.57198803

Figure 75. Parameter setting block

The first parameter of the periodic multilayer is the number of periods  $N = 0, 1, 2 \dots$

The second parameter is the period, i.e. thickness of an unit cell consisting of several layers.

The third parameter is the thickness factor  $\gamma$ . This is the ratio of the thickness of the upper layer of the unit cell to the period. The thickness factor appears only when the number of layers in a period is two. With more layers, it becomes meaningless.

#### 4.2.5.4 Structure type management

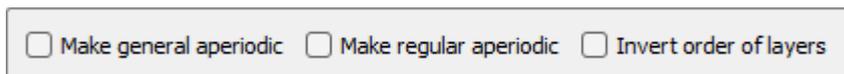


Figure 76. Structure type control block

A periodic multilayer can be turned into a regular or general aperiodic by selecting the appropriate option. In this case, the number of layers in the aperiodic will correspond to the total number of layers in the periodic structure, taking into account the number of periods. An exception is if there are 0 periods in the periodic structure, then the number of periods will first be increased to 1 and only then the periodic will be turned into aperiodic.

"**Invert order of layers**" allows you to quickly change the order of the layers in the unit cell to the opposite.

#### 4.2.5.5 Regular aperiodic

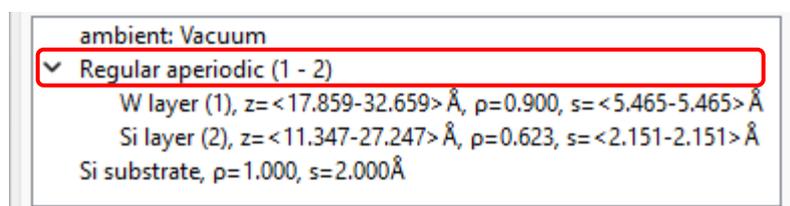


Figure 77. Regular aperiodic in the structure tree

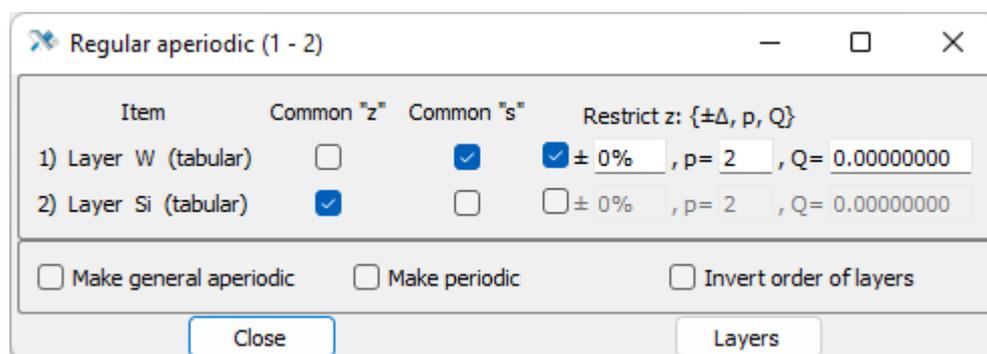


Figure 78. Window "**Regular aperiodic**"

Structurally, the "**Regular aperiodic**" window consists of the following parts: title, parameter limit block, structure type control block.

The "**Layers**" button opens the [detailed layer table](#).

#### 4.2.5.5.1 Title

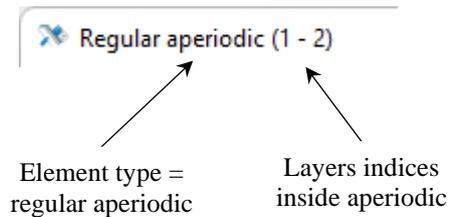


Figure 79. "Regular aperiodic" window header

The title of the window indicates that you are dealing with a regular aperiodic. The range of indexes of layers inside this structure is indicated in brackets.

#### 4.2.5.5.2 Parameters

Item	Common "z"	Common "s"	Restrict z: {±Δ, p, Q}
1) Layer W (tabular)	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> ± 4% , p= 2 , Q= 12.34500000
2) Layer Si (tabular)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/> ± 0% , p= 2 , Q= 0.00000000

Figure 80. Parameter setting block

In this window you cannot work directly with the parameters of the layers, but it is possible to impose connections and restrictions on the thicknesses and interfaces of "same" layers in different unit cells of the aperiodic. For each layer, the material is indicated, as well as whether this material is composed of chemical elements – "(composed)" – or taken from a library of ready-made materials – "(tabular)".

"Common "z"" indicates that all layers with the given index will have the same thickness in all unit cells.

"Common "s"" indicates that all layers with the given index will have the same diffuse interfaces in all unit cells.

If "Common "z"" and "Common "s"" are enabled for all layers, then the structure is periodic.

"Restrict z: {±Δ, p, Q}" indicates that a "soft" restriction will be applied during automatic optimization of thicknesses: if the thickness of any layer differs by more than Δ from the average thickness of layers of this type, then to the value a "penalty" will be added to the minimized function, namely the following value:  $Q \times \left| z - \langle z \rangle - \Delta \right|^p$ , where z is the layer thickness,  $\langle z \rangle$  is the average thickness of layers of this type, p is the exponent responsible for the rate of increase of the penalty with increasing deviation, and Q is the weight factor. Thus, it is "unfavorable" for thicknesses to go far beyond the indicated limits ±Δ.

#### 4.2.5.5.3 Structure type management

<input type="checkbox"/> Make general aperiodic	<input type="checkbox"/> Make periodic	<input type="checkbox"/> Invert order of layers
---	--	---

Figure 81. Structure type control block

A regular aperiodic can be turned into a periodic structure or a general aperiodic by selecting the appropriate option.

#### 4.2.5.6 General aperiodic

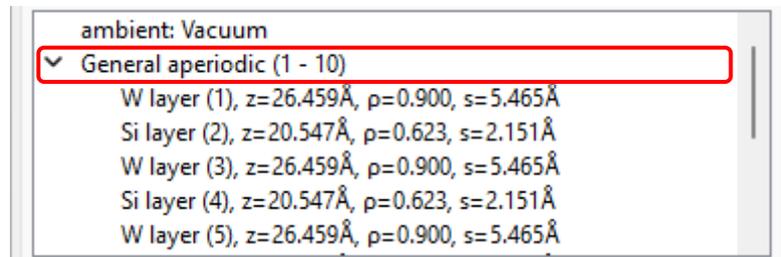


Figure 82. General aperiodic in the structure tree

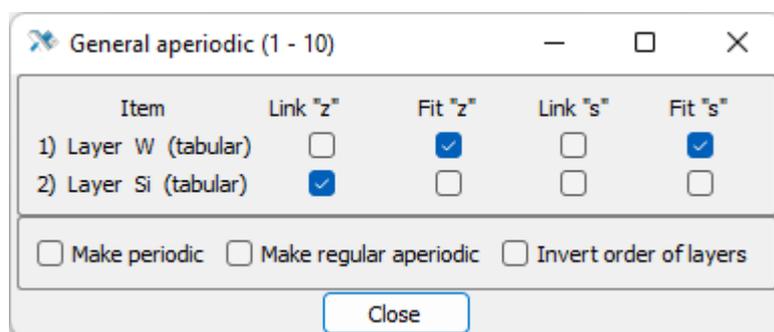


Figure 83. Window "General aperiodic"

Structurally, the "General aperiodic" window consists of the following parts: title, parameter restriction block, structure type control block.

##### 4.2.5.6.1 Title

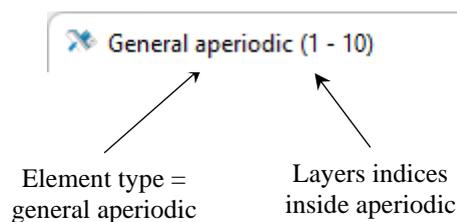


Figure 84. "General aperiodic" window header

The title of the window indicates that you are dealing with general aperiodic. The parentheses indicate the range of layer indices within this structure. In contrast to a periodic structure or regular aperiodic, here all layers are present as separate elements. The structure is "unwrapped".

##### 4.2.5.6.2 Parameters



Figure 85. Parameter setting block

The general aperiodic does not control the parameters of the layers contained in it, but it allows you to massively apply and remove links between the thicknesses or interfaces and massively turn their fitting on and off. Unlike regular aperiodic, there is no concept of an unit cell; layers can be absolutely arbitrary. Therefore, the various "types" of layers listed in this box are determined solely by the material of the layer. This takes into account the use of tabular data for the finished material "(tabular)" or compositions of individual chemical elements "(composed)".

"Link "z"" indicates that all the thicknesses of all layers with this material will be dependent on the thickness of the top layer. The linking function can be set individually in the parameter table. Likewise, "Link "s"" links layer interfaces.

"Fit "z"" turns on/off the thickness fitting for all layers of the corresponding material. "Fit "s"" does the same for interfaces.

#### 4.2.5.6.3 Structure type management

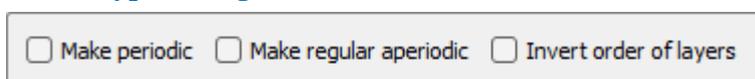


Figure 86. Structure type control block

A general aperiodic can be turned into a regular or periodic structure by selecting the appropriate option. If, in addition, the aperiodic contains a periodic subsequence of materials, then this subsequence will become an unit cell. Otherwise, the structure cannot be "folded" and the unit cell will be the size of the entire common aperiodic.

#### 4.2.6 Window access bar

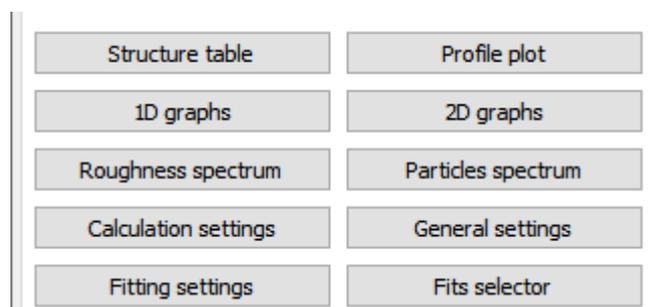


Figure 87. Access to other instruments

Next are the buttons for accessing auxiliary tools that allow you to control the structure parameters in detail, build graphs, make automatic fitting and change various settings. All of them are described in the corresponding paragraphs of this chapter.

## 4.2.7 Independent curves

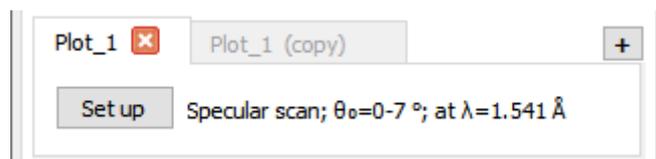


Figure 88. Tabs with curves for calculations without an experimental grid

Next are the controls of so-called "independent" curves. To set and calculate independent curves, you do not need to involve any external data, just specify the type of measurement, instrumental parameters, set the type and range of argument values, and the number of points for calculation.

Each independent curve corresponds to a tab. You can create new, duplicate, delete in the same way as [Structure tabs](#). Double clicking on the tab allows you to set the name of the curve. To the right of the "Set up" button, the basic information is written: the type of measurement, ranges or values of angles and wavelengths.

The "Set up" button opens the curve settings window. If this happens in a new tab where the measurement type has not yet been set, then a window will open with a choice of options:

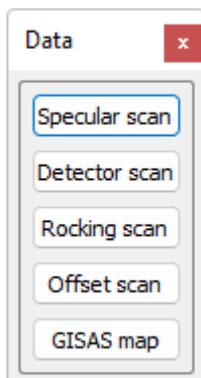


Figure 89. Scan type selection

After setting the curve type, the corresponding settings window will open.

### 4.2.7.1 Specular scan

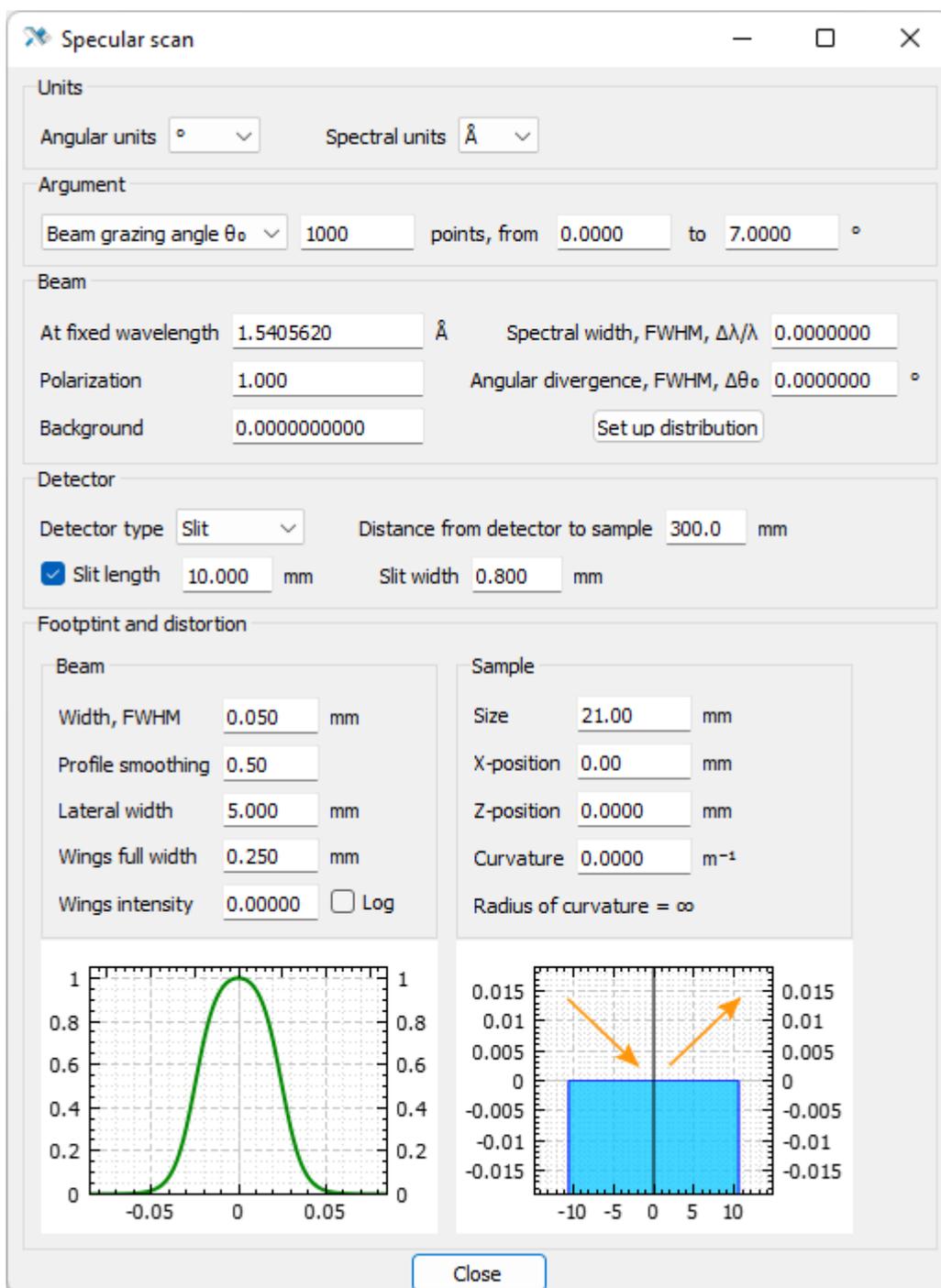


Figure 90. Reflectometric curve settings

All settings are divided into several groups arranged vertically: "Units", "Argument", "Beam", "Detector", "Footprint and distortion". You can close the window by clicking "Close" or pressing the "Escape" key.

#### 4.2.7.1.1 Units

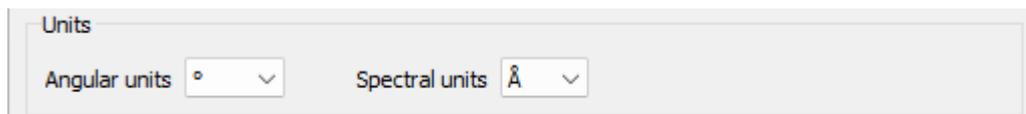


Figure 91. Block "Units"

Angular and spectral units are set here. When the units are changed, the displayed parameter values are recalculated. This block is the same for all types of curves.

#### 4.2.7.1.2 Argument

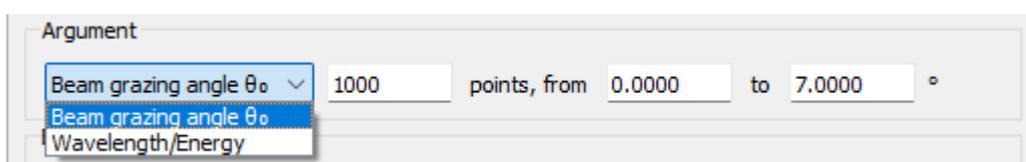


Figure 92. Block "Argument"

The argument type (beam grazing angle or wavelength), number of points, and range are specified.

#### 4.2.7.1.3 Beam

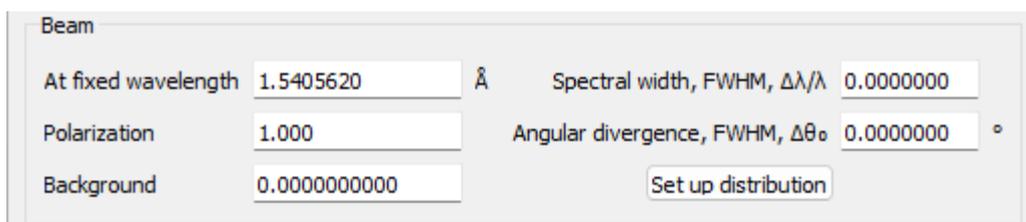


Figure 93. Block "Beam"

If the argument is the beam grazing angle, then a fixed wavelength is specified here. If the argument is the wavelength, then a fixed grazing angle is specified here. You can also specify the spectral width of the beam and the angular divergence in the plane of incidence. The FWHM value is set – full width at half maximum.

Additionally, you can specify the polarization of the incident beam: 1 is the s-polarization, -1 is the p-polarization, and intermediate values correspond to their mixture in the appropriate proportion.

Background is the amount of intensity that is added to all points of the calculated curve. It does not affect the calculations and the automatic fitting process. It is intended for the convenience of comparing the calculated and measured curves.

#### 4.2.7.1.4 Detector

Figure 94. Block "Detector" with slit (a) or crystal (b) detector type

The type and parameters of the detector are specified here. The parameters are the sample-detector distance, the azimuth size of the detector window ("Slit length"). If the detector is slit, then the polar size of the detector is given by the width of the slit. If the detector contains an analyzer crystal – then by the peak width and shape. This block is the same for all one-dimensional curves (i.e. except GISAS).

#### 4.2.7.1.5 Footprint and distortion

Figure 95. Block "Footprint and distortion"

This block is the same for all types of curves. Here the geometrical parameters of the beam and the sample are specified. The width in the plane of incidence, profile ("Profile smoothing"), the size in the direction perpendicular to the plane of incidence ("Lateral width"), is set for the beam. In addition to the main bell-shaped form, the profile section may have an additional wide elevation of low intensity ("Wings"). The beam profile in the plane of incidence is shown on the graph in a linear or logarithmic scale.

The sample has a size in the direction of the beam, a displacement along the beam ("X-position"), vertical displacement towards the surface ("Z-position"), curvature. These parameters are illustrated by the sample image with beam.

#### 4.2.7.2 Detector scan

Blocks "[Units](#)", "[Detector](#)", "[Footprint and distortion](#)" are exactly the same as for specular geometry.

##### 4.2.7.2.1 Argument

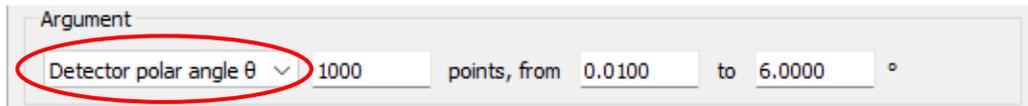


Figure 96. Block "Argument"

The argument is the polar angle of the detector, for which the number of points and the range are specified.

##### 4.2.7.2.2 Beam

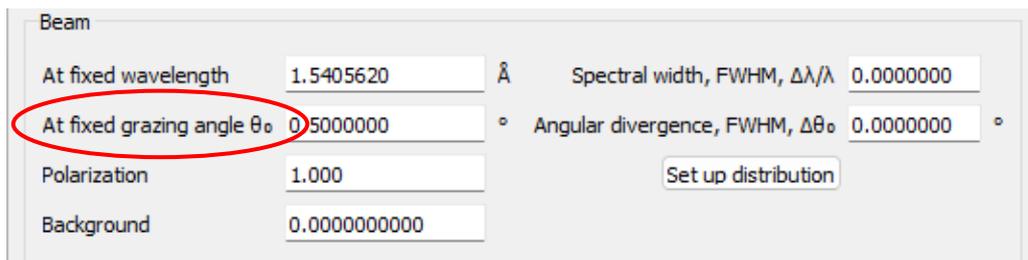


Figure 97. Block "Beam"

Almost all parameters are the same as in [specular geometry](#). An additional parameter is a fixed beam grazing angle (or specular angle).

#### 4.2.7.3 Rocking scan

Blocks "[Units](#)", "[Detector](#)", "[Footprint and distortion](#)" are exactly the same as for specular geometry.

##### 4.2.7.3.1 Argument

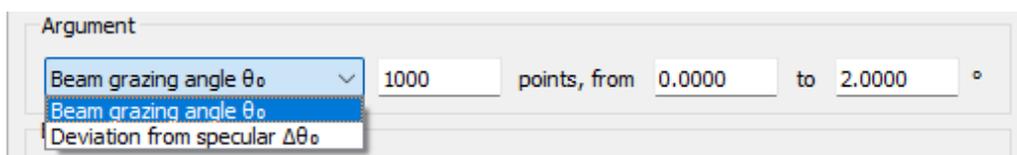


Figure 98. Block "Argument"

When calculating the rocking curve, both the beam grazing angle and the scattering angle change. As an argument, one can choose either the beam grazing angle or the deviation of the sample from the specular position.

#### 4.2.7.3.2 Beam

Beam				
At fixed wavelength	1.5405620	Å	Spectral width, FWHM, $\Delta\lambda/\lambda$	0.0000000
Specular position	1.0000000	°	Angular divergence, FWHM, $\Delta\theta$	0.0000000
Polarization	1.000		Set up distribution	
Background	0.0000000000			

Figure 99. Block "Beam"

Almost all parameters are the same as in [specular geometry](#). An additional parameter is the specular position, i.e. the angle of the incident beam at which the reflected beam arrives at the detector.

#### 4.2.7.4 Offset scan

Blocks "[Units](#)", "[Argument](#)", "[Detector](#)", "[Footprint and distortion](#)" are exactly the same as for specular geometry.

##### 4.2.7.4.1 Beam

Beam				
At fixed wavelength	1.5405620	Å	Spectral width, FWHM, $\Delta\lambda/\lambda$	0.0000000
At fixed detector offset	0.0000000	°	Angular divergence, FWHM, $\Delta\theta$	0.0000000
Polarization	1.000		Set up distribution	
Background	0.0000000000			

Figure 100. Block "Beam"

Almost all parameters are the same as in [specular geometry](#). An additional parameter is a constant angular shift of the detector from the specular position.

#### 4.2.7.5 GISAS map

Blocks "[Units](#)", "[Detector](#)", "[Footprint and distortion](#)" are exactly the same as for specular geometry.

##### 4.2.7.5.1 Argument

Argument					
Detector polar angle $\theta$	1000	points, from	0.0100	to	6.0000
Detector azimuthal angle $\phi$	501	points, from	-1.3000	to	1.3000

Figure 101. Block "Argument"

Scattering is two-dimensional, so there are two arguments here: the polar and azimuthal angles of the detector. Each is given by a number of points and a range of values.

#### 4.2.7.5.2 Beam

Figure 102. Block "Beam"

Almost all parameters are the same as in [specular geometry](#). Additionally, the beam grazing angle and the azimuthal angular divergence of the beam are specified.

#### 4.2.7.5.3 Detector

Figure 103. Block "Detector" with spherical (a) or pixel (b) detector type

Here the sample-detector distance and, if necessary, the angular or linear size of the pixel and the instrumental function are specified.

### 4.2.8 Experimental curves

Target curves		
Import	1: R08; Reflectance; $\theta_0=0.005-6.995^\circ$ ; at $\lambda=1.541 \text{ \AA}$	Add Row <input type="button" value="x"/>
Import	2: R03; Reflectance; $\theta_0=0.005-7.995^\circ$ ; at $\lambda=1.541 \text{ \AA}$	Add Row <input type="button" value="x"/>
Import	3: Ro03 br; Rocking scan; $\theta_0=0.010-3.940^\circ$ ; at $\lambda=1.541 \text{ \AA}$ , specular=1.975°	Add Row <input type="button" value="x"/>
Import	4: Ro1 br2; Rocking scan; $\theta_0=0.025-7.825^\circ$ ; at $\lambda=1.541 \text{ \AA}$ , specular=3.925°	Add Row <input type="button" value="x"/>
Import	<no description> <input type="button" value="Duplicate curve"/>	Add Row <input type="button" value="x"/>

Figure 104. List of loaded data

At the very bottom of the main window there is a list of loaded experimental curves with a brief description. Brief information in the line includes: serial number, name (if any), measurement type, angle and wavelength ranges. The "Add row" and  buttons respectively add and remove a row. The

experimental curve with all its settings can be duplicated by calling the context menu with the right mouse button.

To load data or change measurement parameters, click the "Import". » button. As for an independent curve, if this is a new curve for which the measurement type has not yet been set, then a window will open with a choice of options:

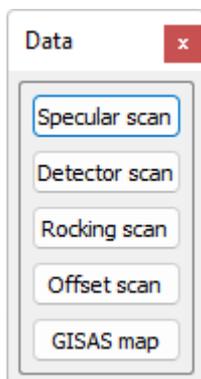


Figure 105. Measurement type selection

After setting the curve type, the corresponding window will open.

## 4.2.8.1 Specular scan

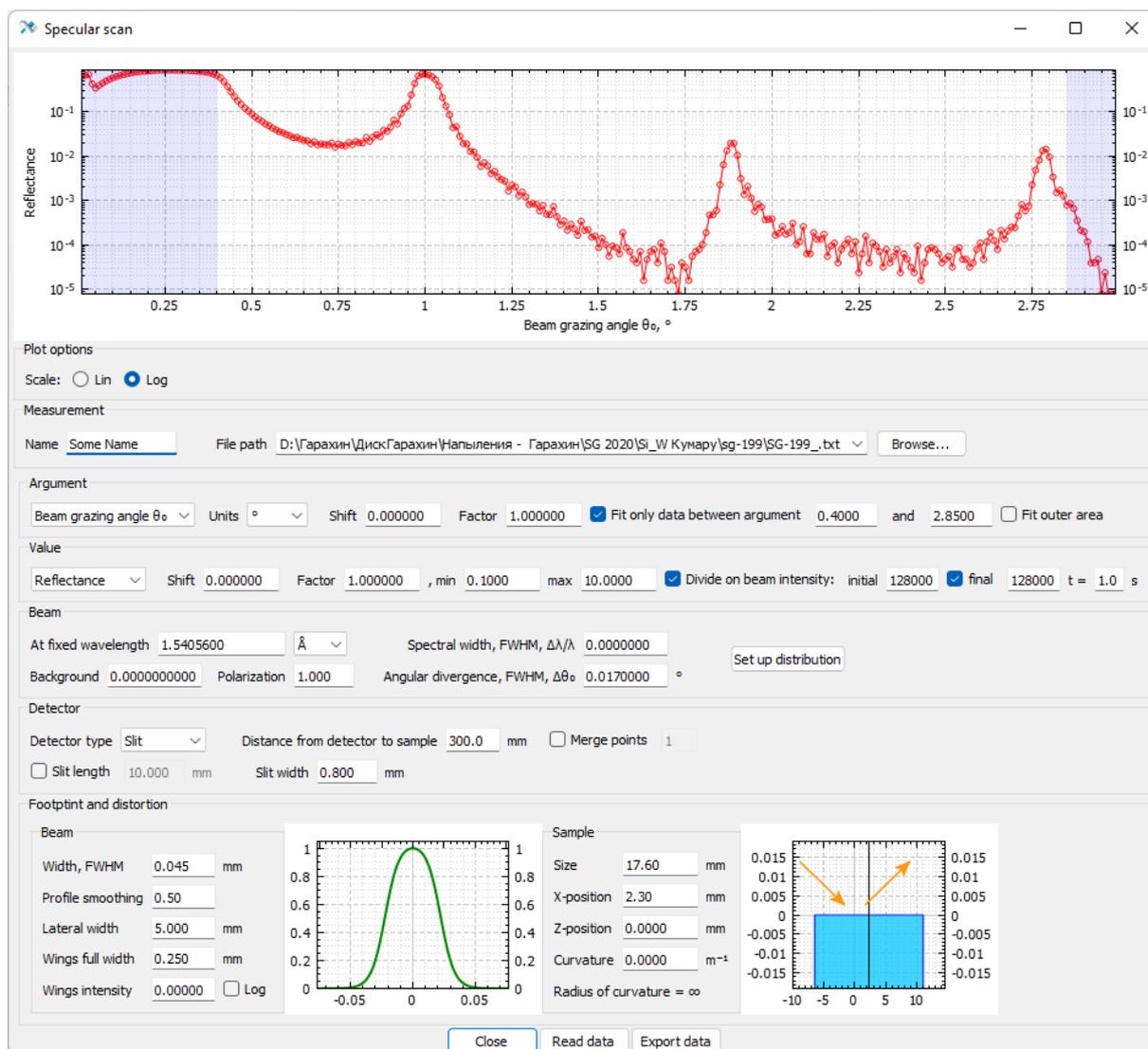


Figure 106. Experimental reflectometric curve settings

The upper part shows a graph of the loaded curve, taking into account the units of measurement, scaling, argument shifts and function values specified in this window. When the "Fit only data between argument" option is enabled in the "Argument" » block, the area excluded from the fit is indicated in purple. In the "Plot options" block, you can switch between linear and logarithmic scale along the vertical axis.

### 4.2.8.1.1 Measurement

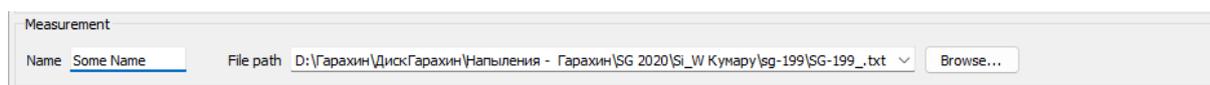


Figure 107. Block "Measurement"

In the left part of the block, you can set the name of the curve, this can be useful in further work, especially if there are several curves. In the remaining part, you can specify the data file to be loaded.

The path can be written manually or pasted, you can use the file dialog box by clicking the "**Browse...**" button. Or you can drag and drop the desired file into the settings window with the mouse.

#### 4.2.8.1.2 Argument

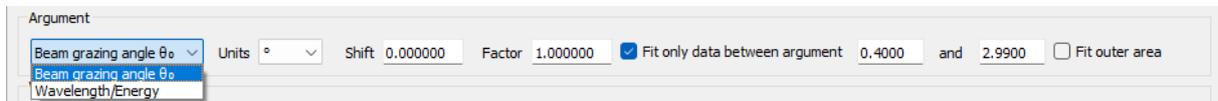


Figure 108. Block "**Argument**"

The argument type is set: beam grazing angle or wavelength. The next item is the units of measurement. It is here that you should specify in which units the values of the argument should be read. The "**Shift**" parameter is a value added to all argument values, the shift of the entire curve along the horizontal axis. In turn, "**Factor**" is the factor by which each value of the argument is multiplied; it scales the curve horizontally.

The "**Fit only data between argument**" option allows you to set the area excluded from automatic fitting. Enabling "**Fit outer area**" does not exclude the outer area between the specified arguments, but the inner one. The excluded area is shown in purple on the graph.

#### 4.2.8.1.3 Value

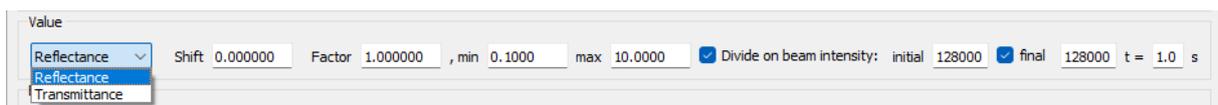


Figure 109. Block "**Value**"

The value type is set: reflection or transmission. As with the argument, "**Shift**" is a constant addition to the curve, and "**Factor**" is the scaling of the curve along the vertical axis. The "**min**" and "**max**" values limit the "**Factor**" parameter in automatic fitting.

*Attention:* Although the normalization parameter "**Factor**" can be adjusted automatically, you should not do this without good reasons. This may be acceptable in cases where the measurements have not been normalized to the beam intensity, but the result obtained should be treated with great care.

The "**Divide on beam intensity**" option allows you to normalize the measurement to the probing beam intensity and exposure time. If the beam intensity changed during the measurement, then in the simplest (linear) case this can be taken into account by turning on the "**Final**" checkbox and specifying in addition to the initial value also the final one.

#### 4.2.8.1.4 Beam

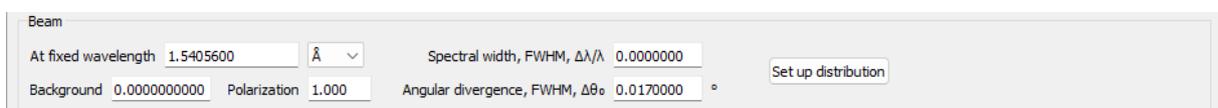


Figure 110. Block "**Beam**"

Almost all parameters are the same as for the [independent curve](#). Wavelength/grazing angle units are specified here, in the drop-down menu.

#### 4.2.8.1.5 Detector

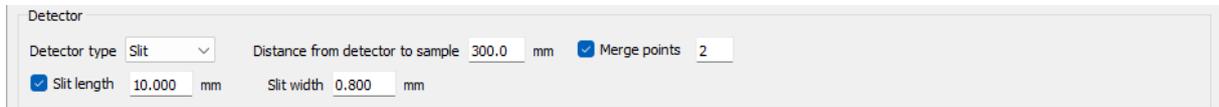


Figure 111. Block "Detector"

Almost all parameters are the same as for the [independent curve](#). But since we are dealing with a fixed dataset here, the "Merge points" option has been added. It allows you to reduce the dimensions of the array of points by combining them (binning). The number of points to merge can be specified. The result is immediately represented in the graph.

#### 4.2.8.1.6 Footprint and distortion

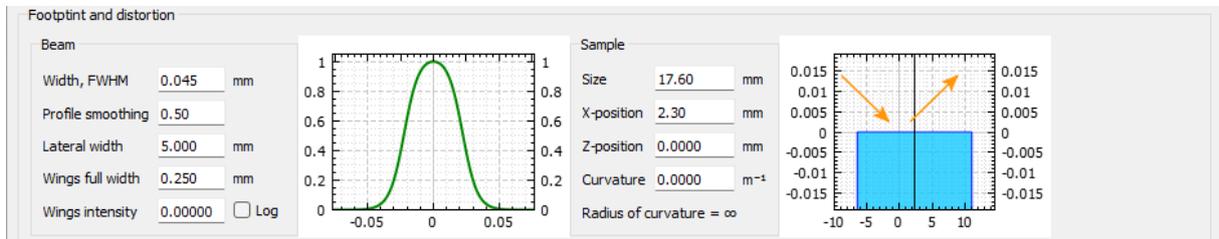


Figure 112. Block "Footprint and distortion"

The parameters are exactly the same as for the [independent curve](#).

#### 4.2.8.1.7 Bottom panel

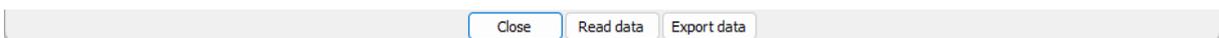


Figure 113. Bottom panel

The "Close" button closes the window (you can also close the window with the «[Escape](#)» key).

"Read data" re-reads data from the file specified in the "File path" field of the [Measurement](#) block.

"Export data" allows you to save the previously loaded curve to a file. The data is stored in the project file and can be exported even if the source file (specified in the "File path" field) no longer exists.

#### 4.2.8.2 Detector scan

The [Measurement](#), [Detector](#), [Footprint and distortion](#) blocks and the [bottom panel](#) are exactly the same as for the specular geometry. The [Value](#) block differs only in the immutable function type: "Scattering".

### 4.2.8.2.1 Argument

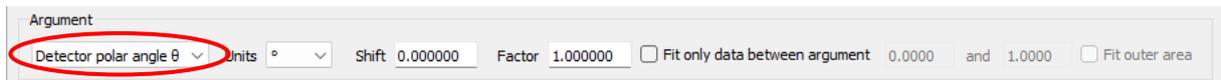


Figure 114. Block "Argument"

The argument is the polar angle of the detector. The rest of the parameters are the same as for the [specular measurement](#).

