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Diagnostics of Structure and Composition of Binary Crystals from Dynamical X-ray Scattering in the Region of Anomalous Dispersion

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Abstract—The analysis of thickness (Pendellösung oscillations) and energy (depending on the radiation wavelength) dependences of X-ray diffraction intensities allows one to apply the dynamical theory of X-ray diffraction and extract the information on the static Debye–Waller factor, extinction coefficient, and parameter which characterizes nonstoichiometry of binary crystals. The corresponding diffraction experiments on gallium arsenide crystals were performed in a single-crystal spectrometer with the use of the Bremsstrahlung radiation in the region of anomalous X-ray dispersion in which the Hönl corrections to the atomic factors of components are important. We considered quasi-forbidden reflection sensitive to low deviations from nonstoichiometry. The values of the static Debye–Waller factor, extinction coefficient, and nonstoichiometry parameter determined by two independent methods indicated above agree quite satisfactorily. *© 2004 MAIK "Nauka/Interperiodica".*

INTRODUCTION

Below we analyze the possibilities of an X-ray diffraction study of a real structure (defects) and chemical composition of binary crystals with the use of the X-ray Bremsstrahlung radiation and superstructural reflections. This approach allowed us to eliminate the contributions of the undesirable scattering components to the total diffraction pattern and increase the sensitivity of the diffraction maxima to slight variations in the chemical composition of the binary crystals.

The composition and defect structure of binary crystals with the lattice consisting of the atoms of two species, *A* and *B*, considerably influence the mechanical, optical, electrical, and other properties of these materials. Thus, metal crystals of binary solid solutions are characterized by ordering processes which influence the plastic properties of the alloys. The degree of lattice order is characterized by the parameter η of the long-range order [1]:

$$\eta = \frac{n_A - n_B}{1 - p_A} \tag{1}$$

which changes the intensity *I* of the superstructural line in the kinematical theory of scattering as

$$I \propto \eta^2 (f_A - f_B)^2. \tag{2}$$

In expressions (1) and (2), n_A is the fraction of *A* species occupying their sites as in the state of the complete order, p_A is the atomic concentration of this component, and f_A and f_B are the atomic formfactors. Analysis of the intensities of the superstructural lines in $Fe_{22.5}Ni_{77.5}$ and $Fe_{0.53}Cr_{0.47}$ single crystals [3] obtained with the use of the synchrotron radiation provides the unique possibility for determining the short-range order coefficients, which describe the chemical order in solid solutions, and, in final analysis, also the static displacements of atoms and cluster formation. The idea of the so-called zero contrast of superstructural lines was suggested in [2, 3]. The selection of an appropriate energy (8 keV) of the synchrotron radiation allowed Ice *et al.* [2] and Reinhard *et al.* [3] to eliminate the phonon contribution and components of the static displacements of higher orders to the total X-ray diffuse-scattering pattern of $Fe_{22.5}Ni_{77.5}$ crystals. These studies were performed within the kinematical theory of X-ray scattering, which, despite the unique information obtained in these studies, did not allow the authors to determine the defect structure of the samples.

The analogous theoretical basis was used by Fujimoto [4, 5] who experimentally studied the changes ΔI_{200} in the intensities of the so-called quasi-forbidden reflections (very small $f_{Ga} - f_{As}$ difference) with respect to the intensity *I* in the stoichiometric GaAs crystal. The structure factor of the 200 reflection is $F_{200} = 4(C_{Ga}f_{Ga} - C_{As}f_{As})$ and, therefore, in the first approximation, it is possible to assume that, in accordance with [4, 5], an increment in the intensity δI for this diffraction maximum in a nonstoichiometric crystal is

