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Physics

FEATURES OF DIFFRACTION FOCUSING OF A SPHERICAL X-RAY WAVE ON A SHORT PERIOD SUPERLATTICE

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The problem of a dynamic diffraction of spherical X-ray wave on a short period superlattice is considered theoretically. It is shown that a focusing of satellites occurred both at different depths of the superlattice and at different distances from the crystal in vacuum depending on the structural factors of the superlattice. The larger the structural factor of the satellite, the more deeply the wave in the crystal is focused and, respectively, the less is the focal length out of the crystal in vacuum.

***Keywords*:** dynamical diffraction, spherical X-ray wave, superlattice.

Introduction. Being important in applications, the artificial superlattices (SL) have been investigated by various methods of X-ray and electron microscopy analysis [1–5]. The consequence of a plane monochromatic X-ray wave diffraction for a SL with short period is the appearance of non-overlapping satellites around the principal diffraction maximum, the location of which is defined by an average over the SL period parameters. In the case of Laue geometry, the dynamical X-ray diffraction of a spherical wave on a perfect crystal is characterized by focusing of weakly absorbable mode of diffracted wave both inside and outside of the crystal [6–9]. In [10] it was shown that for short period SL within the m-th satellite one may consider the SL as an ideal crystal with modified Fourier components of the crystal polarizability. Therefore, the spherical X-ray wave diffraction on the SL for each satellite can be described in the same way as for single crystal with introduction of the corresponding Bragg angles and focus lengths both inside and outside of the SL. In this paper we theoretically study the dynamic diffraction of a spherical X-ray wave on a short-period heteroepitaxial SL, where owing to interdiffusion, different materials overlapped throughout the layer.

Theory. For symmetrical Laue case the intensity of diffracted wave inside the crystal at the depth z near the focal area, when the reflecting atomic planes correspond to x=const planes, approximately expressed by the formula:

$$I_h(x,z)=\frac{\exp\left(-\frac{\mu z}{\cos\theta}\left(1-C\frac{|\chi_{hi}|}{\chi_{0i}}\right)\right)\exp\left(-\pi\frac{zC\,|\chi_{hi}|}{\lambda\cos\theta}\cdot\frac{x^2\cot^2\theta}{\left(\frac{L_1}{\Gamma}-z\right)^2+\left(z\left|\frac{\chi_{hi}}{\chi_{hr}}\right|\right)^2}\right)}{4L_1\Gamma\left(\left(\frac{L_1}{\Gamma}-z\right)^2+\left(z\left|\frac{\chi_{hi}}{\chi_{hr}}\right|\right)^2\right)^{1/2}}, \quad (1)$$

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where

$$\Gamma = \frac{\sin\theta \sin 2\theta}{C|\chi_{hr}|}, \qquad (2)$$

λ is the radiation wavelength; L_1 is the distance between point source and crystal; θ is the Bragg angle; $\mu = 2\pi\chi_{0i}/\lambda$ is the linear absorbance; χ_0 and χ_h are the Fourier-components of the crystal polarizability $\chi = \chi_r + i\chi_i$; C is the polarization factor ($C = 1$ and $\cos 2\theta$ for σ- and π-polarizations respectively).

Since for X-rays $|\chi_{hi}| \ll |\chi_{hr}|$ [11], then according to Eq. (1) we can obtain the focus depth in the crystal

$$z_F = \frac{L_1}{\Gamma}. \qquad (3)$$

The expression for diffracted wave intensity outside of the crystal is similar to (1), with the z coordinate replaced by the thickness of the crystal, D, and the source-crystal distance, L_1, replaced with the sum of distances source-crystal-detector, $L_1 + L_h$. Since the focus outside of the crystal corresponds to the distance crystal-detector L_h, then the focus distance in the vacuum satisfies the condition

$$L_{hF} = \Gamma(D - z_F). \qquad (4)$$

As noted above, if $z_0 \ll \bar{\Lambda}$ (z_0 is the period of SL, $\bar{\Lambda}$ is the mean extinction length of the crystal), it is sufficient to replace the Fourier-component of the crystal polarizability χ_h by the modified Fourier-component χ_{hm}:

$$\chi_{hm} = M_m \bar{\chi}_h, \qquad (5)$$

where m is the number of the diffraction maximum (satellite), M_m is the model dependent structural factor of SL, $\bar{\chi}_h$ is the Fourier-component of the crystal polarizability averaged over SL period.