### 4.2.8.2.2 Beam

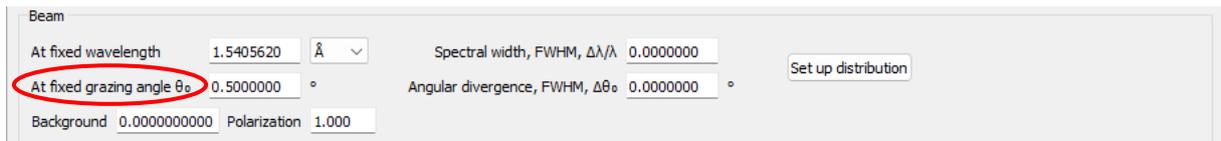


Figure 115. Block "Beam"

Almost all parameters are the same as in the [specular measurement](#). An additional parameter is a fixed beam grazing angle (or specular angle).

## 4.2.8.3 Rocking scan

The "[Measurement](#)", "[Detector](#)", "[Footprint and distortion](#)" blocks and the [bottom panel](#) are exactly the same as for the specular geometry. The "[Value](#)" block differs only in the immutable function type: "[Scattering](#)".

### 4.2.8.3.1 Argument

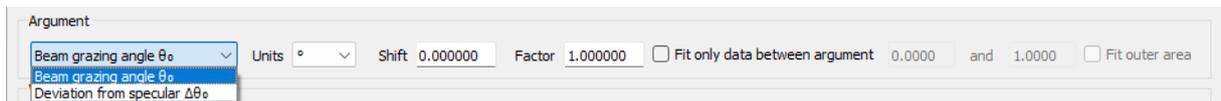


Figure 116. Block "Argument"

The argument can be the grazing angle of the incident beam or the deviation of the sample from the specular position. The rest of the parameters are the same as for the [specular measurement](#).

### 4.2.8.3.2 Beam



Figure 117. Block "Beam"

Almost all parameters are the same as in the [specular measurement](#). An additional parameter is the specular position, i.e. the grazing angle of the incident beam at which the reflected beam arrives at the detector.

#### 4.2.8.4 Offset scan

The "[Measurement](#)", "[Detector](#)", "[Footprint and distortion](#)" blocks and the [bottom panel](#) are exactly the same as for the specular geometry. The "[Value](#)" block differs only in the immutable function type: "[Scattering](#)".

##### 4.2.8.4.1 Argument

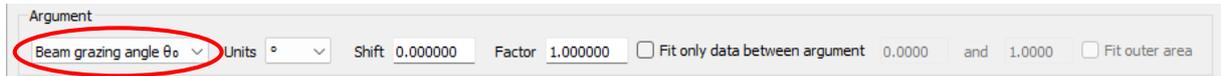


Figure 118. Block "[Argument](#)"

The argument is the grazing angle of the incident beam. Other parameters are the same as in the [specular measurement](#).

##### 4.2.8.4.2 Beam

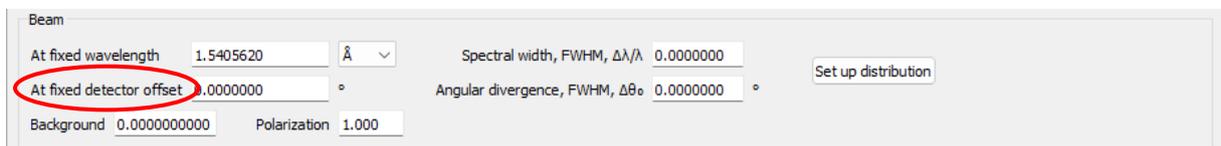


Figure 119. Block "[Beam](#)"

Almost all parameters are the same as in the [specular measurement](#). An additional parameter is the offset of the detector from the specular direction. A positive offset means that the angle from the plane of the sample to the detector is greater than the grazing angle of the beam. If it is equal to zero, then measurements are made in the specular direction, but, unlike the reflectometric curve, here you can get a plot of the amount of scattering in the specular direction.

## 4.2.8.5 GISAS map

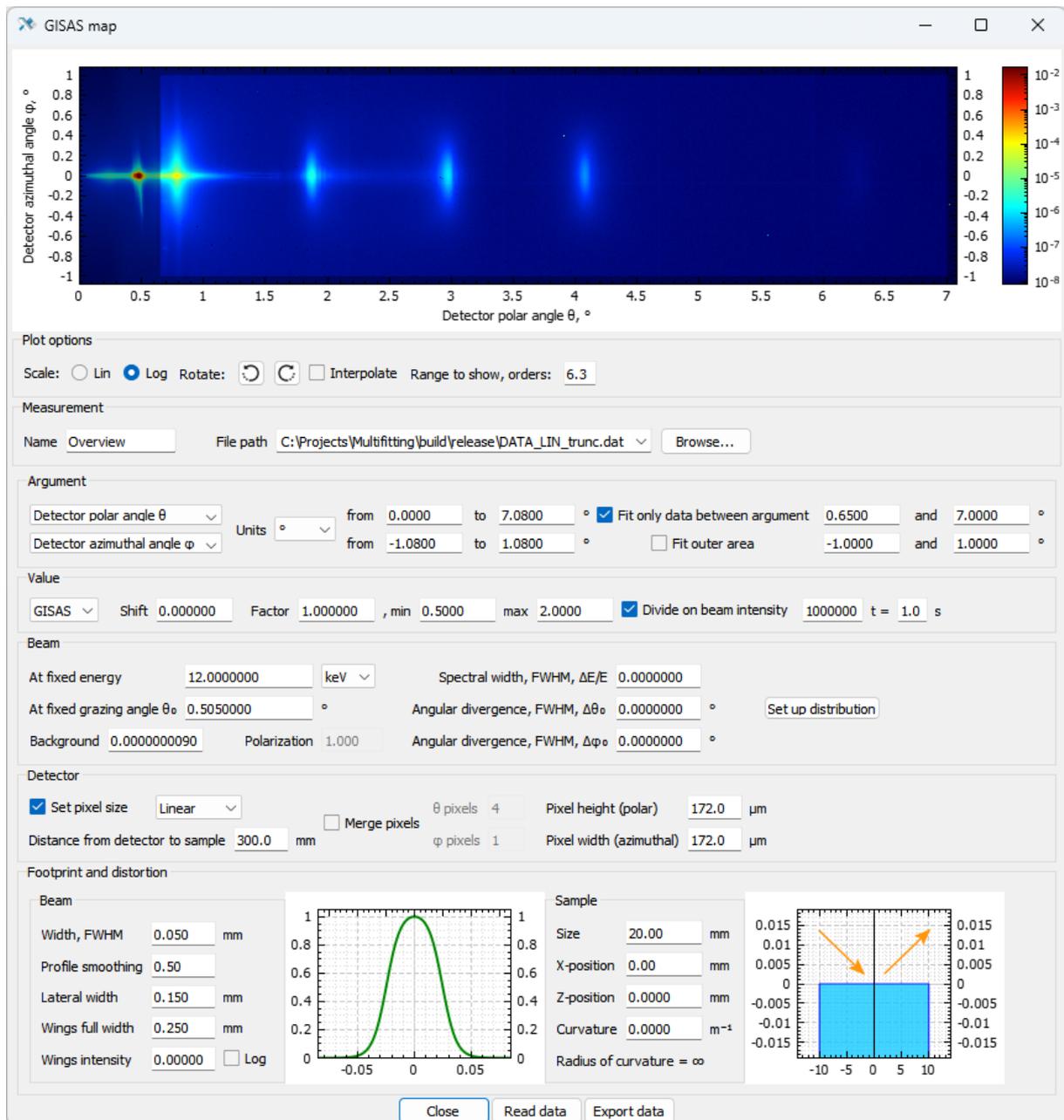


Figure 120. GISAS measurement settings

The top part shows a color map of the loaded data. When the "Fit only data between argument" option is enabled in the "Argument" block, the area excluded from the fit is displayed in a darker color. In the "Plot options" block you can switch between linear and logarithmic scale along the vertical axis, turn interpolation on and off, specify the values range for displaying on a logarithmic scale – these are the display settings. There are also buttons to rotate the image counterclockwise and clockwise. With their help, you should orient the data relative to the coordinate axes. This is where the data is linked to the coordinate axes for further use in calculations.

The "Measurement", "Footprint and distortion" blocks and the bottom panel are exactly the same as for the specular geometry. The rest is described below.

### 4.2.8.5.1 Argument

Argument

Detector polar angle  $\theta$  from 0.0000 to 7.0800 °  Fit only data between argument 0.6500 and 7.0000 °

Detector azimuthal angle  $\phi$  from -1.0800 to 1.0800 °  Fit outer area -1.0000 and 1.0000 °

Units °

Figure 121. Block "Argument"

Here the units and range of arguments for each axis are determined. Unlike the case of one-dimensional curves, here the data is a matrix of numbers without information about the coordinates, so the argument here is not read, but set. The arguments are of azimuthal and polar angles of the detector. The pixel grid is assumed to be equidistant.

The "Fit only data between argument" allows you to set the rectangular area involved in the automatic fit. Enabling "Fit outer area" leaves not the outer area, but the inner one. In the image, the excluded area is shown in a darker color.

### 4.2.8.5.2 Value

Value

GISAS Shift 0.000000 Factor 1.000000 , min 0.5000 max 2.0000  Divide on beam intensity 1000000 t = 1.0 s

Figure 122. Block "Value"

The scattering value is read from the file and can be modified by adding a shift and scaling. "Shift" is a constant addition to the values, and "Factor" is a scaling. There was a [methodological note](#) concerning the automatic adjustment of the normalization factor.

The "Divide on beam intensity" option allows you to normalize the measurement to the probing beam intensity and exposure time.

### 4.2.8.5.3 Beam

Beam

At fixed energy 12.0000000 keV Spectral width, FWHM,  $\Delta E/E$  0.0000000

At fixed grazing angle  $\theta_g$  0.5050000 ° Angular divergence, FWHM,  $\Delta \theta_g$  0.0000000 °

Background 0.0000000090 Polarization 1.000 Angular divergence, FWHM,  $\Delta \phi_g$  0.0000000 °

Figure 123. Block "Beam"

The parameters are the same as for the [independent curve](#).



For convenient work with the structure, all its parameters are summarized in one table, and this table is the main way to change these parameters. In addition to the current value, for each parameter, the upper and lower limits for automatic fitting, participation or non-participation of the parameter in fitting, as well as the relationship with other parameters of this or another structure (if there are several structure tabs in one project) can be specified.

### 4.3.1 Menu

The "File" and "Calculate" menus are exactly the same as in the main window. "Length units" allows you to change the main units of length, including the thickness of layers and interfaces and particle sizes. "Other units" allows you to change other units used in the table. In the "Precision" menu, you can change the number of decimals used to represent parameter values.

### 4.3.2 Table content

#### 4.3.2.1 Header

The top three lines show the color legend, as well as the tools for setting the limits for the adjusted parameters as a percentage of the current value. The latter can be convenient to set the range of values for several layers at once, if, for example, it is known that the uncertainty in the thickness of the layers can be  $\pm 30\%$  of the nominal value. By pressing the "Reset" button, the parameters in the corresponding column for which fitting is enabled will update the limits.

Setting the limits for variables:

Legend			density	thickness of layer/period	transitional region
pure slave	confidence interval	active fit	$\rho, -\%$	$z/d, \pm\%$	$s, \pm\%$
master/slave	master/confidence	use particles	Reset	Reset	Reset
pure master	free parameter	not parameter	10.000	20.000	10.000

Figure 126. Table header

#### 4.3.2.2 Modifiers

The underlying block of the table is also heterogeneous. On the left are the modifier checkboxes.

<input checked="" type="checkbox"/> Mouse wheel	<input checked="" type="checkbox"/> Change dependent
<input checked="" type="checkbox"/> Recalculate	Set model

Figure 127. Modifiers and the choice of the imperfections model of the structure

The "Mouse wheel" modifier determines the ability to change values in spin boxes by scrolling the mouse wheel. You can always change values by entering numbers or using the arrows keys  $\uparrow$  and  $\downarrow$ .

If the "Recalculate" modifier is enabled, then on any change in the current parameter values the curves are immediately recalculated and a new result is displayed.

The "Change dependent" modifier blocks the possibility of manual changing dependent parameters, they are immediately recalculated as a function of the master parameter instead. Dependent parameters are always recalculated during automatic fitting, regardless of this modifier.

The "Set model" button opens the window for setting the structure imperfection model.

### 4.3.2.3 Set imperfections model

In "Set imperfections model" window, it is indicated which "imperfections" should be included in the structure model: the presence of interlayer transition regions, the presence of thickness drift in a periodic multilayer, the roughness model and intralayer inhomogeneities (particles).

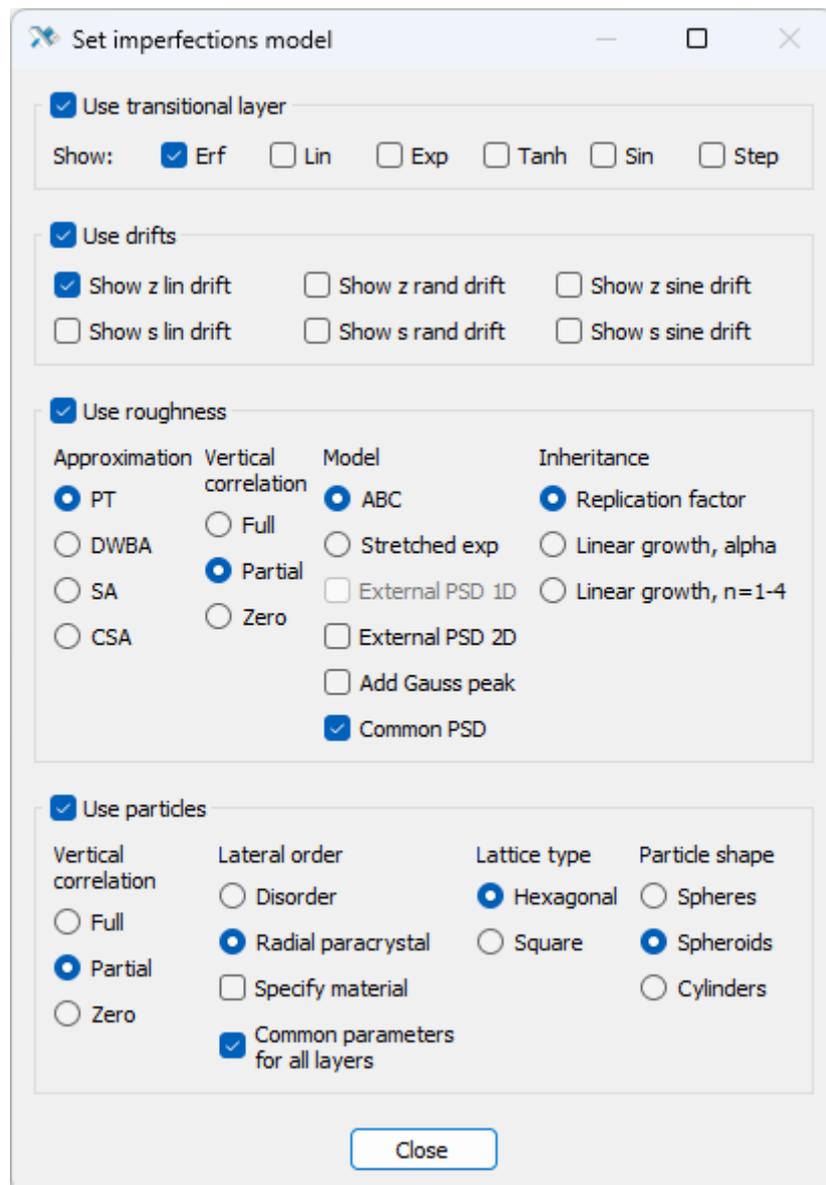


Figure 128. Structure imperfections models

Enabling and disabling blocks and their parameters affects which parameters will be shown in the main table.

#### 4.3.2.3.1 Transitional layer

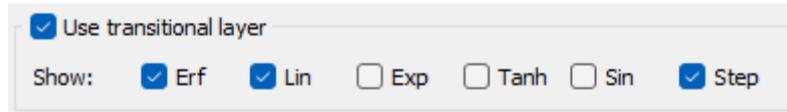


Figure 129. Block "Use transitional layer"

The block determines which transition layer profile functions to display in the table. If the function is disabled, then it is hidden from the table and is not used in calculations. If enabled, the feature is visible in the table, but is disabled by default for use in a calculation. It can be finally enabled and configured from the table.

#### 4.3.2.3.2 Drifts



Figure 130. Block "Use drifts"

The block determines which of layer thicknesses and transition regions drift models to show in the table: linear drift, random deviation, harmonic modulation. Drift can only be shown for layers that are part of a periodic multilayer. If the model is disabled, then it is hidden from the table and is not used in calculations. If enabled, it is visible in the table, but disabled by default for use in a calculation. It can be finally enabled and configured from the table

#### 4.3.2.3.3 Roughness

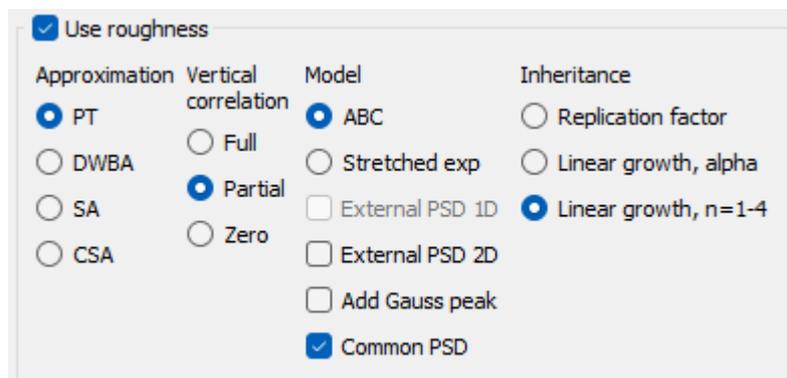


Figure 131. Block "Use roughness"

The block determines which roughness models are used in the calculations and which parameters can be changed in the table.

"**Approximation**" determines the type of approximation used in the scattering calculation. For "**PT**" (Perturbation Theory) the largest choice of options is available.

"**Vertical correlation**" determines the presence or absence of cross-layer roughness correlation.

- **"Full"** – the roughness is fully replicated from layer to layer, the scattering is completely coherent. Roughness parameters are the same for all layers.
- **"Partial"** – the roughness is not fully inherited, depending on the parameters of the **"Inheritance"** column.
- **"Zero"** – roughness is not inherited, scattering on different interfaces is incoherent. Interfaces can have different roughness parameters.

**"Model"** determines the type of lateral correlation function.

- **"ABC"** – ABC-model or K-correlation function.
- **"Stretched exp"** – another fractal roughness model.
- **"External PSD 1D"** – the ability to load an arbitrary one-dimensional PSD function from a file. Beyond the uploaded data, the PSD continues as a model.
- **"External PSD 2D"** – the ability to load an arbitrary two-dimensional isotropic PSD function from a file. Beyond the uploaded data, the PSD continues as a model.
- **"Add Gauss peak"** – in addition to the main model, add a Gaussian peak to the PSD function in the vicinity of the specified spatial frequency.
- **"Common PSD"** – make the roughness and replication model the same for all layers or leave the possibility to customize each layer.

**"Inheritance"** determines the type of roughness inheritance from the underlying interface to the overlying interface with the type of vertical correlation **"Partial"**.

- **"Replication factor"** – the roughness PSD is the same for all interfaces, but some part is inherited coherently and some – incoherently.
- **"Linear growth, alpha"** – a linear growth model with a single power law is used.
- **"Linear growth, n=1-4"** – a linear growth model with the sum of several power laws is used.

#### 4.3.2.3.4 Particles

Vertical correlation	Lateral order	Lattice type	Particle shape
<input type="radio"/> Full	<input type="radio"/> Disorder	<input checked="" type="radio"/> Hexagonal	<input type="radio"/> Spheres
<input checked="" type="radio"/> Partial	<input checked="" type="radio"/> Radial paracrystal	<input type="radio"/> Square	<input checked="" type="radio"/> Spheroids
<input type="radio"/> Zero	<input type="checkbox"/> Specify material		<input type="radio"/> Cylinders
	<input checked="" type="checkbox"/> Common parameters for all layers		

Figure 132. Block "Use particles"

The block determines which particle models and their correlations are used in the calculations and which parameters can be changed in the table.

"**Vertical correlation**" determines the presence or absence of interlayer particle correlation. Material, particle geometry, vertical displacement can be different for each layer.

- "**Full**" – particles in different layers are located strictly one above the other, the scattering is completely coherent. The parameters of the lateral distribution are common to all layers.
- "**Partial**" – particles in different layers are located not strictly one above the other, but with some random lateral shift, the same for the whole layer. The parameters of the lateral distribution, except for the vertical displacement of individual particle, are common to all layers.
- "**Zero**" – particles in different layers are not connected with each other, scattering between layers is incoherent. The parameters of the lateral distribution are individual for each layer.

"**Lateral order**" determines the lateral correlation of particles in the layer. In the table, you can set the lateral order of particles individually for each layer with a vertical correlation of "**Zero**".

- "**Disorder**" – particles in the layer are located randomly, there is no correlation.
- "**Radial paracrystal**" – particles in the layer are located in a paracrystal averaged over lattice orientations.

"**Specify material**" – sets the material of the particle separately or use the material of the layer.

"**Common parameters for all layers**" – makes the parameters of particles and their distribution the same for all layers or leave the possibility of setting each layer. The particle material density can be set for each layer anyway.

"**Lattice type**" sets the basic geometry (before statistical and directional averaging) of the lateral arrangement of particles. It also affects the density of particles in the layer. In the table, you can set the lattice type individually for each layer with a vertical correlation of "**Zero**".

- "Hexagonal" – the particles in the layer are arranged in a paracrystal with a hexagonal lattice.
- "Square" – particles in the layer are arranged in a paracrystal with a square lattice.

"Particle shape" sets the particle shape. When you change the shape of particles here, the result is applied to all layers. In the table, you can set the shape of the particles individually for each layer. Particles are made up of a homogeneous substance.

- "Spheres" – particles are spheres.
- "Spheroids" – particles are spheroids, i.e. ellipsoids of revolution around a vertical axis.
- "Cylinder" – particles are vertical cylinders with a round base.

#### 4.3.2.4 Parameter change step

In the right part of the block there are fields for setting the step for changing parameters when they are changed using the keyboard arrows or the mouse wheel. The step is set in the same units as the parameter values. Some parameters of roughness and particles do not have a fixed step, in which case the step is adaptive: when scrolling, changes occur in the second digit.

Set increase/decrease steps							
	$\rho$	$z/d$ [Å]	$s$ [Å]	$\gamma$	interl		dz lin
	0.010	0.0100	0.010	0.0010000	0.100		0.0010

Figure 133. Parameter change step for the underlying part of the table

*Note:* While holding down the «Ctrl» key, the parameters change in x10 increments.

#### 4.3.2.5 Parameters of the layered structure

Next comes the layered structure with its own parameters. To set the material of the layer, you need to write in the text field the appropriate name of the file with the refractive index or select the file by clicking "Browse". If the material is composed of individual chemical elements, then you should select the elements in the drop-down menu and set the stoichiometry.

		Be		
		Browse		
<input checked="" type="checkbox"/> Be layer (1)				

		Ga ▾	Al ▾	As ▾
		1.000	0.300	0.700
<input checked="" type="checkbox"/> GaAl0.3As0.7 layer (2)		<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
		0.000	0.000	0.000
		1.000	1.000	1.000

Figure 134. Materials of layers

*Note:* To find the element faster, you can press the letter on the keyboard that begins the name of the chem. element. Elements can also be scrolled with the mouse wheel or the ↑ and ↓ arrows.

Most of the table is occupied by vertical boxes corresponding to specific parameters. Parameters are mainly indicated by symbols, next to them the units of measurement are indicated in square brackets. For most parameters, you can call up the context menu by right-clicking on the light blue header. It is also a way to see the full name of a given parameter. The figure below shows the purpose of the fields in the block.

	context menu			
		z [Å]		
current value	→	34.5028		
fitting on/off	→	<input checked="" type="checkbox"/> fit	<input checked="" type="checkbox"/> fit	<input type="checkbox"/> fit
min	→	26.9330	1.000	s erf
max	→	40.3994	20.000	6.684

Figure 135. Field block for one parameter

*Attention:* For stoichiometry parameters " $\zeta$ " and periodic drift "sine drift" the context menu is called up on the "fit". field. The "N" (number of periods) parameter does not have a context menu.

Optional parameters that have a checkbox in the header can be turned on and off with it:

<input checked="" type="checkbox"/> dz sin : $A \cdot \sin(2\pi n v + \varphi)$		
1.0000	0.3433	0.3433
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
0.0000	0.1667	0.0000
0.0000	0.5000	1.0000

Figure 136. Layer thickness harmonic modulation parameters: A, v, φ

An exception is the thickness of the interlayer transition region. It can be set by a single parameter "s" or thicknesses of individual profile functions. In the second case, the effective thickness is calculated as the mean square of the individual values, taking into account the weight. You can switch between these models with the flag marked in the figure:

<input type="checkbox"/> s [Å]	<input checked="" type="checkbox"/> erf	<input checked="" type="checkbox"/> lin
2.7386	0.300	0.700
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
1.0000	s erf	s lin
5.0000	2.0000	3.0000

Figure 137. Switch between a single transition region thickness and individual for each profile

The particles in the structure can be turned on and off individually for each layer. You can also customize the particle shape, lateral correlation and geometry model.

<input checked="" type="checkbox"/> on/off
Spheroid
Radial PC
Square

Figure 138. Managing particles in a layer

It is worth mentioning the possibility of [uploading from file](#) the external PSD in addition to the model one. Instead of the light blue "header" of the parameter, here is the download button. If the external PSD is not loaded, then the button is white, if it is loaded, then it is green.

<input checked="" type="checkbox"/> PSD 1D	<input type="checkbox"/> PSD 2D
$\sigma_z$ [Å]	$\sigma_z$ [Å]
3.8707	0.0000
rf 1D	rf 2D
0.800	1.000

Figure 139. External roughness PSD

The parameter to be changed is the "roughness factor" "rf 1D" or "rf 2D" which is the multiplier for the root-mean-square roughness. Accordingly, the PSD depends on "rf 1D"/"rf 2D" quadratically. The resulting roughness in the frequency range of the loaded PSD is displayed in the " $\sigma_e$ " field.

#### 4.3.2.5.1 Parameter list

Multilayer:

- number of periods in the multilayer
- period thickness
- the ratio of the thickness of the upper layer to the period

Layer:

- chemical element and its stoichiometric index
- material (file name)
- absolute density of material
- relative density of material
- layer thickness
- root-mean-square diffuse interface thickness

Diffuse interface profile features:

- erf error function *erf* and weighting factor
- lin linear profile *lin* and weighting factor
- exp exponential profile *exp* and weighting factor
- tanh hyperbolic tangent *tanh* and weighting factor
- sin sinusoidal profile *sin* and weighting factor
- step step profile *step* and weighting factor
- root-mean-square *erf* profile thickness

- $s_{lin}$  root-mean-square *lin* profile thickness
- $s_{exp}$  root-mean-square *exp* profile thickness
- $s_{tanh}$  root-mean-square *tanh* profile thickness
- $s_{sin}$  root-mean-square *sin* profile thickness
- $s_{step}$  root-mean-square *step* profile thickness

Layer thickness drift:

- $dz_{lin}$  linear thickness drift
- $dz_{ran}$  random fluctuations in thickness
- $dz_{sin} : A \cdot \sin[2\pi(nv + \varphi)]$  sinusoidal thickness modulation

Diffuse interface thickness drift:

- $ds_{lin}$  linear drift of interface thickness
- $ds_{ran}$  random fluctuations in interface thickness
- $ds_{sin} : A \cdot \sin[2\pi(nv + \varphi)]$  sinusoidal modulation of interface thickness

Roughness:

- $\sigma [\text{\AA}]$  root mean square height
- $\xi [\mu\text{m}]$  correlation radius
- $\alpha$  fractal parameter
- $\sigma_v [\text{\AA}]$  root-mean-square roughness peak height
- $\nu_0 [\mu\text{m}^{-1}]$  central spatial frequency of the roughness peak
- $\delta\nu [\mu\text{m}^{-1}]$  width of roughness peak in spatial frequency
- $L_v [\text{\AA}]$  correlation depth at the base frequency
- $\nu_0 [\mu\text{m}^{-1}]$  base frequency for correlation depth

$\beta$	exponent of the frequency exponent in the correlation factor PSD
$\Omega$ [ $\text{\AA}^3$ ]	particle volume in the linear growth model
$a_1$	coefficient at the first power of frequency in the linear growth model
$a_2$ [nm]	coefficient at the second power of frequency in the linear growth model
$a_3$ [nm <sup>2</sup> ]	coefficient at the third power of frequency in the linear growth model
$a_4$ [nm <sup>3</sup> ]	coefficient at the fourth power of frequency in the linear growth model
rf 1D	"roughness factor", coefficient when one-dimensional outer PSD is loaded
rf 2D	"roughness factor", coefficient when 2D outer PSD is loaded

Particles:

$\rho_o$ [g/cm <sup>3</sup> ]	absolute density of particle material
$\rho_o$ [r.u.]	relative density of particle material
$R$ [ $\text{\AA}$ ]	particle lateral radius
$H$ [ $\text{\AA}$ ]	particle height
$r$ [ $\text{\AA}$ ]	average distance between particles
$\delta r$ [ $\text{\AA}$ ]	particle spacing variation
$D$ [ $\mu\text{m}$ ]	domain size – size of particle correlation region
$\Delta$ [ $\text{\AA}$ ]	random shift of particles in a layer relative to an adjacent layer
$z_o$ [ $\text{\AA}$ ]	vertical shift of all particles relative to the center of the layer
$\delta z_o$ [ $\text{\AA}$ ]	random scattering of particles in a layer vertically

#### 4.3.2.6 Coupling editor

If you click on the only item of the parameter's context menu, the "**Coupling editor**", window will open, which is intended for setting relationships between parameters, as well as for estimating the confidence interval of parameter values based on the residual.

Figure 140. Window "Coupling editor"

Parameters can be linked to each other by a functional dependency. In the process of fitting, the values of the dependent parameters are calculated in accordance with the given function. The hierarchy of related parameters is displayed in color according to the legend: the **red** parameter is dependent, while no one depends on it; the **green** parameter is independent, but other parameters depend on it; the **yellow** parameter is dependent, but other parameters also depend on it. Each parameter can have no more than one "master" and as many "slaves" as desired. To assign a new parameter as "master" or "slave" in relation to the given parameter for which this window is open, you need to put the cursor in the corresponding field in the "Master" or "Slaves" block and right-click in the table (as a call to context menu) by the target parameter.

The figure above shows an example where the thickness of the Al layer depends on the thickness of the W layer, and determines the thicknesses of the Be and Mo layers. The function written in the editable field can be not only linear. The ExprTk library used in Multifitting (<https://www.partow.net/programming/exprtk/>) can parse and recognize a wide range of mathematical expressions. For example, following can be used

- Mathematical operators (+, -, \*, /, %, ^)
- Functions (*min, max, avg, sum, abs, ceil, floor, round, roundn, exp, log, log10, logn, pow, root, sqrt, clamp, inrange, swap*)
- Trigonometric functions (*sin, cos, tan, acos, asin, atan, atan2, cosh, cot, csc, sec, sinh, tanh, d2r, r2d, d2g, g2d, hyp*)

In the notation of expressions, the master parameter is denoted by the letter "x", and the dependent parameter is the function f(x).

**Attention:** Consider the dimension and current units indicated in the table! Both the value of the function and the argument "x" are calculated in *angstroms* for all parameters that have the length units, or  $\text{\AA}^n$  for the units of  $[\text{length}]^n$ . The internal value of the remaining parameters corresponds to their value displayed in the table.

**Note:** You can link parameters not only within the same structure, but also between structures of the same project located in different tabs.

The dependency mechanism can be useful, for example, for linking the stoichiometry of a structure and its density, or for linking the parameters of several initially identical structures, with which various technological operations were then carried out.

Multifitting does not limit you in writing expressions, but you yourself must monitor the correctness and physical relevance of the resulting values, for example, avoiding negative thicknesses, division by zero, calculating the root of a negative number, etc. Otherwise, you will get an incorrect result or a program crash.

Also in this window, you can configure data generation for further calculation of the confidence interval for a specific parameter. The principle here is as follows: for each fixed value of a parameter from a given grid, all other fitting parameters of the structure are adjusted. As a result, a set of pairs "parameter value – the best residual value found" is obtained, saved in the file "confidence.txt". If we build a graph from these points, then we will see the dynamics of the increase in the value of the discrepancy when the value of the studied parameter deviates from the optimal one.



Figure 141. Grid setting for confidence interval

#### 4.3.2.7 Elements of the layered structure

The left part of the table shows the elements of the structure with their nesting depth. All elements, except for the substrate and layers as part of a regular aperiodic, can be "switched on and off". A disabled element is not taken into account in the calculations, as if it simply does not exist. For a periodic multilayer, you can call the context menu if it does not contain layers with a dependent thickness (red or yellow).

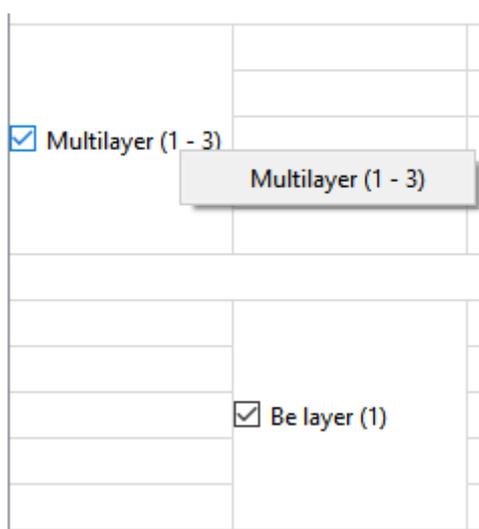


Figure 142. Элементы структуры с возможностью отключения

### 4.3.2.8 Redistribution of layer thicknesses within a period

The only item of the context menu allows you to open a window where you can redistribute the thickness between the layers of the elementary cell without changing the thickness of the period.

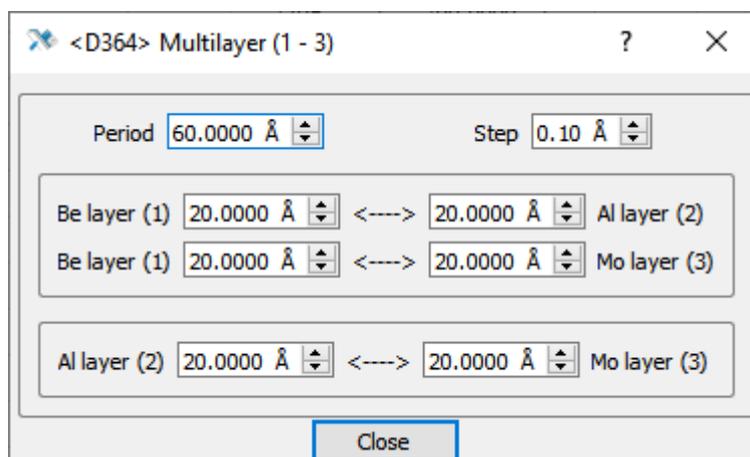


Figure 143. Redistribution of thickness between layers of periodic structure

In the case of a two-component multilayer, this can also be done in the main table by changing the parameter "Y". Here you can redistribute the thickness for any number of layers in the period.

### 4.3.3 Regular aperiodic

The creation of a regular aperiodic is described in the section [Defining a layered structure](#). A regular aperiodic can contain an integer number of elementary cells, as in a periodic structure. Layers of the same type can have different thicknesses and different transition regions. In this regard, the layers have new parameters and conditions: the ability to set all layers of a given type to the same thickness ("common z" checkbox) and the same interface ("common s" checkbox). Also, when optimizing the aperiodic stack, you can impose a "soft" restriction on the layer thicknesses distribution. If the thickness of some layer differs from the average thickness of this type of layers in the structure by more than  $\Delta$ , then the quantity  $Q \times \left| z - \langle z \rangle - \Delta \right|^p$  is added to the residual function. Thus, the magnitude of the spread and the need to fit into this limit can be varied over a wide range, depending on the practical restrictions on the synthesis of a multilayer mirror. And of course, the absolute values of the thicknesses are also limited by the minimum and maximum specified for the layer in the main table.