$$\delta I/I \cong K(C_{Ga} - C_{As}). \tag{3}$$

The coefficient *K* depends on the diffraction parameters of the crystal and the radiation wavelength. Assuming that structural defects (dislocations) do not affect the intensities of the quasi-forbidden reflections, Fujimoto [4, 5] determined the nonstoichiometry level $\Delta = C_{Ga} - C_{As}$ in GaAs crystals. This assumption is justified if all the intensity variations δI depend on Δ. Indeed, the total crystal reflectivity, R_Σ, which has the coherent, R_B, and diffuse, R_{DS}, components, does not depends on the presence of defects [6]. It was shown [4, 5] that the character of the variations of the parameter Δ correlates with the *W*-like variation of the dislocation density along the ingot diameter (Fig. 1). It seems that excessive As atoms in the crystal studied with the concentration at a level of $\Delta \sim 5 \times 10^{-3}$ are located at dislocations which are the effective sinks of point defects. Of course, the assumption that the crystal scatters the radiation as a mosaic object is only a rough approximation of the real situation in the structures of most semiconductor materials. It is more justified to assume that the scattering power of the sample has the value lying between the values calculated in the first (kinematical theory) and second (dynamical theory) approximations of the Born problem of radiation scattering. In this situation, like in the kinematical theory, the total scattering power R_Σ of a real crystal has the Bragg (R_B) and diffuse (R_{DS}) components and is not constant any more—it varies depending on the defect concentration and the extension of their deformation fields. This approach allowed Molodkin and Gudzenko [7, 8] to calculate, for the first time, the effect of the parameter η in the β-brass-type alloys within the distance t' between the Pendellösung intensity oscillations for superstructural lines and also on the additions to the interference absorption coefficient due to alloy ordering. Ignoring small corrections to diffuse scattering from thermal vibrations and static distortions, we have $t' = 2\pi\gamma/\lambda\eta(f_A - f_B)N\sin\alpha$, where N is the number of the unit cells in the crystal, λ is the wavelength, γ is the cosine of the Bragg angle, and α is the wedge angle.

The aim of the present publication is to discuss the experimental results obtained for real binary crystals with relatively large (GaP) and small (GaAs) differences between the atomic formfactors during the measurements of the intensities of quasi-forbidden reflections in the Laue and Bragg diffraction in the region of anomalous X-ray dispersion in two cases: in the vicinity of the *K*-edges of component absorption and at such frequencies of the Bremsstrahlung radiation that the real part of the structure factor becomes close to zero. This approach allowed us, for the first time, to determine both parameters of the defect structure (dislocation density, mean size and concentration of Coulomb deformation centers) and crystal nonstoichiometry [9]. We also managed to show that there exists the satisfactory correlation between these parameters obtained in independent X-ray diffraction experiments in the wavelength range, where the Hönl corrections to the real and imaginary parts of the atomic formfactors are rather important.

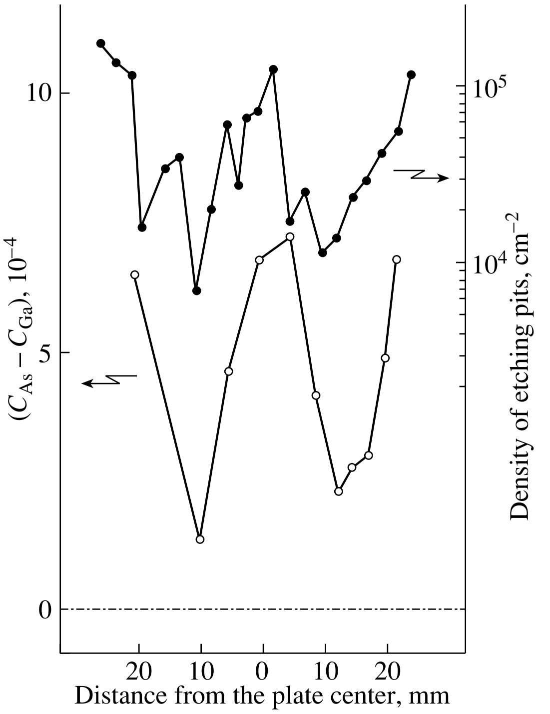

Fig. 1. Density profiles of etching pits and the nonstoichiometry parameter ($C_{As} - C_{Ga}$) are given for a the sample grown by the Bridgman horizontal melting method [4, 5].

