Influence of absorption on the X-ray diffraction by the trapeziform model of superlattice with a stacking fault

H M Manukyan[1] **and S M Manukyan**[2]
[1]Faculty of Physics, Yerevan State University, 1Alex Manoogian,
Yerevan 0025, Armenia
[2]Faculty of Informatics and Applied Mathematics, Yerevan State University,
1Alex Manoogian, Yerevan 0025, Armenia

E-mail: hasmikm@ysu.am

Abstract. The problem of a dynamic diffraction of a plane monochromatic X-ray wave at the absorbing superlattice with a stacking fault between the layers for the trapeziform model of superlattice is considered. It is shown, that presence of stacking fault reduces the anomalous absorption. The interference absorption depends on the shift vector and depth of the stacking fault and the structural factor of superlattice.

1. Introduction

When a plane monochromatic X-ray wave is incident on a superlattice (SL) double diffraction occurs, first by atomic planes causing the formation of a modulated X-ray wave, and then by diffraction of the latter by the interfaces between layers, since the layer structure acts as a diffraction grating. Consequence of this diffraction is appearance of satellites around the principal maximum of X-ray diffraction in SL.

SL based on heterojunction are applied widely in microelectronics and computer techniques [1–3]. Dynamic diffraction of X-ray radiation has been applied in [4] for harmonic SL. Work [5] develops dynamical theory of X-ray diffraction on one-dimensional perfect SL of arbitrary model. Obtained results are employed for different models [6]. Being important in applications, superlattice perfection has been investigated by various methods of X-ray analysis [7–11].

One of the possible defects impairing superlattice parameters is a stacking fault. Work [12] develops the theory of X-ray dynamic diffraction on one-dimensional SL with a stacking fault between the layers if a absorption by the medium is neglected. In [13] X-ray dynamic diffraction on a SL with a stacking fault between the layers is considered theoretically in the case of interdiffusion of SL components if a absorption by the medium is neglected. In [14] we obtained the reflectivity in the exact directions of diffraction maxima for SL with a stacking fault between the layers when absorption is taken into account. The results are used for square-wave model of SL.

In this paper we develop the theory of X-ray diffraction on trapeziform model of SL with a stacking fault between the layers when absorption is taken into account.

2. Absorption in the superlattice with a stacking fault

Let us consider a superlattice of thickness Nz_0 (z_0 period of SL, N number of identical layers). Let a stacking fault be located at the depth N_1z_0 in SL (figure 1). In this case, the fault plane divides the

crystal into two SLs of thicknesses $N_1 z_0$ and $N_2 z_0$ ($N_1 + N_2 = N$). Let a plane monochromatic X-ray wave of unit amplitude be incident at this SL. The waves emerging from the first SL are incident on the second one and for reflection amplitude of SL one obtains [15]

$$\Phi_{h,N} = r_{hN_1} t_{\bar{0}N_2} + e^{-i\alpha} t_{0N_1} r_{hN_2}, \tag{1}$$

where r_{hN_1}, r_{hN_2} and t_{0N_1}, $t_{\bar{0}N_2}$ are, respectively, the reflection and transmission amplitudes of two parts of SL; $\alpha = 2\pi \mathbf{hu}$ (**h** is the diffraction vector, **u** is the shift vector characterizing the displacement of second SL lattice with respect to the lattice of the first part of SL) and the dash corresponds to incidence from the back of the reflecting planes.
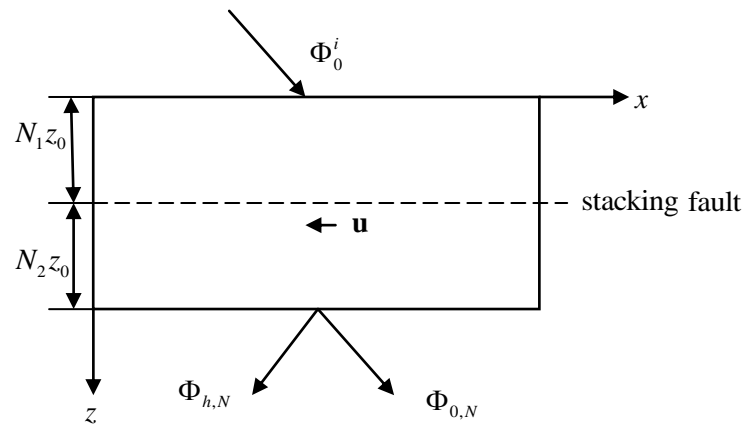

Figure 1. The geometry of diffraction.