<input checked="" type="checkbox"/> erf	<input checked="" type="checkbox"/> lin	<input type="checkbox"/> exp	<input type="checkbox"/> tanh	<input type="checkbox"/> sin	<input type="checkbox"/> step
0.004	0.996	0.001	0.001	0.695	0.081
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
<input checked="" type="checkbox"/> common z		<input checked="" type="checkbox"/> restrict z: { $\pm\Delta$ , p, Q}			
<input checked="" type="checkbox"/> common s		$\pm 0\%$	p = 2	Q = 0.00000000	

Figure 144. Special parameters of regular aperiodic

Для детальной работы с большим количеством индивидуальных слоёв аперериодики существует специальная таблица. Чтобы её открыть, вызовите контекстное меню и нажмите единственный пункт:

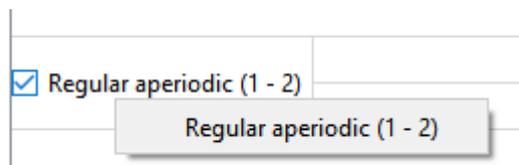


Figure 145. Контекстное меню регулярной аперериодики

A table will open in which you can see and change the thicknesses and interfaces of the layers. Density can only be changed for all layers of a given type. Interface fitting can only be collective, for all layers of this type, and thickness fitting can be individual or collective. You can enable the "Fit z" checkbox for all thicknesses by holding down the "Shift" key or from the main table. The limits of variation are set in the main table. Depending on the parameters "common z" and "common s" the corresponding layers will have the color according to the legend. Changes between the main table and the table for aperiodic are synchronized.

Regular aperiodic (1 - 2)					
File Length units Precision					
common s		common z		active fit	common z and s
<input checked="" type="checkbox"/> Mouse wheel	z step			s step	
<input checked="" type="checkbox"/> Recalculate	0.10 Å			0.10 Å	
Cell #	Material	z [Å]	Fit z	s [Å]	ρ
1	Be	39.3360	<input checked="" type="checkbox"/>	0.000	1.000 [r.u.]
2	Mo	39.3360	<input type="checkbox"/>	0.000	1.000 [r.u.]
3	Be	39.3360	<input checked="" type="checkbox"/>	0.000	1.000 [r.u.]
4	Mo	39.3360	<input type="checkbox"/>	0.000	1.000 [r.u.]
5	Be	39.3360	<input checked="" type="checkbox"/>	0.000	1.000 [r.u.]
6	Mo	39.3360	<input type="checkbox"/>	0.000	1.000 [r.u.]
7	Be	39.3360	<input checked="" type="checkbox"/>	0.000	1.000 [r.u.]
8	Mo	39.3360	<input type="checkbox"/>	0.000	1.000 [r.u.]
9	Be	39.3360	<input checked="" type="checkbox"/>	0.000	1.000 [r.u.]
10	Mo	39.3360	<input type="checkbox"/>	0.000	1.000 [r.u.]

Figure 146. Table of layers of regular aperiodic

## 4.4 Profile plot

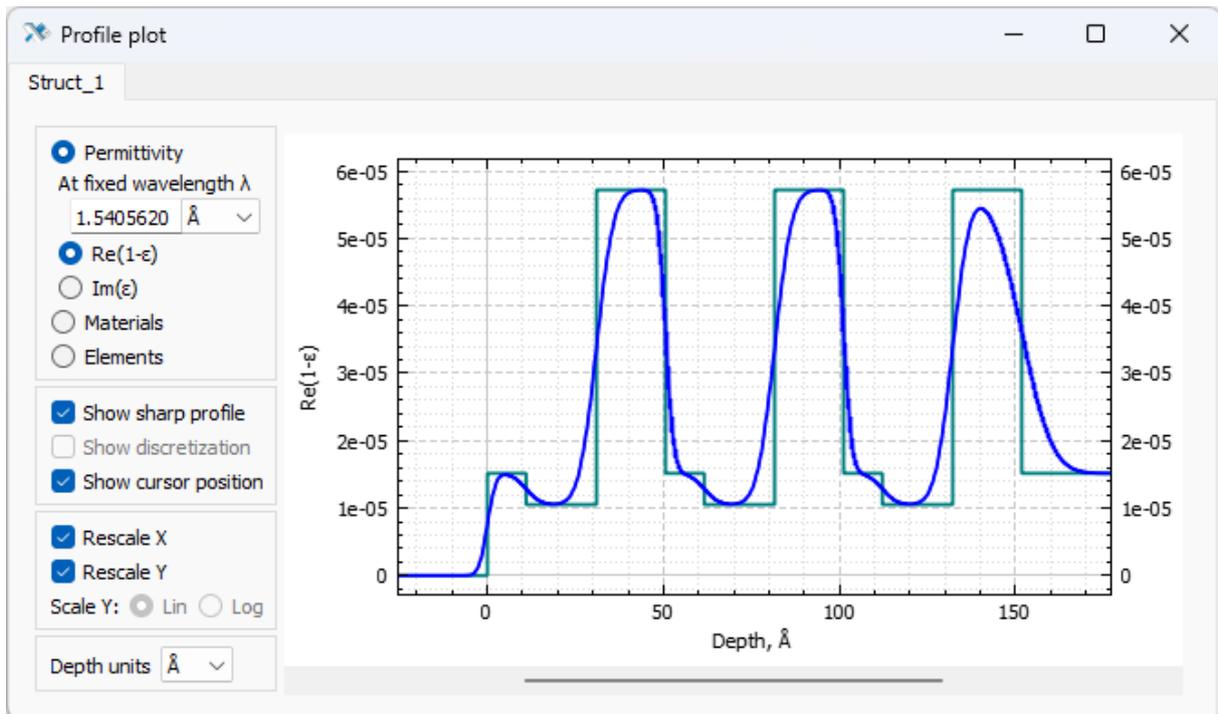


Figure 147. Real part profile of permittivity

In this window, you can see the profile of the real or imaginary part of the permittivity at a given wavelength, the distribution of a particular material, or the concentration of atoms of different kinds. The profile is based on materials and densities of layers and substrate, layer thicknesses, thickness and shape of interlayer transition regions. Roughness and particles do not affect the profile. The displayed profile is automatically changed when the mentioned parameters in the "**Structure table**" are changed, regardless of the "**Recalculate**" modifier. You can shift the visible area by dragging the pointer, and the display scale can be changed using the mouse wheel. If the pointer is in the inner area of the graph, then the scaling on both axes changes synchronously. If the pointer is located near the left axis or the lower axis, then only its scale changes.

On the left side there is a panel with chart display options. In the first block, the displayed value is selected. If you select "**Materials**" or "**Elements**", different components will be shown in different colors according to the legend. A single click on one of the profiles will make it thicker, and a double click will remove all materials from the chart, except for this one. You can return them by double-clicking again, or by changing any parameter of the structure, or by recalculating it.

The permittivity depends on the wavelength/energy of the photon. You can change it, as well as the units of measurement, in the corresponding field.

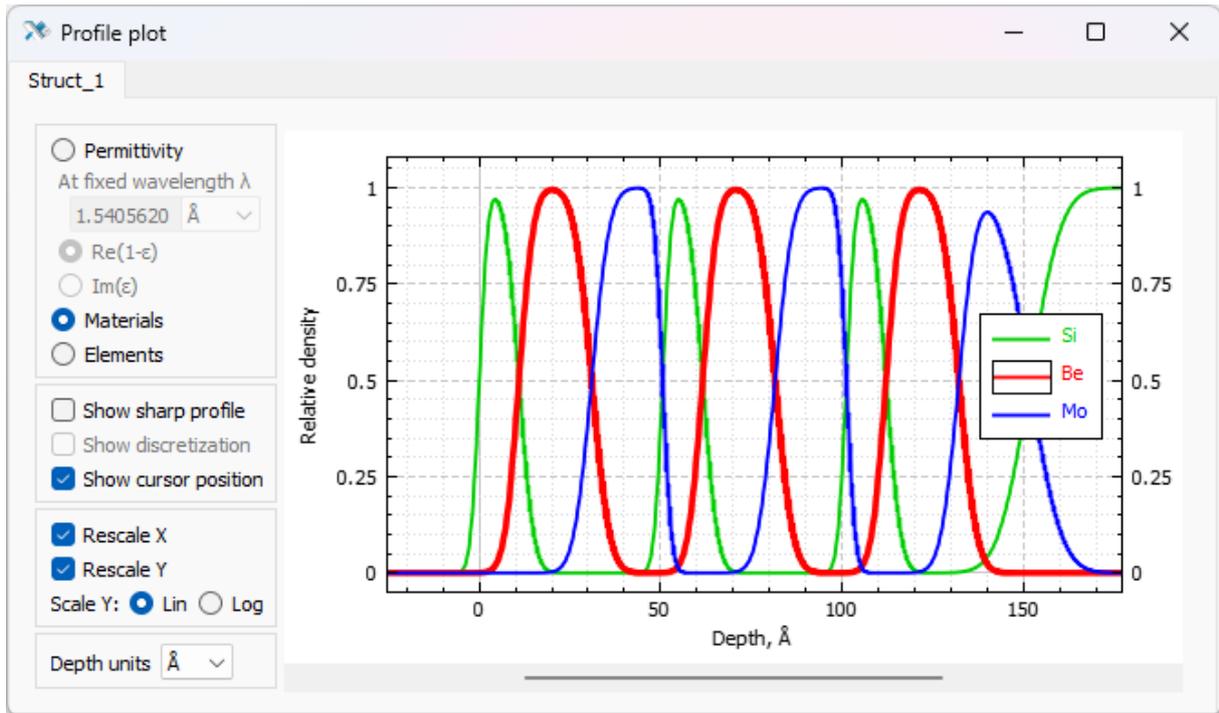


Figure 148. Distribution of materials in the structure

If you select "**Materials**" the relative density of each material will be plotted along the vertical axis. It depends on the density given in the table and on the smearing of the material over adjacent layers. When selecting "**Elements**", the vertical axis will be the absolute concentration of atoms per  $1 \text{ cm}^3$ . It depends not only on the parameters of the structure, but also on the internal properties of the element.

The second block allows you to show additional information on the chart. "**Show sharp profile**" shows what the profile would look like if there was no mixing of materials at the interfaces. "**Show discretization**" shows the splitting of the profile into thin homogeneous sublayers, if discretization is enabled for the structure and its step is specified. The sampling setting is located in the "[Calculation settings](#)" window. "**Show cursor position**" shows the coordinates cursor.

The third block contains scaling settings. The options "**Rescale X**" and "**Rescale Y**" indicate automatic scaling along the corresponding axes when recalculating curves or when changing the structure. If there are many layers in the structure, then it makes sense to turn off horizontal scaling and manually change the scale to see the details of the profile. The type of scaling, linear or logarithmic, can be chosen for non-negative values, that are all but the real part of the polarizability.

In the last block, you can change the units of depth plotted along the horizontal axis.

All display settings, including the current coordinates of the axes (if there is no autoscaling) are saved for the structure. When closing and opening the "**Profile plot**" window, they are restored automatically. For this to happen when you reopen the project, you need to save the project.

## 4.5 1D graphs

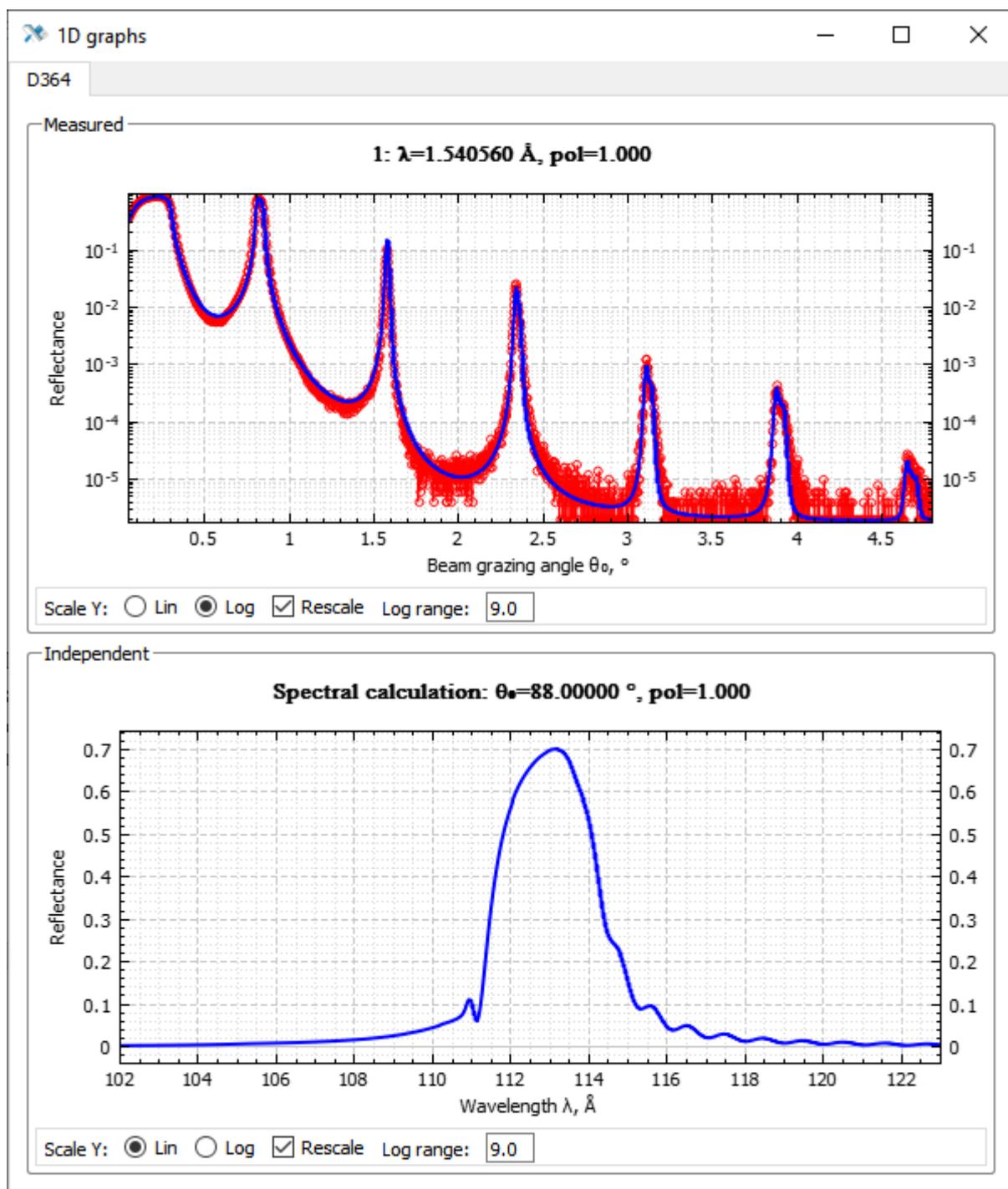


Figure 149. Window "1D graphs": calculation on experimental grid and independent calculation

The "1D graphs" window is designed to visualize the calculation results. Here you can see one-dimensional curves: reflection, transmission, diffuse scattering. The number of curves to display is determined by how many of them are set (see the figure with the [structure of the main window](#)) and how many are "enabled" in the ["Calculation settings"](#) window. The window contains two sections. The upper one, "Measured", is for loaded experimental data and calculation on the same experimental grid. The lower one, "Independent", is for calculations on a uniform grid, which is set directly in Multifitting.

If one of the sections is empty, it is hidden. Between the sections there is an invisible horizontal separator, which allows you to manually redistribute the height between the sections in the window using the mouse.

Each section can have multiple curves. By default, they are arranged in a line, but if there are more than two curves, then this is very inconvenient, because requires huge screen width. You can arrange graphs in several lines by specifying the appropriate number in the window settings called through the context menu. The settings are discussed below.

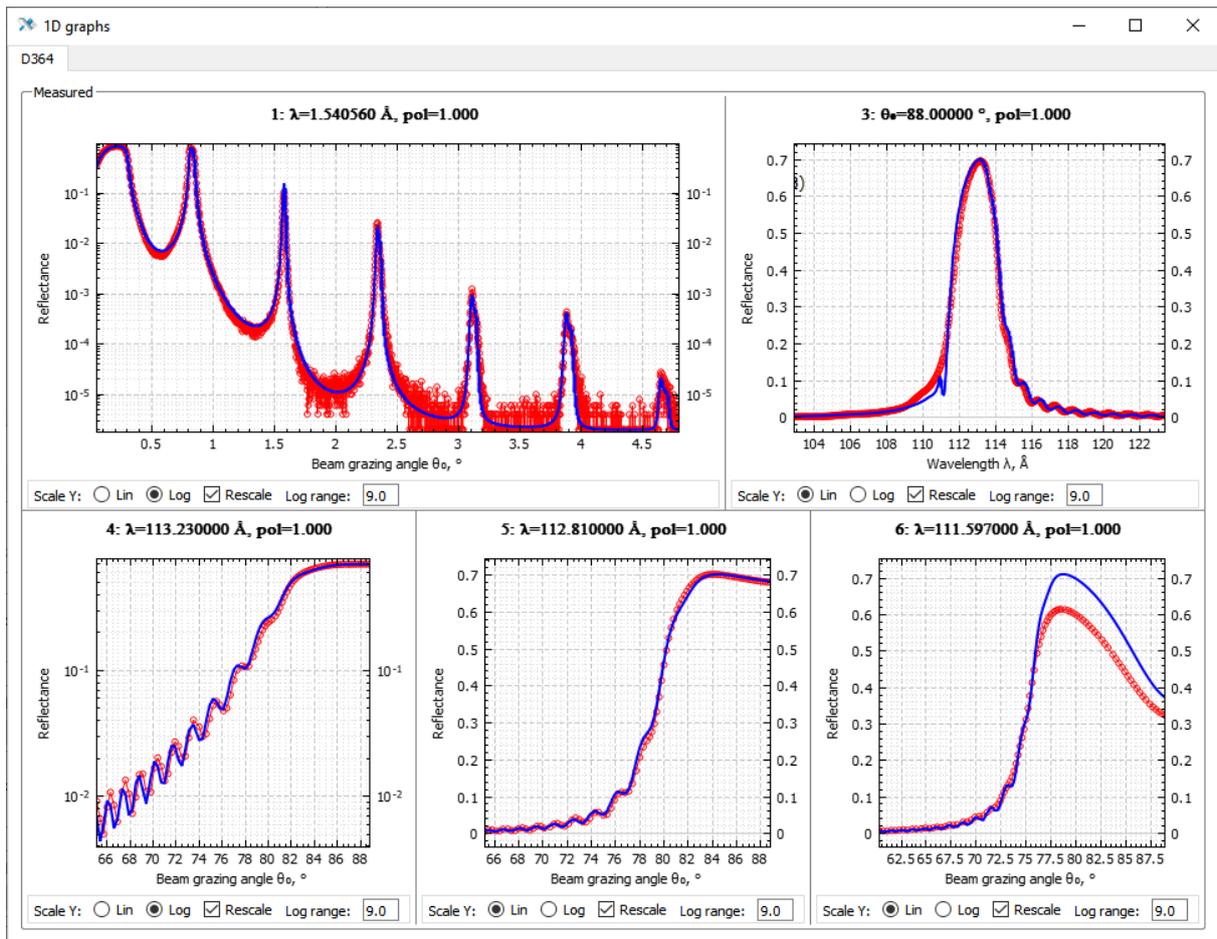


Figure 150. Arranging multiple curves in a section

There are also separators between the graphs, with which you can distribute the window space along individual curves. Horizontal separators adjust the height of the rows, while vertical separators control the space within the row.

#### 4.5.1 Settings

The context menu can be called in the area outside the graphs (including the title and labels of the axes), i.e. outside the outer frame of the section or in the free space of the control panel of each graph. There is only one item in the menu – the "Settings" window.

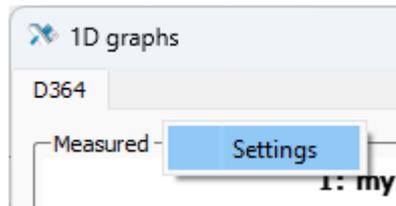


Figure 151. Context menu "1D graphs"

The upper block of settings allows you to arrange charts in several lines, separately for the "Measured" and "Independent" sections.

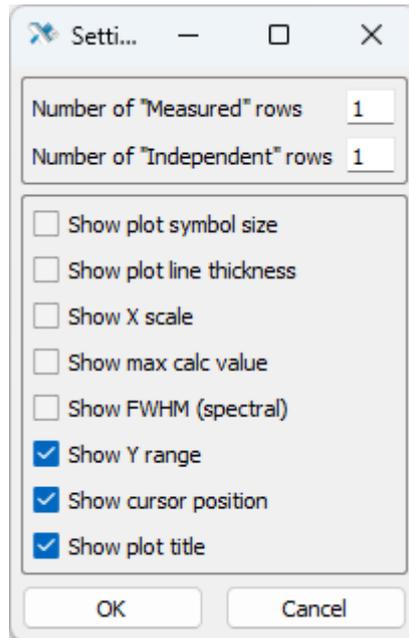


Figure 152. "1D graphs" settings

A further list of options concerns the display of controls in a row below each graph. Permanently displayed options below each graph are:

"Scale Y" allows you to select a linear or logarithmic scale for the vertical axis.

"Rescale" enables rescaling the plot on both axes with each curve calculation to show the full curves.

"Show plot symbol size" shows the "Scatter" option to change the size of the experimental curve symbols. The experimental curve must first be selected by clicking on it with the pointer. It has no effect on the calculated curve.

"Show plot line thickness" shows the "Line" option to change the line thickness. The desired curve must first be selected by clicking on it with the pointer. Applies to any curve.

"Show X scale" shows the "Scale X" option to select linear or logarithmic scale on the horizontal axis.

"Show max calc value" displays the maximum value and its position on the calculated curve.

"Show FWHM (spectral)" displays the spectral width of the peak for the calculated curve.

"Show Y range" shows the "Log range" option, in which you can specify the number of magnitude order displayed on the vertical axis during automatic rescaling. Those. this parameter is in addition to the "Rescale" option and only works with the "Scale Y" logarithmic scale.

"Show cursor position" shows the coordinates of the cursor on the graph.

"Show plot title" shows the title and basic information about the plot.

## 4.5.2 Curve color setting

By default, the experimental curves are red, the calculated curves are blue. Double clicking on a curve allows you to change its color. Changes are saved with the project.

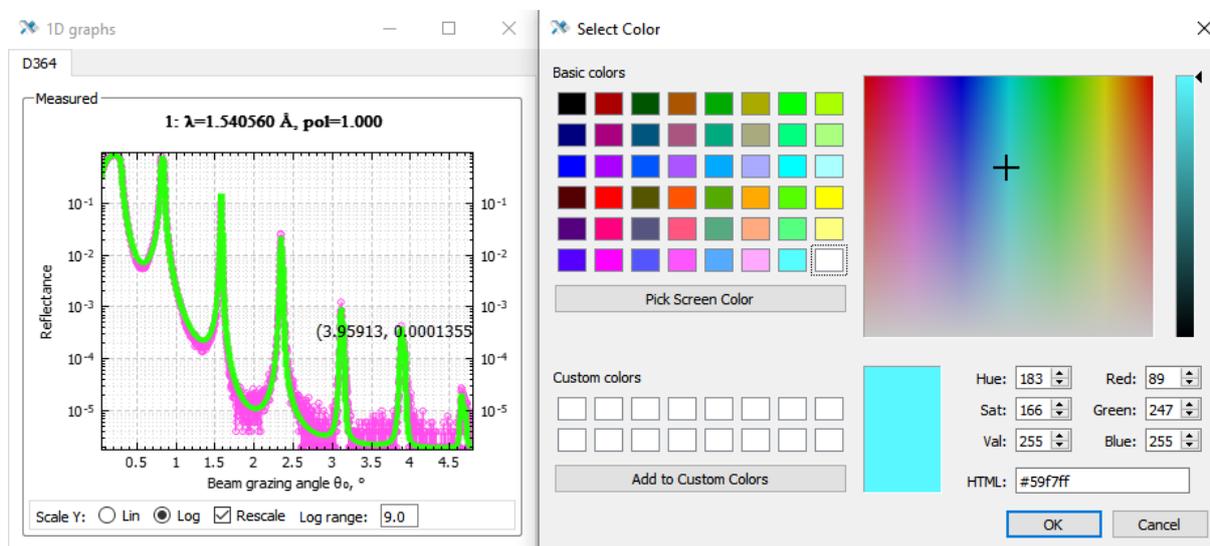


Figure 153. Change the color of the curve by double clicking

## 4.5.3 Additional curves

Sometimes it is convenient to compare the calculated curve not only with the only loaded experimental curve, but also with several others. This can be done by dragging the text file with the additional curve onto the plot area. Additional curves will be displayed along with the main ones. You can also customize the line color and thickness for them. The argument will be read in the same units that are specified on the axes at the time the file is dragged.

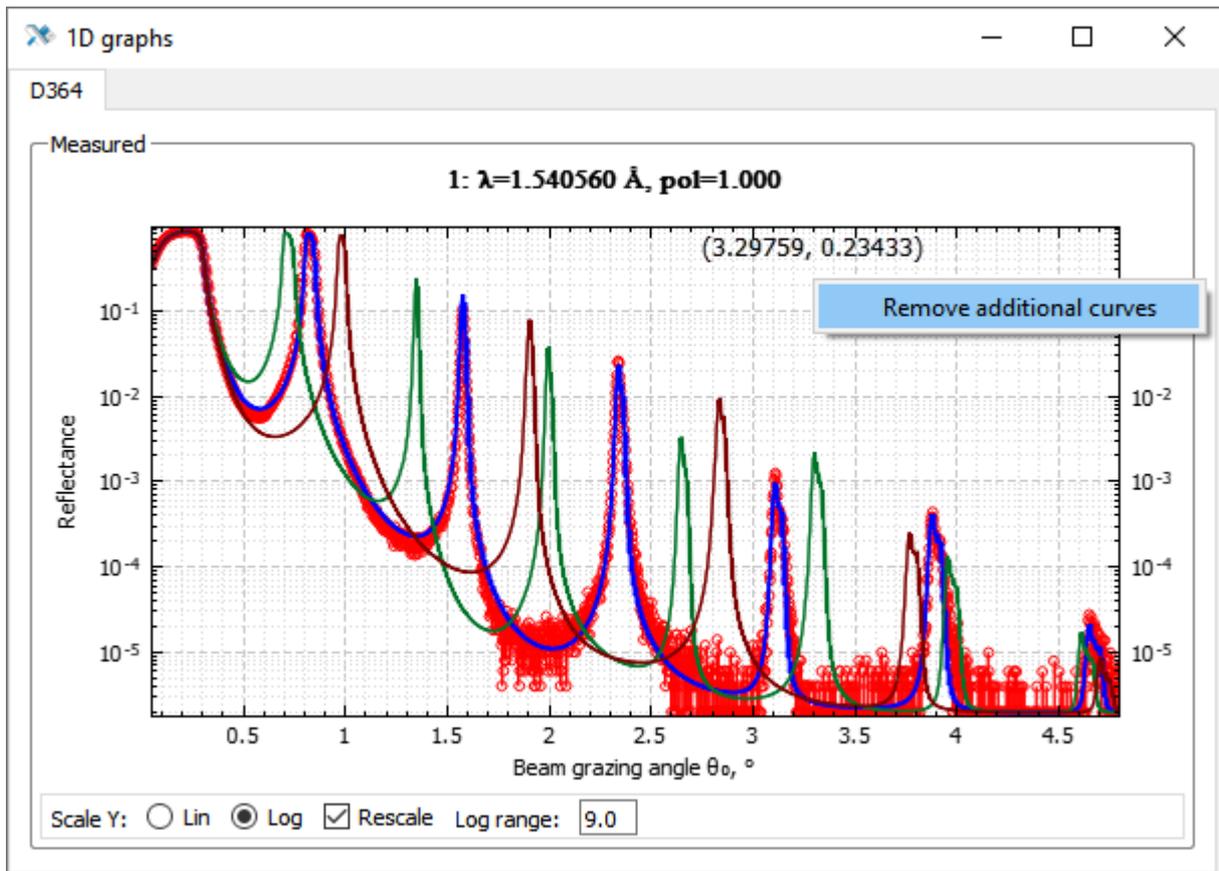


Figure 154. Additional curves on the graph

These additional curves are not saved with the project and disappear when the project is reopened. You can remove them by reopening the project, or by calling the context menu in the graph area and clicking "Remove additional curves".

## 4.6 2D graphs

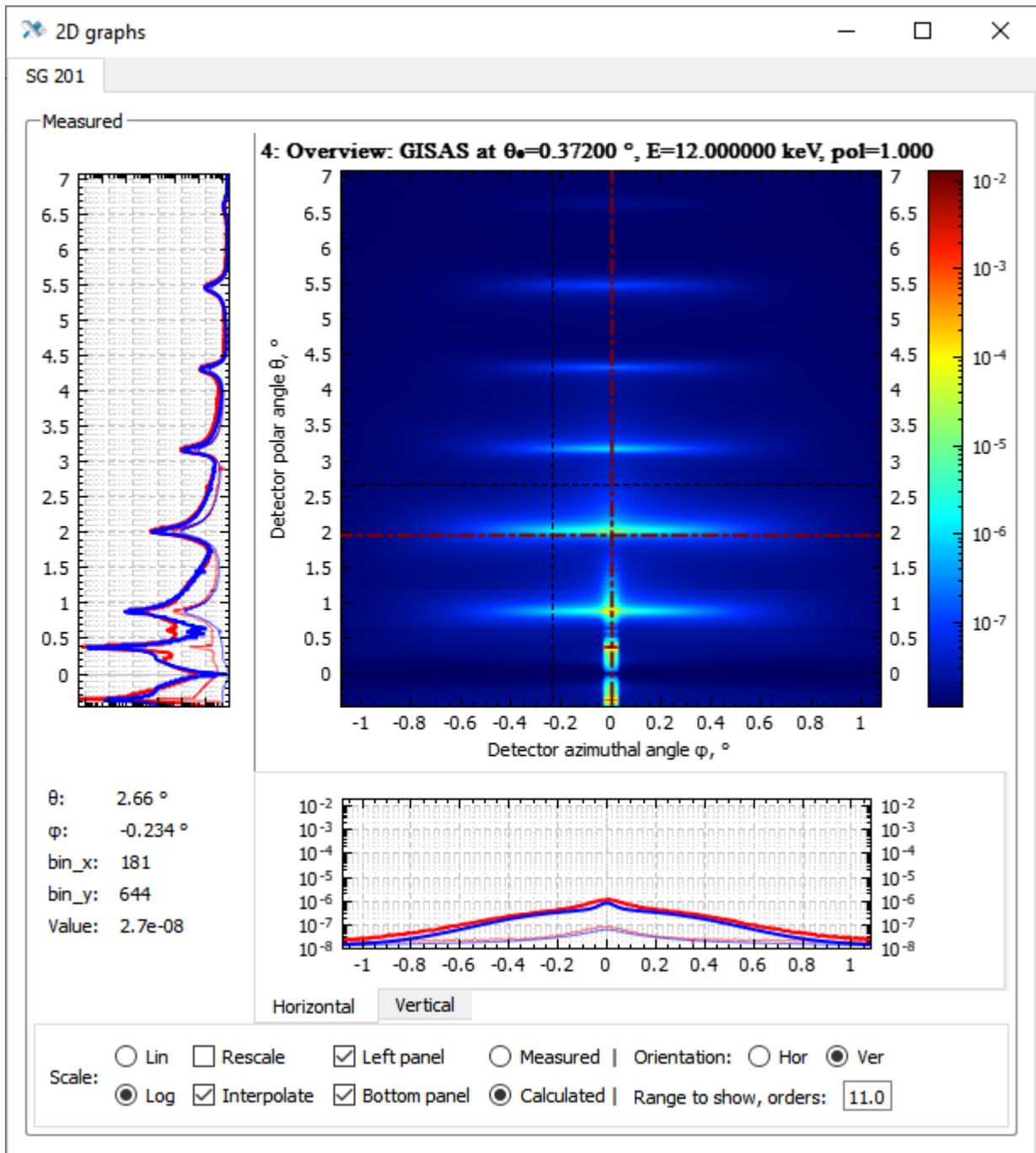


Figure 155. GISAS: measurement and calculation

There are two 2D types of data in Multifitting. These are GISAS, depending on the polar and azimuth angles, and the field intensity distribution, depending on the depth coordinate and the angle of incidence/wavelength of the probing radiation. As in the one-dimensional case, the window is divided into "Measured" and "Independent" sections, and only GISAS can be in the experimental section. The number of graphs is determined by how many of them are set in the main window and how many are "enabled" in the "Calculation settings". The redistribution of space between graphs is done in the same way as in the "1D graphs" window.

## 4.6.1 Settings

Similarly, the context menu can be called in the area outside the plots, i.e. outside the outer frame of the section or in the free space of the control panel of each chart. There is only one item in the menu – the "Settings" window.

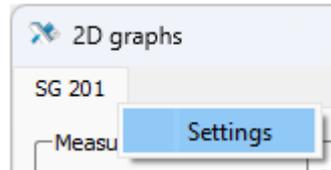


Figure 156. Context menu "2D graphs"

The upper block of settings allows you to arrange charts in several lines, separately for the "Measured" and "Independent" sections. There are two options in the bottom block:

"Show value near cursor" shows the value near the cursor.

"Show plot title" shows the title and basic information about the plot.

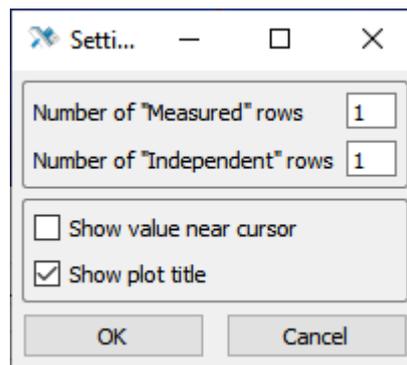


Figure 157. "2D graphs" settings

All other controls are located on the panel below each plot.

The graphs themselves are color maps with a scale of displayed values and additional blocks on which you can see the current coordinates and values, as well as one-dimensional section plots.

The sections displayed in the left and bottom blocks are shown for the current cursor position, as well as for a fixed point, which can be selected with a single left mouse button click. You can clear a fixed section by right-clicking anywhere on the map. If there is an experimental and calculated map, the experimental profile is red, and the calculated profile is blue.

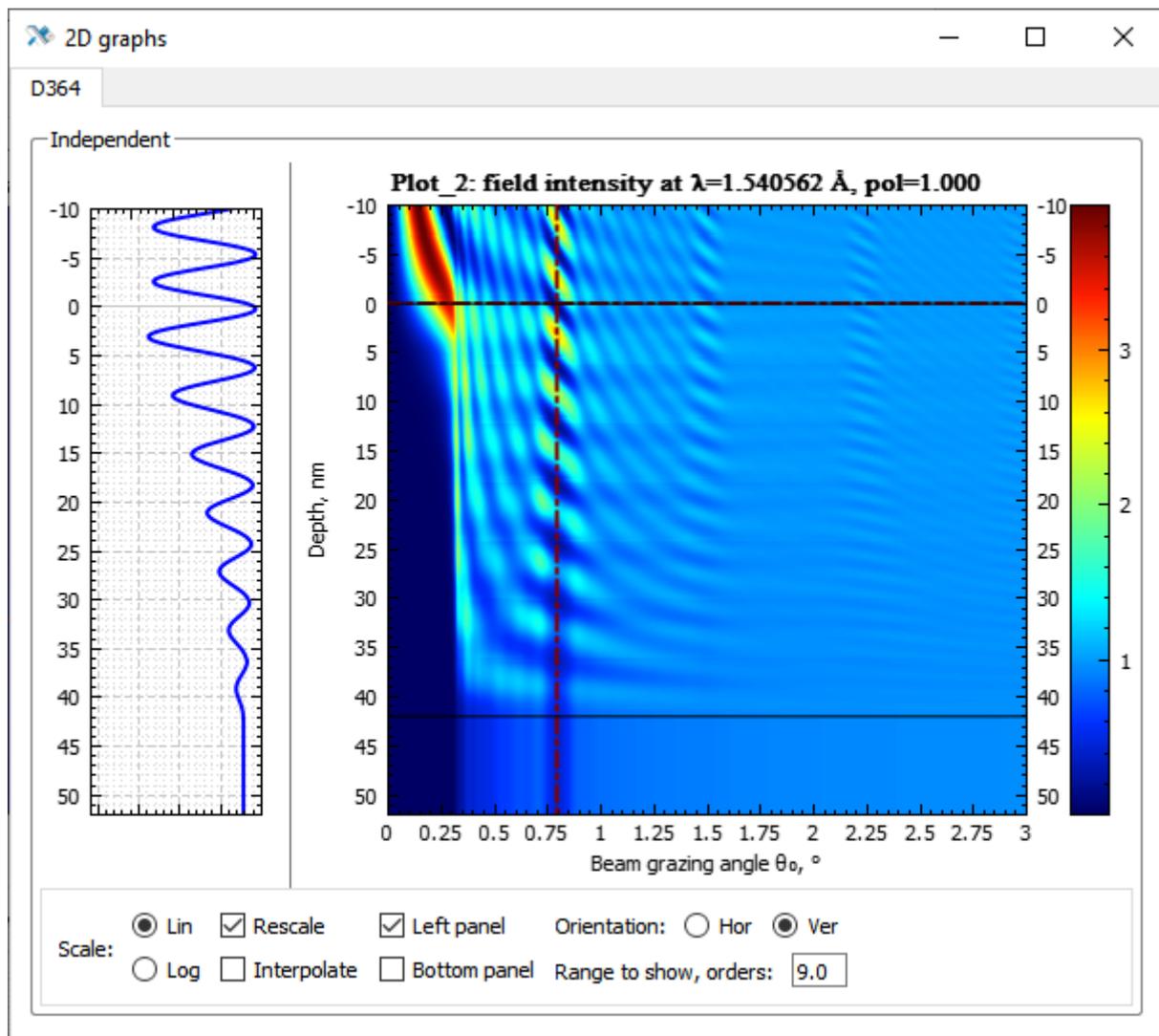


Figure 158. Field intensity in the structure

The controls should be considered in more detail. Some of them are completely similar to those for one-dimensional graphs:

"Scale" allows you to select a linear or logarithmic scale for the color scale.