INTEGRAL REFLECTIVITY OF A BINARY CRYSTAL IN THE REGION OF ANOMALOUS X-RAY DISPERSION

The most important parameter characterizing the intensity of the diffraction maximum in the dynamical theory of X-ray scattering is the Fourier coefficient of crystal polarizability χ_h [10], which depends on the structure factor F_h or the atomic formfactor f_h as

$$\chi_h = -\frac{e^2\lambda^2}{\pi mc^2 V}F_h = -\frac{e^2\lambda^2}{\pi mc^2 V}8f_h. \qquad (4)$$

The Laue formulas, which describe the integral reflectivity of a crystal at frequencies close to the frequency ν_K of the *K* absorption edge, with due regard for the imaginary part χ_h, were refined in [11]. In this case, one has also to take into account the resonance Hönl correction to f_h

$$f_h = f_0 + \Delta f'_{rh} + i\Delta f''_{ih}, \qquad (5)$$

where $\Delta f'_{rh}$ and $\Delta f''_{ih}$ are the real and imaginary parts of f_h, respectively.

The variation of the Hönl corrections f' and f'' in the vicinity of the *K* absorption edge of Ga in GaAs crystal calculated in accordance with [12] and [13] is illustrated by Fig. 2. It is seen that in both approaches, f'' varied in the jumpwise manner in the vicinity of the Bremsstrahlung-spectrum energy corresponding to the

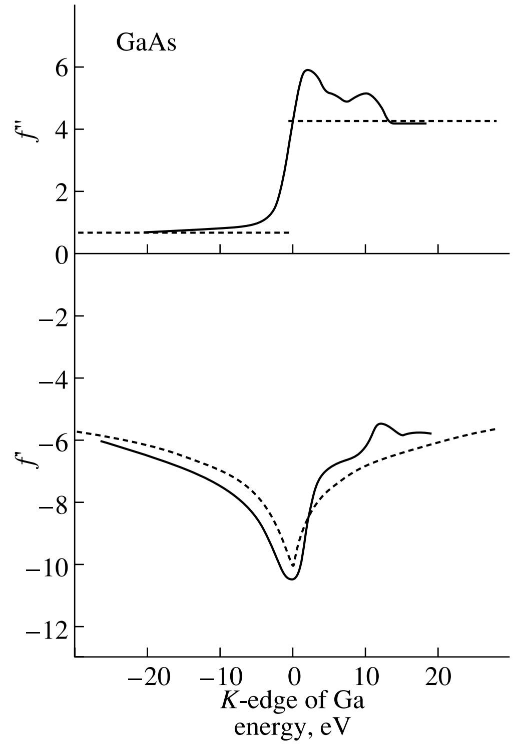

Fig. 2. Calculated values of dispersion corrections for the K edge of Ga in GaAs. Solid curves are calculated according to [13], dashed curves, according to Hönl [12].

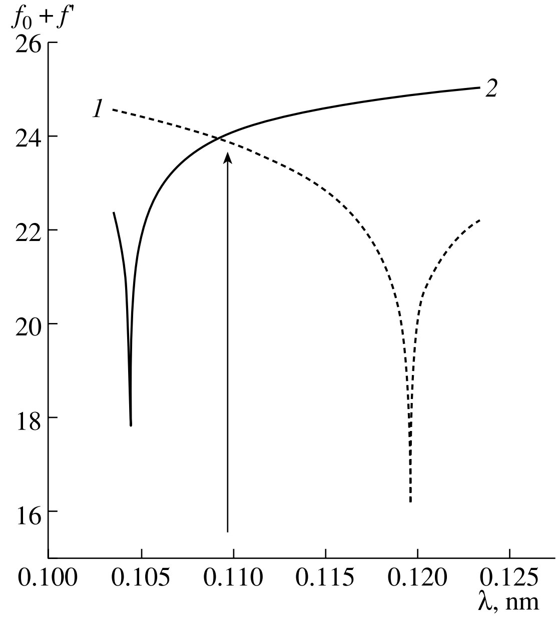

Fig. 3. Energy dependence of the real parts of the atomic formfactors for the Ga(1) and As(2) atoms. The arrow indicates the wavelength at which $(f_0 + f')_{Ga} = (f_0 + f')_{As}$.

K absorption edge of Ga, whereas the real part of the correction to the of the atomic-formfactor function f' is practically symmetric with respect to E_K. The calculation of this quantity yields close values for both approaches.

