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ABSORPTION AT X-RAY DIFFRACTION BY THE ONE-DIMENSIONAL SUPERLATTICE WITH A STACKING FAULT

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The problem is considered of a dynamic reflection of a plane monochromatic X-ray wave at the superlattice with a stacking fault between the layers when absorption is taken into account. It is shown, that taking absorption into account reduces the reflectivity in the direction of satellites. At the same time, the closer stacking fault is to the crystalline surface, the less impact it has on the reflectivity.

Keywords: X-ray diffraction, superlattice, defects.

Introduction. Modulated structures are crystals, where a periodical function of displacement exists with the period of distortions much exceeding the lattice constant. In this case, electrons undergo, besides the periodic potential of crystal lattice, also to the additional potential with much larger period. Such crystals are conventionally called superlattices (SL). Presence of the additional potential in SL leads to a number of specific properties of the crystal, which are absent in homogeneous samples. Since the X-ray wavelength is much shorter than the period of additional potential, diffraction is possible at small angles of incidence. But when X-ray radiation undergoes Bragg diffraction, modulated waves are excited in the crystal, with period much exceeding the X-ray wavelength, and the periodic distortions serve as diffraction grating for these modulated waves. Consequence of this diffraction is appearance of satellites around the principal maximum of X-ray diffraction in SL.

SL based on heterojunction are especially important. These are artificial SL with preselected parameters, which are applied widely in microelectronics and computer techniques [1–3] due to their unique properties (regions of negative differential conductivity in the current-voltage characteristic, sharp anisotropy of intraband optical absorption, and so on).

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].

Heteroepitaxial SL are obtained by in turn, one-upon-another, deposition of thin layers of different semiconductors with close interplane distances. In this case,

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addition of different defects to SL is possible, deteriorating its parameters. In this connection, it is very important to study the influence of defects on the diffraction pattern, at diffraction of X-rays on SL. Studies of heteroepitaxial SL by different X-ray techniques have been performed in [7–11]. In order to interpret experimental results, works [7, 11] take into account non-constancy of SL period and diffuse scattering on thermal phonons and SL imperfections. Works [9, 10] study formation in SL of quantum dots and wires. Influence of interdiffusion of heteromaterials in a bilayer on the diffraction pattern at annealing of an ideal SL has been investigated in [8].

One of possible defects in producing heteroepitaxial SL is stacking fault between the layers. In work [12] we develop the theory of X-ray dynamic diffraction on one-dimensional superlattice with a stacking fault between the layers, if a absorption by the medium is neglected. We develop expressions for reflection and transmission amplitudes depending on the shift vector and depth of the stacking fault. For comparison with a perfect superlattice, relative change of the reflectivity coefficient is calculated. We show that the existence of a stacking fault is reducing satellite intensity. At the same time, the closer stacking fault is to the crystalline surface, the less impact it has on diffraction pattern.

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

Absorption in the Superlattice with Stacking Fault. Let us consider a superlattice of thickness Nz_0 (z_0 is the period of SL, N is number of identical layers). Let a stacking fault be located at the depth N_1z_0 in SL. In this case, the fault plane divides the crystal into two SL of thicknesses N_1z_0 and N_2z_0 ($N_1 + N_2 = N$), in-between which the waves suffer a phase jump $\alpha = 2\pi\,\mathbf{hu}$ with $\mathbf{h}$ the diffraction vector and $\mathbf{u}$ the shift vector. Let a plane monochromatic X-ray wave of unit amplitude be incident at this SL.

As shown in [5], if $z_0 \ll \overline{\Lambda}$ ($\overline{\Lambda}$ is the mean extinction length of the crystal) for obtaining the reflection and transmission amplitudes in SL in the directions of diffraction maxima, it is sufficient to replace the Fourier-component of crystal polarizability χ_h by the modified Fourier-component χ_{hm}:

$$|\chi_{hm}| = M_m |\chi_h|, \tag{1}$$

where M_m is structural factor of SL; m is number of the diffraction maximum (satellite).

In [12] for the reflectivity in the direction of m-th satellite for non-absorptive superlattice we obtain

$$R_m = R_{m0} - |f|^2 \left(\sin^2(\alpha/2)\sin(2A_{1m})\sin(2A_{2m}\right). \tag{2}$$

Here the following notations are introduced:

$$R_{m0} = |f|^2 \sin^2(A_m) \tag{3}$$

is coefficient of reflection of X-ray wave from one-dimensional perfect SL of thickness Nz_0 in the direction of m-th satellite;

$$A_m = \pi N z_0 \beta M_m, \tag{4}$$

$$A_{1m} = \pi N_1 z_0 \beta M_m, \tag{5}$$

$$A_{2m} = \pi N_2 z_0 \beta M_m , \tag{6}$$

$$\beta = kC(\chi_h \chi_{\bar{h}})^{1/2} / (\gamma_0 \gamma_h)^{1/2}, \tag{7}$$

$$f = (\chi_h / \chi_{\bar{h}})^{1/2}, \tag{8}$$

γ_0 and γ_h are the direction cosines of incidence and reflection angles respectively.