"Rescale" enables plot rescaling on all axes with each calculation.

"Range to show, orders" allows you to specify the number of orders displayed on the value axis during automatic rescaling. This parameter is in addition to the "Rescale" option and only works with the "Scale" logarithmic scale.

Other options are specific to 2D maps:

"Interpolate" enables 2D interpolation for a smoother picture. Disabled option allows to estimate the sufficiency of points density to describe intensity gradients.

Switch "Measured" – "Calculated" allows you to show the corresponding map. This option is only present in the "Measured" section.

"Orientation" swaps the axes and allows you to rotate the map to the appropriate orientation, horizontal or vertical.

"Left panel" and "Bottom panel" open the left and bottom blocks, respectively, where sections of the map are shown. The left box shows only the vertical section, while the bottom box allows you to choose between the "Horizontal" and "Vertical" tabs. If both panels are open, then a block with information about the coordinates, cell number and value at the current cursor position also appears in the lower left corner.

## 4.6.2 Setting the color scheme

You can shift the visible area by dragging it with by mouse pointer, and you can scale the axes using the mouse wheel. If the pointer is in the inner area of the graph, then the scaling on both axes changes synchronously. If the pointer is located near the left axis or the lower axis, then only its scale changes. To adjust the value axis, you need to move the pointer to the color scale.

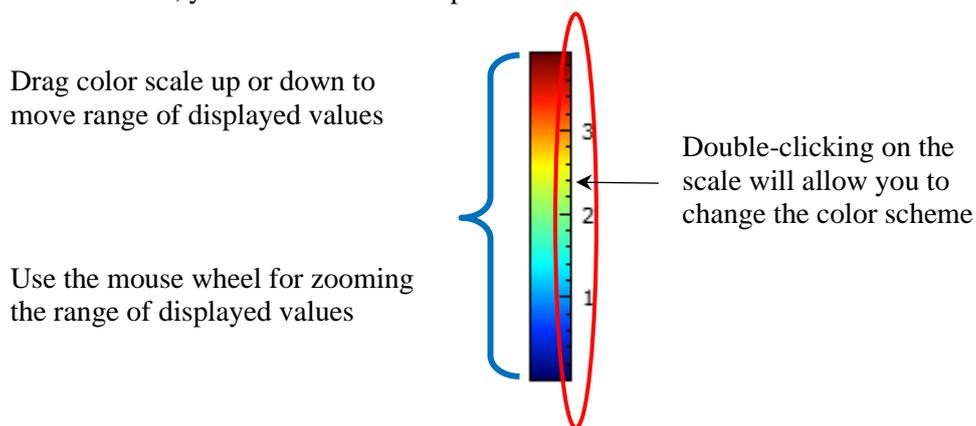


Figure 159. Working with the color scale

To change the color scheme, double-click on the right side of the color scale.

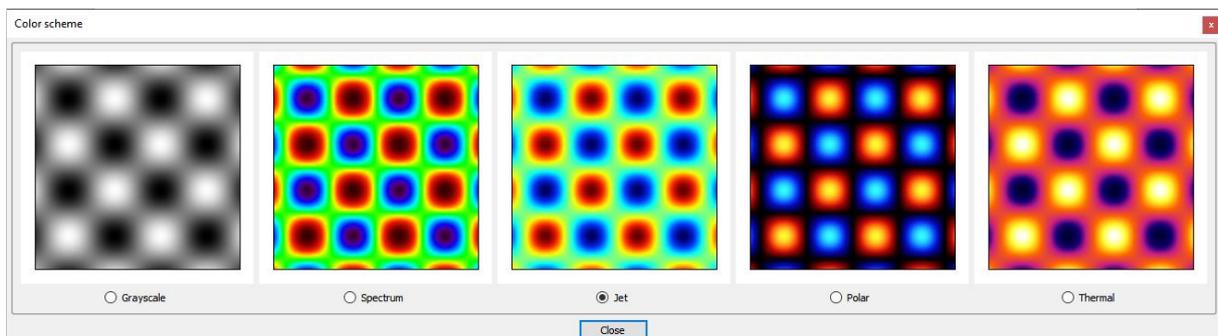


Figure 160. Change color scheme

## 4.7 Roughness spectrum

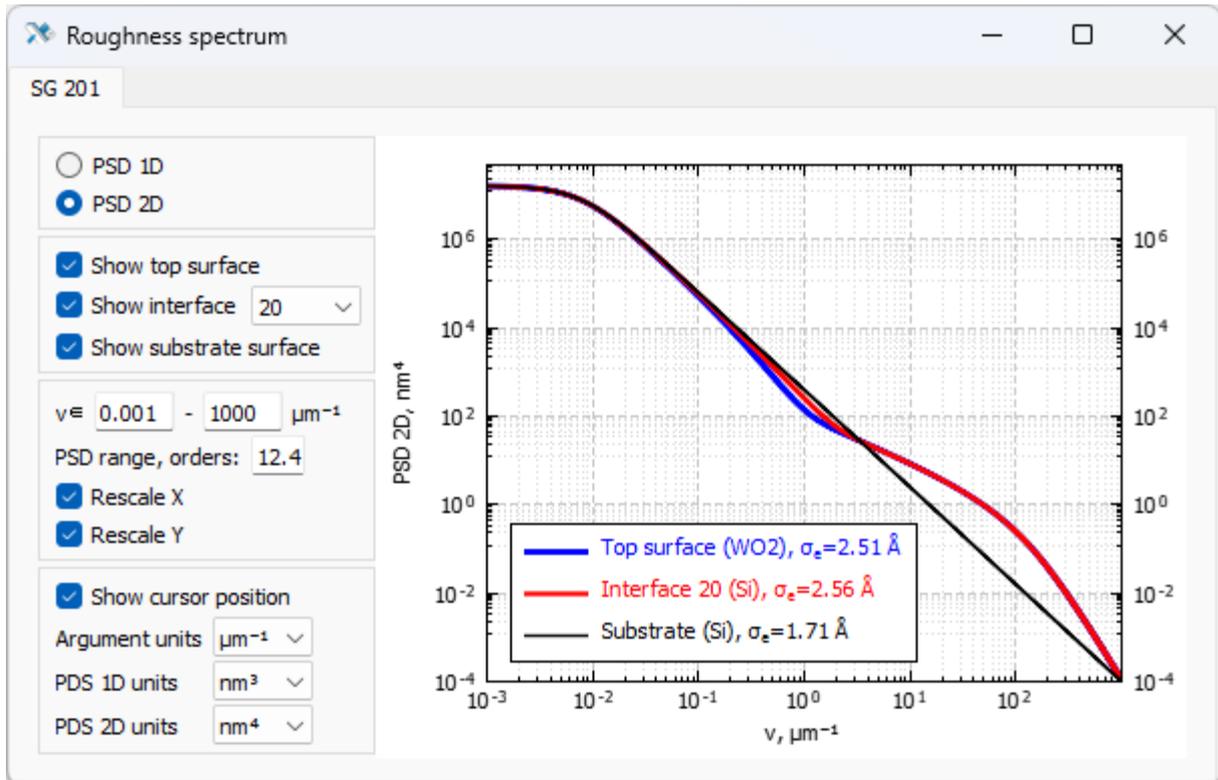


Figure 161. Roughness PSD on interfaces

Like the "Profile plot", the "Roughness spectrum" window is designed to visualize structural parameters, namely roughness. Here you can see the PSD function of the roughness in the selected model, given by several parameters in the structure table, and the effective roughness, i.e. integral of PSD over the specified spatial frequency range.

The PSD is automatically resized when changing the roughness parameters in the "Structure table" regardless of the "Recalculate" modifier. You can shift the visible area by dragging it, the display scale can be changed using the mouse wheel. If the pointer is in the inner area of the graph, then the scaling on both axes changes synchronously. If the pointer is located near the left axis or the lower axis, then only its scale changes.

On the left side is a panel with display options. In the first block, the displayed function is selected – one-dimensional or two-dimensional PSD.

The second block allows you to select the interfaces to display. If the PSD is the same throughout the depth of the structure, then interface selection is not available. In other cases, you can see up to three PSDs at the same time: substrates, surfaces, and any intermediate boundary. Interfaces are numbered starting from the substrate.

The third block contains scaling settings. The options "Rescale X" and "Rescale Y" indicate automatic scaling along the corresponding axes when recalculating curves or when changing the structure. The axes have only a logarithmic scale. For the vertical axis, you can specify the dynamic range – "PSD range", and for the horizontal axis – the minimum and maximum value of the spatial frequency  $\nu$ .

In the last block, you can specify the units of the argument and separately the units of PSD<sub>1D</sub> and PSD<sub>2D</sub>. The "Show cursor position" option shows the numerical coordinates of the cursor on the plot. The units of effective roughness correspond to the units of length in the "Structure table" (angstroms or nanometers).

All these settings are saved for the structure. When you close and open the "Roughness spectrum" window, they are played automatically. For this to happen when you reopen Multifitting, you need to save the project.

## 4.8 Particles spectrum

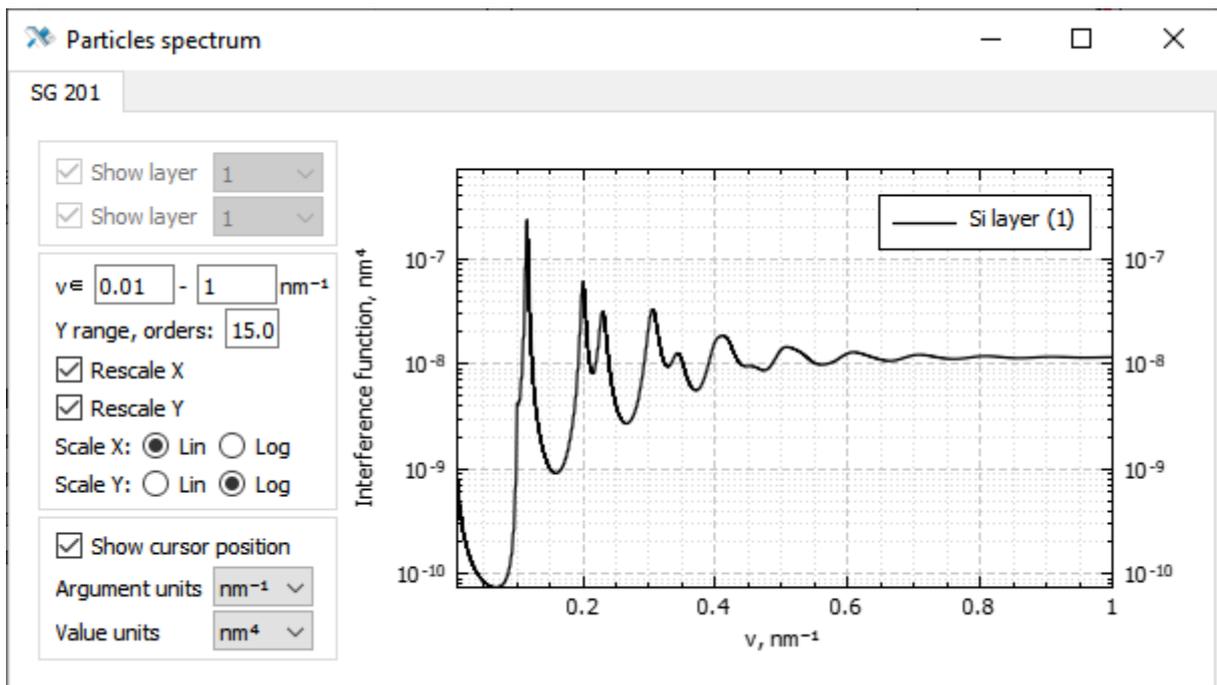


Figure 162. Interference function of particles

The "Particles spectrum" window performs the same role as the "Roughness spectrum", but for the distribution of particles in layers. The analogue of PSD here is the interference function of particles, which is specified by the parameters in the structure table. The interference function shows the ordering of the particles; in the absence of an order, it is not shown.

The interference function is automatically changed when changing the particle distribution parameters in the "Structure table" regardless of the "Recalculate" modifier. You can shift the visible area by dragging it with the pointer, and the display scale can be changed using the mouse wheel. If the pointer is in the inner area of the graph, then the scaling on both axes changes synchronously. If the pointer is located near the left axis or the lower axis, then only its scale changes.

B On the left side is a panel with display options. The first block allows you to select layers to display. If the distribution of particles is the same in all layers of the structure, then the layer selection is not available. In other cases, you can see up to two plots at the same time.

The second block contains scaling settings. The options "Rescale X" and "Rescale Y" indicate automatic scaling along the corresponding axes when recalculating curves or when changing the structure. Both axes can be scaled linearly or logarithmically. For the vertical axis, you can specify the dynamic range "Y range", and for the horizontal axis – the minimum and maximum value of the spatial frequency.

In the last block, you can specify the units of the argument and the value. The "Show cursor position" option shows the numerical coordinates of the cursor on the graph.

All these settings are saved for the structure. When closing and opening the "Particles spectrum" window, they are played automatically. For this to happen when you reopen Multifitting, you need to save the project.

## 4.9 Calculation settings

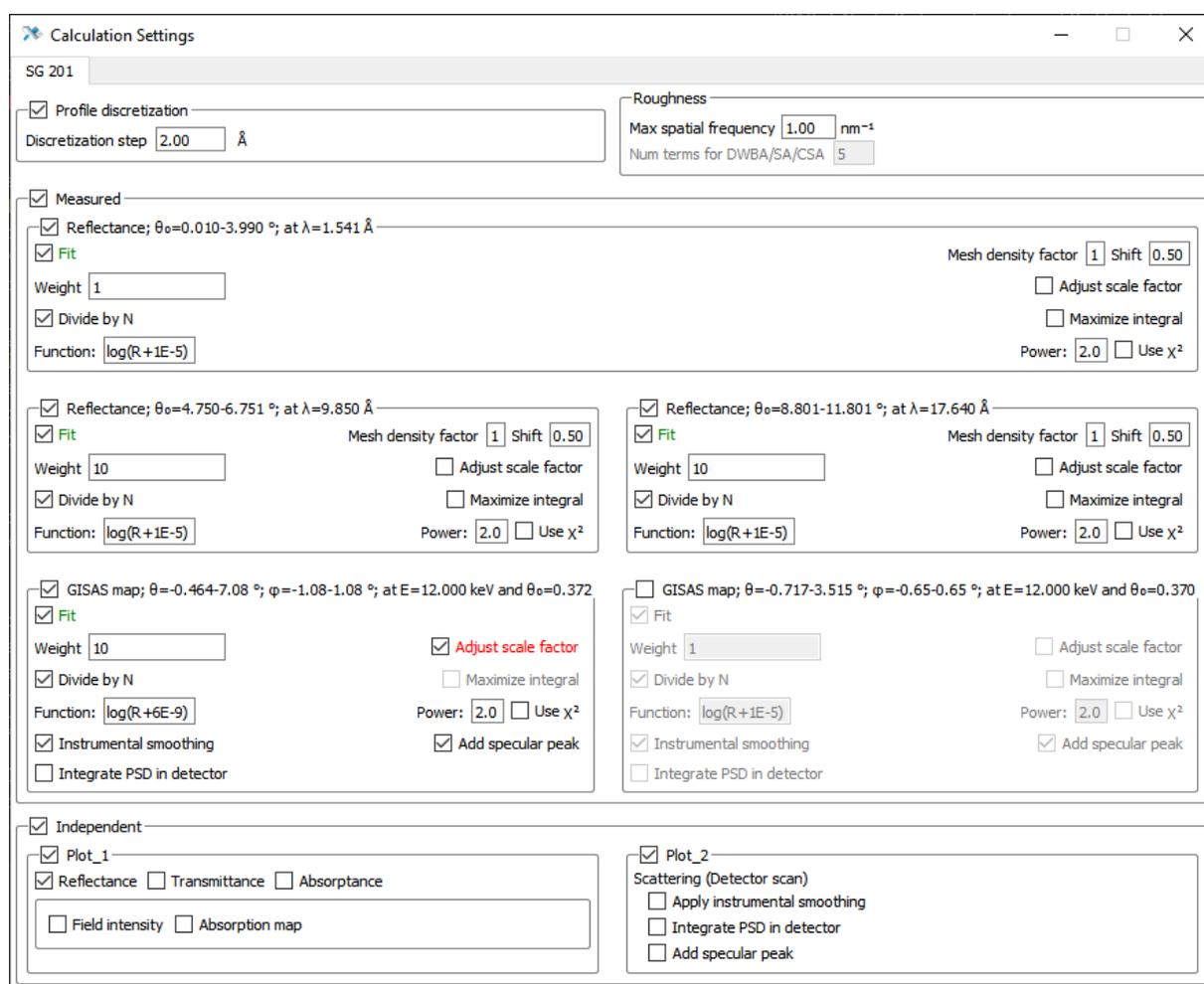


Figure 163. Window "Calculation settings"

In the main window of the program many curves can be created, but not all of them are needed at the same time. To "turn on" and "off" individual curves, as well as to select curves to participate in the fitting and their individual parameters, Multifitting has a special window – "Calculation settings".

The number of curves to display is determined by how many of them are set in the main window. As in the "1D graphs" and "2D graphs" windows, there are "Measured" and "Independent" sections. "Measured" is for loaded experimental data and the lower one, "Independent" is for calculations on a uniform grid, set directly in Multifitting. By clicking on the section heading, you can turn it on and off in its entirety. The corresponding sections will immediately turn on or off in the "1D graphs" and "2D graphs" windows. In the same way, you can enable and disable curves individually.

#### 4.9.1 Structure model parameters

In the upper part of the window there are two blocks related to the computational model of the structure, and not to specific curves: "Profile discretization" and "Roughness".



Figure 164. Additional model parameters for calculations

In the "Profile discretization" block, the partitioning of the permittivity profile into thin homogeneous layers is set to calculate the field in the structure by the method of recurrence relations. You can turn this mode on and off by clicking on the block header. The sampling step can be changed by entering a value from the keyboard or by scrolling with the mouse wheel. The actual discretization step is individual for each layer and is made in such a way that an integer number of "sublayers" fit in this layer, but not exceeding a given value. You can observe the actual discretization of the profile in the "[Profile plot](#)" window with the "Show discretization" checkbox on.

In the "Roughness" block, two parameters are set. "Max spatial frequency" is an upper limit on the spatial frequency of roughness. It should be set from general physical considerations or from external data on the high-frequency part of the roughness spectrum. This constraint is needed so that for models with a slowly diminishing PSD to the high-frequency region, the integral over frequencies converges. In calculations, it will be assumed that  $PSD(\nu > \nu_{\max}) = 0$ . "Num terms for DWBA/SA/CSA" is the number of terms in the power series of the correlation function, which is taken into account when using the appropriate approximation. The approximation itself is selected in the "Structure table", in the "[Set imperfections model](#)" window.

#### 4.9.2 Window settings

The position of the blocks within each section can also be customized. To do this, in any free area of the window, you need to right-click the context menu and select the only item "Settings". In the window that opens, specify the number of lines in the "Measured" and "Independent" sections.

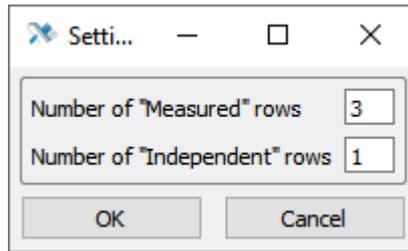


Figure 165. "Calculation settings" window settings

### 4.9.3 Specular curve with experimental grid

Now let's see what parameters should be set for each curve. In the case of reflection or transmission of radiation, these are:

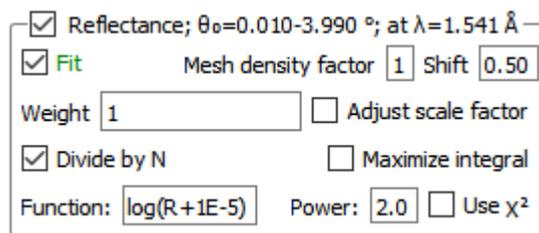


Figure 166. Parameters for calculating the experimental reflection curve

"Fit" determines whether the curve participates in automatic fitting. Non-participation in automatic fitting does not mean non-participation in single calculations! Even if the checkbox is unchecked, the calculated curve is updated with manual changes in the structure parameters and recalculations.

"Weight" is the factor by which the residual value for this particular curve is multiplied. It needs to be changed to increase or decrease the relative weight of this curve in the total residual in order for this particular curve to fit better, even to the detriment of other curves. The current residual values can be seen in console when manually recalculating («Ctrl+Shift+C»).

"Divide by N" – the residual of this curve is divided by the number of points in it. It is used so that the residuals of the curves are determined primarily by the actual mismatch between the measurement and calculation, and not by the different number of points in them.

"Mesh density factor" is an option that allows you to reduce the moiré effect on the calculated curve. It can arise if the frequency of interference oscillations is significantly higher than the density of points on the experimental grid, but is not a multiple of it. Then, "slow" oscillations are observed on the calculated curve, which significantly distort the real behavior of the curve. To eliminate the effect, the number and density of points for calculation are increased by the specified number of times, the curve is calculated, the instrumental function is applied, and only after that the result is projected onto the original grid. The "Shift" parameter, which can be changed from 0 to 1, allows you to put additional points between the initial points of the grid not equidistantly, but with a shift by the corresponding fraction of a step. The figure below schematically shows the arrangement of points of the densified mesh with "Mesh density factor" = 3 and "Shift" >0.

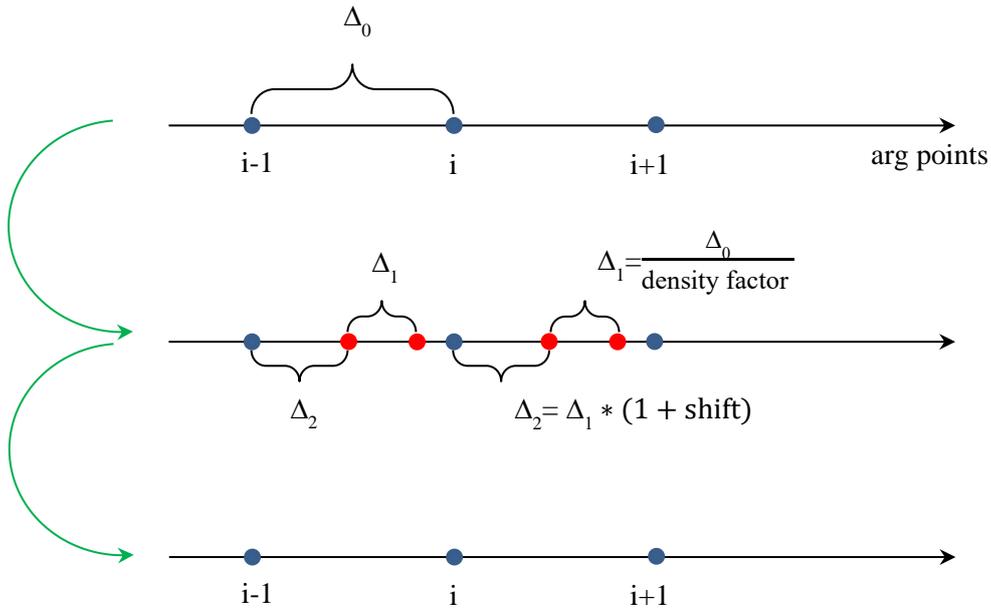


Figure 167. Method for arranging additional points in a densified grid

"Adjust scale factor" includes "Factor" in the list of fitting parameters when the curve is loaded. Variation limits are set in the import/instrument settings window for each curve. Can be used in cases where there is no absolute calibration of the measured data.

"Maximize integral" changes the aim of the automatic fitting from the best match between the loaded and calculated curve to maximizing the integral of the loaded curve with a given function from the calculated curve. This is an option for reflection/transmission only. Used to find the structure with the maximum energy efficiency (including for a multimirror layout) for a given source spectrum.

"Function" and "Power" set the type of user-defined function of the residual, which in general is arranged as follows:  $residual = \sum_i |f(calc\_value_i) - f(meas\_value_i)|^{power}$ . Accordingly, the function is given as a mathematical expression of the argument R (although we are talking not only about reflection, but also about transmission and scattering). The ExprTk library (<https://www.partow.net/programming/exprtk/>) is used to interpret the formula. In particular, one can use:

- Mathematical operators (+, -, \*, /, %, ^)
- Functions (min, max, avg, sum, abs, ceil, floor, round, roundn, exp, log, log10, logn, pow, root, sqrt, clamp, inrange, swap)
- Trigonometric functions (sin, cos, tan, acos, asin, atan, atan2, cosh, cot, csc, sec, sinh, tanh, d2r, r2d, d2g, g2d, hyp)

"Use  $\chi^2$ " switches between the residual described in the previous paragraph and the residual of the form

$$residual = \frac{beam\_counts\_per\_s}{N - p} \sum_{i=1}^N \left( \frac{calc\_value_i - meas\_value_i}{calc\_value_i} \right)^2, \text{ where } N \text{ is the number}$$

of points,  $p$  is the number of fitting parameters, and  $beam\_counts\_per\_s$  is the intensity of the probing beam, which affects the noise level and, accordingly, the reliability of the final signal.

#### 4.9.4 Independent specular curve

For an "independent" specular scan, the settings are different. Here you can select the type of quantity to be calculated: reflection R, transmission T and absorption A, which is calculated as  $A=1-R-T$ . You can also see the field functions: the field intensity distribution in the F structure and the absorption distribution in the J structure, which is simply the product of the intensity and the imaginary part of the permittivity  $J=F*Im(\epsilon)$ .

The screenshot shows a settings dialog for an independent specular scan. It includes checkboxes for 'just scan R,F', 'Reflectance', 'Transmittance', 'Absorptance', 'Field intensity', and 'Absorption map'. Below these are numerical input fields for 'Z-spacing' (2.00 Å), 'Calculation depth into ambient' (0.00 Å), 'Calculation depth from surface' (500.00 Å), and 'Calculation depth into substrate' (0.00 Å). There are also checkboxes for 'Show surface' and 'Show substrate', and radio buttons to select the calculation depth reference point.

Figure 168. Independent specular scan settings

Selecting a field function "Field intensity" or "Absorption map" opens additional options:

"Z-spacing" is step along the depth of the structure, between the points at which the field is calculated.

"Calculation depth into ambient" – the height at which the field is calculated from the surface.

"Calculation depth from surface" – the depth at which the field is calculated from the surface.

"Calculation depth into substrate" calculates the field over the entire depth of the layered structure plus the specified depth into the substrate.

"Show surface" shows the position of the surface with a line on a two-dimensional graph.

"Show substrate" shows the position of the substrate with a line on a two-dimensional graph.

#### 4.9.5 Scattering

Scattering is described by the same parameters as for [specular curve](#) as well as additional ones described below.

GISAS map;  $\theta = -0.464-7.08^\circ$ ;  $\varphi = -1.08-1.08^\circ$ ; at  $E = 12.000$  keV and  $\theta_0 = 0.372^\circ$

Fit

Weight:

Divide by N

Function:

Instrumental smoothing

Integrate PSD in detector

Adjust scale factor

Maximize integral

Power:   Use  $\chi^2$

Add specular peak

Figure 169. Parameters for calculating the scattering curve over the experimental grid

"**Instrumental smoothing**" includes taking into account the finite angular and spectral width of the beam and the finite resolution of the detector.

"**Integrate PSD in detector**" is an approximation that makes it possible in some cases to avoid the obviously non-physical amount of scattering in the specular direction in a situation where the PSD has a very sharp peak at zero spatial frequency. Multiplying the PSD value by the width of the angular size of the detector is replaced by the integral of the PSD over the spatial frequencies, resulting in scattering within the detector.

"**Add specular peak**" shows on the calculated curve not only scattering, but also a specularly reflected spot, the size and shape of which are determined by the size and shape of the beam, the distance from the sample to the detector, the angular divergence, and the size of the detector.

## 4.10 General settings

The "**General settings**" window contains settings that are common not only for the open project, but for Multifitting as a whole. They are applied immediately and do not change when you close one project and open another. Settings are grouped into several thematic tabs.

## 4.10.1 Input/Output

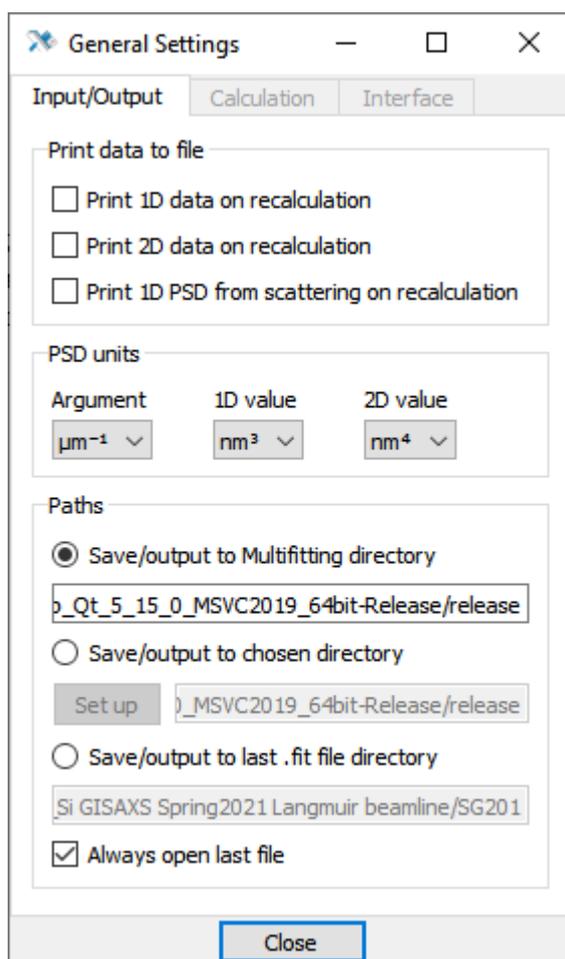


Figure 170. Tab "Input/Output"

Here are the settings related to loading and saving projects, as well as the output of structural data and the results of calculating the objective functions: reflection, transmission, scattering.

The first block indicates which calculation results will be output to the file during each manual recomputation, i.e. pressing "Ctrl+Shift+C": 1D curves, 2D curves and PSD derived directly from intensity. The latter only works for 1D scatter curves and assuming that the PSD is the same for all interfaces.

In the second block, the argument units and PSD values are selected, which are used when exporting or as default units when importing an external PSD from a file in the structural table.

In the third block, the working directory for input and output is configured. The working directory is the starting directory in the save and open dialog box.

"**Save/output to Multifitting directory**" sets the working directory to the location of the Multifitting executable.

"Save/output to chosen directory" enables selecting an any directory as a working directory by writing the address manually or by selecting the "Set up" button.

"Save/output to last .fit file directory" working directory is the directory from which the project file was last loaded last time.

"Always open last file" is an option that allows immediately after starting Multifitting by quick opening ("Ctrl+O") to load the last loaded file, regardless of the selected working directory. If the previous file does not exist, Multifitting will notify about it. If the option is disabled, then pressing "Ctrl+O" immediately after launch will open a dialog box with the working directory.

## 4.10.2 Calculation

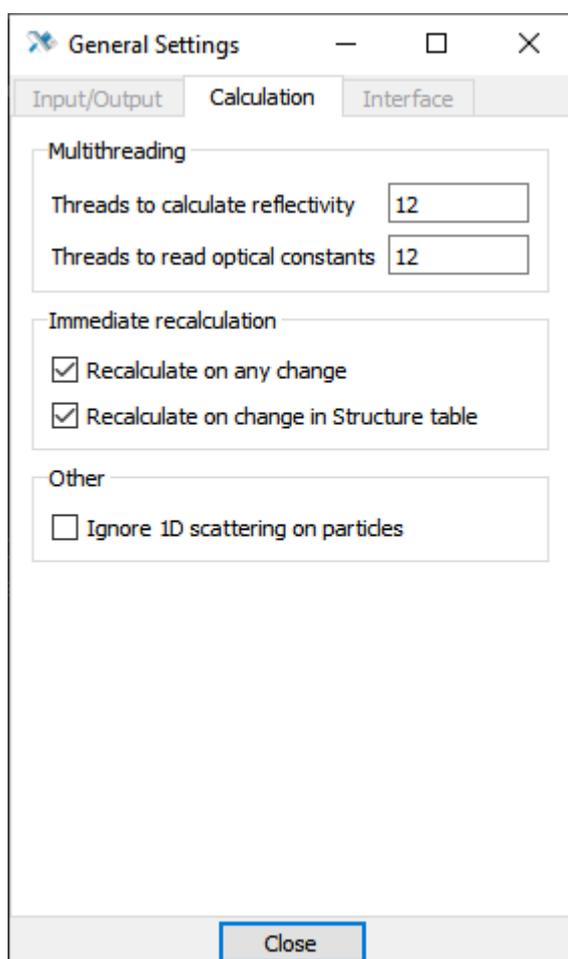


Figure 171. Tab "Calculation"

Here are the settings for the global calculation parameters.

The first block indicates the parallelization of calculations. The number of threads can be set from one to the number of logical processor cores. Routine calculations are determined by the "Threads to calculate reflectivity" item, this is what affects the speed of calculating curves.

"**Threads to read optical constants**" affects the speed of loading the optical constants database into random access memory during the Multifitting startup or when manually reloading the database from the main window menu ("**Optical constants**" → "[Reload optical constants](#)").

The second block concerns the response of Multifitting to changing parameters.

"**Recalculate on any change**" – if enabled, then when changing any parameter (except for the "**Structure table**" window), the curves are immediately recalculated.

"**Recalculate on change in Structure table**" duplicates the "**Recalculate**" modifier in the "**Structure table**" window. The curves are recalculated when any parameter in the table is changed.

The last option "**Ignore 1D scattering on particles**" allows you to ignore particle scattering in 1D curves even if particles are present and affect 2D scattering.

### 4.10.3 Interface

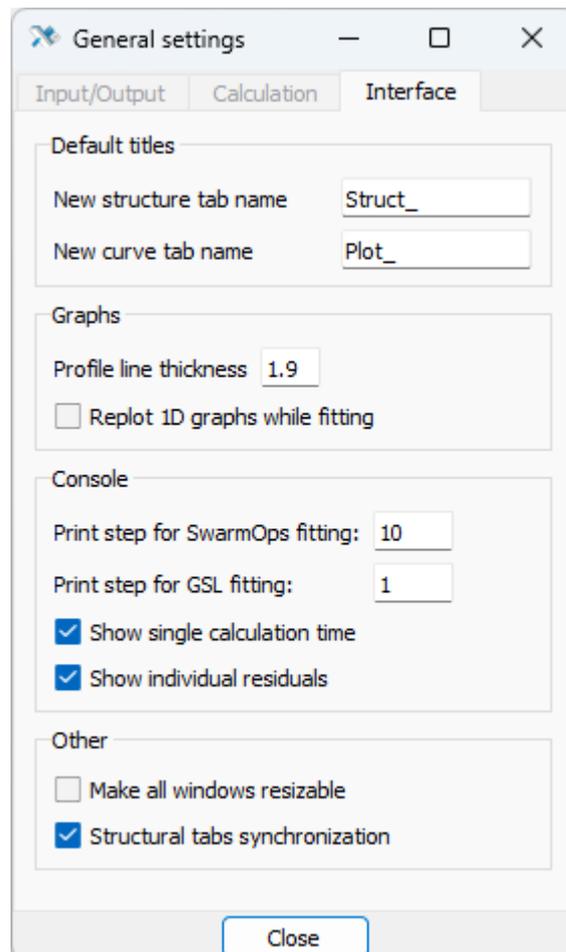


Figure 172. Tab "**Interface**"

Here are some settings for the appearance and behavior of windows.

The first block specifies the default titles that are assigned to new tabs when adding a structure or adding an independent curve in the main window.

The second block concerns charts. Here are some settings for the appearance and behavior of windows.

"**Replot 1D graphs while fitting**" – if enabled, then during the automatic fitting process, the calculated curves in the "[1D graphs](#)" window, for which the "**Fit**" parameter is set, will be automatically updated, illustrating the path that the algorithm goes through.

"**Profile line thickness**" sets the thickness of all structure profile lines in the "[Profile plot](#)". window. This parameter has been moved to the global settings for the convenience of quickly changing it when you need to get a clear, well-defined profile picture and take a screenshot.

Items in block "**Console**":

"**Print step for SwarmOps fitting**" sets the update period N during automatic fitting. The console displays information about each N-th calculation of the residual when using algorithms from the SwarmOps group.

"**Print step for GSL fitting**" sets the update period N during automatic fitting. The information about each N-th iteration is displayed in the console when using the algorithms of the GSL group.