Simultaneous consideration of f_{Ga} and f_{As} (Fig. 3) shows that the region of anomalous X-ray dispersion located between the λ_K Ga and λ_K As for the 200 quasi-forbidden reflection is characterized by another interesting feature. It follows from Fig. 3 that at the wavelength $\lambda \sim 0.110$ nm (indicated by an arrow), $f_{Ga} + \Delta f'_{Ga} = f_{As} + \Delta f'_{As}$. At this point, the real part χ_h is zero and the reflectivity is described by the imaginary part χ_h alone [14]

$$R_h = (|\cos\theta_2|\cos\theta_1)^{1/2}(|\chi_h|/\sin 2\theta)\int(P_h/P_0)dy, \quad (6)$$

where the differential ratio of the reflected wave P_h to the incident wave P_0 at the given deviation y,

$$y = -(\sin 2\vartheta)/\lfloor |(\cos\vartheta_1)\cos\vartheta_2|^{1/2} K_{0_r}|\chi_h| \rfloor, \quad (7)$$

in the case of Bragg diffraction is

$$P_h/P_0 = K\lfloor \Pi - (\Pi^2 - 1)^{1/2} \rfloor. \quad (8)$$

The parameter Π in Eqs. (6)–(8) is a complex function of the important characteristics of the diffraction conditions $p = |\chi_{rh}||\chi_{ih}|/|\chi_h|^2$, $b = 2^{1/2}|\chi_{ih}|/|\chi_h|$, and $d = \chi_{i0}/|\chi_h|$, and also the phase difference between the imaginary and real parts of polarizability χ. Similar formulas were obtained in [15] for the Laue diffraction. All these formulas allow one to determine the shapes of the rocking curves in this interesting case and also the Pendellösung oscillations of intensity.

To describe scattering by real crystals with uniformly distributed defects in the case $F_{rh} = 0$, one has to transform Eqs. (6) and (8) in accordance with the theory developed in [16–18]. The total integral reflectivity of a real crystal, R_Σ, in this case has the Bragg (coherent) R_B and diffuse R_{DS} components. The coherent component may be determined from Eq. (6) by replacing χ_h by $\chi_h \exp(-L_h)$ (where L_h is the static Debye–Waller factor) and χ_{i0} (absorption) by $(|\chi_{i0}| + \mu_{ds}/K)$ (where μ_{ds} is the coefficient of additional energy losses due to diffuse scattering by defects (extinction) in a sample with the thickness t). According to [17, 18], the diffuse component after integration over the Ewald sphere in the vicinity of the point H is

$$\begin{aligned} R_D(\Delta\vartheta) &= \int\limits_{K' = K} R_{DS}(k)dS_{K'}/K^2 \\ &= F_{dyn}(\Delta\vartheta)\mu_{00}^{\partial}(\Delta\vartheta)t/\gamma_0. \end{aligned} \quad (9)$$

Here, the differential diffuse scattering $R_{DS}(k)$ at $k = K' - K - H$ (deviation of the wave vector K' of a diffusely scattered wave from the reciprocal-lattice point

H) may be written as

$$R_{DS} = \frac{1}{\gamma_0 S}\left(\frac{PVK^2}{4\pi}\right)^2 F_{dyn}S(q). \qquad (10)$$

where $S(q) = \langle|\delta\chi_{H=q}|^2\rangle$ and F_{dyn} is the extinction factor that describes the modulation of rescattering of diffusely scattered intensity, $S(q)$ is the area of the entrance slit of the counter, and $dS_{k'} = K^2 d\Omega_{K'}$ is the surface element in the reciprocal space.

The formulas for integral reflectivity of a quasi-forbidden reflection for a real crystal allow one to calculate not only the characteristics of the defect structure but also the nonstoichiometry parameter of binary crystals.

