Laue diffraction of X-ray microbeams by multilayers

V I Punegov
Institute of Physics and Mathematics, Federal Research Center "Komi Scientific Center", the Ural Branch of the Russian Academy of Sciences, 167982, Syktyvkar, Russia

E-mail: vpunegov@dm.komisc.ru

Abstract. Laue diffraction theory of X-ray microbeams in multilayers (MLs) is developed. The solution for calculating X-ray reciprocal space maps is obtained. The pendulum (Pendellösung) effect for perfect and imperfect MLs is shown. The numerical simulation of Laue diffraction in Mo/Si multilayers with boundary conditions in the case of geometrical optics and the Fresnel approximation is carried out. It is shown that for X-ray microbeams one should take into account the diffraction of X-ray waves at the edges of slits (collimators) of the diffraction scheme.

1. Introduction
Multilayers (MLs) are used in synchrotron radiation installations for a transportation of X-ray beams, for a focusing of radiation, in EUV lithography and in astronomy. Such MLs are mainly related to grazing X-ray reflectors. To focus hard X-rays, it was proposed to create multilayer Laue lenses (MLLs) [1]. Such lenses belong to a new class of X-ray optics elements and, according to [1], have great prospects for a hard X-ray focusing with a focus size of several nanometers. A magnetron sputtering predominantly is used to fabricate MLLs according to the configuration of the Fresnel zones. Despite their similarity to Fresnel zone plates, due to Laue diffraction, MLLs should exhibit different focusing properties. The diffraction of the hard X-ray radiation by multilayer Laue lenses has been studied by numerical simulation [2]. It is shown that the focusing by MLLs is the collimation of the X-ray beam due to the variation of the multilayer period [2].

A manufacture of multilayer Laue lenses is a rather complicated problem; therefore, the first step in this direction is the study of Laue diffraction in multilayers with a constant period [3]. Hence, in this work, the Laue diffraction theory of X-ray microbeams in MLs is considered using the formalism for spatially restricted X-ray fields [4, 5].

2. Dynamical Laue diffraction of restricted X-ray beams in a multilayer
Using the equations of X-ray diffraction in periodic structures [4, 5], taking into account the Laue diffraction boundary conditions, we obtain the solution for the amplitude of the diffracted microbeam in reciprocal space

\[
E_i(q_x, q_z) = \frac{ia_f \exp(i \hat{\psi} L_s)}{2\pi} \int_{-\infty}^{\infty} d\kappa \sin\left(\frac{\xi L_s}{\xi/2}\right) \hat{Y}_\xi(\kappa) \hat{Y}_{ex}(\kappa - q_z),
\]
where \( \hat{w} = -\sqrt{[(q_x - \xi)^2 + 4a_x a_x f^2]} \), \( a_0 = \pi \chi_0 / (\lambda \cos \theta_B) \), \( a_1 = C \pi \chi_1 / (\lambda \cos \theta_B) \), \( \alpha_i = \alpha_i \).

\( \theta_B \) is the Bragg angle; \( \chi_0 \) and \( \chi_1 \) are the Fourier coefficients of X-ray polarizability in the direction of transmission and diffraction, respectively; \( \lambda \) is the wavelength of X-ray radiation in vacuum; \( C \) is the polarization factor; and \( f \) is the attenuation factor depending on defects in the multilayer.

The triple-axis registration of X-ray waves in reciprocal space depends on the angular position of the sample \( \omega \) and the analyzer (position-sensitive detector) \( \varepsilon \) [6,7]. In the symmetrical Laue geometry, these angles are related to the projections of the diffraction vector deviation in the horizontal and vertical directions by relations \( q_x = k \sin \theta_B (2 \omega - \varepsilon) \) and \( q_z = -k \cos \theta_B \varepsilon \).

In the solution (1) the factor \( \hat{Y}_{\omega}(\kappa) = P(\kappa, L_{S1}) \sin(\kappa L_{z1}^{(in)} / 2) / (\kappa / 2) \) is the boundary function of the incident X-ray wave in Fourier space, where \( L_{z1}^{(in)} = w_1 / \cos \theta_B \); \( w_1 \) is the width of the incident X-ray microbeam (Fig.1).

![Schematic representation of Laue diffraction in a multilayer with depth \( L \) and thickness \( L_c \). The size of the incident beam is \( w_1 \), the projection of which to the input face of the multilayer is \( L_{z1}^{(in)} \approx L_c \). The distance from the slit \( S_1 \) to the input face \( (x = 0) \) of the multilayer is \( L_{S1} \). Distance from exit edge \( (x = L_c) \) to position sensitive detector (PSD) is \( L_{PSD} \). The transverse width of the outgoing beam is \( w_2 \), the vertical size of which is \( L_{z2}^{(ex)} \).](image)

The coefficient \( P(\kappa, L_{S1}) = \exp(-i \lambda \kappa^2 L_{S1}^{(in)} / 4\pi (\cos \theta_B)^2) \) is the propagator in Fourier space in the Fresnel approximation [8]; \( L_{S1} \) is the distance from the slit \( S_1 \) to the input surface of the multilayer. In the case of geometrical optics, the propagator is always equal to unity.

The second factor in (1)

\[ \hat{Y}_{\omega}(\kappa - q_z) = P(\kappa - q_z, L_{PSD}) \frac{\sin(L_{z2}^{(ex)} |\kappa - q_z| / 2)}{|\kappa - q_z| / 2} \]

is the transmission coefficient of the diffracted wave in Fourier space; \( L_{z2}^{(ex)} \) is the width of the diffracted X-ray beam. The propagation of the reflected X-ray wave from the multilayer to the position sensitive detector (PSD) or the analyzer is described by the propagator

\[ P(\kappa - q_z, L_{PSD}) = \exp(-i \lambda \kappa^2 L_{PSD}^{(in)} / 4\pi (\cos \theta_B)^2 |\kappa - q_z|^2) \],

where \( L_{PSD} \) is the distance from the exit surface of the multilayer to the PSD.