"**Show single calculation time**" shows in the console the time of curves calculation on manual recalculation ("Ctrl+Shift+C").

"**Show individual residuals**" shows in the command line the residuals for each curve and the total residual on manual recalculation ("Ctrl+Shift+C").

Items in block "**Other**":

"**Make all windows resizable**" makes the size of all windows unfixed and gives the opportunity to make the window size smaller than the content size. Needed to save screen space.

"**Structural tabs synchronization**" – if your project has several tabs with structures, then when switching between tabs in one window, the tabs in all other open windows also switch. It is necessary not to confuse which structure is open in which window.

## 4.11 Fitting settings

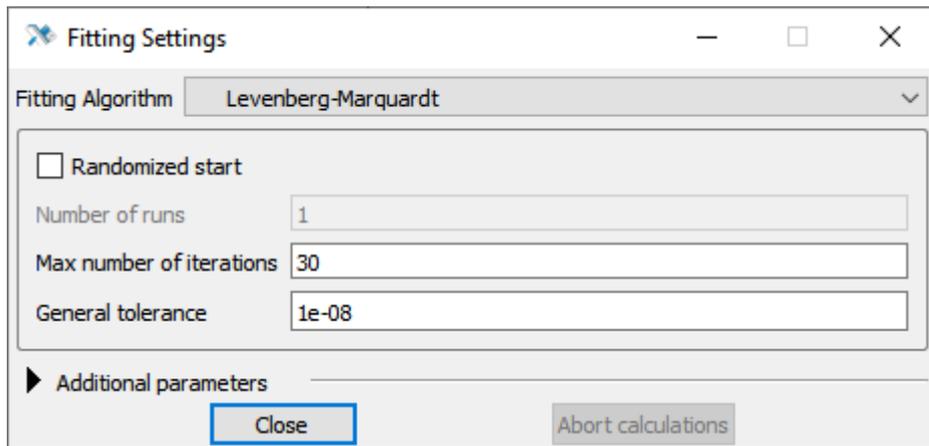


Figure 173. Window "Fitting settings"

The selection of the automatic fitting algorithm and changing its parameters is done in the "Fitting settings".

The algorithm is selected from the drop-down list. The two main groups of algorithms are distinguished by the libraries from which they are taken. Gradient algorithms are used from the GSL library (GNU Scientific Library (<https://www.gnu.org/software/gsl/doc/html/nls.html#nonlinear-least-squares-fitting>)), and predominantly stochastic algorithms are from the SwarmOps library ([https://github.com/Hvass-Labs/swarmops-other/blob/master/SwarmOpsC1\\_1.pdf](https://github.com/Hvass-Labs/swarmops-other/blob/master/SwarmOpsC1_1.pdf))

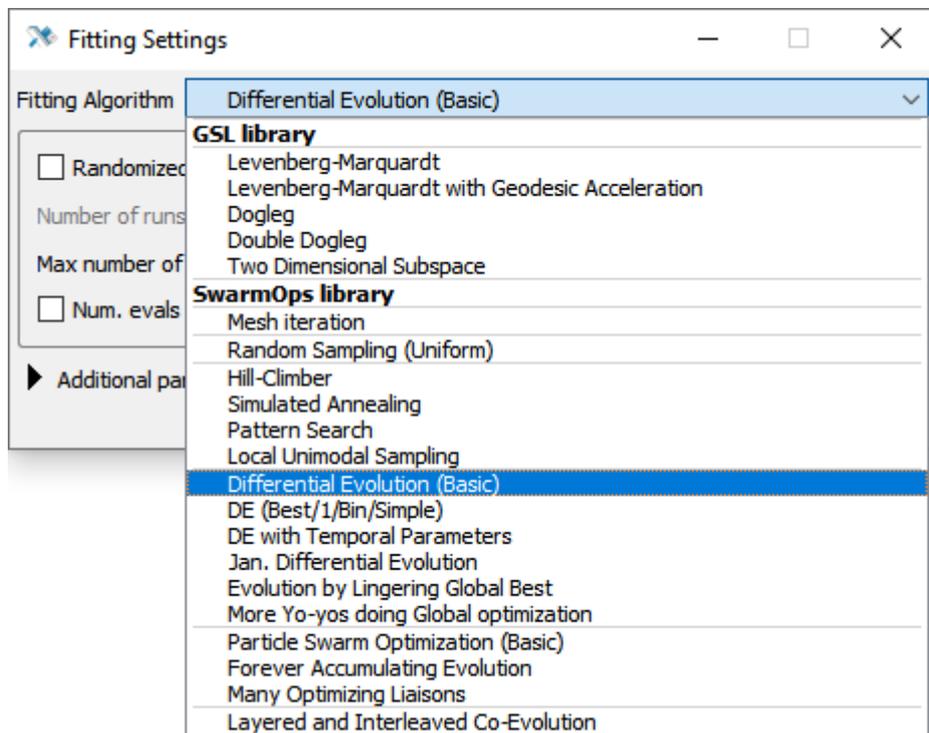


Figure 174. Algorithm list

There are few basic fitting parameters, and they are in plain sight. For algorithms from GSL, these are:

"**Randomized start**" starts a series of fittings in turn with random initial values of the adjusted parameters. The number of such runs is determined by the "**Number of runs**" parameter, and the results are written to the "`fits.txt`" file. This approach is used to cover most of the parametric space and more likely to find a sufficiently deep residual minimum.

"**Number of iterations**" is the number of iterations in each individual fitting procedure, after which the algorithm is forced to stop.

"**General tolerance**" simultaneously sets the minimum gradient, the minimum residual value and the minimum parameter step, below which the algorithm stops.

For algorithms from SwarmOps, some of the parameters are different, namely:

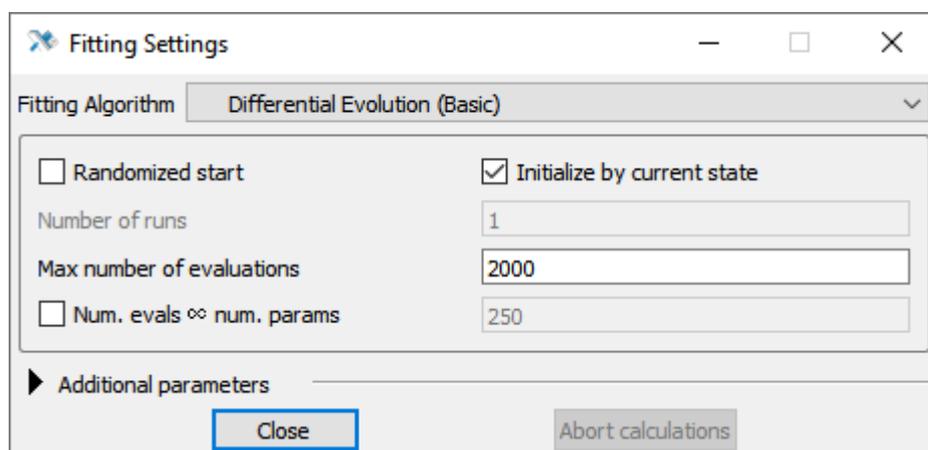


Figure 175. Window "**Fitting settings**"

"**Initialize by current state**" – the first residual calculation will be done on the structure in its current state, to ensure that the initial state is included in comparison with all other parameter sets that arise during the fitting process.

"**Max number of evaluations**" is the number of residual calculations after which the algorithm is forcibly stopped.

"**Num. evals  $\propto$  num. params**" sets the proportionality coefficient, which is multiplied by the number of fitted parameters to obtain the maximum number of residual calculations. Even within the same algorithm, the number of calculations after which convergence begins may depend on the number of parameters, so this alternative constraint can be used.

The "**Abort calculations**" button (or "Alt+,") aborts the current fitting procedure.

In addition to the described basic parameters, there are additional ones. You can see and change them by opening the bottom block by pressing the "**Additional parameters**":

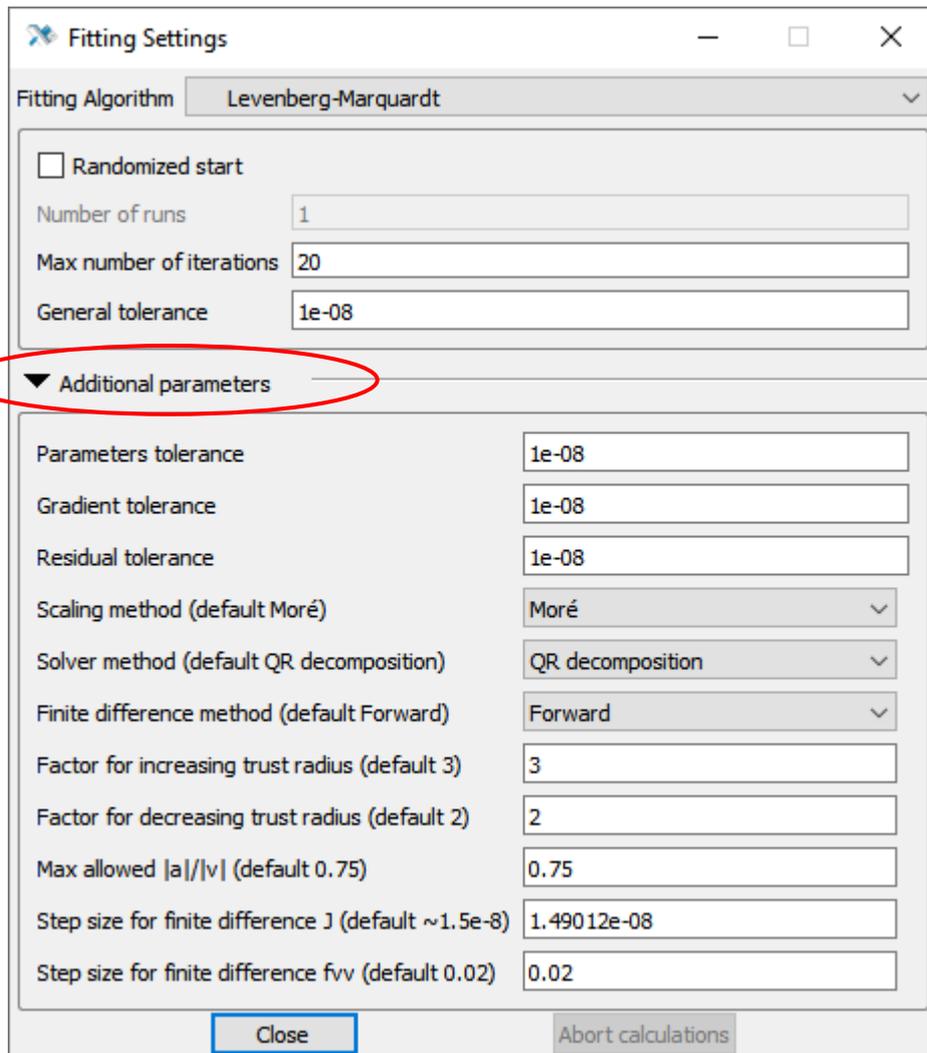


Figure 176. Additional algorithm parameters

I do not recommend changing these parameters without understanding what is happening, however, understanding the principle of the algorithm and finding out which parameters are responsible for what, you can find a more optimal combination that will give better stability and better convergence for your tasks.

## 4.12 Fits selector

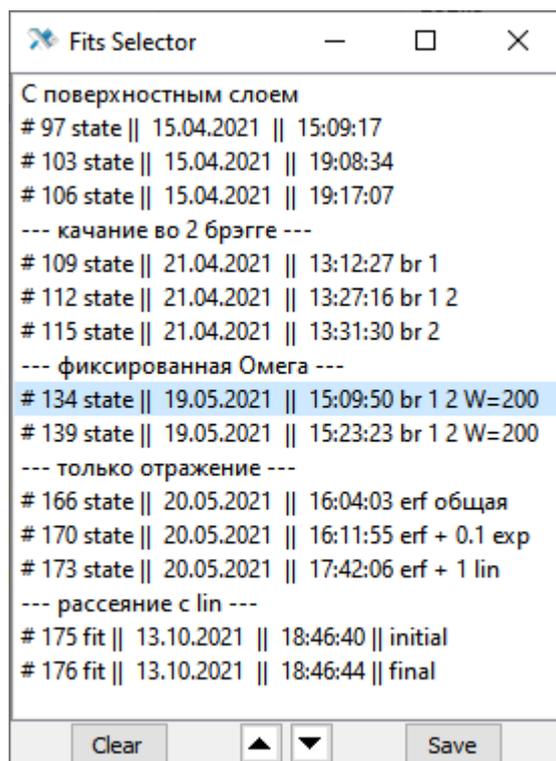


Figure 177. Window "Fits selector"

A special place is occupied by a tool for saving snapshots of the state of the structure – the "Fits selector" window. In the process of finding the right structure and the right parameters, you often need to save successful configurations so that you can return to them later if necessary.

*Attention:* Only the structure model itself and its parameters presented in the table are saved in the «Fits selector» Curve settings, instrumental parameters, calculation settings are not saved in fits and remain the same when switching between fits!

The configurations are automatically saved before the start of the new automatic fit and at the end of it, in this case the entry name is generated as "#<number> fit || <date> || <time> || initial/final". You can save the state manually by pressing the "Save" button, then its name is generated in the form "#<number> state || <date> || <time>". The number assigned to a record always increments within a saved project. Records can be renamed by selecting the record and pressing "F2" on the keyboard:

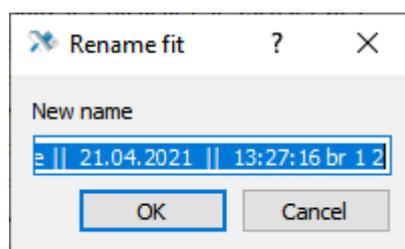


Figure 178. Renaming an entry

*Note:* To divide the fits into groups, you can enter "separators" by saving the current state (unnecessary on its own) and renaming it to something like "-----" or "- - - one more group started - -".

The "**Clear**" button clears all entries. To delete one entry, you need to select it with the mouse (or run the arrows on the keyboard) and press the "Delete" key on the keyboard. Entries can be swapped by selecting the desired entry and moving it up or down using the ▲ or ▼ buttons at the bottom of the window.

To load a saved state, double-click on it. If at the same time the "[Structure table](#)" window was open, it will close and reopen. Other windows that display structure parameters or design curves will simply update their contents.

*Note:* The «**Structure table**» window reopens slowly. If you do not need to track changes directly in the table, but need to track, for example, the reflection curves in different states and compare them, then it makes sense to close the «**Structure table**». Then switching between states will be faster.

## 5 Defining a layered structure

When starting Multifitting, the new structure by default consists of two half-spaces: the ambient (vacuum) and the substrate. Therefore, the first thing to do is to add layers to the structure and set their parameters.

### 5.1 Layer

You can add a new layer using the "Add layer" button on the [toolbar](#). The layer will be created under the currently selected structure element, but in any case between the ambient and the substrate.

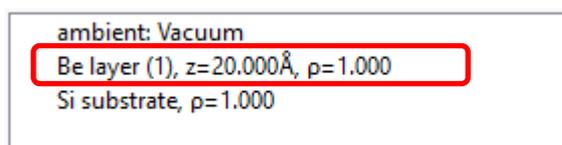


Figure 179. A layer in the structure

Layers can be copied , cut , pasted , deleted , moved up  or down  across the structure. Double-clicking the layer or "Edit"  button clicking for the selected item opens [basic properties editing window](#). Here you can specify the thickness, material and interface.

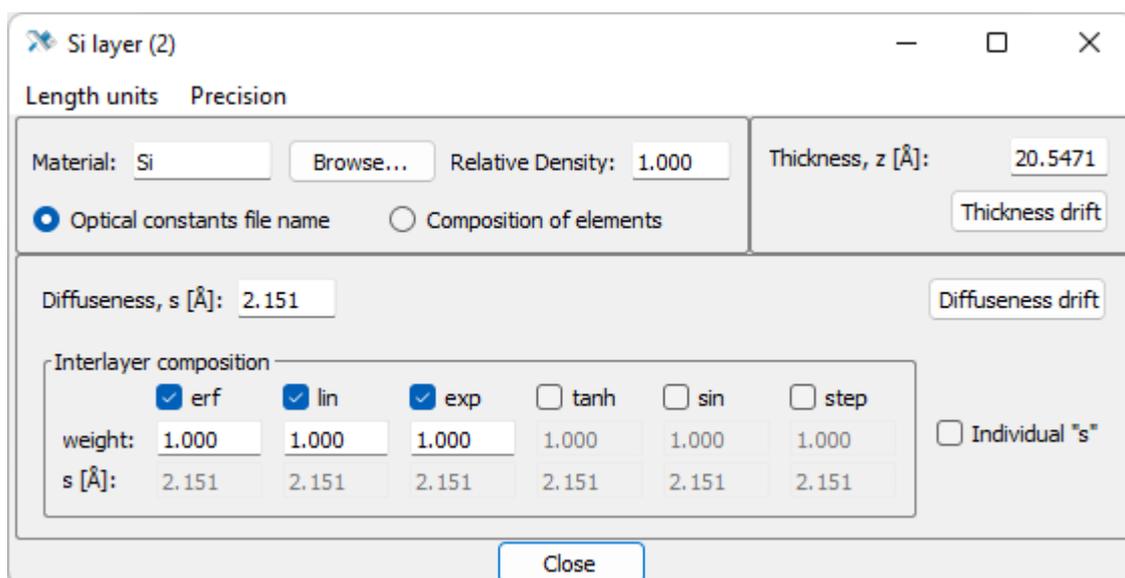


Figure 180. Window "Layer"

All these parameters can be changed from [the main table](#), except for using the material as a composition of chemical elements or as a tabular file in the database.

#### 5.1.1 Material

The material can be specified for the ambient, substrate and layers. The choice of a material model – from the database of finished materials or as a composition of individual chemical elements – can be made only in the above window. [Here](#) is a detailed description of the process of setting the material.

If the model of the material and the number of chemical elements in the composition are specified, then further work can be carried out in [structure table](#): changes in the material, elemental composition, stoichiometry, density.

Al	O	$\rho$ [g/cm <sup>3</sup> ]
2.00	3.00	3.950
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
0.00	0.00	2.500
1.00	1.00	2.700

W		$\rho$ [r.u.]
Browse		1.000
		<input type="checkbox"/> fit
		0.700
		1.000

Figure 181. Material parameters in the table

### 5.1.2 Thickness

The thickness can be set in the layer window or in a table where the parameter is indicated by the letter "z".

z [Å]
20.0000
<input type="checkbox"/> fit
10.0000
30.0000

Figure 182. Layer thickness in the table

### 5.1.3 Diffuseness

A diffuse interface can be specified for the layer and the substrate. there are two ways to do this: from [the layer properties window](#) or from the table. In the first case, you just need to enable the required profile functions, set their thickness and relative weight.

To work with the diffuse interface in the table, you must first open the [configuration window of the structure model](#) and already there enable [the corresponding block](#) and the required types of profile.

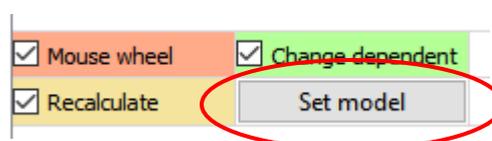


Figure 183. Accessing structure model settings in the table

Addition the profile to the table does not automatically add a profile to the calculation model. Parameter headers allow you to quickly turn profile functions on and off, affecting the shape of the transition region.

The total profile is constructed as a normalized linear combination [3]:

$$f(z) = \frac{\sum \alpha_j f_j(z, s_j)}{\sum \alpha_j}, \quad \alpha_j \geq 0, \sum_j \alpha_j > 0, \quad j = erf, lin, exp, tanh, sin, step$$

Parameter with short title "s" responsible for the uniform root-mean-square thickness of the transition region.

<input checked="" type="checkbox"/> s [Å]	<input checked="" type="checkbox"/> erf	<input type="checkbox"/> lin	<input checked="" type="checkbox"/> exp	<input checked="" type="checkbox"/> tanh	<input checked="" type="checkbox"/> sin	<input type="checkbox"/> step
0.0000	0.250	1.000	0.250	0.250	0.250	1.000
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
1.0000	s erf	s lin	s exp	s tanh	s sin	s step
20.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Figure 184. Diffuse interface in the table

The thickness of each component can also be set individually in the bottom row, but to do this [you need to click](#) on the heading "s".

## 5.2 Periodic multilayer

A new periodic multilayer is created by the button  "Add multilayer" on the [toolbar](#). Similarly, the periodic multilayer will be created under the currently selected structure element. Multilayers can be copied , cut , pasted , deleted , moved up  or down  in structure. They can also be disbanded with the button  "Ungroup" on the toolbar.

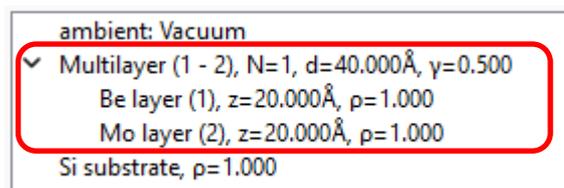


Figure 185. Periodic multilayer in the structure

Double-click on the multilayer or press the button  "Edit" opens the [window for editing basic properties](#). Here you can specify the number of periods, the thickness of the period and, if there are exactly two layers in the composition, the thickness factor.

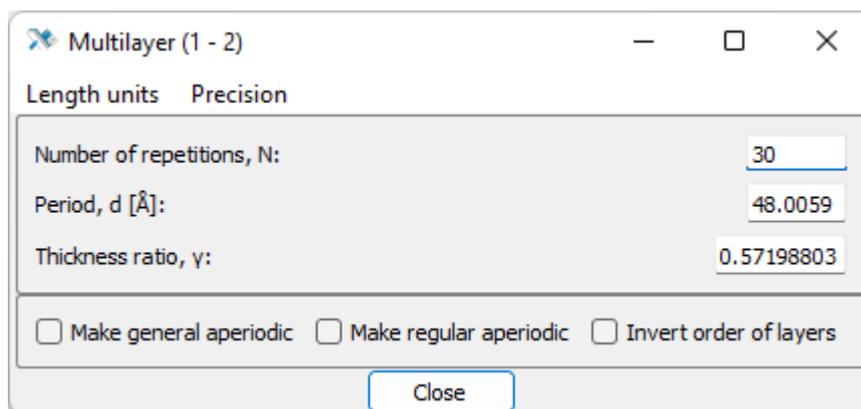


Figure 186. Window "Multilayer"

The options in the bottom block allow you to invert the order of the layers in the unit cell and turn the periodic stack into an aperiodic stack.

these parameters can be set in a "Multilayer" window or in the structure table. "N" is a number of periods, "d" is a period thickness, "γ" is a thickness factor, i.e. the ratio of the thickness of the top layer to the period.

N	d [Å]		γ
10	40.0000		0.6600000
<input type="checkbox"/> fit	<input type="checkbox"/> fit		<input type="checkbox"/> fit
1	20.0000		0.0000000
100	60.0000		1.0000000

Figure 187. Number of periods, period thickness and thickness factor in the table

By default, the layering period consists of two layers. If more is needed, new layers can be created (or deleted) within an existing multilayer. Moreover, other periodic or aperiodic multilayers can be created within the current periodic multilayer, i.e. the periodic structure can be with several levels of nesting.

### 5.2.1 Redistribution of layer thicknesses within a period

if there are three or more layers in a period you must open [a separate window](#) to change their thickness without changing the thickness of the period. you can do this by calling the context menu on the item "Multilayer":



Figure 188. Opening the window to work with the thicknesses of the unit cell layers

### 5.2.2 Thickness drift

In reality, even in nominally periodic structures the parameters of the layers are not fully repeated. First of all, deviations in the thicknesses of individual layers from the average value over all periods become

noticeable. In Multifitting it is possible to simulate linear depth drift, random deviations and periodic modulation for layer thickness and interface thickness.

With linear drift, the thicknesses of the layers are replaced  $z \rightarrow z \times \left[ 1 + \frac{dz_{lin}}{100} \left( n - \frac{N}{2} \right) \right]$

In case of random deviations:  $z \rightarrow z \times \left[ 1 + gauss\_rand \left( \frac{dz_{ran}}{100} \right) \right]$

In harmonic modulation:  $z \rightarrow z \times \left[ 1 + \frac{A}{100} \sin(2\pi(n\nu + \varphi)) \right]$

You can also read about the drift parameters [here](#). An important point: linear drift is cumulative, i.e. the more periods, the more different the thicknesses at the top and bottom of the stack. You can adjust the drift in two ways.

**The first one** – in the [editing window](#) of the layer in unit cell:

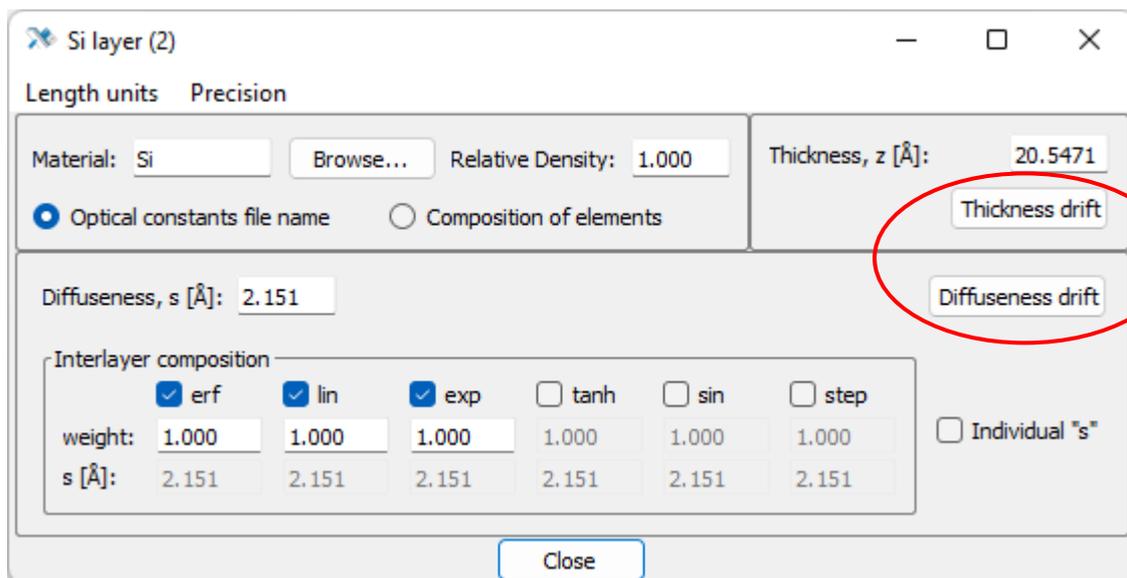


Figure 189. Access to layer thickness drift settings

**The second one** – in the structural table. To do this, you need to open "[Structure table](#)", and inside it – the [window for setting up the structure model](#), and already there to enable [the corresponding block](#) and the required types of drift. Adding them to a table does not automatically add drift to the computational model. You must enable drift by clicking on the header. Similarly, you can quickly turn off drift from the calculation.

<input checked="" type="checkbox"/> dz lin	<input checked="" type="checkbox"/> dz ran	<input checked="" type="checkbox"/> dz sin : $A \cdot \sin[2n(nv + \varphi)]$		
0.0010	1.0000	1.0000	0.3333	0.0000
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
-0.0100	0.0000	0.0000	0.0100	0.0000
0.0100	1.0000	1.0000	1.0000	1.0000

Figure 190. Thickness drift: linear, random, harmonic

<input checked="" type="checkbox"/> ds lin	<input checked="" type="checkbox"/> ds ran	<input checked="" type="checkbox"/> ds sin : $A \cdot \sin[2n(nv + \varphi)]$		
0.0370	1.1600	0.3500	0.3534	0.1120
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
-0.0100	0.0000	0.0000	0.0100	0.0000
0.0100	1.0000	1.0000	1.0000	1.0000

Figure 191. Interface drift: linear, random, harmonic

### 5.3 General aperiodic

General aperiodic is, in essence, the union of a set of elements into one container, allowing some group operations. It can contain not only individual layers, but also other periodic and aperiodic stacks. You can create it in two ways.

**The first** way is to create a periodic structure and convert it to an aperiodic one by selecting the [appropriate option](#):



Figure 192. Structure type control block

The periodic structure will be expanded into a sequence of layers, which can now be edited independently of each other. New layers or multilayers can be added to an existing general aperiodic. The general aperiodic can be disbanded by the "Ungroup"  button.

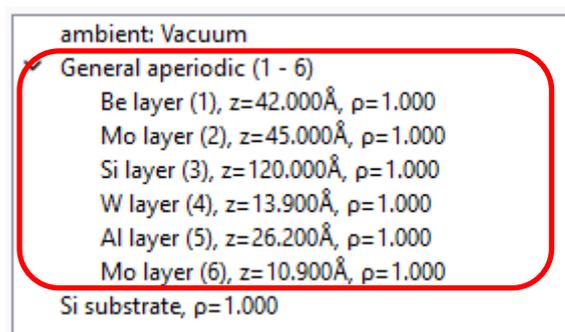


Figure 193. General aperiodic in the structure

**The second** way is to load a text file with a list of layers by clicking the "Add aperiodic multilayer"  button on the [toolbar](#) and follow [the import instructions](#).

Double-click on aperiodic or press "Edit"  button opens the [edit properties window](#).

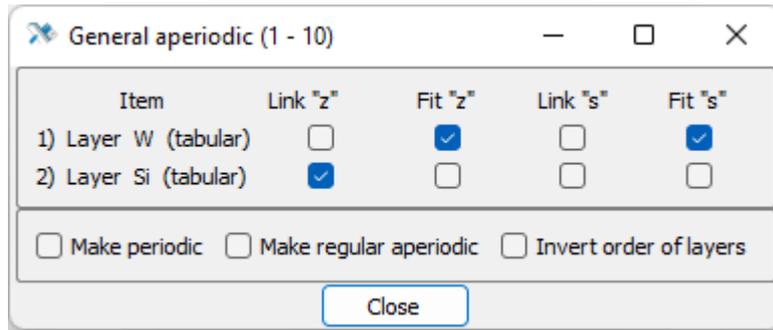


Figure 194. Window "General aperiodic"

General aperiodic can be turned into regular aperiodic or into periodic stack. It is also possible to enable and disable fitting and impose relations on the thicknesses and interfaces of all layers made of the same material. When you turn on "Link "z"" or "Link "s"" the thickness of the underlying layers/interfaces begins to depend on the top layer of the same material.

## 5.4 Regular aperiodic

Regular aperiodic is an intermediate type of structure between periodic stack and general aperiodic. It is distinguished from periodic stack by the fact that the layers can have an individual thickness and interface. But otherwise, the layers are grouped into quasi-periods or elementary cells, and have repeating material, density, and other properties. Unlike periodic and general aperiodic, regular aperiodic can only contain layers, and layers cannot be added or deleted dynamically. To change the number of layers, regular aperiodic must be recreated.

You can create a regular aperiodic by transforming from a periodic structure or from a general aperiodic. After you create it, you can [load layer thicknesses from a file](#), if there is such a need.

Double-click on aperiodic or press "Edit"  button opens the [properties window](#).

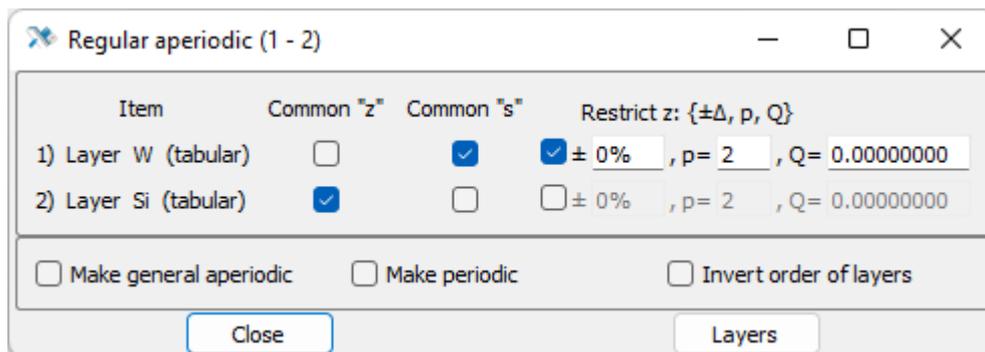


Figure 195. Window "Regular aperiodic"

You can do all of the following from the aperiodic window or from the main table.

The "Layers" button opens a [detailed table of layers](#) where you can work with individual layers, change thicknesses and interfaces, turn fitting on and off. The layers are colored to indicate whether they can be changed individually. Thickness fitting can be enabled for individual layers or for all at once if click "Fit z" while holding "Shift".

Length units		Precision				
<input type="checkbox"/>	common s	<input type="checkbox"/>	common z			
<input checked="" type="checkbox"/>	Mouse wheel	<input type="checkbox"/>	z step			
<input checked="" type="checkbox"/>	Recalculate	0.10 Å	s step			
			0.10 Å			
Cell #	Material	z [Å]	Fit z	s [Å]	ρ	
1	1	Be	75.7000	<input type="checkbox"/>	52.0000	1.000 [r.u.]
2	1	Mo	62.9000	<input type="checkbox"/>	23.0000	1.000 [r.u.]
3	2	Be	75.7000	<input type="checkbox"/>	52.0000	1.000 [r.u.]
4	2	Mo	62.9000	<input type="checkbox"/>	23.0000	1.000 [r.u.]

Figure 196. Table of regular aperiodic layers

Regular aperiodic can be turned into general aperiodic or into periodic stack. In the first case, the layer parameters will be preserved; in the second case, the layer thickness values will be replaced with averaged over the structure.

You can also turn on and off fit and link thicknesses and interfaces of all layers of the same type. "Common z" or "Common s" makes the thicknesses of all layers/interfaces of this type exactly the same. That is, if they are enabled for all layers in the cell, then this will be equivalent to the periodic structure.

[Parameters](#) in a group "Restrict z: {±Δ, p, Q}" allow you to set "soft" limiting the spread of layer thicknesses with automatic structure optimization. If the thickness of any layer will differ by more than the Δ from the average thickness of the layers of this type, then to the value of the minimized function will be added a "penalty", namely:  $Q \times ||z - \langle z \rangle - \Delta|^p$ , where z – layer thickness, <z> – average thickness of layers of this type, p – exponent responsible for the rate of increase of the penalty with an increase in deviation, Q – weight factor. Thus, it is "unprofitable" for thicknesses to go far beyond these limits ±Δ.

In the main table these parameters are located under the interface profiles.

<input checked="" type="checkbox"/> erf	<input type="checkbox"/> lin	<input checked="" type="checkbox"/> exp	<input type="checkbox"/> tanh	<input checked="" type="checkbox"/> sin	<input type="checkbox"/> step
1.000	1.000	1.000	1.000	1.000	1.000
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
<input checked="" type="checkbox"/> common z	<input checked="" type="checkbox"/> restrict z: {±Δ, p, Q}				
<input checked="" type="checkbox"/> common s	±10%	p = 4	Q = 123455.00000000		

Figure 197. Parameters of regular aperiodic

If some type of layer has common thickness/interface throughout the structure, then they can be set directly from the main table.

You can open the layer table through the context menu on the item "Regular aperiodic"

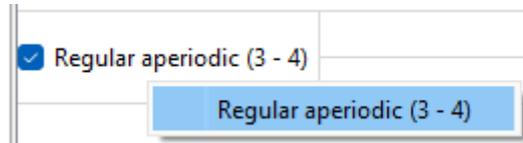


Figure 198. Context menu for layer table

## 5.5 Roughness

Roughness, unlike the diffuse interface, is set exclusively from the main table. To do this, you need to open "[Structure table](#)", there – [imperfection model settings window](#), and already there turn on the [corresponding block](#) and configure the roughness model in it.

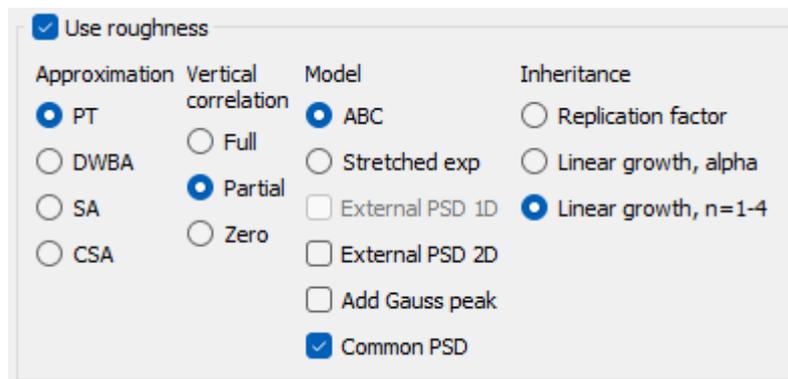


Figure 199. Block "Use roughness"

### 5.5.1 Approximation

Main model for real use – "PT", it does not use a specific kind of height statistics, but is more limited in height of roughness. "DWBA", "SA", "CSA" are reference approaches, allowing you to compare the correctness of the method.

Presence of cross-layer correlation "Full"/"Partial"/"Zero" is chosen for general physical reasons. it also determines which lateral correlation functions can be used.