EXTRACTION OF INFORMATION ON THE STRUCTURE AND COMPOSITION FROM THE THICKNESS DEPENDENCE OF INTEGRAL REFLECTIVITY OF QUASI-FORBIDDEN REFLECTIONS

One of the promising methods of the experimental determination of the parameter Δ is analysis of the Pendellösung oscillations of integral reflectivity for quasi-forbidden reflections:

$$R_i = (C\pi|\chi_{rh}|/2\sin 2\theta(1+K^2)^{1/2} \times \exp(-\mu t/\gamma)\left[\int_0^{2A} I_0(x)dx + I_0(h) - 1\right]. \qquad (11)$$

Here $\chi_{rh} = \chi_{rh}^{\mathrm{Ga}} - \chi_{rh}^{\mathrm{As}}$ consists of the polarizabilities of two GaAs sublattices $K = \chi_{ih}/\chi_{rh}$. The Bessel function is calculated in the conventional way for the dynamical parameter $\Lambda = \pi t/\Lambda$, where Λ is the extinction length for the radiation with the wavelength λ. The parameter h equals $h = \mu t\varepsilon/\gamma$, where ε is the quantity which characterizes the local absorption of Bloch waves in the crystal.

To observe the Pendellösung fringes, one has to determine the effective value of the parameter A such that two types of Bloch waves would coexist in the crystal. Moreover, since the extinction length Λ of quasi-forbidden reflections may considerably exceed the value of this parameter for a structural reflection (e.g., 400), one has to select such a wavelength from the Bremsstrahlung spectrum that the spacings between the Pendellösung fringes with due regard for the Hönl corrections $\Delta f'_{rh}$ would not exceed the sample thickness. The calculation of the extinction length Λ_{200} and absorption coefficients showed [19, 20] that the two above conditions are satisfied by the wavelength from the Bremsstrahlung spectrum which is located in the long wavelength range λ_K.

Experimentally, it is convenient to observe the reflectivity oscillations [21, 22] when normalizing the R_i values in (11) to the kinematical integral reflectivity R_K multiplied by the parameter $2A$, i.e., $r_i = R_i/(R_K \times 2A)$ (Fig. 3). One can readily see that the experimental r_i values (points) obtained in a GaAs crystal with dislocations at the wavelength $\lambda = 0.1198$ nm are located above curve *1* for an ideal crystal because of diffuse scattering. The fitted curve *2*, which satisfactorily describes the experimental data, is displaced to the right with respect to curve *1* along the abscissa because of the influence of the static Debye–Waller factor ($L = 0.052$).

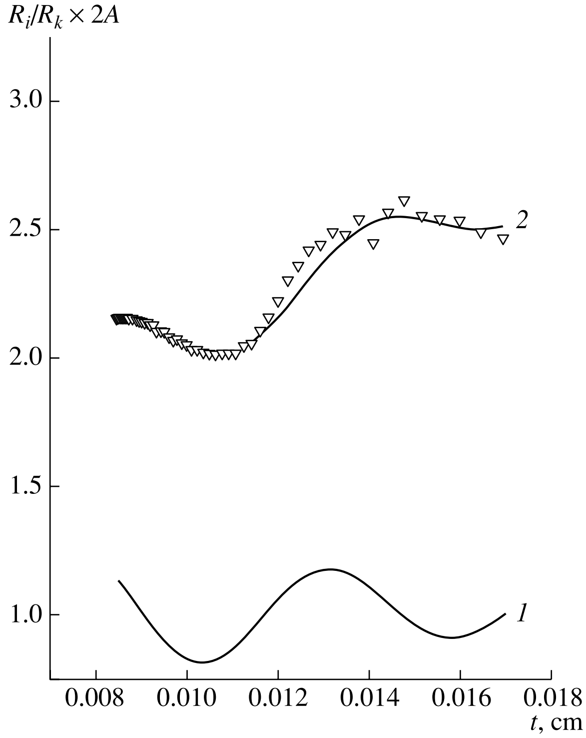

Fig. 4. Thickness dependences of the reduced intensity r_i for the quasi-forbidden 200 reflection of GaAs ($\lambda = 0.1198$ nm): *1* calculation for an ideal crystal, *2* the calculated dependence for a real crystal with the L and μ_{DS} parameters. Points indicate the experimental data.

The latter effect also depends on the crystal nonstoichiometry, because no agreement between the calculated parameters (solid curve) and the experimental η value can be achieved without allowance for the parameter Δ. Thus, the use of Pendellösung oscillations of the integral reflectivity for the quasi-forbidden 200 reflection allowed us, for the first time, to determine not only the characteristics of dynamical scattering (L and μ_{ds}) of a real crystal but also the nonstoichiometry value (Fig. 4).