As known, consequence of X-ray diffraction for SL with short period $z_0 \ll \bar{\Lambda}$ ($\bar{\Lambda}$ the mean extinction length of the crystal) is appearance of non-overlapping satellites around the principal diffraction maximum, the location of which is defined by an average over the superlattice period parameters. It is shown in [5], that for short-period SL within the limits of the mth reflection one may consider the SL as an ideal crystal with the modified Fourier component of the crystal polarizability:

$$\chi_{hm} = M_m \bar{\chi}_h, \tag{2}$$

where $\bar{\chi}_h$ is the Fourier component of the polarizability of crystal averaged over SL period and M_m the SL model-dependent structural factor of SL.

Substituting (2) in dynamical formulas of the reflection and transmission amplitudes of ideal crystal for symmetrical Laue case [16], we can write:

$$r_{hN_i,m} = i(\bar{\chi}_h / \bar{\chi}_{\bar{h}})^{1/2} M_m \frac{\sin(\pi Z_0 N_i (p^2 + M_m^2)^{1/2})}{(p^2 + M_m^2)^{1/2}}, \tag{3}$$

$$t_{0N_i, \bar{0}N_i, m} = \cos(\pi Z_0 N_i (p^2 + M_m^2)^{1/2}) \mp ip \frac{\sin(\pi Z_0 N_i (p^2 + M_m^2)^{1/2})}{(p^2 + M_m^2)^{1/2}}, \tag{4}$$

where

$$Z_0 = z_0 / \bar{\Lambda} = \frac{C |\bar{\chi}_h|}{\lambda \cos \bar{\theta}_B} z_0, \tag{5}$$

$$p = (\sin 2\bar{\theta}_B / C |\bar{\chi}_h|)(\theta - \theta_m) \tag{6}$$

is a dimensionless parameter proportional to the deviation from the mth reflection direction θ_m, λ the wavelength of an incident wave, C the polarization factor, $\bar{\theta}_B$ the Bragg angle, averaged over SL

period, and $i = 1; 2$.

In [12] we develop expressions for reflectivity within the limits of the mth satellite for non-absorptive SL with a stacking fault between the layers, depending on the shift vector and depth of the stacking fault. We show, that the existence of a stacking fault is reducing satellite intensity. In [13] X-ray dynamic diffraction on a SL with a stacking fault between the layers is considered theoretically in the case of interdiffusion of superlattice components if a absorption by the medium is neglected.

The procedure of taking absorption into account based on the method used in the classical theory of dispersion, i.e. on the introduction of complex parameters of polarizability and its Fourier components:

$$\overline{\chi} = \overline{\chi}_r + i\overline{\chi}_i, \quad \overline{\chi}_h = \overline{\chi}_{hr} + i\overline{\chi}_{hi}, \quad \overline{\chi}_0 = \overline{\chi}_{0r} + i\overline{\chi}_{0i}. \tag{7}$$

Since for X-rays the dynamic absorption is usually small, i.e. $|\chi_{hi}| << |\chi_{hr}|$, neglecting terms of the order of $(|\overline{\chi}_{hi}|/|\overline{\chi}_{hr}|)^2$, for symmetrical reflection one can write:

$$Z_{0r} = C|\overline{\chi}_{hr}|z_0 / \lambda \cos\overline{\theta}_B, \qquad Z_{0i} = Z_{0r}\text{æ}\cos\nu_h, \tag{8}$$

$$p_r = (\sin 2\overline{\theta}_B / C|\overline{\chi}_{hr}|)(\theta - \theta_m), \qquad p_i = -p_r\text{æ}\cos\nu_h, \tag{9}$$

where $\text{æ} = |\chi_{hi}|/|\chi_{hr}|$ and for crystals with a centre of symmetry $\cos\nu_h = \pm 1$.

In [14] we obtained the reflectivity in the direction of mth satellite $\theta = \theta_m$ (i.e. for $p = 0$) for SL with a stacking fault between the layers when absorption is taken into account. The results are used for square-wave model of SL.