<b>PT approximation</b>
<b>ABC model + external PSD + Gauss peak</b>
<b>partial vertical correlation</b>

Figure 200. Information about the selected roughness model in the table header

Next, two models are chosen: the model of the basic roughness, i.e. the roughness of the substrate, and the model of inheritance. If the cross-layer correlation is full, only the basic roughness is set, which is completely replicated to the top of the structure. If the correlation is zero, then depending on the

"Common PSD" option either one model is set for all interfaces, or for each interface individually. For partial correlation you must specify how to replicate PSD.

## 5.5.2 Substrate roughness

### 5.5.2.1 Main model

The first model is the so-called "ABC" or K-correlation model [4], describing a large number of measured spectra of polished substrates:

$$C(\rho) = \sigma^2 \frac{2^{1-\alpha}}{\Gamma(\alpha)} \left(\frac{\rho}{\xi}\right)^\alpha K_\alpha\left(\frac{\rho}{\xi}\right)$$

Its PSD is calculated analytically:

$$PSD_{2D}(\nu) = \frac{4\pi\sigma^2\xi^2\alpha}{(1 + \xi^2(2\pi\nu)^2)^{\alpha+1}}$$

The second is "Stretched exp" correlation function model [4–6] with the same three parameters:

$$C(\rho) = \sigma^2 \exp\left[-\left(\frac{\rho}{\xi}\right)^{2\alpha}\right]$$

At " $\alpha$ " = 0.5 these two models are the same.

"ABC" and "Stretched exp" have one set of parameters: total root-mean-square roughness " $\sigma$ ", for spatial frequencies from 0 to  $+\infty$ , fractal dimension " $\alpha$ ", determining the rate of descent of the spectrum into the region of high frequencies, and the correlation radius " $\xi$ ", meaning the lateral distance between the points of the relief, closer to which the heights are correlated. Big " $\xi$ " means that the main contribution to the roughness is made by the low-frequency part of the relief, small " $\xi$ " means a greater contribution of the high-frequency part.

$\sigma$ [Å]	$\xi$ [µm]	$\alpha$
2.9000	2.600	0.55
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
1.0000	0.100	0.10
20.0000	50.000	1.00

Figure 201. Parameters of "ABC" and "Stretched exp" models

### 5.5.2.2 External PSD

Along with the model roughness, it is possible to use an experimentally measured one. Loading PSD from the file is described in [another section](#). For a loaded curve, the root mean square factor "rf 1D" or "rf 2D" can be adjusted.

PSD 1D	PSD 2D
$\sigma_z$ [Å]	$\sigma_z$ [Å]
3.8707	0.0000
rf 1D	rf 2D
0.800	1.000

Figure 202. External PSD of roughness

The loaded PSD will replace the model one in its spatial frequency domain. Beyond these limits, it will be continued by the model function "ABC" or "Stretched exp". You can clearly see this PSD stitching in the window "[Roughness spectrum](#)".

### 5.5.2.3 Gaussian peak

Model PSDs are monotonous, they decrease with increasing spatial frequency. But in reality, it may be necessary to simulate the roughness with some lateral scale, in the vicinity of which a PSD peak can be observed. For this purpose, a model PSD in the form of a Gaussian peak has been added to Multifitting:

$$PSD_{2D}(v) = f \sigma_v^2 \exp\left[-\left(\frac{v-v_0}{\delta v}\right)^2\right]$$

where  $f$  is the normalization factor, such that  $\int_0^{\infty} PSD_{2D}(v) 2\pi v dv = \sigma_v^2$

This peak is **summed up** with the already existing basic model PSD and loaded experimental PSD.

The peak has three parameters: " $\sigma_v$ " – full root mean square roughness of the peak, " $v_0$ " – central spatial frequency, " $\delta v$ " – frequency peak width at half-height.

$\sigma_v$ [Å]	$v_0$ [ $\mu\text{m}^{-1}$ ]	$\delta v$ [ $\mu\text{m}^{-1}$ ]
0.0000	0.00000	0.00900
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
0.0000	0.00000	0.00090
2.0000	90.00000	0.90000

Figure 203. Gaussian peak of roughness

### 5.5.3 Replication model

If the vertical correlation type is "Partial", then the PSD correlation model must be additionally configured. There are three models.

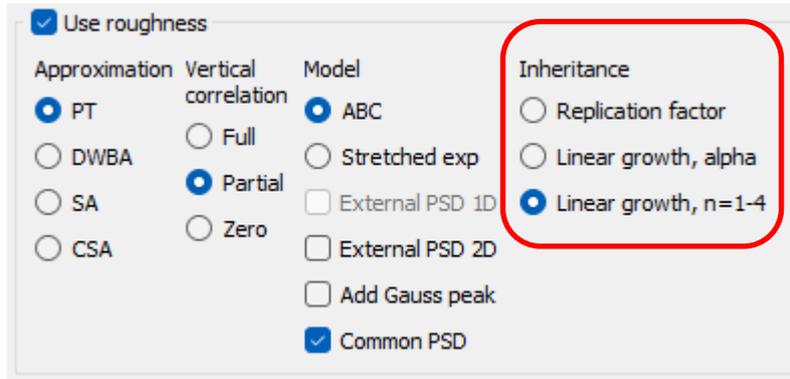


Figure 204. Vertical correlation models

#### 5.5.3.1 Replication factor

The PSD on all interfaces is considered to be the same, but the correlation between the interfaces is frequency-dependent and drops with the thickness of the layer. Cross-correlation factor is:

$$e^{-\left(\frac{\nu}{\nu_l}\right)^\beta \frac{z}{L_v}}$$

There are two main parameters here: " $L_v$ " – correlation depth at frequency " $\nu_l$ ", " $\beta$ " – frequency exponent, determining the decay rate of correlation into the region of high frequencies.

$L_v$ [Å]	$\beta$
200.000	3.00
<input type="checkbox"/> fit	<input type="checkbox"/> fit
10.000	1.00
1000.000	5.00

Figure 205. Replication parameters

Parameter " $\nu_l$ " is auxiliary, it cannot be varied automatically and is common for all interfaces. It is also located in the table separately:

PT approximation		
ABC model		
partial vertical correlation		
$\sigma$ [Å]	$\nu_l$ [ $\mu\text{m}^{-1}$ ]	$\alpha$
0.1000	10.00	0.01

Figure 206. Frequency for which the correlation depth is set

### 5.5.3.2 Linear growth, alpha

Here, a film growth model [7–9] is used to model the roughness of a multilayer structure. PSD on subsequent interfaces is partially inherited from the previous ones, and partially replaced by a growth one with a single fractal parameter " $\alpha$ ":

$$PSD_{up}(\nu) = PSD_{low}(\nu)e^{-b(\nu)z} + \Omega \frac{1 - e^{-b(\nu)z}}{e^{-b(\nu)z}}, \text{ where } b(\nu) = \left( \frac{\nu}{\nu_l} \right)^\alpha \frac{1}{L_\nu}$$

There are three main parameters here: " $\Omega$ " – the volume of particles falling during the growth process, " $L_\nu$ " – correlation depth at frequency " $\nu_l$ ", " $\alpha$ " – fractal parameter that determines the rate of the spectrum decay and cross-correlation to the region of high frequencies.

$\Omega$ [Å <sup>3</sup> ]	$L_\nu$ [Å]	$\alpha$
100.000	200.000	0.50
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
20.000	10.000	0.10
2000.000	1000.000	1.00

Figure 207. Growth parameters

As in the [previous model](#), " $\nu_l$ " is an auxiliary parameter that cannot be varied automatically and is common for all interfaces.

### 5.5.3.3 Linear growth, n=1-4

Here, a film growth model [7–9] is also used to model the roughness of a multilayer structure. PSD on subsequent interfaces is partially inherited from the previous ones, and partially replaced by a growth one. But the growth here occurs simultaneously within the framework of several processes corresponding to the frequency exponents:

$$PSD_{up}(\nu) = PSD_{low}(\nu)e^{-b(\nu)z} + \Omega \frac{1 - e^{-b(\nu)z}}{e^{-b(\nu)z}}, \text{ where } b(\nu) = \sum_{n=1}^4 a_n \nu^n$$

The model contains five parameters: " $\Omega$ " – the volume of particles falling during the growth process, " $a_1$ ", " $a_2$ ", " $a_3$ ", " $a_4$ " – growth coefficients.

$\Omega$ [ $\text{\AA}^3$ ]	$a_1$	$a_2$ [nm]	$a_3$ [ $\text{nm}^2$ ]	$a_4$ [ $\text{nm}^3$ ]
100.000	0.600	2.000	6.000	20.000
<input type="checkbox"/> fit				
20.000	0.000	0.000	0.000	0.000
2000.000	10.000	90.000	900.000	900.000

Figure 208. Growth parameters

## 5.6 Intralayer particles

Parameters of intralayer particles are set in the main table. To do this, you need to open "[Structure table](#)" and there [imperfections model settings window](#), enable [corresponding block](#) and configure the particle model.

Use particles

<p>Vertical correlation</p> <p><input type="radio"/> Full</p> <p><input checked="" type="radio"/> Partial</p> <p><input type="radio"/> Zero</p>	<p>Lateral order</p> <p><input type="radio"/> Disorder</p> <p><input checked="" type="radio"/> Radial paracrystal</p> <p><input type="checkbox"/> Specify material</p> <p><input checked="" type="checkbox"/> Common parameters for all layers</p>	<p>Model</p> <p><input checked="" type="radio"/> Hexagonal</p> <p><input type="radio"/> Square</p>	<p>Particle shape</p> <p><input type="radio"/> Spheres</p> <p><input checked="" type="radio"/> Spheroids</p> <p><input type="radio"/> Cylinders</p>
---	--	--	---

Figure 209. Block "Use particles"

Cross-correlation of particles located in different layers can be selected from the set "**Full**"/"**Partial**"/"**Zero**" basing on general physical considerations.

Lateral correlation may be absent ("**Disorder**") or correspond to an orientationally averaged two-dimensional paracrystal ("**Radial paracrystal**"). "**Disorder**" can also be understood as the limiting case of a paracrystal with infinite large random particle displacements.

The type of lattice affects not only the interference of particles, but also the density of the particles in the layer, and hence the scattering intensity.

**DWBA approximation**

**radial paracrystal, hexagonal lattice**

**partial vertical correlation**

Figure 210. Information about the selected particle model in the table header

The "**Specify material**" option allows you to choose whether the material of the particle differs from the material of the layer. Even if not, the density may differ.

Unlike roughness, particles can be individually switched on and off in each layer. Depending on the type of interlayer correlation and the "**Common parameters for all layers**" option, the particle shape, lattice and lateral order settings for individual layers are also available.



Figure 211. Managing particles layout

### 5.6.1.1 Particle parameters

The material of the particle is specified in the same way as the material of the layer.

Al	Al	$\rho_0$ [g/cm <sup>3</sup> ]
1.00	1.00	2.699
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
0.00	0.00	2.500
0.00	0.00	2.700

Figure 212. Material of particles

Parameters that determine the shape of the particles: radius in the plane of the layer and height in the perpendicular direction.

R [Å]	H [Å]
10.000	20.000
<input type="checkbox"/> fit	<input type="checkbox"/> fit
0.000	0.000
20.000	20.000

Figure 213. Particle dimensions

### 5.6.1.2 Distribution parameters

If there is no lateral order ("**Disorder**"), then only the average distance between the particles in the base lattice is specified.

$r_s$ [Å]
100.000
<input type="checkbox"/> fit
10.000
200.000

Figure 214. Average distance between the particles

If "**Radial paracrystal**" is selected: "**r**" is average lattice parameter, " **$\delta r$** " is a root mean square variation of this distance (Gaussian distribution), "**D**" is the diameter of the paracrystalline domain, which determines the maximum number of particles involved in interference.

r [Å]	$\delta r$ [Å]	D [ $\mu\text{m}$ ]
100.000	5.000	500.000
<input type="checkbox"/> fit	<input type="checkbox"/> fit	<input type="checkbox"/> fit
10.000	0.500	0.010
200.000	90.000	900.000

Figure 215. Lattice parameters

With partial vertical correlations ("Partial") the root mean square random displacement of the whole particle layout relative to the underlying layout is specified. The distribution is Gaussian.

$\Delta$ [Å]
5.000
<input type="checkbox"/> fit
0.000
50.000

Figure 216. Random particle layout displacement relative to the underlying layout

By vertical coordinate, the default center of the particles coincides with the center of the layer. This position can be changed by the parameter " $z_p$ ": positive value lifts up the layout to the surface, negative – lowers to the substrate. " $\delta z_p$ " specifies the root mean square vertical spread of individual particles with Gaussian distribution.

$z_p$ [Å]	$\delta z_p$ [Å]
0.000	0.000
<input type="checkbox"/> fit	<input type="checkbox"/> fit
-10.000	0.000
10.000	5.000

Figure 217. Vertical arrangement of particles in a layer

If the values are such that the particles begin to go beyond the layer boundaries, then the calculation becomes incorrect, because the intersection of particles by the layers boundaries is not accounted in the model.

*Attention:* When calculating the field of the unperturbed scattering problem, the particles do not change the average dielectric constant of the layer. But when calculating the reflection from the system containing the particles, the permittivity changes to the average taking into account the particles.

## 6 Calculation of curves and loading of experimental data

Before you get the result of the calculation, you need to specify what exactly should be calculated, i.e. set the geometry of the simulation and instrumental parameters. Multifitting offers five scan geometries:

- Specular geometry: reflection and transmission, distribution of field intensity in the structure
- Detector scan: one-dimensional scattering at a fixed angle of beam incidence
- Rocking curve: one-dimensional scattering at a fixed angle between beam and detector
- Offset scan: one-dimensional scattering with fixed angular offset between detector and specular direction
- GISAS map: two-dimensional scattering pattern at a fixed angle of beam incidence

Each type of simulation can be used in one of two modes: calculation from a given equidistant grid ("independent curve") or calculation from a grid of loaded data ("experimental curve"). Let's describe how to create and configure a new simulation.

In accordance with the [structure of the main window](#), you need to add a new or duplicate an existing curve, [independent](#) or [experimental](#).

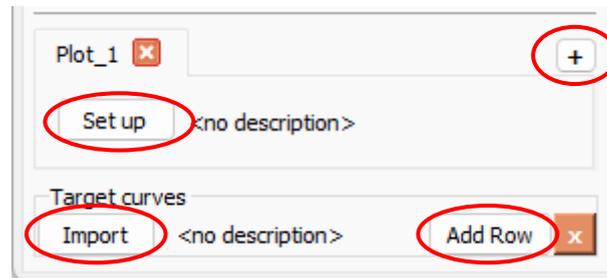


Figure 218. Adding a new curve

When you click on "Set up" for an independent curve, or "Import" for experimental, the window for choosing the type of simulation will open

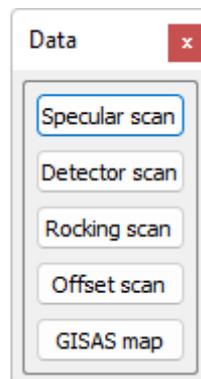


Figure 219. Choosing the simulation type

## 6.1 Specular scan

### 6.1.1 Independent curve

The window structure of the specular independent curve is discussed in detail in the chapter [User interfaces](#). You can go through each of the blocks "[Units](#)", "[Argument](#)", "[Beam](#)", "[Detector](#)", "[Footprint and distortion](#)", and set the required values.

It is worth paying attention to the block "[Argument](#)" because it is here that you can choose the type of curve – spectral or angular.

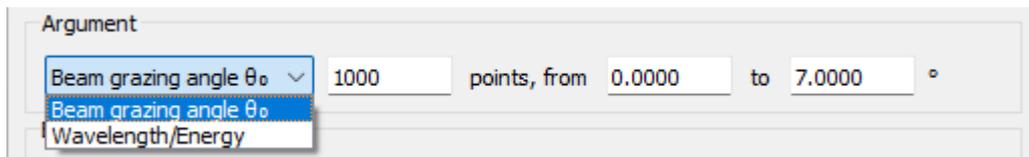


Figure 220. Block "[Argument](#)"

In the block "[Beam](#)" the angular and spectral width of the beam shall be specified. The value is set directly in the window, and additional parameters can be set by clicking the "[Set up distribution](#)".

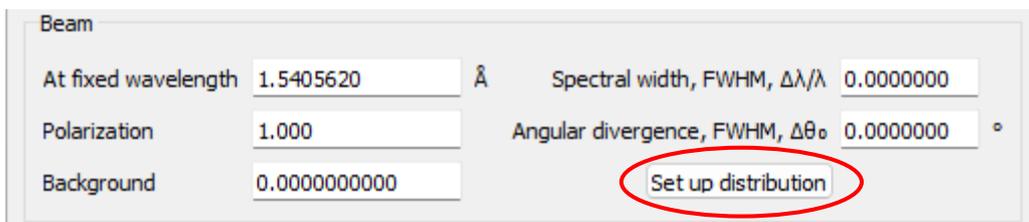


Figure 221. Block "[Beam](#)" and distribution setting

A separate window will open with graphs of the distribution of radiation intensity by wavelength or angle. The options here are as follows::

Value "[Spectral width](#)"/"[Angular divergence](#)" – full width at half the maximum of the distribution (FWHM).

"[Distribution](#)" – distribution function.

"[Use sampling](#)" – calculate several curves with different values from the distribution and sum them with the corresponding weights. The most direct and accurate way to take into account the non-monochromaticity and non-collimation of the beam, but requiring a sufficiently large number of calculations. The options below concern the setting of the sampling of points for the calculation:

"[Coverage](#)" – specify the width of the area within which the points will be selected.

"[Number of samples](#)" – how many angle/wavelength values to take for calculation.

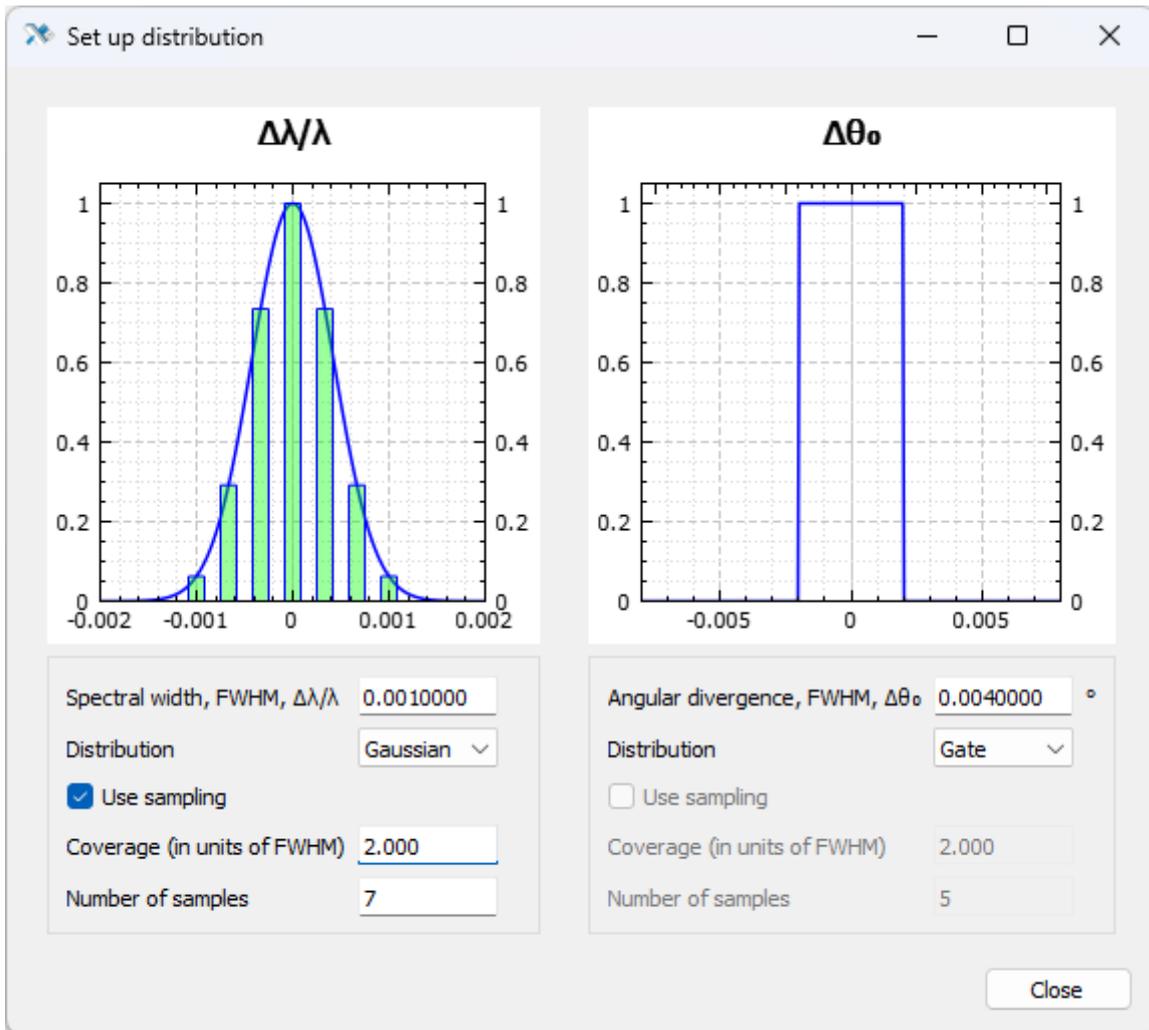


Figure 222. Window of angular and spectral distribution of incident intensity

If the "Use sampling" option is turned off or unavailable, the divergence is taken into account in a simpler way: the "clean" curve is replaced by a convolution with an appropriate distribution. In this case, the spectral distribution still affects the angular curve, and the angular distribution affects the spectral curve. This is done in accordance with the following consideration: in the presence of angular widening, spectral widening is applied, which gives the same distribution of the wave vector.

$$k = \frac{2\pi}{\lambda} \sin(\theta + \delta\theta) = \frac{2\pi}{\lambda - \delta\lambda} \sin \theta$$

A distribution with enabled sampling and a sufficient number of points gives a reference curve against which the result of using a less accurate but faster convolution can be compared.

### 6.1.2 Experimental curve

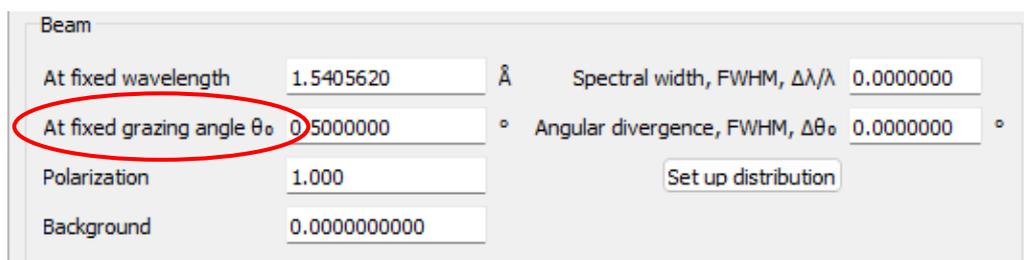
The structure of the experimental curve window is discussed in detail in the chapter [User interface](#). The window consists of blocks "[Measurement](#)", "[Argument](#)", "[Value](#)", "[Beam](#)", "[Detector](#)", "[Footprint and distortion](#)" and [bottom block](#) with data import and export buttons.

The process of loading data is described in the section "[Import](#)" of chapter "[Export and import data](#)". The data format is described in the [corresponding section](#).

After the curve appears on the graph, pay attention to the axes ranges, check the correctness of the data.

## 6.2 Detector scan

The structure of the [independent](#) and [experimental](#) curve window is discussed in detail in the chapter **User interface**. The approach is the same as in the previous section, but here is an additional parameter – a fixed grazing angle of the beam, it is also a specular angle for the detector.

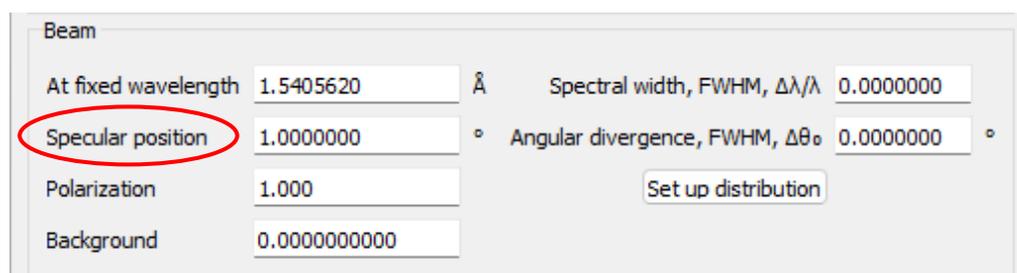


Beam			
At fixed wavelength	1.5405620	Å	Spectral width, FWHM, $\Delta\lambda/\lambda$ 0.0000000
At fixed grazing angle $\theta_0$	0.5000000	°	Angular divergence, FWHM, $\Delta\theta_0$ 0.0000000 °
Polarization	1.000		Set up distribution
Background	0.0000000000		

Figure 223. Fixed grazing angle

## 6.3 Rocking scan

The structure of the [independent](#) and [experimental](#) curve window is discussed in detail in the chapter **User interface**. Almost all parameters are the same as for [specular geometry](#), but the argument type can be chosen: the grazing angle of the incident beam or the deviation of the sample from the specular position. An additional parameter is the grazing angle of the beam, at which the reflected beam enters the detector.



Beam			
At fixed wavelength	1.5405620	Å	Spectral width, FWHM, $\Delta\lambda/\lambda$ 0.0000000
Specular position	1.0000000	°	Angular divergence, FWHM, $\Delta\theta_0$ 0.0000000 °
Polarization	1.000		Set up distribution
Background	0.0000000000		

Figure 224. Specular position angle

## 6.4 Offset scan

The structure of the [independent](#) and [experimental](#) curve window is discussed in detail in the chapter **User interface**. Almost all parameters are the same as for [specular geometry](#). An additional parameter is the constant offset of the detector from the specular direction.

Beam			
At fixed wavelength	1.5405620	Å	Spectral width, FWHM, $\Delta\lambda/\lambda$ 0.0000000
At fixed detector offset	0.0000000	°	Angular divergence, FWHM, $\Delta\theta_0$ 0.0000000 °
Polarization	1.000		Set up distribution
Background	0.0000000000		

Figure 225. Offset from the specular direction

## 6.5 GISAS map

### 6.5.1 Independent curve

The window structure of an independent GISAS measurement is discussed in detail in the chapter [User interface](#).

The data on the detector is two-dimensional, but the grazing angle of the beam is set only for the polar coordinate  $\theta_0$ . There is no azimuthal beam coordinate  $\phi_0$ , it is considered to be zero. But angular divergence  $\Delta\phi_0$  in the azimuthal plane can be specified.

Beam			
At fixed wavelength	1.5405620	Å	Spectral width, FWHM, $\Delta\lambda/\lambda$ 0.0000000
At fixed grazing angle $\theta_0$	0.5000000	°	Angular divergence, FWHM, $\Delta\theta_0$ 0.0000000 °
Polarization	1.000		Angular divergence, FWHM, $\Delta\phi_0$ 0.0000000 °
Background	0.0000000000		Set up distribution

Figure 226. Block "Beam"

### 6.5.2 Experimental curve

The structure of the experimental curve window is discussed in detail in the chapter [User interface](#).

The process of loading data is the same as for one-dimensional curves and is described in "Import" section of chapter [Export and import data](#). That is, you just need to drag and drop the data file onto the curve window. The format of the two-dimensional data is also described in the [corresponding section](#).

After data loading, a color map will be shown. Based on it, you should not only adjust the already described tool parameters, but also orient the data along the axes using the buttons for rotating the image counterclockwise ↺ and clockwise ↻.

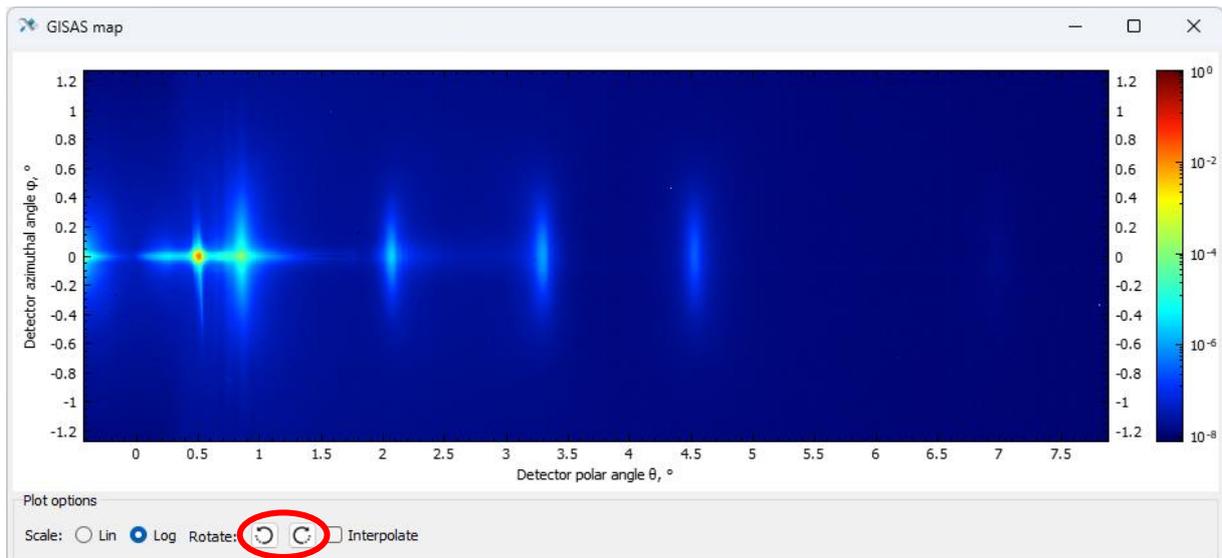


Figure 227. Adjust the orientation of two-dimensional data

Unlike one-dimensional data here the range of arguments is not read from the file. The argument is specified separately in the corresponding [block](#), and the grid of values is assumed to be uniform.

Figure 228. Block "Argument"

## 6.6 Visualization of calculation results

When the scan parameters are set you can start a calculation ("Ctrl+Shift+C") and open a window "[1D graphs](#)" or "[2D graphs](#)" or both depending on the set of curves.

Part of the settings related to the calculation of the curve is located in the window "[Calculation settings](#)". For scattering, you can specify [additional settings](#) for the instrumental function and the accounting of the specular component.

For an independent specular scan in "[Calculation settings](#)" the type of calculated value [is specified](#): "[Reflectance](#)", "[Transmittance](#)" or "[Absorptance](#)", distribution of field intensity in the structure "[Field intensity](#)" and the distribution of absorption in the structure "[Absorption map](#)".

Figure 229. "Independent" specular scan settings

When you simultaneously select the checkboxes corresponding to "Reflectance", "Transmittance" or "Absorptance" on the graph of the one-dimensional curve only one value will be displayed – the rightmost. Similarly, if simultaneously enabled "Field intensity" and "Absorption map" – the "Absorption map" will be shown in the "2D graphs" window.

## 7 Optimization and fit

Automatic or at least automated finding of suitable structure parameters is one of the main requirements for programs like Multifitting. It makes sense to distinguish two classes of tasks faced by researchers and technologists for which this functionality is required.

The first problem is the problem of **analysis** or reconstruction. In this case, a sample and the results of its measurements on the reflectometer and diffractometer are given. The nominal structure of the sample is known and the task is to find quantitative parameters of the model, allowing to explain all the essential features of the experimental data. In cases where the appropriate set of parameters is not unique, it is highly desirable to find all such sets. The experimental data here are , one-dimensional scattering scans, and GISAS..

The second problem is the problem of **synthesis** or optimization. It is required to obtain a structure with certain optical characteristics, for example, with a specific reflection spectrum. Only those parameters can be varied that technologists can control during the synthesis of the structure. First of all, this is the number of layers, their thickness and chemical composition. Interlayer interfaces and the internal microstructure of layers are much more difficult to control and change, so they are often fixed, relying on them to be known for a proven technological process. In the formulation of the problem, there may be additional conditions that facilitate the creation of the structure: limiting the number of layers, limiting the spread of layer thicknesses. As a result, it is enough to have only one set of structure parameters that allow you to solve the original problem. External data to be adjusted can be simulated – for example, a reflection curve of a certain shape, or experimental – for example, the radiation spectrum of a source.

The synthesis problem is easier to automate than the structure analysis problem. In synthesis, there is a clear set of parameters to be varied, there is a clear criterion by which we evaluate the result. When analyzing a structure, you have to consistently complicate its model by introducing new parameters for fine-tuning. You almost always have to manually consider different options and intersperse manual changes with automatic adjustment.

### 7.1 Selecting target curves

After all the necessary data is loaded, you can choose which one to use for fit. This is done in the window "[Calculation settings](#)". The desired curves must 1) be enabled for the calculation and 2) have a "Fit" checkbox enabled:

Reflectance;  $\theta_0=0.010-3.990^\circ$ ; at  $\lambda=1.541 \text{ \AA}$   
 Fit Mesh density factor  Shift   
Weight   Adjust scale factor  
 Divide by N  Maximize integral  
Function:  Power:   Use  $\chi^2$

Figure 230. Participation of the curve in the fit

If these two checkboxes are enabled the residual value will be calculated for this curve, which in turn will affect the evolution of the values of the structure parameters. In order for the fit to be more effective,

you should configure several additional parameters. The section "[Specular curve with experimental grid](#)" gives a brief description of the parameters in the block of the curve.

First of all, you should pay attention to the type of residual function. Fields "**Function**" and "**Power**" define the custom residual function, which is arranged as follows:

$residual = \sum_i |f(calc\_value_i) - f(meas\_value_i)|^{power}$ . Checkmox "**Use  $\chi^2$** " allows using another

$$function: residual = \frac{beam\_counts\_per\_s}{N - p} \sum_{i=1}^N \left( \frac{calc\_value_i - meas\_value_i}{calc\_value_i} \right)^2$$

If there are several curves, you may need to adjust the parameters "**Weight**" and "**Divide by N**", to balance the contribution of each curve to the overall residual. You can see the current residual values with each recalculation ("**Ctrl+Shift+C**"), if in the "**General settings**" window on the "[Interface](#)" tab checkbox "**Show individual residuals**" is enabled:

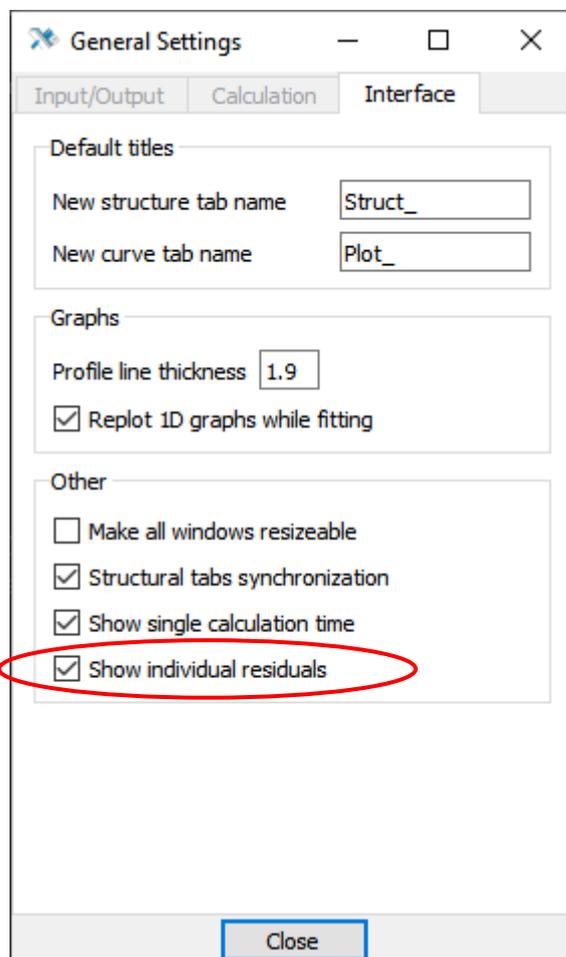


Figure 231. "**Interface**" tab

Then the console will display the residual of each individual curve and the total residual.

```

PowerShell 7
-----
Calculation...      0.016012  seconds
-----
struct 0      curve 0      residual    0.813042
struct 0      curve 1      residual    0.677707
common residual ..... 1.49075
-----

```

Figure 232. Residuals: total and individual

"Adjust scale factor" allows you to vary the normalization factor "[Factor](#)" of target curve. This may be required only if the experimental curve is not normalized, in other cases it is not necessary!

For the problem of optimizing the energy efficiency of the mirror at a given source spectrum, there is a switch "**Maximize integral**". With it, the integral of the loaded curve with a given function of the calculated curve will be maximized.

## 7.2 Structure parameters

### 7.2.1 Enabling parameter

Parameter fitting is turned on and off in the [main table](#) of the structure. Each [parameter](#) has a check box "**fit**" below the field with the current value. Enabling adds a parameter to the fitting list and makes the fields for setting the upper and lower bounds editable.