The thickness oscillations of the intensity of the superstructural lines (quasi-forbidden 222 reflection) were also used to determine the nonstoichiometry value in GaP crystals, where $f_{\mathrm{Ga}} \gg f_{\mathrm{P}}$ [23].

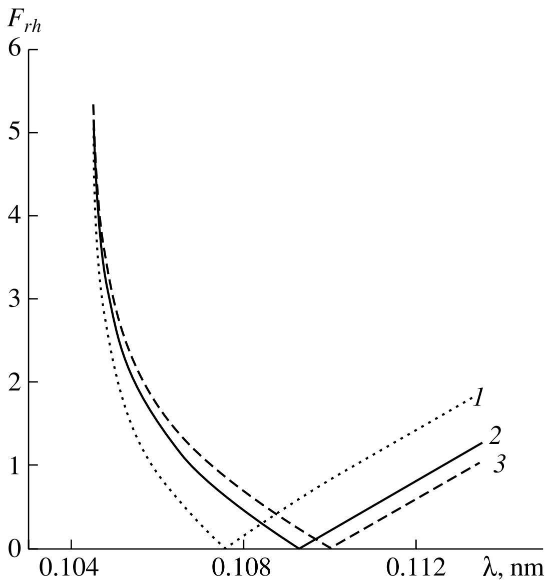

Fig. 5. Position of the point $F_{rh} = 0$ as a function of the deviation of the crystal composition from stoichiometric. $C_{Ga} - C_{As}$ is equal (*1*) 0.01, (*2*) 0, (*3*) –0.01.

ANALYSIS OF ENERGY DEPENDENCE OF INTEGRAL REFLECTIVITY IN THE REGION OF ANOMALOUS X-RAY DISPERSION

It was indicated [24] that the maximum sensitivity of the diffraction-maximum intensity of a quasi-forbidden reflection to the nonstoichiometry of binary crystals should be expected in the case of Bremsstrahlung-radiation diffraction at the point, where the real part of the structure factor with due regard for the corrections for anomalous dispersion is zero (Fig. 3). The variation of the structure factor F_{rh} depending on the wavelength was analyzed for the quasi-forbidden 200 reflection of GaAs (Fig. 5) in [25]. It is easy to see that at $C_{Ga} - C_{As} = 0.01$, the curve for a nonstoichiometric crystal (*1*) is displaced to the left in comparison with the curve in the case $C_{Ga} = C_{As}$. On the contrary, if $C_{As} > C_{Ga}$ (i.e., $C_{Ga} - C_{As} = -0.01$), the curve is displaced in the opposite direction. The calculation of the effect of excessive Ga ($C_{Ga} - C_{As} = 0.05$) or excessive As ($C_{Ga} - C_{As} = -0.05$) on the integral reflectivity for the quasi-forbidden 200 reflection (Fig. 6) was studied in [26, 27]. It is seen from Fig. 6 that the minimum of the curve $R_i = f(\lambda)$ changes its position on the wavelength scale. Thus, the point, where R_i attains its minimum value, may also be used for determining the parameter Δ.

Now, the question arises what role is played by the diffusion component R_{iD} in R_i for both structural (curve *1* in Fig. 7) and quasi-forbidden (curve *2*) reflections from GaAs crystals with $n_0 = 2.5 \times 10^8$ cm^{-3} clusters with the average radius $R_0 = 1$ μm [27, 28]. The behavior of these curves shows that the diffuse- component contribution to the integral reflectivity for the 200 reflection is considerably less than for the struc-