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 dynamical scattering.

Neglecting terms of the order of $(|\chi_{hi}|/\chi_{hr})^2$ for symmetrical reflection one can write

$$Z_{0r} = \frac{kC|\chi_{hr}|}{\cos\overline{\theta}_B} z_0, \quad Z_{0i} = Z_{0r}\frac{|\chi_{hi}|}{|\chi_{hr}|}\cos\nu_h , \tag{9}$$

where $k = 1/\lambda$ is the wave number in vacuum; C is the polarization factor; $\overline{\theta}_B$ is the mean Bragg angle; χ_{hr} and χ_{hi} are the real and imaginary parts of Fourier coefficients of crystal susceptibility respectively. For crystals with a centre of symmetry $\cos\nu_h = \pm 1$.

In the direction of m-th satellite we obtain the following expression:

$$\begin{aligned} R_m = \frac{e^{-\mu D/\cos\overline{\theta}_B}}{2}&(\sin^2\frac{\alpha}{2}(\text{ch}(2a_i\Delta N) - \cos(2a_r\Delta N)) + \\ &+ \cos^2\frac{\alpha}{2}(\text{ch}(2a_i N) - \cos(2a_r N)) + \\ &+ \sin\alpha(\sin(2a_r N_1)\,\text{sh}(2a_i N_1) - \sin(2a_r N_2)\,\text{sh}(2a_i N_2))), \end{aligned} \tag{10}$$

where $\Delta N = |N_1 - N_2|$, $N = N_1 + N_2$, N_1 is the number of layers before the stacking fault, N_2 is the number of layers after the stacking fault, $D = Nz_0$ is the thickness of the superlattice, $a_r = \pi M_m Z_{0r}$, $a_i = \pi M_m Z_{0i}$, μ is the linear absorption factor.

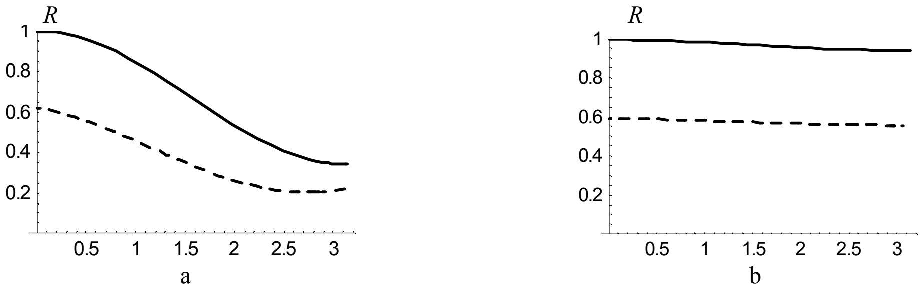
It follows from expression (10) that reflectivity in the direction of m-th satellite depends on both the phase jump on the stacking fault and the depth of its position, and the specific SL model and the number of satellite.

Square-Wave Model. Artificial SL crystals based on heterojunctions are one-after-another layers of different compositions with close interplane distances (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.

Structural factor of SL has in square-wave model the following form [6]:

$$M_m = \begin{cases} (\varepsilon_0/\pi)\left|\sin(\pi\varepsilon_0/4)/(m^2 - \varepsilon_0^2/4)\right|, & m = 2n, \\ (\varepsilon_0/\pi)\left|\cos(\pi\varepsilon_0/4)/(m^2 - \varepsilon_0^2/4)\right|, & m = 2n+1, \end{cases}$$

where $\varepsilon_0 = 2kz_0 \sin\overline{\theta}_B \text{tg}\overline{\theta}_B \, \Delta d/\overline{d}$ is a parameter characterizing the degree of misfit of heteromaterials, Δd is the difference in interplane distances of heterostructures, and the bar denotes the averaging over the SL period.



α -Dependence of the reflectivity: solid curve is for nonabsorbing superlattice with stacking fault; dashed curve is for absorbing superlattice with stacking fault: a) $m=0$; b) $m=\pm 1$.

It is seen in the Figure, that taking absorption into account decreases magnitude of both principal maximum and satellites. On the other hand, shift vector of stacking fault more affects on the principal maximum.

Conclusion. We obtained, that taking absorption into account reduces the reflectivity in the direction of satellites. At the same time, the closer stacking fault is to the crystalline surface, the less impact it has on the reflectivity.

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