**X-Ray Calc**

v. 2.4

**Getting Started**

**Tutorial**

***X-Ray Calc*** is a software for computer simulation of X-ray reflectivity, including normal incidence and grazing incidence X-ray reflectometry (NIXR and GIXR).

The X-Ray Calc distribution contents several demonstration projects located in the ***Examples*** folder:

* ***mo-si\_multilayer.xrcx*** contents a simplified model of Mo/Si X-Ray mirror (***Model 1***). It demonstrates the effect of the layer’s thickness on GIXR. ***Data1.dat*** and ***Data2.dat*** content computed diffraction curves for thinner and thicker Si layers.
* ***mo-b4c\_multilayer\_67.xrcx***contents a simplified model of Mo/B X-ray mirror. It demonstrates the calculation of reflectivity as a function of wavelength (NIXR). The project also contents a reference curve (Mo-B).
* ***mo-b.xrcx ­***demonstrates how to work with several different models and data-files in the same project.
* ***n\_stacks.xrcx­*** demonstrates the effect of the number of bilayers in a stack on GIXR.
* ***roughness.xrcx*** shows how the surface roughness changes GIXR of a silicon wafer.

To see the demos, click the ***Open*** button, navigate to the ***Examples*** folder, and select a project. Go to the ***Computation*** tab and click the **Run** button (Or press F5). You can also use **Run all** command (F12)

The projects items could be easily modified:

* *Double-click* on a model in the **Project Items** list will show ***Properties*** dialog, which allows changing its name, color, and description. Or the dialog could be called from the right-click menu
* *Double-click* on a layer will show ***Layer Properties*** dialog. The dialog allows changing of material, thickness, roughness, and density of the layer.
* To change the number of stacks, *double-click* on it. **Stack Properties** dialog allows renaming the stack and changing its name.
* Commands on ***Stack*** and ***Layer*** panes allow manipulating the structure of a model (add or delete stacks and layers).

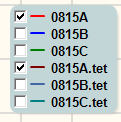
A screenshot of a social media post

Description automatically generated

***O*ptions *pane*** of the ***Computation tab*** allows for choosing the calculation mode. Reflectivity could be calculated as a function of grazing angle or wavelength. Depending on the selected ***Mode***, one of the panes ***By angle*** or **By wavelength** would be activated. These panes allow changing the parameters of calculation.

* **Polarization –** should be both types of polarization used in the calculation. Using of s polarization is preferable when the calculation is performed at hard x-rays and low grazing angles (below 20°). In this case, the calculation speed would be significantly faster. In the cases of larger angles and softer irradiation, ***sp*** mode should be used.
* ***Number of points*** defines the precision of calculation. The time of calculation linearly increased with the rising of the number.
* ***Θ1*** and ***Θ2*** define the range of angles for calculation. The ***2Θ*** check-box enables calculation for Θ-2Θ geometry. **ΔΘ** implements the instrumental divergence of the incident beam.
* The similar settings for adjustment of the wavelength range are used in the ***Wavelength*** mode.

A picture containing screenshot

Description automatically generated******These controls allow switching between the Linear/Log scale of the reflectivity plot and set the background level.

The ***Legend*** on the ***Plot*** could be used to control the visibility of curves.

The ***Export*** button on the ***Result*** pane allowed to export the calculated curve to an ASCII file or copy it to the clipboard. The ***Save*** button on the ***Plot*** pane saves the graph as a graphical file (\*.bmp).