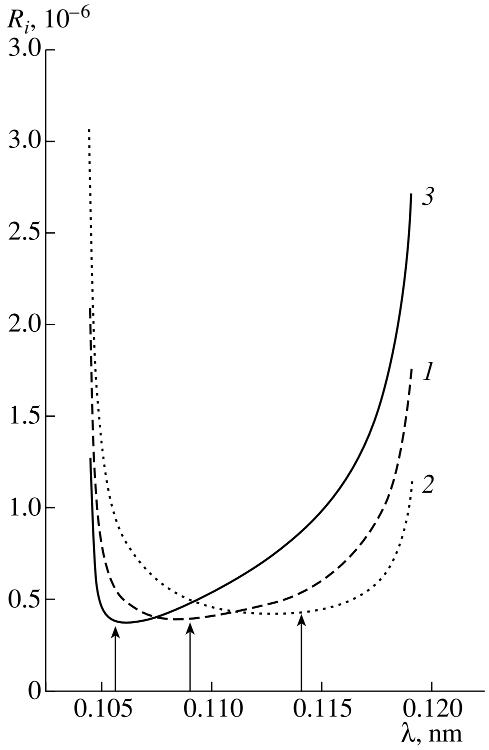

Fig. 6. Energy dependences of the coherent component of the integral reflectivity for quasi-forbidden 200 reflection of GaAs calculated for (*1*) stoichiometric composition, (*2*) composition with an excess in Ga ($c_{Ga} - c_{As} = 0.05$), and (*3*) composition with an excess in As ($c_{Ga} - c_{As} = -0.05$).

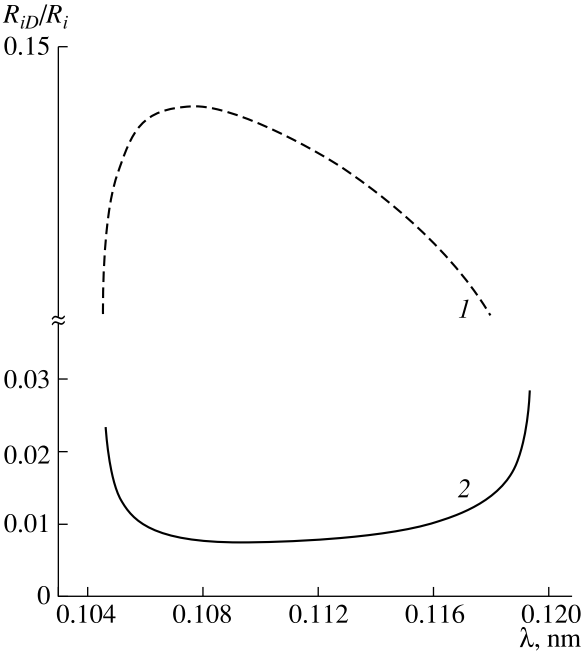

Fig. 7. Comparison of the relative contributions R_{iD} to the integral reflectivity for the (*1*) 400 and (*2*) 200 reflections of GaAs (calculation for $n = 2.5 \times 10^8$ cm^{-3}, $R_0 = 1$ μm).

tural 400 reflection in the whole wavelength range between λ_K Ga and λ_K As. Nevertheless, when performing the rigorous calculations of integral reflectivity, one should not ignore the effect of the diffuse component on quasi-forbidden reflections.

The examples of the measured and calculated energy dependences of the integral intensity R_i (points) for the Bragg 200 reflection are shown in Fig. 8. Curve *1* in Fig. 8 corresponds to R_i calculated for an ideal stoichiometric crystal. Curve *2* is obtained by fitting the integral reflectivities calculated by Eqs. (6)– (9) to the experimental values (points). The values of the static Debye–Waller factor *L*, the parameters of the defect structure R_0, and n_0 values obtained by fitting the integral intensities for the structural and quasi-forbidden reflections are listed in Table 1 (method 1). The right-hand column of the table lists the nonstoichiometry parameter Δ, whose values and signs are different for samples 1–3. The defect-structure parameters of samples 2 and 3 with different signs of the deviation from the stoichiometry have the same orders of magnitude.