In accordance with approach, mentioned above, after some transformations for the reflectivity within the limits of the mth reflection, depending on the deviation from the mth reflection direction θ_m, we obtain the following expression:

$$R_m = \frac{e^{-\mu D/\cos\overline{\theta}_B}}{(p_r^2 + M_m^2)}\left| \sin(A_m + i\beta_m) + \frac{1 - \exp(-i\alpha)}{2}\left\{ i\frac{p_r[\cos(B_m + i\gamma_m) - \cos(A_m + i\beta_m)]}{(p_r^2 + M_m^2)^{1/2}} \right.\right.$$

$$\left.\left. + \sin(B_m + \upsilon_m + i\gamma_m) - \sin(A_m + \upsilon_m + i\beta_m)\right\}\right|^2, \tag{10}$$

where

$$A_m = \pi Z_{0r}N\sqrt{p_r^2 + M_m^2}, \qquad \beta_m = \text{æ}A_m/(p_r^2 + M_m^2), \tag{11}$$

$$B_m = \pi Z_{0r}(N_1 - N_2)\sqrt{p_r^2 + M_m^2}, \qquad \gamma_m = \text{æ}B_m/(p_r^2 + M_m^2), \tag{12}$$

$$\upsilon_m = \text{æ}/(p_r^2 + M_m^2)^{3/2}, \tag{13}$$

$D = Nz_0$ is the thickness of the superlattice, $\mu = -2\pi\overline{\chi}_{0i}/\lambda$ is the coefficient of linear absorption.

Since the p_r dependence of the reflectivity (10) is very lengthy, let us present it for a particular case, when $\alpha = \pi$:

$$R_m = \frac{e^{-\mu D/\cos\overline{\theta}_B}}{(p_r^2 + M_m^2)^2}\left\{ \left[\sqrt{p_r^2 + M_m^2}\left(\sin A_m \operatorname{ch}\beta_m + \sin(B_m + \upsilon_m)\operatorname{ch}\gamma_m - \sin(A_m + \upsilon_m)\operatorname{ch}\beta_m\right)\right.\right.$$

$$\left.+ p_r\left(\sin B_m \operatorname{sh}\gamma_m - \sin A_m \operatorname{sh}\beta_m\right)\right]^2 + \left[p_r\left(\cos B_m \operatorname{ch}\gamma_m - \cos A_m \operatorname{ch}\beta_m\right)\right.$$

$$\left.\left. + \sqrt{p_r^2 + M_m^2}\left(\cos A_m \operatorname{sh}\beta_m + \cos(B_m + \upsilon_m)\operatorname{sh}\gamma_m - \cos(A_m + \upsilon_m)\operatorname{sh}\beta_m\right)\right]^2\right\}. \tag{14}$$

According to (2) the interference absorption factor of m th diffraction maximum for ideal SL has the following form: $\sigma_m = \sigma_0 M_m$, where $\sigma_0 = 2\pi k C |\chi_{hi}| \cos\nu_h / (\cos\theta_B \sqrt{1 + p_r^2})$ is the interference absorption factor for homogeneous crystal [16]. As is shown in [5], $M_m < 1$ for any SL model, therefore the interference absorption factor in SL decreases.

Presence of stacking fault reduces the effect of anomalous absorption. The interference absorption depends on the shift vector and depth of the stacking fault. For the maximum shift ($\alpha = \pi$) the wave field, weakly absorbable in the first part of SL, is strongly absorbable in the second one and vice versa.

3. Trapeziform model

Artificial SL crystals based on heterojunctions are one-after-another layers of different compositions with close interplanar spacings (like GaAs–AlAs). At early stage after fabrication when interdiffusion of semiconductor compounds entering the bilayer composition is absent, SL can be described by a rectangular (square-wave, if layers of different materials have the same thickness) model. Taking into account the interdiffusion of heteromaterials, one may describe SL by trapeziform model. If the SL layers are thin due to the interdiffusion of SL components different materials will be overlapped throughout the layer. One may describe such a SL by either sinusoidal or triangular model.

Assume that in some time after fabrication of SL, a diffusion layer of thickness z_d has been formed. Denote z_1 and z_2 the thicknesses of ideal layers. Then SL is described by a trapeziform model whose structural factor has the following form [6]:

$$M_m = \left| \frac{\sin(\pi p_{1m}\varepsilon_1)}{\pi p_{1m}\varepsilon_0} + (-1)^m \frac{\sin(\pi p_{2m}\varepsilon_2)}{\pi p_{2m}\varepsilon_0} - F_{1m} - (-1)^m F_{2m} \right|, \tag{15}$$

where the following notations are introduced:

$$p_{1m} = \frac{m - \varepsilon_2 - \varepsilon_d}{\varepsilon_0}, \qquad\qquad p_{2m} = \frac{m + \varepsilon_1 + \varepsilon_d}{\varepsilon_0}, \tag{16}$$

$$\varepsilon_j = 2k z_j \sin\overline{\theta}_B \, \mathrm{tg}\overline{\theta} \, \Delta d / \overline{d} \qquad (j = 0; 1; 2; d), \tag{17}$$

$$F_{jm} = \frac{\sqrt{\varepsilon_d}}{\varepsilon_0} (\sin(\pi p_{jm}\varepsilon_j) U_{3/2}(2q_{jm}^2, 0) - (-1)^j \cos(\pi p_{jm}\varepsilon_j) U_{1/2}(2q_{jm}^2, 0)), \tag{18}$$

$$q_{jm} = \sqrt{\pi\varepsilon_d p_{jm}} \qquad\qquad (j = 1, 2), \tag{19}$$

$$U_\nu(2x, 0) = \sum_{k=0}^{\infty} \frac{(-1)^k x^{\nu + 2k}}{\Gamma(\nu + 2k + 1)}, \tag{20}$$

ε_0 is a parameter characterizing the degree of misfit of heteromaterials, Δd the difference in interplanar spacings of heterostructures, and the bar denotes the averaging over the SL period.

By inserting $z_d = 0$ into expressions (15)–(20) the structural factor of rectangular model is obtained. On the other hand, at full interdiffusion of semiconductor materials constituting SL, by substitution of $z_1 = z_2 = 0$ into (15)–(20), the structural factor of triangular model is obtained.

The numerical calculations are carried out for GaAs–AlAs SL, CuK$_\alpha$ radiation, when diffusion layer thickness is 20% of the bilayer thickness. With increasing interdiffusion of heteromaterials, redistribution of intensity of diffraction maxima takes place. In discussed case the magnitude of the principal maximum decreases, while oscillations increase.

Figure 2 shows dependence of reflectivity of the principal maximum ($m = 0$) on dimensionless parameter (p) of deviation from the direction of diffraction maximum at $\alpha = \pi$ and the stacking fault depth $N_1 z_0 = 0.1\, N z_0$. As seen the plot on figure 2(b) becomes asymmetrical. If the depth of the stacking fault satisfies the condition $N_2 z_0 = 0.1\, N z_0$, we obtained the reflectivity of absorbing SL similar to figure 2(b), mirrored with respect to Y-axis.
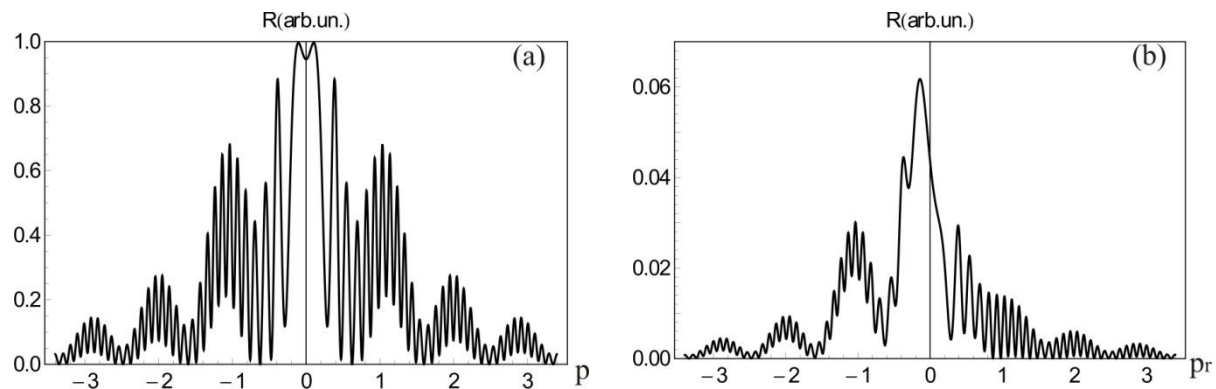

Figure 2. The reflectivity of the principal maximum for $\alpha = \pi$, $N_1 = 0.1\,N$ and $z_d = 0.2\,z_0$
(a) nonabsorbing SL, (b) absorbing SL

