

# **X-Ray Calc**

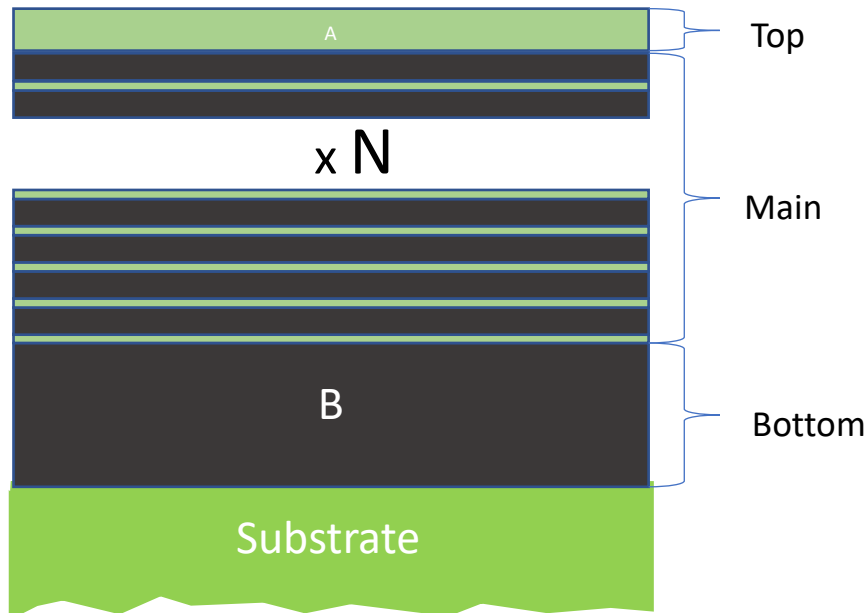
v. 2.4

## **CREATING A MODEL**

### **Tutorial**

This document briefly describes the creation of new models in X-Ray calc. The model represents a layered structure, which also could be periodical. The model consists of a substrate and at least one *Stack*. The Stack is the group of layers.

The following figure demonstrates the general structure of a model of a typical periodical X-Ray mirror.



The model above consists of three stacks – Top, Main, and Bottom. Top and Bottom stacks consists of single layers of materials A and B respectively. Main Stack consists of alternated layers of materials A and B. A/B pairs in Main Stack repeated N times.



Commands on **Stack** and **Layer** panes could be used to manipulate elements of the structure. Some commands could be called from the right-click menu.

**Note: Editing of layers in the model.** To change the properties of any layer or Stack, double-click, or select the layer and press **Enter**, or right-click and select **Edit** from the pop-up menu, or press **Ctrl+E**.

To create such a model in X-Ray calc, do the following steps:

- 1) Click on the **New Model** button at **Project items** pane. The new model will be created. It contents only default substrate. Double-click on the Substrate layer and change the Material to

Structure		Calculation			
Stack / Material		H (Å)	σ (Å)	ρ (g/cm³)	N
.....	SiO2	substrate	3		

SiO<sub>2</sub> and set roughness to 0.3 nm. Because the default density of SiO<sub>2</sub> will be used, leave the field  $\rho$  empty.

- 2) Add stacks. Click **Add** on the pane **Stack**. In the dialog, enter the name of a new stack ("Top"). Repeat for stacks "Main" and "Bottom."

Structure Calculation				
Stack / Material	H (Å)	$\sigma$ (Å)	$\rho$ (g/cm <sup>3</sup> )	N
Top				1
Bottom				1
Main				1
SiO2	substrate	3		

- 3) Select the top Stack. Click **Add** on the **Layer** panel. The new Si layer will be added to the Stack. Double click on the layer and change its properties as follows: Material – B; Thickness – 25; Roughens - 3; Density – empty. Click Ok.

Layer properties

Layer material B

H (Å) 25  $\sigma$  (Å) 3  $\rho$  (g/cm<sup>3</sup>) 0

<< >> OK Cancel

- 4) Select the stack "Main." Add Mo and B layers to the stack "Main" as follows:
- 5) Select the Mo layer. Click **Copy** on **Layer** pane. Then select the stack "Bottom" and click **Paste** on the **Layer** panel. Double-click on the Mo layer in the stack "Bottom" and increase its thickness to

Structure Calculation				
Stack / Material	H (Å)	$\sigma$ (Å)	$\rho$ (g/cm <sup>3</sup> )	N
Top				1
B	25	3		
Main				1
B	25	3		
Mo	15	3	9.5	
Bottom				1
Mo				
SiO2	substrate	3		

100.

- 6) Double click on the stack "Main" and set  $N$  to 300.

The final structure looks as follows:

Structure Calculation				
Stack / Material	H (Å)	$\sigma$ (Å)	$\rho$ (g/cm <sup>3</sup> )	N
Top				1
B	25	3		
Main				300
B	25	3		
Mo	15	3	9.5	
Bottom				1
Mo	15	3	9.5	
SiO2	substrate	3		

Press **F5** to immediately compute the GIXR curve for this model.