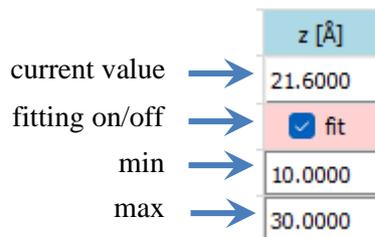


Figure 233. Enabling fit and variation limits

The parameter will not be varied if it is [dependent](#). In this case, its header will not be blue, but red or yellow.

### 7.2.2 Regular aperiodic

In the case of regular aperiodic, the fitting of all parameters except thicknesses can be turned on and off only for all layers of the same type simultaneously. The thicknesses of the layers can be enabled for fitting both together and separately. Enabling "**fit**" from the main table will result in a fit for all layers, which can be seen by opening the [regular aperiodic layer table](#).

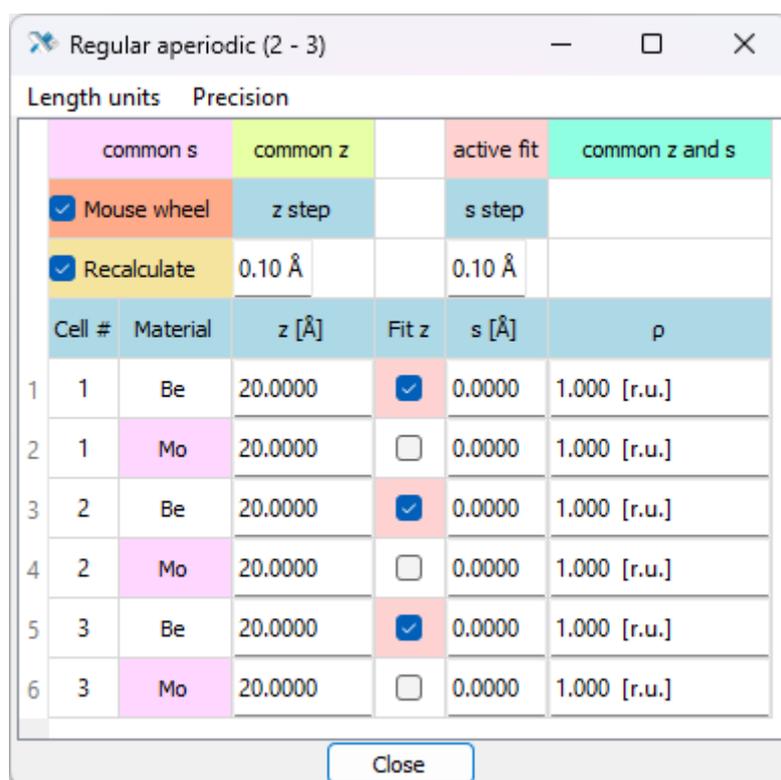


Figure 234. Fitting regular aperiodic layers

"Fit z" this table enables fit for individual layers. If you hold down "Shift" when you turn on, the fit of all layers at once will be enabled.

Variation limits are the same for all layers of the same type, they are set in the main table. But in addition to these limits, you can additionally [limit the spread](#) of thicknesses around the average value. This feature can be enabled from the main table.

### 7.2.3 Coupled parameters

Parameters can be linked to each other by a functional dependency. To do this, you need to [call the context menu](#) by right-clicking on the parameter title. The process is described in the "[Coupling editor](#)".

Зависимые параметры не подгоняются, а рассчитываются из значения "параметра-хозяина" на каждой итерации. В зависимости от модификатора "[Change dependent](#)" зависимые параметры могут быть заблокированы от ручного изменения или нет. При автоматической подгонке они пересчитываются в любом случае.

## 7.3 Fitting algorithm

Before starting the fit, you should select the algorithm in the window "[Fitting settings](#)" and set basic settings.

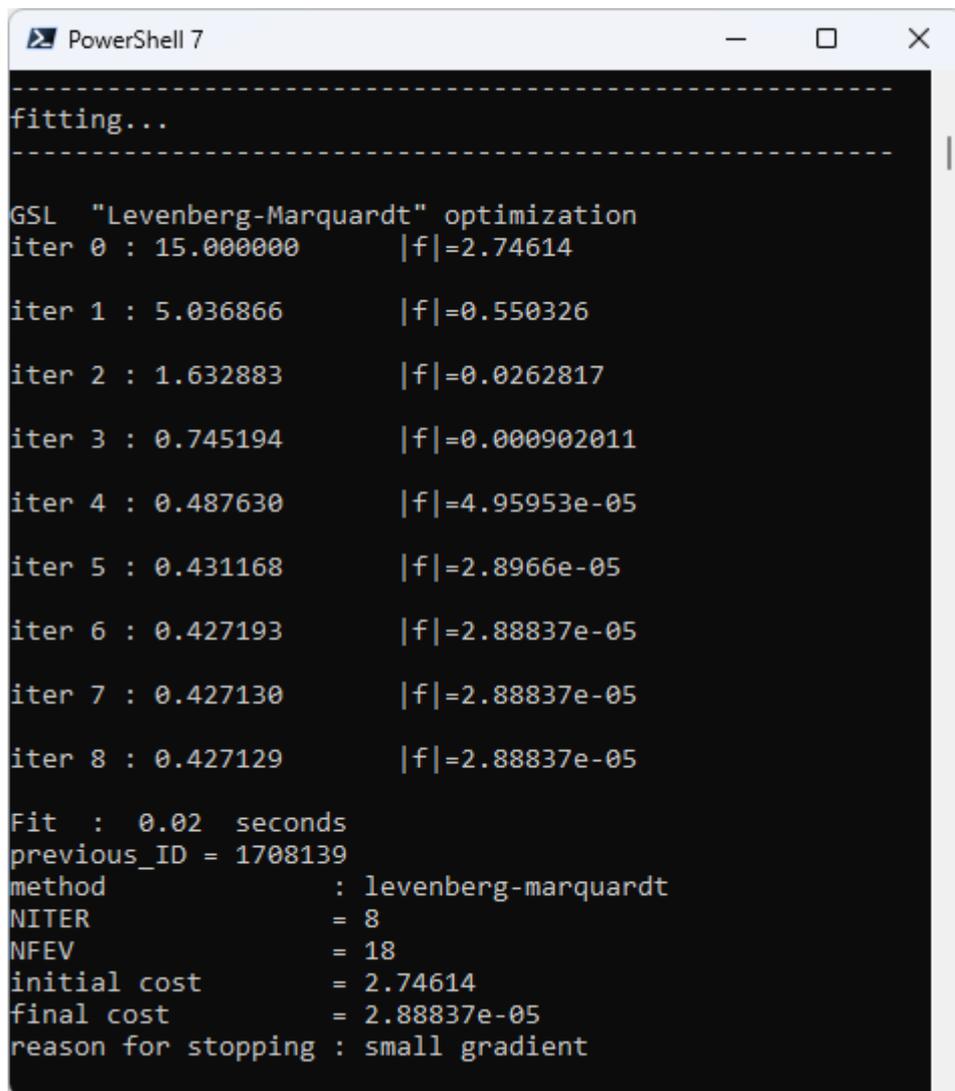
For GSL group algorithms, the parameter "**Number of iterations**" sets the maximum number of iterations that can be achieved if the convergence criterion is not met. For SwarmOps group algorithms this number is equal to the number of residual calculations.

Parameters from the table parameters are used as initial values. For the algorithms of the SwarmOps group, you can initialize the fit with random variables by unchecking the box "Initialize by current state".

If you want to get several sets of parameters, starting not only from the initial value from the table, but from a random variable from the allowed interval, then you need to enable "Randomized start" and set "Number of runs". In this case the first run will still start with the value from the main table.

## 7.4 Launch

To start the fitting process, you need to press "Ctrl+Shift+F" or in the menu "Calculate" of main window select "Start fitting". In the console you can monitor the progress and result of the fit.



```
PowerShell 7
-----
fitting...
-----
GSL "Levenberg-Marquardt" optimization
iter 0 : 15.000000      |f|=2.74614
iter 1 : 5.036866      |f|=0.550326
iter 2 : 1.632883      |f|=0.0262817
iter 3 : 0.745194      |f|=0.000902011
iter 4 : 0.487630      |f|=4.95953e-05
iter 5 : 0.431168      |f|=2.8966e-05
iter 6 : 0.427193      |f|=2.88837e-05
iter 7 : 0.427130      |f|=2.88837e-05
iter 8 : 0.427129      |f|=2.88837e-05

Fit : 0.02 seconds
previous_ID = 1708139
method      : levenberg-marquardt
NITER       = 8
NFEV        = 18
initial cost = 2.74614
final cost   = 2.88837e-05
reason for stopping : small gradient
```

Figure 235. Output information in the process of fitting

The process can be interrupted by pressing "Alt+." or in the menu "Calculate" of main window select "Abort calculation".

## 7.5 After finishing

The results of the fit are saved in "Fits selector" window under automatically generated names. Before the beginning of fitting, a snapshot of the structure is automatically taken and saved with a note "...||**initial**". If the result is unsatisfactory, you can roll back to the previous state.

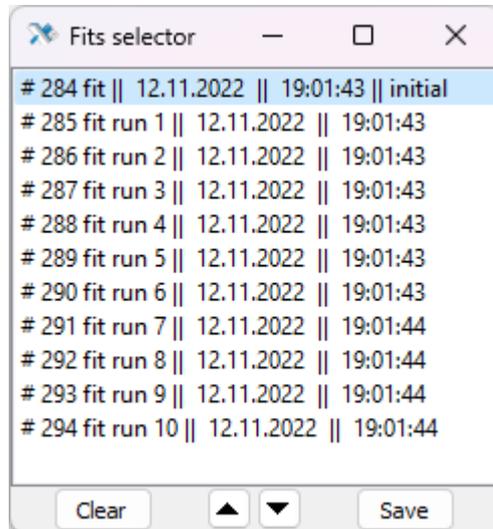


Figure 236. Set of fits in the window "Fits selector"

With a randomized start the results of all runs are saved under the appropriate names "... run 1 ||...", "... run 2 ||..." etc. The results are also exported to a file "fits.txt". The columns are as follows: run number, final residual value, final values of fitted parameters.

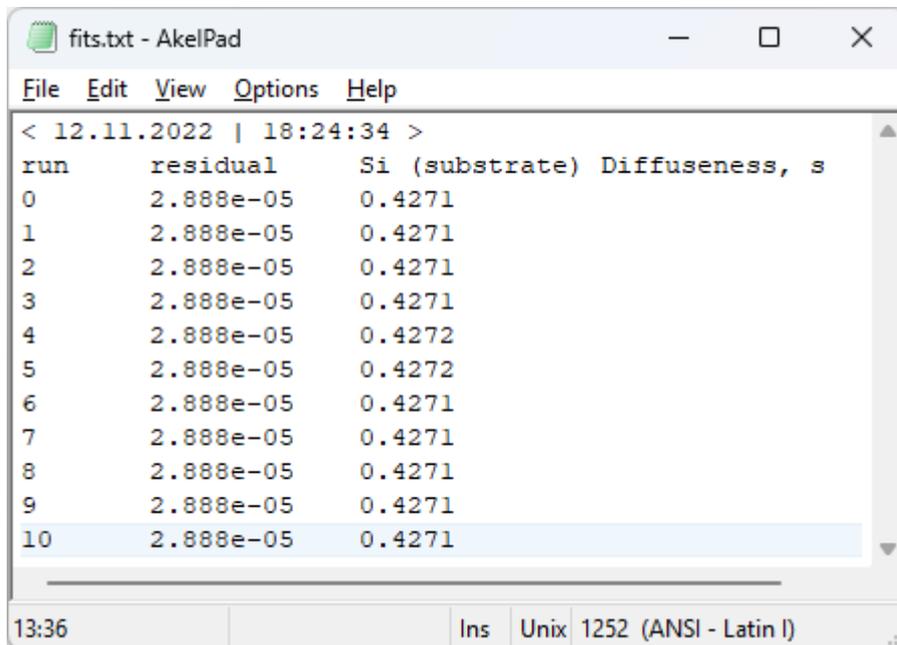


Figure 237. Run results in the file "fits.txt"

If the run is single, then in addition to the initial state, the final state with a mark "...||**final**" will be saved.

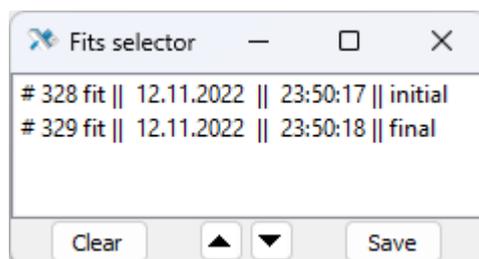


Figure 238. Set of fits in the window "Fits selector"

When the fit is finished or interrupted, a dialog box appears prompting you to update the parameters by replacing the initial values with the final values (in the case of an interruption, the current values). If you refuse, the final state, as in the screenshot above, will not be saved.

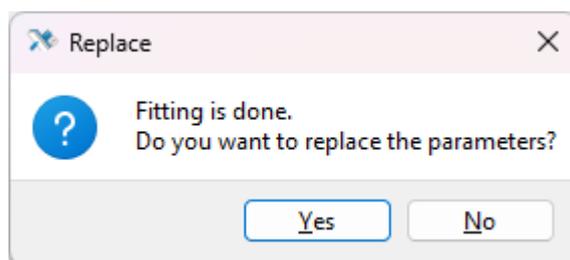


Figure 239. Dialogue at the end of the fit

## 7.6 Confidence interval

Multifitting allows you to estimate the confidence interval of the structure parameters. The task sounds like this: to get the limiting values of the selected parameter, deviations to which can still be compensated by changes in all other parameters. This is not done completely automatically, the final decision on the confidence interval is made by the user. Multifitting only provides information about how much the deviation of the parameter will worsen the coincidence of the calculated and target curves.

The algorithm is as follows. In the main table, for the desired parameter, you should call the "[Coupling editor](#)" window through the [context menu](#). In this window you need to enable the top block "[Calculate confidence interval](#)". If the parameter is dependent you cannot enable this block.

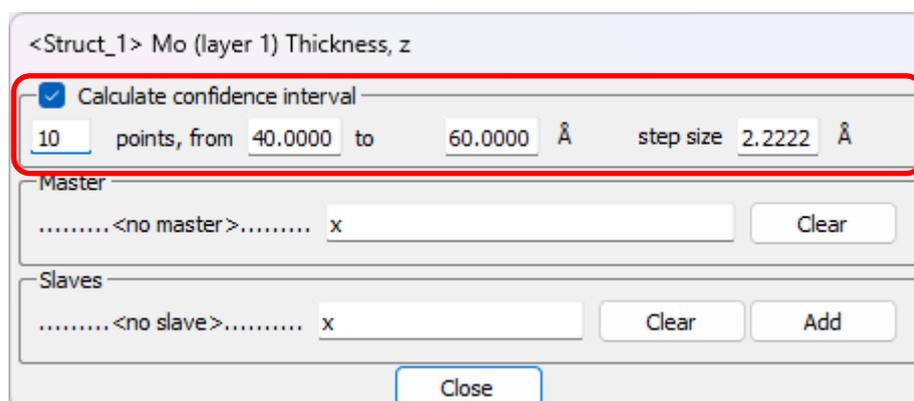


Figure 240. Setting a grid for a confidence interval

Next, the number of points and the range of values are specified. The step is calculated automatically, it is shown for user convenience. "[Coupling editor](#)" can be closed now. The parameter in the table will be indicated by purple or violet:

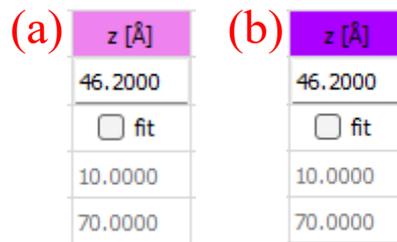


Figure 241. Parameter color designation

The values of the selected parameter will run through the chosen range, and for each value the other (auxiliary) parameters that have the "fit" checkbox enabled will be adjusted. Therefore, now you need to turn on "fit" for these auxiliary parameters. For the estimated parameter "fit" checkbox does not play the role. If "Calculate confidence interval" is enabled for several parameters at once, then they will take on this role one by one.

The calculations start when you press "Ctrl+Shift+A" or click "Calculate confidence intervals" in the menu "Calculate" of main window. The process can be interrupted by pressing "Alt+." or "Abort calculation" in the "Calculate" menu.

The results of the fit for each parameter value from the grid are saved in "Fits selector" under automatically generated names.

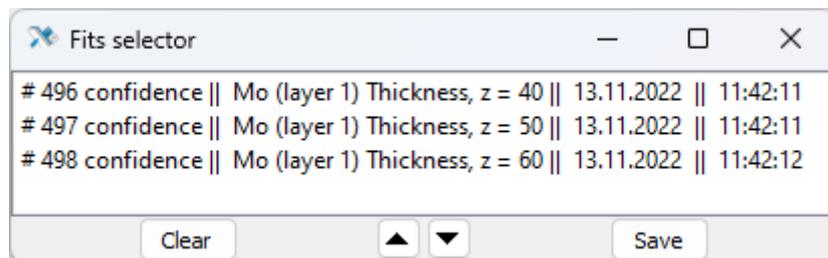


Figure 242. Fits at different values of the estimated parameter

Switching between them, you can see how the calculated curve changes relative to the target and, thus, assess the acceptability of the deviation of the target parameter.

Besides "Fits selector" the results are saved to a file "confidence.txt". They are recorded in two columns: the parameter value and the best found residual value. If we build a graph from these points, we will see the dynamics of the increase in the residual value when the value of the estimated parameter deviates from the optimum.

```

confidence.txt - AkelPad
File Edit View Options Help
< 13.11.2022 | 11:42:11 >
-----
Mo (layer 1) Thickness, z
-----
value      residual
40         1.20851e+00
50         1.56976e-14
60         1.10169e+00

```

Figure 243. Least residual for each parameter value in the file "confidence.txt"

If in the "Fitting settings" window "Randomized start" is enabled, then in "Fits selector" the best result of all runs (with the least residual) will be recorded. To file "confidence.txt" all final runs, sorted by size, will be recorded. The format is as follows: parameter value – least residual – sorted list of residuals:

```

confidence.txt - AkelPad
File Edit View Options Help
< 13.11.2022 | 12:58:22 >
-----
Mo (layer 1) Thickness, z
-----
value      residual
40         1.20671e+00 ( 1.207e+00, 1.207e+00, 1.804e+00)
50         1.56966e-14 ( 1.570e-14, 1.570e-14, 1.570e-14)
60         1.08743e+00 ( 1.087e+00, 1.913e+00, 1.913e+00)

```

Figure 244. The smallest residual and the entire set for randomized starts in the file "confidence.txt"

## 8 Export and import data

For calculations you may need to load the following data to Multifitting: [reflectometric curves](#), [diffuse scattering](#), [GISAS](#), [roughness PSD](#), [general aperiodic](#), [regular aperiodic](#).

You can save simulated intensity distribution as well as dielectric constant and material distribution profiles as text. The files will be created in the directory specified in the tab "[Input/Output](#)" of "[Global settings](#)" window:

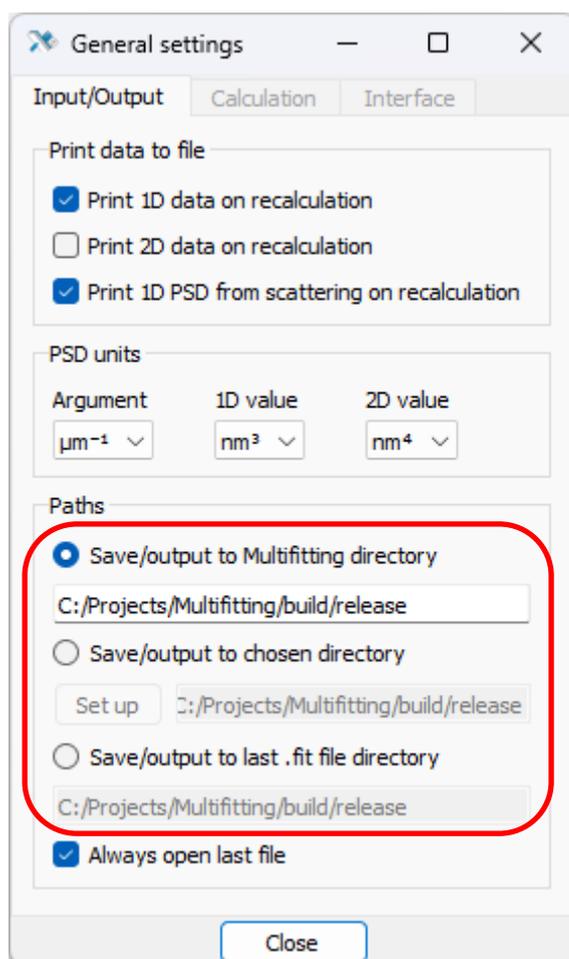


Figure 245. Directory for exporting files

### 8.1 Experimental curves

Data files can contain comments. A line with a comment can begin with any character other than a number (a space or tab is not considered such a character). For example, "; , . : ! ? = /" or any letter. Multifitting ignores such lines. The file is read line by line, so any line can be commented out by adding the appropriate character to the beginning.

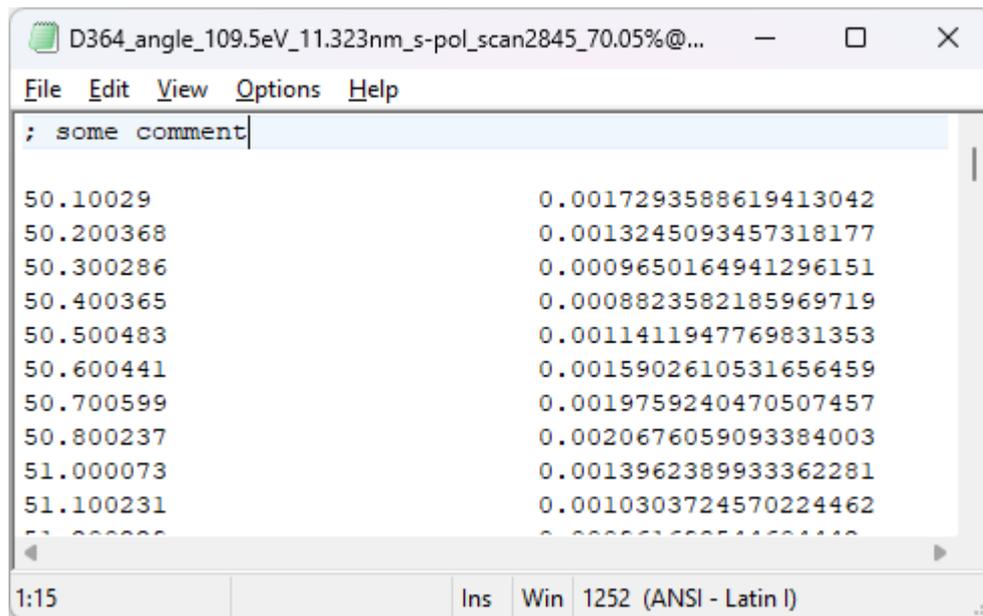
## 8.1.1 Data format

### 8.1.1.1 1D data

One-dimensional data format: two columns:

- argument
- value

If there are more than two columns, the subsequent ones are ignored.



The screenshot shows a text editor window titled "D364\_angle\_109.5eV\_11.323nm\_s-pol\_scan2845\_70.05%@...". The window contains a data file with the following content:

```
; some comment  
  
50.10029          0.0017293588619413042  
50.200368        0.0013245093457318177  
50.300286        0.0009650164941296151  
50.400365        0.0008823582185969719  
50.500483        0.0011411947769831353  
50.600441        0.0015902610531656459  
50.700599        0.0019759240470507457  
50.800237        0.0020676059093384003  
51.000073        0.0013962389933362281  
51.100231        0.0010303724570224462  
51.200200        0.000851600511601110
```

The status bar at the bottom of the window shows "1:15", "Ins", "Win", and "1252 (ANSI - Latin I)".

Figure 246. Example of a data file

### 8.1.1.2 2D data

Two-dimensional data for GISAS can be read in two formats.

The first is pointwise. The file contains three columns:

- row (integer starting with 0)
- column (integer starting with 0)
- value

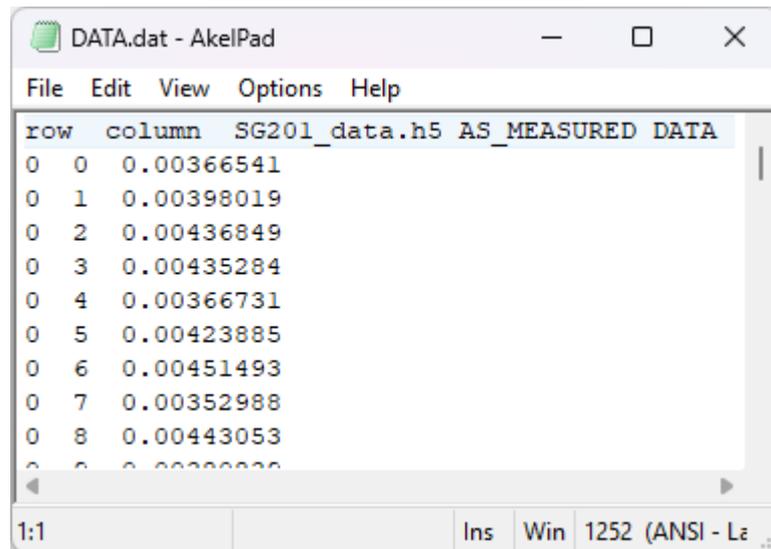


Figure 247. Example of a file with two-dimensional GISAS data, one line – one pixel

The second format is a rectangular matrix of values. The length of each row is equal to the number of columns.

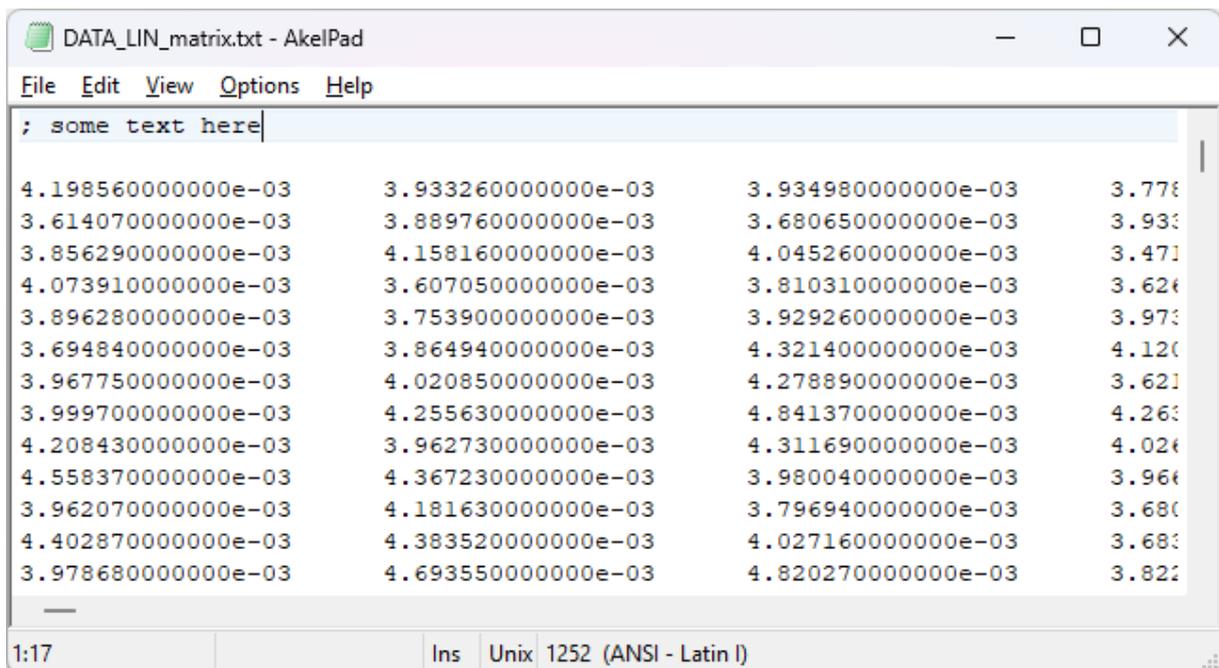


Figure 248. Example of a file with two-dimensional GISAS data in the form of a matrix

## 8.1.2 Import

Experimental (or simulated earlier) data should be loaded in the "[Target curves](#)" section of main window. In the "[Argument](#)" block you must specify the type of argument and its units.

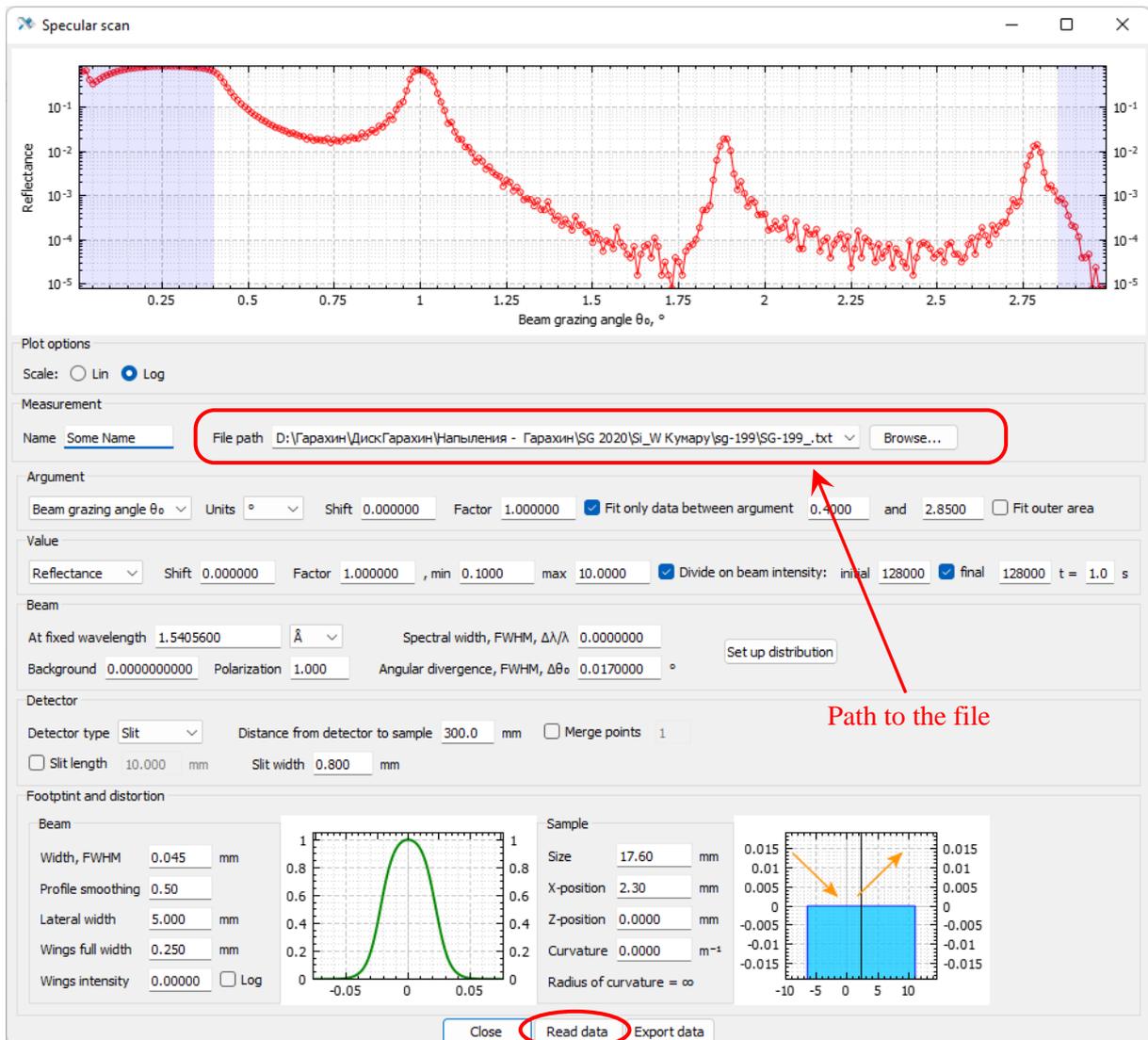


Figure 249. Loaded experimental reflectometric curve

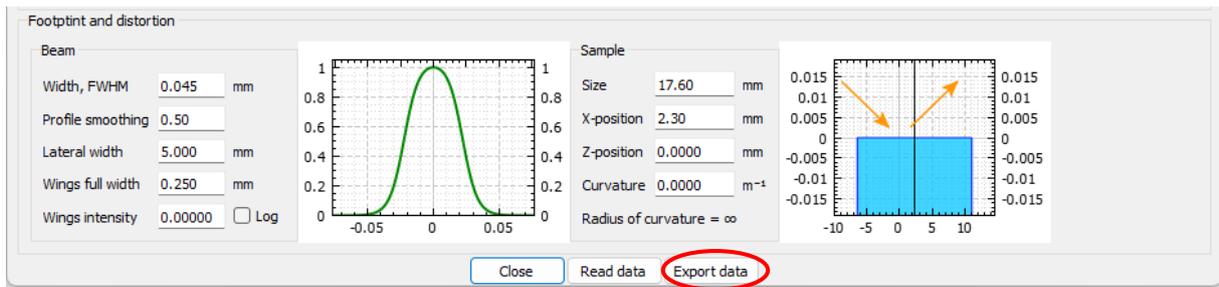
The easiest and most convenient way is to drag the file to the curve window, it will be read automatically.

Alternative – in the block "Measurement" specify the path to the file or select a file in the dialog box.

Button "**Read data**" at the bottom of the window allows you to re-read the already loaded file specified in the field "**File path**".

### 8.1.3 Export previously loaded data

Button "**Export data**" at the bottom of the window allows you to save the previously loaded curve to the file. The original data is stored in the project file and can be exported even if the source file (specified in the "**File path**") no longer exists.



Save all content back to a file

Figure 250. Experimental curve window

The contents of the file will be completely identical to the source, with all comments, additional columns, etc.

## 8.2 Export simulated data

The results of the reflectivity or scattering calculation are saved as text automatically at the end of the calculation, if in the "Input/Output" tab of "Global settings" window there are corresponding flags. In this case, it is enough to make a recalculation by pressing "Ctrl+Shift+C".

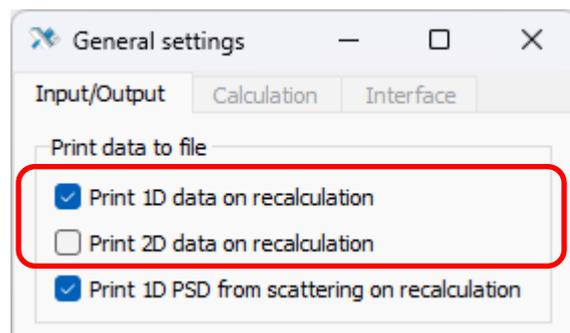


Figure 251. Automatic output to a file

With any settings, you can make a one-time export from the menu item "File" of main window. In this case, all curves will be recalculated.

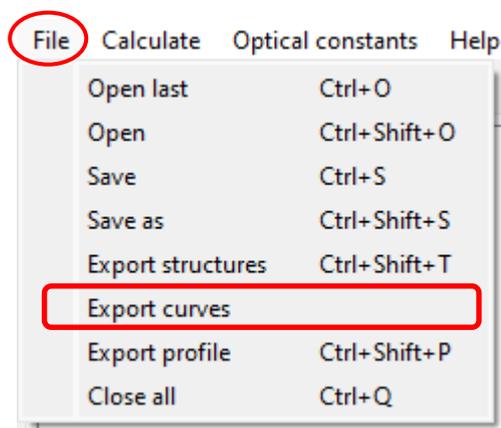


Figure 252. Main menu "File"

The results of the calculations are saved in text files with the name "`<struct_name>_target_<N>_<curve_name>.txt`" or "`<struct_name>_independent_<curve_name>.txt`". "`independent`" or "`target`" means that the curve is calculated from an independent or experimental grid. "`<N>`" is an ordinal number of the curve, counting from 1. "`<curve_name>`" is editable curve name.

For example:

- "`Struct_1_independent_Plot_1.txt`"
- "`Struct_1_target_1_.txt`"

Two-dimensional data has an additional suffix to the name, indicating the data type.