Figure 3 shows dependence of reflectivity of the principal maximum ($m = 0$) on dimensionless parameter (p) of deviation from the direction of diffraction maximum at $\alpha = \pi$ and the stacking fault depth $N_1 z_0 = N_2 z_0 = 0.5\, N z_0$. In this case the plot on the figure 3(b) is symmetrical.
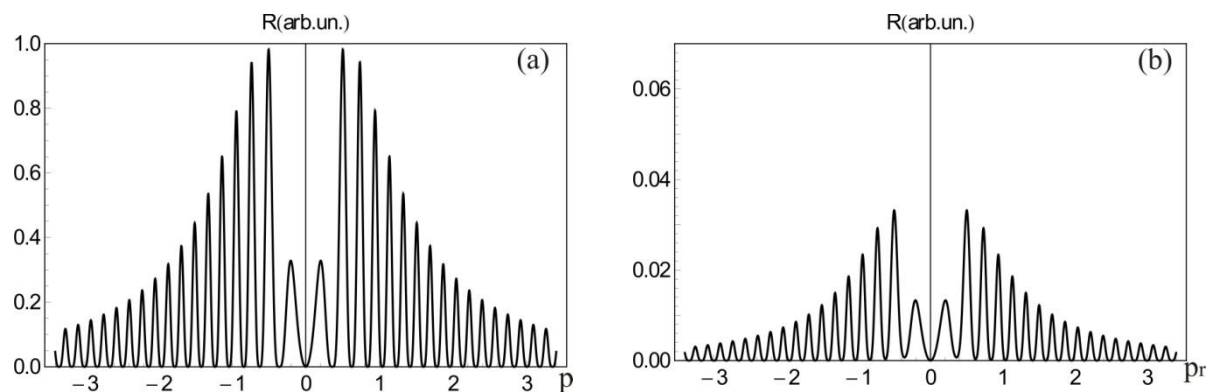

Figure 3. The reflectivity of the principal maximum for $\alpha = \pi$, $N_1 = N_2$ and $z_d = 0.2\,z_0$
(a) nonabsorbing SL, (b) absorbing SL

4. Conclusion
In this study we obtained, that in the case of a short-period SL with a stacking fault between the layers, taking absorption into account decreases the reflectivity of SL. Presence of stacking fault reduces the effect of anomalous absorption. The interference absorption depends on the shift vector and depth of the stacking fault and the structural factor of SL (which in turn depends on the interdiffusion degree of constituent heteromaterials).

References

[1]   Shik A Ya 1974 *FTP* **8** 1841
[2]   Golubev L V and Leonov E I 1977 *Sverkhreshetki* (Superlattices) Moscow: Znaniye
[3]   Maslyuk V T and Fennich P A 1981 *Poluprovodnikoviye sverkhreshetki* (Semiconductor Superlattices) Moscow: Zarubezhnaya Elektronnaya Tekhnika
[4]   Khapachev Yu P and Kuznetsov G F 1983 *Kristallografiya* **28** 27
[5]   Vardanyan D M, Manoukyan H M and Petrosyan H M 1985 *Acta Cryst.* **A41** 212
[6]   Vardanyan D M, Manoukyan H M and Petrosyan H M 1985 *Acta Cryst*. **A41** 218
[7]   Afanasyev A M, Zaytsev A A and Imamov R M 1998 *Kristallografiya* **43** 1
[8]   Engström C, Birch J, Hultman L, *et al* 1999 *J. Vac. Sci. Technol. A* **17** 2920
[9]   Holy V, Stangl J, Springholz G, *et al* 2001 *J. Phys. D: Appl. Phys.* **34** A1
[10] Roch T, Holy V, Daniel A, *et al* 2001 *J. Phys. D: Appl. Phys.* **34** A6
[11] Zaytsev A A, Subbotin I A, Pashaev E M, *et al* 2004 *Plenki-2004 Materiali mezhdunarodnoi nauchnoi konferentsii* (Films-2004 Materials of International Conference) Moscow MIRE 49
[12] Manukyan H M 2007 *Poverkhnost'. Rentgen., sinkhrotron. i neytronniye issledovaniya* **10** 17
[13] Manukyan H M 2014 *Izvestiya NAN Armenii Fizika* **49** 360
[14] Manukyan H M, Manukyan S M 2015 *Proceedings of the Yerevan State University Physical and Mathematical Sciences* **3** 55
[15] Amelinckx S 1964 *The direct observation of dislocations* New York and London: Academic press
[16] Pinsker Z G 1982 *Rentgenovskaya Kristallooptika* (X-ray Crystal Optics) Moscow: Nauka