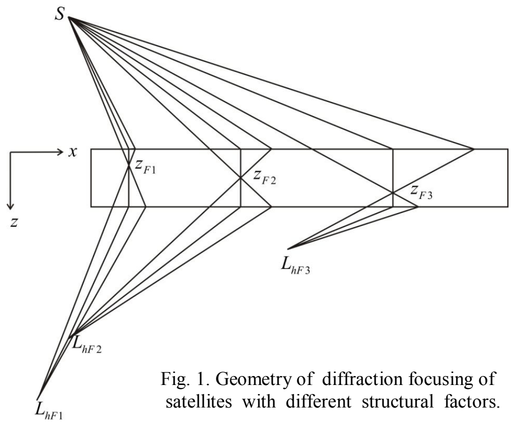

Fig. 1. Geometry of diffraction focusing of satellites with different structural factors.

Fig. 1 schematically shows the geometry of diffraction focusing of satellites with different structural factors $M_{m1} < M_{m2} < M_{m3}$. Accordingly, for the focus depths inside the crystal $z_{F1} < z_{F2} < z_{F3}$ and for corresponding outside focal lengths $L_{hF1} > L_{hF2} > L_{hF3}$.

It is seen in the Fig. 1, that the larger the structural factor of the satellite is, the more deeply the wave in the crystal is focused and, respectively, the focal length out of the crystal in vacuum is shorter.

Artificial superlattices based on heterojunctions are consecutive layers of different compositions with close interplanar spacings. At the early stage after superlattice preparation, when the interdiffusion of heteromaterials is negligible, one may describe it by rectangular model (or quadratic, if layers of different materials have the same thickness). Taking into account the interdiffusion of heteromaterials, SL may be described by trapeziform model. If the superlattice layers are thin due to the interdiffusion of superlattice components, different materials will be overlapped throughout the layer. Such a superlattice may be described by either sinusoidal or triangular model.

The expression for the structural factor for the triangular model of SL has the form [12]:

$$M_m = \frac{1}{(2\varepsilon_0)^{1/2}} \left| U_{1/2}(2q_+^2, 0) - (-1)^m U_{1/2}(2q_-^2, 0) \right|, \tag{6}$$

where $q_\pm = (m \pm \varepsilon_0/2)(\pi/2\varepsilon_0)^{1/2}$, $\varepsilon_0 = 2(z_0/\lambda)\sin\bar{\theta}\tan\bar{\theta}\Delta d/\bar{d}$, Δd is the difference of interplanar spacings of heterostructures, the bar denotes the averaging over the SL period and

$$U_\nu(2x, 0) = \sum_{k=0}^{\infty} \frac{(-1)^k x^{\nu+2k}}{\Gamma(\nu + 2k + 1)} \tag{7}$$

is the two-variable Lommel function [13].

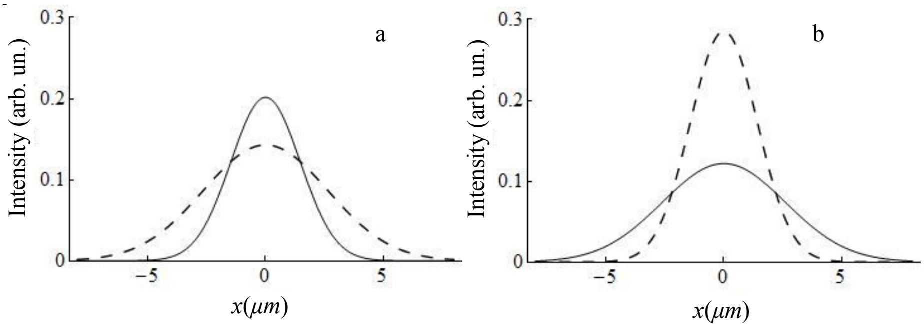

Fig. 2. Intensity of the principal maximum corresponding:
(a) to the focus distance for quadratic model; (b) to the focus distance for triangular model.
Solid curve is for quadratic model, dashed curve is for triangular model.

Fig. 2. shows the influence of the interdiffusion on the intensity distribution of the principal maximum ($m = 0$). Numerical calculations were carried out for SL on the basis of GaAs – AlAs heterojunction with 150 *nm* period in the case of CuK_α radiation for quadratic and triangular models. In this case the structural factor of the principal maximum increases, therefore, according to expressions (1)–(4), its intensity increases and as presented in Fig. 1, the focal length outside of the crystal decreases.

Conclusion. The study of the dynamic diffraction of a spherical X-ray wave on a short-period superlattice shows, that depending on the structural factor of the superlattice, the satellites are focused at different depths both inside and outside of the superlattice. The larger the structural factor of the satellite is, the more deeply the wave in the crystal is focused and, respectively, the focal length out of the crystal in vacuum is shorter. As a consequence of interdiffusion, structural factor of the superlattice changes altering the focal lengths of satellites.

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