For example:

- "`Struct_1_independent_Plot_3_GISAS.txt`"
- "`Struct_1_independent_Plot_1_intensity.txt`"
- "`Struct_1_independent_Plot_1_absorption.txt`"

The header of the file records the type of scan and basic information about the tool settings and the geometry of the measurement. Examples:

```

Struct_1_target_1_test.txt - AkelPad
File Edit View Options Help
; < 31.10.2022 | 09:49:06 >
; Specular scan

; polarization = 1.000
; wavelength = 1.540562 A

; spectral resolution (FWHM) = 0
; beam divergence (FWHM) = 0 deg

; beam width = 0.05 mm
; sample size = 20 mm

; Grazing angle (deg)      R_mixed      R_s      Phase_R_s
0.0000000000000000      5.000000e-01  1.000000e+00  180.0000
0.0020020020020020      1.370352e-02  9.993951e-01  -175.3984
0.0040040040040040      2.738888e-02  9.987903e-01  -170.7962
0.0060060060060060      4.105451e-02  9.981852e-01  -166.1925
0.0080080080080080      5.469881e-02  9.975797e-01  -161.5867
  
```

Figure 253. Output of the reflectometric calculation to the file

```

Struct_1_independent_Plot_1.txt - AkelPad
File Edit View Options Help
; < 31.10.2022 | 09:49:06 >
; Rocking scan

; polarization = 1.000
; wavelength = 1.540562 A
; specular grazing angle position = 1 deg

; spectral resolution (FWHM) = 0
; beam divergence (FWHM) = 0 deg
; detector angular width (FWHM) = 0.01909859317 deg

; beam width = 0.05 mm
; sample size = 20 mm

; Beam grazing angle (deg) S_mixed      S_s
0.000000000000000000      0.000000e+00      0.000000e+00
0.0020020020020020020      0.000000e+00      0.000000e+00
0.0040040040040040040      0.000000e+00      0.000000e+00
0.0060060060060060060      0.000000e+00      0.000000e+00

```

Figure 254. Figure 253. Output of the rocking curve calculation to the file

```

Struct_1_independent_Plot_1_intensity.txt - AkelPad
File Edit View Options Help
; < 31.10.2022 | 09:49:06 >
; Field intensity distribution
; (61 x 1000) points

; polarization      : 1.000000
; depth             : (-50.00 , 70.00) angstrom, step = 2.00 angstrom
; wavelength        : 1.540562 A
; beam grazing angle : (0.000000 , 1.000000) deg

0.000000e+00      0.000000e+00      0.000000e+00      0.000000e+00      0.000000e+
6.134631e-05      5.878593e-05      5.631477e-05      5.393065e-05      5.163138e-
2.453843e-04      2.351434e-04      2.252594e-04      2.157234e-04      2.065268e-
5.521670e-04      5.391351e-04      5.268850e-04      5.154200e-04      5.047371e-

```

Figure 255. Output of the field intensity distribution in the structure to the file

```

Struct_1_independent_Plot_3_GISAS.txt - AkelPad
File Edit View Options Help
; < 31.10.2022 | 09:49:06 >
; GISAS data
; (1000 x 501) points

; polarization           : 1.000000
; beam grazing angle     : 0.500000 deg
; wavelength             : 1.540562 A
; spectral resolution    : 0.000000
; beam polar divergence  : 0.000000 deg
; beam azimuthal divergence : 0.000000 deg
; beam width             : 0.050000 mm
; sample size           : 20.000000 mm

; detector point size Theta : 0.005996 deg
; detector point size Phi   : 0.005200 deg

; detector Theta range : (0.010000 , 6.000000) deg
; detector Phi range   : (-1.300000 , 1.300000) deg

0.000000e+00  0.000000e+00  0.000000e+00  0.000000
0.000000e+00  0.000000e+00  0.000000e+00  0.000000
0.000000e+00  0.000000e+00  0.000000e+00  0.000000
1:28 Ins Unix 1252 (ANSI - Latin I)

```

Figure 256. Output of GISAS to the file

For one-dimensional curves, the values for each of the involved polarizations and the total result are printed ( $R_{mixed}$ ,  $R_s$ ,  $R_p$ ). The reflectometric curve also contains a phase for the reflected wave for the polarization involved ( $Phase_{R_s}$ ,  $Phase_{R_p}$ ) in range  $(-180^\circ, 180^\circ]$ .

### 8.3 Import roughness PSD

Loading the roughness PSD from the file can be done in the [main table](#). To do this, click on the button located in the header of the parameter. If the external PSD is not loaded, the button is white, if loaded, then green.

PSD 1D	PSD 2D
$\sigma_z$ [Å]	$\sigma_z$ [Å]
3.8707	0.0000
rf 1D	rf 2D
0.800	1.000

Figure 257. Roughness PSD load button

When you press the button "PSD 1D" or "PSD 2D" a window will open to load the data. You can drag and drop the PSD file into the window or specify the path to it through the button "Browse...". You should also specify the units of argument and value. You can also delete data here.

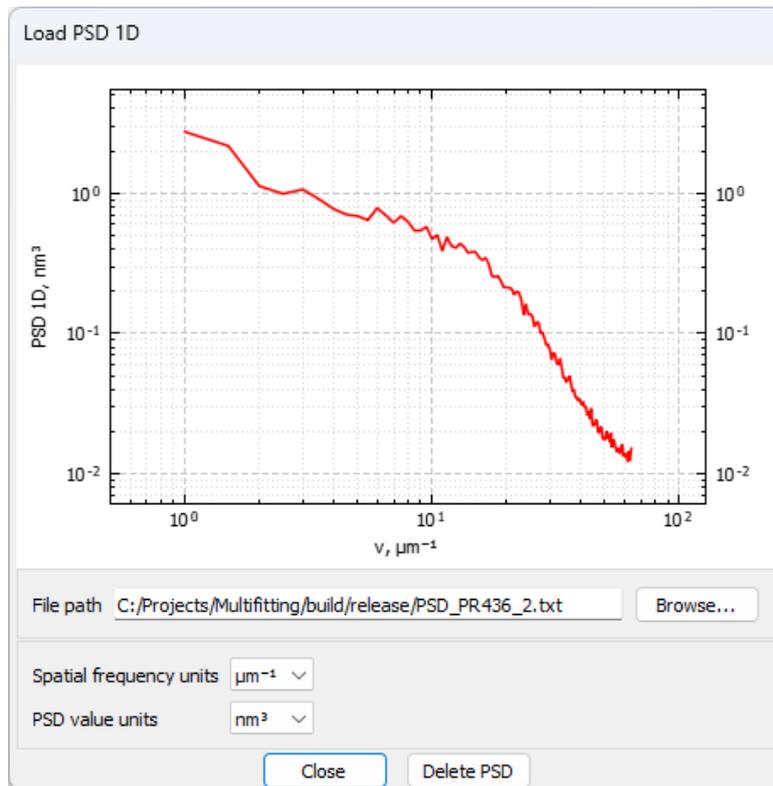


Figure 258. Loading a one-dimensional PSD

The data must be organized into two columns: the argument (spatial frequency) and the value (PSD).

## 8.4 Structure

### 8.4.1 Export the entire structure

Information about the entire structure can be saved in a text file in human-readable form. You cannot automatically load this file back to Multifitting; the file is intended only to quickly share the information or use it for some other purpose.

To save the structure to a file, you can select the item in menu "[File](#)" or click "[Ctrl+Shift+T](#)".

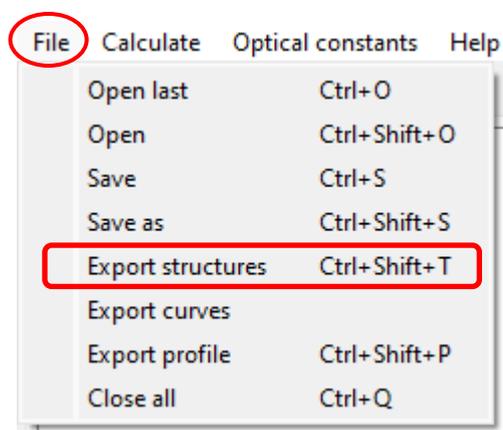
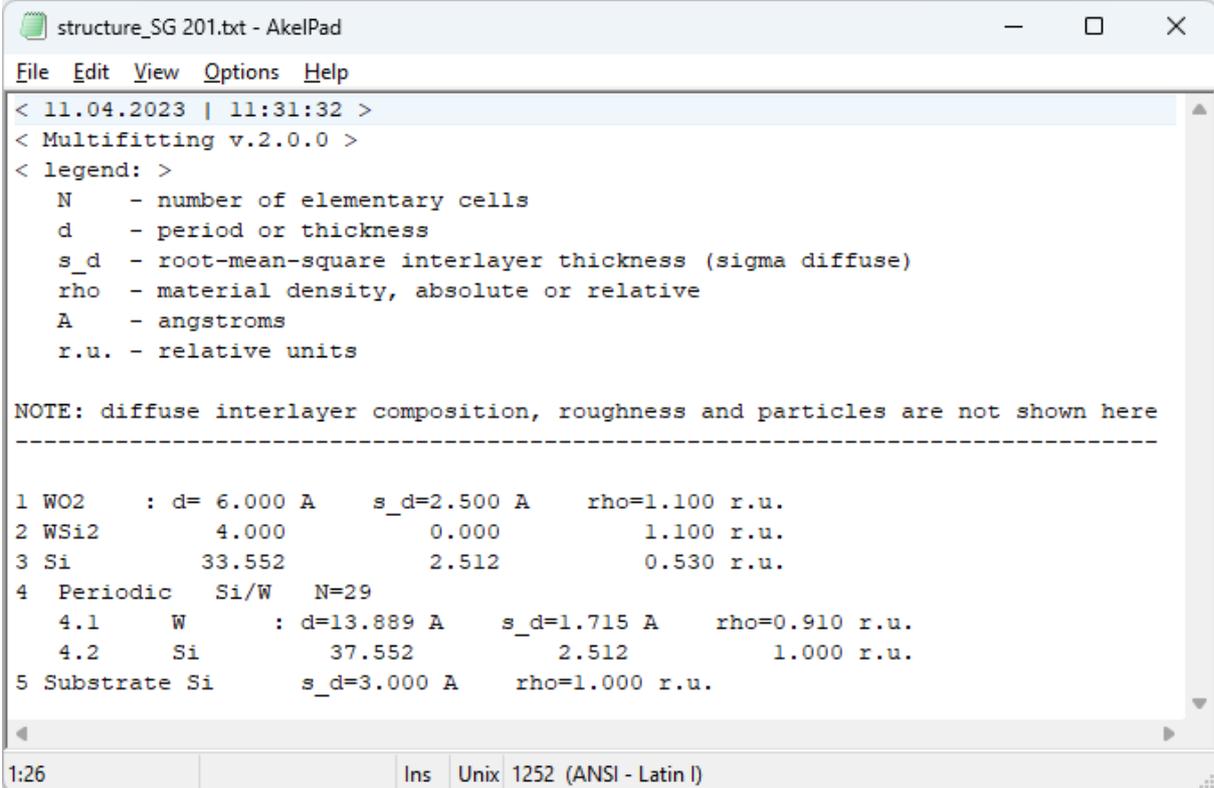


Figure 259. Export structure from the main menu "[File](#)"

The result is saved to a file with the name "`structure_<struct_name>.txt`".

"<struct\_name>" is editable structure name written on the tab. Its content is something like this:



```
structure_SG 201.txt - AkelPad
File Edit View Options Help
< 11.04.2023 | 11:31:32 >
< Multifitting v.2.0.0 >
< legend: >
  N - number of elementary cells
  d - period or thickness
  s_d - root-mean-square interlayer thickness (sigma diffuse)
  rho - material density, absolute or relative
  A - angstroms
  r.u. - relative units

NOTE: diffuse interlayer composition, roughness and particles are not shown here
-----

1 WO2      : d= 6.000 A    s_d=2.500 A    rho=1.100 r.u.
2 WSi2     4.000         0.000         1.100 r.u.
3 Si       33.552        2.512         0.530 r.u.
4 Periodic Si/W    N=29
  4.1 W      : d=13.889 A    s_d=1.715 A    rho=0.910 r.u.
  4.2 Si     37.552        2.512         1.000 r.u.
5 Substrate Si    s_d=3.000 A    rho=1.000 r.u.
```

Figure 260. Basic structure parameters in a text file

## 8.4.2 Aperiodic structure

Aperiodic stacks are stored in the structure file on a common basis. However, aperiodic can be filled with values read from a file. For regular and general aperiodic, this is done a little differently.

### 8.4.2.1 Export of regular aperiodic

If there is a regular aperiodic in the structure, then when you export the structure to a file ("Ctrl+Shift+T") in addition to the general structure file, another one is created with the name of the form "`structure_<struct_name>_Aperiodic_#<N>.txt`". Here "<N>" is ordinal number of regular aperiodic in the structure, because there may be several of them. The counting goes from the surface.

The file includes the following columns of values:

- unit cell number (from the surface) "**cell**"
- layer substance "**material**"
- layer thickness "**d**"
- thickness of the upper diffuse interface "**sigma**"

```

; < 31.10.2022 | 19:02:19 >
; < Multifitting v.1.11.30 >
;cell   material   d (A)      sigma (A)
1       Be         12.700     3.000
1       Mo         15.500     4.400
2       Be         20.200     7.000
2       Mo         23.200     9.700
3       Be         22.400     4.000
3       Mo         21.500     10.100
4       Be         23.200     4.200
4       Mo         19.700     1.900
5       Be         31.200     11.300
5       Mo         13.700     12.400

```

Figure 261. Parameters of regular aperiodic layers

A file of this format can be imported back into Multifitting.

#### 8.4.2.2 Import of regular aperiodic

You can create a regular aperiodic from a periodic structure by specifying the composition of the elementary cell and their number. But you can also set the thicknesses and interfaces of the layers by loading the appropriate file. The format and contents of the file correspond to the figure above. At the same time, the column №4 (*sigma*) is optional, i.e. interfaces can be skipped. The first two columns play an auxiliary role, allowing you to check the data and not get confused, but the information from them is not directly used.

You can read the file by dragging it to the previously opened aperiodic [layer table](#):

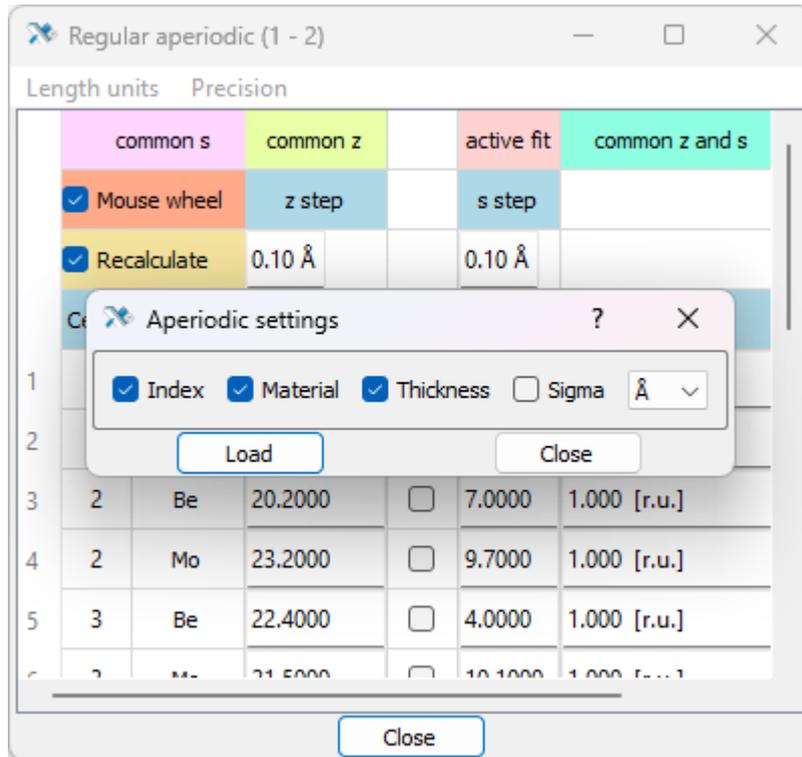


Figure 262. Loading regular aperiodic from a file

Here you select the thickness units in which the values in the file will be read, and also choose whether or not to read the interfaces in the fourth column.

If the number of layers in the file is not equal to the number of layers in the table, a warning will be shown. If you think this is how it should be, the warning can be ignored and the file will be read. Moreover, if the file has fewer layers than the table, then the last layers in the table will not be affected. If there are more layers in the file, only the corresponding part of the file will be read.

### 8.4.2.3 Import of general aperiodic

Generic aperiodic can be created by loading materials, densities, thicknesses and layer interfaces from a file. The file format is [almost the same](#) as for regular aperiodic, but may include material densities:

- layer number (from surface)
- material
- layer thickness
- thickness of the upper diffuse interface
- relative density of the material

The last two columns are optional and may be omitted if they are not intended to be read.

index	material	thickness	sigma	density
1	Mo	23.4	1.32	0.95
2	Si	43.1	4.94	1
3	Ru	21.3	2.38	0.9
4	Al	120.7	3.52	0.98
5	Si	5.2	5.67	0.87
6	Zr	13.2	3.97	0.99
7	Ni	10.2	1.41	1
8	SiO2	56.2	2.47	1

Figure 263. Parameters of layers of general aperiodic

To create an aperiodic in this way, you need to click on the toolbar "Add aperiodic multilayer"  button and configure the import. After pressing the "Load" button a dialog box will open to select a file.

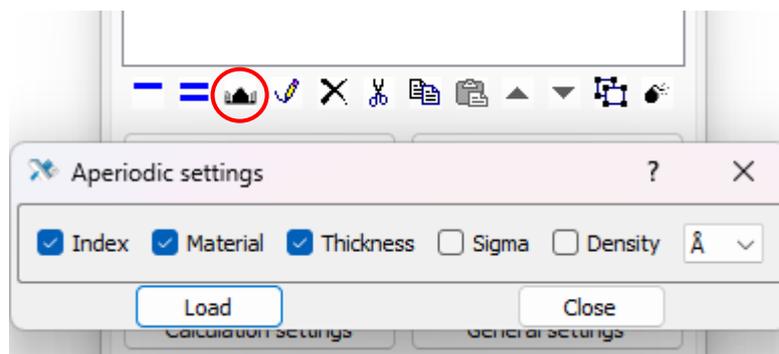


Figure 264. Loading general aperiodic from a file

## 8.5 Structure profile

Profile of the structure in depth, which can be seen in the window "[Profile plot](#)", can be saved to a text file for further work or to prepare for publication. You can export the profile by selecting the menu "[File](#)" item or by pressing "Ctrl+Shift+P":

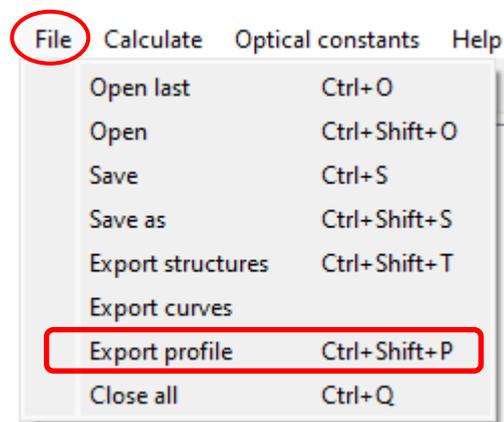


Figure 265. Export profile in the main menu "File"

In this case, several files will appear in the corresponding directory. their names are as follows:

"profile\_<data\_type>\_<sharpness>\_<struct\_name>.txt". Here "<struct\_name>" is structure name.

"<data\_type>" takes values "Permittivity", "Materials", "Elements".

"<sharpness>" takes values "Sharp", "Discretized" or remains empty.

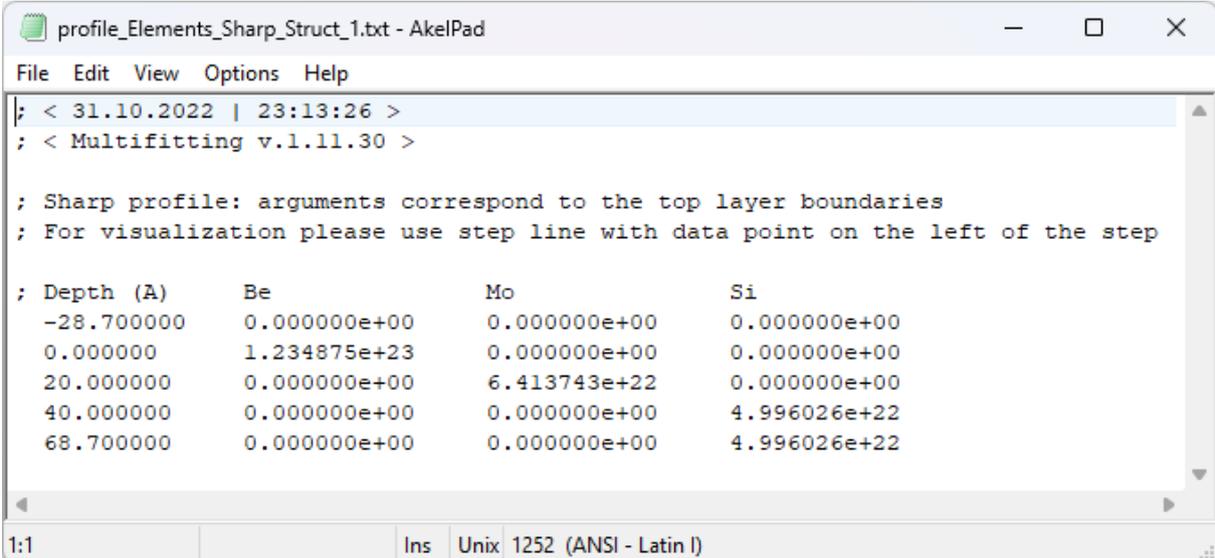
For example:

- "profile\_Elements\_Sharp\_Struct\_1.txt"
- "profile\_Permittivity\_Discretized\_Struct\_1.txt"
- "profile\_Materials\_Struct\_1.txt"

If the structure contains a layer/substrate whose material is composed from individual chemical elements, then a file with a concentration profile of these elements will be created.

If the structure contains a layer/substrate whose material is specified by the file name ".nk", then a file with a relative density profile of the materials will be created.

Presence of "Sharp" in the file name means that this is profile of a structure with zero mixing at the boundaries. Layer thicknesses can be different, so the coordinates of the upper boundary of the layer are indicated as an argument.



```
profile_Elements_Sharp_Struct_1.txt - AkelPad
File Edit View Options Help
|: < 31.10.2022 | 23:13:26 >
; < Multifitting v.1.11.30 >

; Sharp profile: arguments correspond to the top layer boundaries
; For visualization please use step line with data point on the left of the step

; Depth (A)      Be          Mo          Si
-28.700000      0.000000e+00  0.000000e+00  0.000000e+00
0.000000        1.234875e+23  0.000000e+00  0.000000e+00
20.000000       0.000000e+00  6.413743e+22  0.000000e+00
40.000000       0.000000e+00  0.000000e+00  4.996026e+22
68.700000       0.000000e+00  0.000000e+00  4.996026e+22

1:1                               Ins Unix 1252 (ANSI - Latin I)
```

Figure 266. An example of the contents of a file with a sharp profile of chemical elements

Presence of "Discrete" in the file name means that this is a structure profile with discretization specified in the window "[Calculation settings](#)".

```

profile_Materials_Discrete_Struct_1.txt - AkelPad
File Edit View Options Help
; < 31.10.2022 | 23:28:29 >
; < Multifitting v.1.11.30 >

; Discretized profile: arguments correspond to the top slice boundaries
; For visualization please use step line with data point on the left of the step

; Depth (Å)      Be                Mo                Si
-29.000000      0.000000e+00      4.141450e-10      0.000000e+00
-28.000000      0.000000e+00      9.115599e-10      0.000000e+00
-27.000000      0.000000e+00      1.975266e-09      0.000000e+00
-26.000000      1.108999e-16      4.213857e-09      0.000000e+00
-25.000000      1.330798e-15      8.850229e-09      0.000000e+00
-24.000000      1.718948e-14      1.830023e-08      0.000000e+00
-23.000000      1.961264e-13      3.725577e-08      0.000000e+00
-22.000000      2.021826e-12      7.467464e-08      0.000000e+00

```

Figure 267. Example of the content of a file with a discretized material profile

As for a sharp profile, the thicknesses of the sublayers change from layer to layer, so the coordinates of the upper boundary of the each sublayer are also specified as an argument. To export a discretized profile, check that the checkbox "Show discretization" in "Profile plot" options is **enabled**

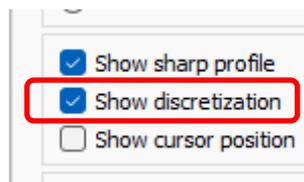
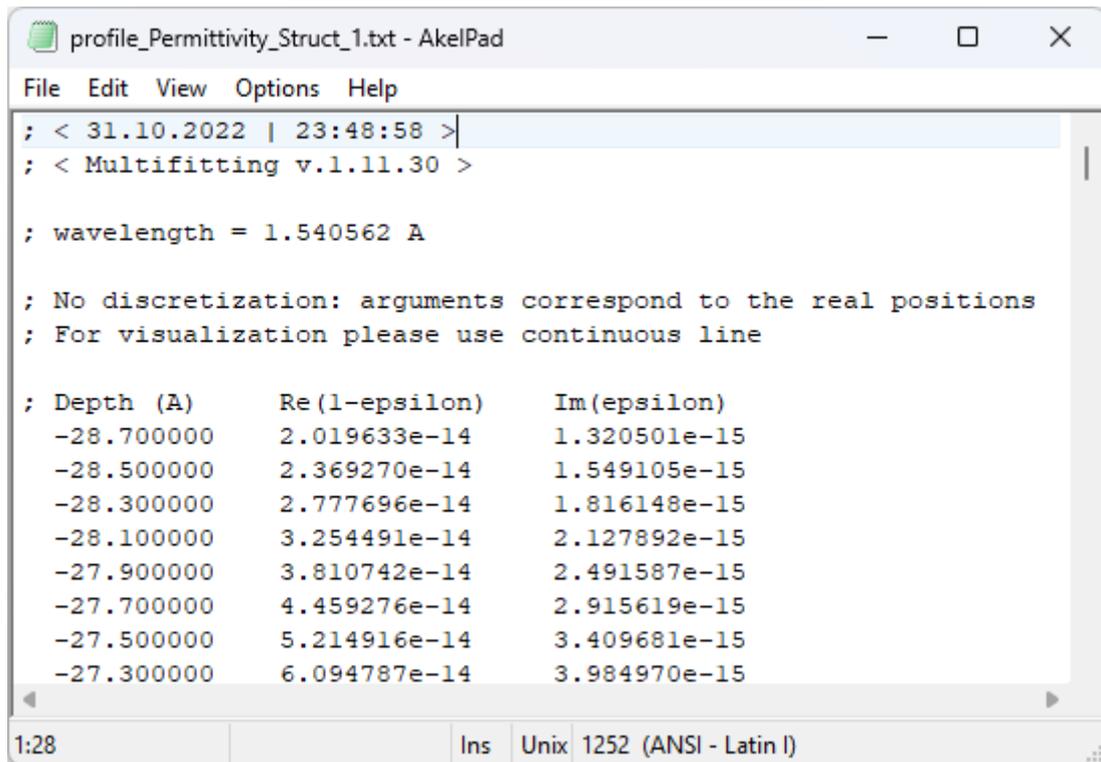


Figure 268. Profile presentation options in "Profile plot" window

The absence of additional indicators in the file name means that this is a "continuous" structure profile. However, to output data to a file, you need to get a set of points. A fixed sampling step  $0.2 \text{ \AA}$  is set for a continuous profile, which is smaller than the physically meaningful size of any profile feature. Since the step is constant, and the profile is intended to be represented in an interpolated form, here the argument is the coordinate of the **center of the sublayer**.



The screenshot shows a text editor window titled "profile\_Permittivity\_Struct\_1.txt - AkelPad". The window contains the following text:

```
; < 31.10.2022 | 23:48:58 >
; < Multifitting v.1.11.30 >

; wavelength = 1.540562 A

; No discretization: arguments correspond to the real positions
; For visualization please use continuous line

; Depth (A)      Re(1-epsilon)    Im(epsilon)
-28.700000      2.019633e-14    1.320501e-15
-28.500000      2.369270e-14    1.549105e-15
-28.300000      2.777696e-14    1.816148e-15
-28.100000      3.254491e-14    2.127892e-15
-27.900000      3.810742e-14    2.491587e-15
-27.700000      4.459276e-14    2.915619e-15
-27.500000      5.214916e-14    3.409681e-15
-27.300000      6.094787e-14    3.984970e-15
```

The status bar at the bottom of the window shows "1:28", "Ins", "Unix", and "1252 (ANSI - Latin I)".

Figure 269. Example of file contents with a "continuous" dielectric constant profile

To export a continuous profile, you must have a check that checkbox "Show discretization" in "[Profile plot](#)" option is **disabled**.

## 9 Optical constants of materials

Calculating the reflection and scattering of radiation requires knowledge of the dielectric constant of substances. It depends on the wavelength or energy of the photon, so for each material involved, a number of values in the corresponding spectral range are needed. Multifitting uses the database of optical constants of the IMD program [1] with minor additions. This database consists of two directories: "nk" and "f1f2". The first contains refractive indices of substances, the second – atomic factors of chemical elements.

Optical constants are automatically loaded when you open Multifitting, but you can reload them manually from the [main window menu](#) if some material file has been updated.

Data files can contain comments. A line with a comment can begin with any character other than a number (a space or tab is not considered such a character). For example, "; , . : ! ? = /" or any letter. Multifitting ignores such lines. The file is read line by line, so any line can be commented out by adding the appropriate character to the beginning.

### 9.1 Material library "nk"

Each material corresponds to a text file, for example, "GaAs.nk". The material name in Multifitting is the name of the file before the extension ".nk".

The file header usually contains a comment with information. Auxiliary information about the substance can be indicated: density, allotropic modification (amorphous, crystalline material). A data origin (measurement, calculation, or mixture) may be mentioned. If the data is a combination, then the names of the source files are indicated. Almost always a link to the data source is given.

The data is arranged in three columns:

- wavelength in angstroms:  $\lambda[\text{\AA}]$ ,
- real part of the refractive index:  $\text{Re}(n)$
- imaginary part of the refractive index:  $\text{Im}(n)$

The wavelength must change monotonously, i.e. either increase or decrease. The direction of the argument change is determined by the first two lines. Values falling out of a monotonic relationship are skipped.

Values between spectral points are interpolated. If the calculated wavelength is outside the data range for any of the materials of the structure, then Multifitting will warn about this and the calculation will not be made! In this case you need to use a file with material properties in the appropriate part of the spectrum.

If the file contains only one spectral point, then it is applied for all  $\lambda \in (0, \infty)$ .

```

GaAs.nk - AkelPad
File Edit View Options Help
; Optical constants for GaAs
;
; Concatenation of:
;
; GaAs_llnl_cxro + GaAs_windt + GaAs_palik
;
;   Lambda (A)           n           k
; -----
;   0.12398425          0.99999990    2.0156681e-10
;   0.12460729          0.99999990    2.0567769e-10
;   0.12523662          0.99999990    2.0989399e-10
;   0.12651454          0.99999990    2.1865512e-10
;   0.12848109          0.99999990    2.3267137e-10
;   0.13050974          0.99999989    2.4782712e-10
;   0.13189814          0.99999989    2.5862025e-10
;   0.13331640          0.99999989    2.7000658e-10
;   0.13550191          0.99999988    2.8828555e-10
;   0.13776028          0.99999988    3.0813545e-10
;   0.13930815          0.99999988    3.2229708e-10
;
1:1                               Ins Win 1252 (ANSI - Latin I)

```

Figure 270. "GaAs.nk" file content

The list of library files with single-line comments is given in the file "AAACATALOG.TXT".

```

AAACATALOG.TXT - AkelPad
File Edit View Options Help
FILE          DESCRIPTION, with [wavelength range in angstroms]
-----
Ac            =Ac_llnl_cxro [.12398425-423.15444]
Ac_llnl_cxro LLNL + CXRO (1997) 10.07 g/cm3 [.12398425-423.15444]
-----
Ag            =Ag_llnl_xro [.12398425-423.15444]+Ag_palik [428-99190]
Ag_llnl_cxro LLNL + CXRO (1997) 10.50 g/cm3 [.12398425-423.15444]
Ag_hagemann  Hagemann et al. (Palik + DESY) [1.24-1378]
Ag_leveque   Leveque et al. (Palik) [460-1348]
Ag_palik     Palik (1985) [1.24-99190]
Ag_windt     Windt et al. (1988) evap. Ag [24-1216]
-----
Ag2O         =Ag2O_cllnl_xro [.12398425-423.15444]
Ag2O_llnl_cxro LLNL + CXRO (1997) 7.143 g/cm3 [.12398425-423.15444]
-----
Al            =Al_llnl_xro [.12398425-423.15444]+Al_palik [427-12398]
Al_llnl_cxro LLNL + CXRO (2013) 2.6989 g/cm3 [.12398425-423.15444]
Al_palik     Palik (1985) [165-12398]
Al_shiles    Shiles et al. (Palik) [12.4-1305]
-----
1:1                               Ins Win 1252 (ANSI - Latin I)

```

Figure 271. "AAACATALOG.TXT" file content

## 9.2 Atomic factors library "f1f2"

Materials can be composed by combining any of the first 92 chemical elements. The dielectric constant of the material will depend on the stoichiometric ratio of the elements and the absolute density of the substance, which is converted to an atomic concentration. The refractive index is calculated as follows:

$$n = 1 - \delta - i\beta = 1 - \frac{r_0}{2\pi} \lambda^2 \sum_i N_i f_i(\lambda)$$

where  $r_0$  is classical electron radius,  $\lambda$  is wavelength,  $N_i$  is atomic concentration, and  $f_i$  is atomic scattering factor of the  $i$ -th element.

The files have a name that exactly matches the chemical element, plus an extension ".ff", for example "Si.ff".

The file header usually contains a comment with information, usually a link to the data source.

The data is arranged in three columns:

- energy in electronvolts: E[eV],
- real part of the scattering factor: f1
- imaginary part of the scattering factor: f2

Energy must increase strictly. Values falling out of this dependency are skipped. If the value of the real part of the scattering factor is -9999, then it is undefined. Lines with  $f1 \leq -8888$  are not taken into account.

Values between spectral points are interpolated. If the calculated wavelength is outside the data range for any of the chemical elements, Multifitting will warn you and no calculation will be made.

```
; Atomic scattering factors for Si.
;
; Concatenation of data from CXRO <http://www-cxro.lbl.gov>
; and LLNL <http://www-phys.llnl.gov/V Div/scattering/asf.html>
;
; E (eV) f1 f2
;-----
10.0000 -9999. 3.94851
10.1617 -9999. 3.95531
10.3261 -9999. 3.96212
10.4931 -9999. 3.96894
10.6628 -9999. 3.97577
10.8353 -9999. 3.98262
11.0105 -9999. 3.98948
11.1886 -9999. 3.99635
11.3696 -9999. 4.00322
11.5535 -9999. 4.01012
11.7404 -9999. 4.01702
11.9303 -9999. 4.02394
```

Figure 272. "Si.ff" file content

## 10 Version history

- Multifitting v.1.9.2 – release (06.07.2019)
- Multifitting v.1.10.0 (19.10.2019)
  - The graphical interface now supports scaling from the operating system.
  - Updated angular and spectral resolution. Now the resolution values that were set in versions  $\leq 1.9.2$  should be multiplied by 2. Now the thin line is blurred into a wide one with FWHM  $\approx$  the given resolution.
  - Angular and spectral resolution each act on both types of curves: spectral and angular (according to a simplified scheme)
  - The initial and final intensities of the probe beam with linear interpolation between them can be specified.
  - Warning when overwriting files from previous versions is added.
  - Additional options are available for graphs: header with measurement parameters, logarithmic scale for the X axis.
  - Information can be shown/hidden in the "Settings" window of the context menu of the "Plots" window.
  - Instant recalculation when switching on/off structural items in the table if the "Recalculate" modifier is enabled.
  - The plots in the "Plots/Measured" window have got ordinal numbers that allow you to match the curve with the loaded data.
  - Added the ability to maximize the integral of the reflection curve with the source function.
  - Added settings for fitting algorithms.
  - Decimal separators in data files – dots and commas.
  - Files added to the database of optical constants: "Cr\_delmotte.nk", "Pt\_soufli.nk", "Be\_svechnikov.nk".
  - Various bugs are fixed.
- Multifitting v.1.10.2 (21.02.2020)
  - Files "Sc\_larruquert.nk", "ScSi.nk", "Sc5Si3.nk", "Sc3Si5.nk" are added to the database of optical constants, the ranges of "MoSi2.nk" and "Sc.nk" are extended
  - Subrange of experimental data can be set for fitting.
  - The ability to duplicate structure tabs has been added.
  - Visualization of structure profile has been added.
  - The ability to calculate the permittivity profile with its discretization into thin sublayers has been added.
  - The ability to export an already loaded experimental curve back to a text file has been added.
  - The ability to fit a scaling intensity factor for experimental curves has been added.
  - It is possible to eliminate the moiré distortions of the calculated curve arising when the period of oscillations of reflection from thick structures is almost a multiple of the step of the experimental curve.
  - An automatic calculation of the spectral width of the reflection peak when calculating the corresponding curve has been added.
  - Various bugs are fixed, including a fitting bug for a scaled experimental curve.

- Multifitting v.2.0.0 (17.04.2023)
  - Redesigned user interface.
  - Added the ability to simulate 1D and 2D scattering by roughness and particles.
  - Added visualization of the field intensity distribution in the structure.
  - Lots of small changes and fixes.

## **11 List of abbreviations**

GISAS – Grazing Incidence Small-Angle Scattering.

PSD – Power Spectral Density, roughness spectrum.

## 12 References

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