The angular distribution of the diffracted intensity in reciprocal space from multilayers with a restricted front of X-ray waves is found as

\[ I(q_x, q_z) = |\hat{E}_{\omega}(q_x, q_z)|^2 \].

Solution (1) taking into account (2) is the main relation for calculations of reciprocal space maps (RSMs).
3. Numerical Simulation

We performed a numerical simulation of the angular distribution of the X-ray scattered intensity from Mo/Si multilayers. The structural parameters of the multilayers and the characteristics of the incident synchrotron radiation correspond to the experimental work [3]. The wavelength of the incident synchrotron radiation was $\lambda = 0.1305$ nm. The period of the Mo/Si multilayer is $d = d_{Mo} + d_{Si} = 7$ nm, where $d_{Mo} = d_{Si} = 3.5$ nm; Bragg's angle is $2.25$ mrad. The optical constants for this multilayer were obtained using an X-ray server [9].

![Figure 2](image1)

**Figure 2.** Calculated distributions of transmission [$I_0(x)$, $I_{0,f}(x)$] and diffraction [$I_1(x)$, $I_{1,f}(x)$] intensities within (a) perfect $I_{0,1}(x)$ and (b) imperfect ($f = 0.8$) $I_{0,1,f}(x)$ Mo/Si multilayers.

Dynamical Laue X-ray diffraction in multilayers is associated with the so-called pendulum (Pendellösung) effect, when the intensity of the X-ray beam of the transmission wave is transmitted into the diffraction beam and then, with increasing depth, on the contrary, the intensity of the diffraction wave is transmitted into the transmission beam. The period of such Pendellösung oscillations in symmetric Laue geometry is equal to $l_{Pen} = \frac{\lambda \cos \theta_B}{|C|\chi_1}$. At small Bragg angles $\cos \theta_B \approx 1$, the Pendellösung distance is inversely proportional to the Fourier coefficient of X-ray polarizability $\chi_1$. The Pendellösung period for Mo/Si is equal $l_{Pen}^{Mo/Si} = 38.2 \mu m$.

![Figure 3](image2)

**Figure 3.** Calculated RSMs of diffraction intensity from a Mo/Si multilayer with a synchrotron radiation energy of 9.5 keV for sectioned depths in the case of the boundary conditions in the geometrical optics approximation; (a) $L_x = l_{Pen}^{Mo/Si} / 2$ and (b) $L_x = l_{Pen}^{Mo/Si}$.
Figure 2 shows the Pendellösung effect of perfect and imperfect Mo/Si multilayers. The presence of defects in the multilayer leads to an increase in the period of the Pendellösung oscillations (Fig. 2b).

We made numerical calculations of RSMs for Mo/Si multilayers with sectioned depths \( L_s = \frac{L_{\text{Pen}}}{2} = 19.2 \mu m \) and \( L_s = \frac{l_{\text{Pen}}}{2} = 38.2 \mu m \). The width of the incident X-ray microbeam is \( w_1 \approx L_s = 14 \mu m \) (Fig. 1). Results of calculations within the framework of geometrical optics are shown in Fig. 3. Note that for a sectional depth equal to the period of the Pendellösung oscillations, a splitting of the main diffraction peak is observed (Fig. 3b).

Figure 4 shows calculated RSMs for boundary conditions in the Fresnel approximation. Comparing the results in Figs. 3 and 4, it is easy to see that angular distributions of the X-ray scattered intensity for boundary conditions in the case of geometrical optics and the Fresnel approximation are different.

Figure 4. Calculated RSMs of diffracted intensity with the synchrotron radiation energy of 9.5 keV from a Mo/Si multilayer with sectioned depths taking into account boundary conditions in the Fresnel approximation; (a) \( L_s = \frac{l_{\text{Pen}}}{2} \) and (b) \( L_s = \frac{l_{\text{Pen}}}{2} \). \( L_{\text{PSD}} \) is 30mm and \( L_{\text{PSD}} \) is 40 mm.

4. Conclusion

Thus, we theoretically investigated the Laue diffraction of X-ray microbeams in sectioned multilayers. As in the Bragg geometry [4], in the case of Laue diffraction of microbeams, when performing calculations of RSMs, it is always necessary to choose boundary conditions in the Fresnel approximation. Note that solution (1) is valid only for multilayers with a constant period. For aperiodic multilayer structures, it is necessary to numerically integrate the X-ray diffraction equations [2].

References

[1] Maser J, Stephenson G B, Vogt S et al. 2004 Proc. SPIE. 5539 185
[2] Punegov V I 2020 JETP Letters. 111 376
[3] Kang H C, Stephenson G B, Liu C at el. 2005 Appl. Phys. Lett. 86 151109
[4] Punegov V I and Karpov A V 2021 Acta Cryst. A 77 117
[5] Punegov V I, Pavlov K M, Karpov A V and Faleev N N 2017 J. Appl. Cryst. 50 1256
[6] Punegov V I 2015 Physics-Uspekhi. 58 419
[7] Iida A and Kohra K 1979 Phys. Stat. Sol. A 51 533
[8] Kohn V G, Snigireva I and Snigirev A 2000 Phys. Stat. Sol B 222 407
[9] Stepanov S and Forrest R 2008 J. Appl. Cryst. 41 958