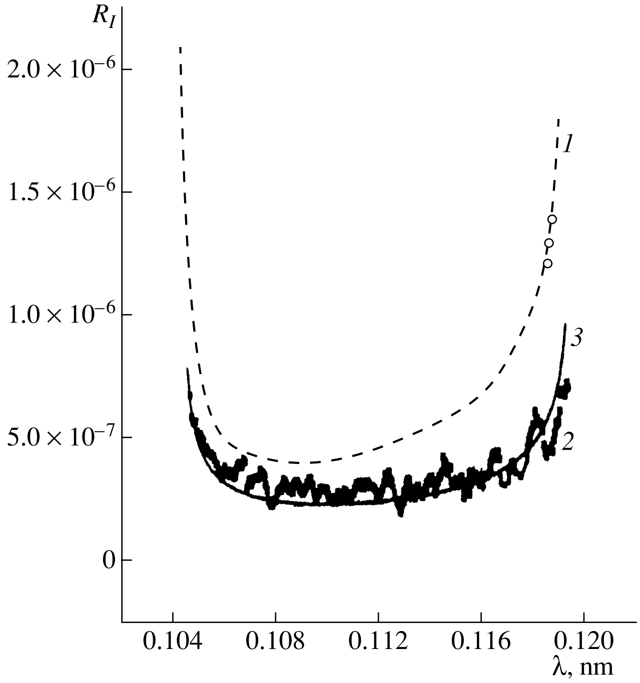

Fig. 8. Energy dependences of $R_{i200}(\lambda)$ for a GaAs crystal. (*1*) calculated dependence for an ideal stoichiometric crystal, (*2*) experimental dependences, 200 reflection. Solid curve *3* is the result of fitting.

COMPARISON OF DATA ON STRUCTURE AND COMPOSITION FOR GALLIUM ARSENIDE OBTAINED IN INDEPENDENT DIFFRACTION EXPERIMENTS

Unlike [26, 27], we studied the defect structure and the composition of a GaAs crystal in Laue diffraction of the Bremsstrahlung spectrum of the X-ray radiation in independent experiments (observation of Pendellösung oscillations of intensity and analysis of the energy dependences of integral reflectivity) with the aim to prove the possibility of obtaining reliable structural and composition parameters (Table 2) [22]. In these experiments, the quasi-forbidden 200 and 600 reflections and the allowed 400 reflection were used. It is seen that the static Debye–Waller factors for the 200 and 400 reflections in samples 4 (with the dislocation density $N_d = 8 \times 10^3$ cm^{-2}) and 5 ($N_d = 8 \times 10^{-4}$ cm^{-2}) are close to one another. The deviation from the stoichiometry $\Delta = C_{\rm As} - C_{\rm Ga}$ in sample 4 (see note to Table 2) are close in the case of the Bremsstrahlung and characteristic CuK_α radiations. The reasonable values of the parameter Δ were also obtained for the 600 reflection.

Thus, the use of the Laue diffraction for quasi-forbidden reflections in independent experiments with the variations of the sample thickness by the inclination method (method 1) and the Bremsstrahlung-radiation wavelength at t = const (method 2) gave rather close values of the parameters sought. The Δ parameter in both samples correlates with the dislocation density. In sample 5 with a higher parameter *L*, the Δ value is higher than in sample 4.

DETECTION OF MACROINCLUSIONS OF COMPONENTS IN BINARY CRYSTALS BY ANALYSIS OF INTENSITY JUMPS IN THE VICINITY OF *K* ABSORPTION EDGES

The region of anomalous X-ray dispersion turned out to be rather important also for the qualitative and quantitative analysis of the structural homogeneity of binary crystals (presence of macroinclusions of the components).

Analysis of the dynamical X-ray scattering in the Laue diffraction for the structural reflections of thin

Table 1. Characteristics of defects and nonstoichiometry parameters for various GaAs samples obtained by method 1

Sample	400 reflection			200 reflection			
	L	R_0, μm	$n_0 \times 10^{-8}$, cm^{-3}	L	R_0, μm	$n_0 \times 10^{-8}$, cm^{-3}	$\Delta = c_{\rm Ga} - c_{\rm AS}$
1	0.22	0.57	200	0.075	0.7	29	−0.0037
2	0.029	0.20	3000	0.005	0.31	2800	−0.0003
3	0.14	1.0	5	0.035	4.0	6	+0.0012

Table 2. Parameters of structural perfection of GaAs crystals obtained by methods 1 and 2

Method	Reflection	Sample 4		Sample 5	
		L	μ_{DS}, cm^{-1}	L	μ_{DS}, cm^{-1}
Thickness oscillations of intensity (method 1)	400	0.005 ± 0.0003	20 ± 3	0.0052 ± 0.0004	27 ± 4
	200	0.052 ± 0.004	31 ± 3	0.067 ± 0.004	21 ± 5
Analysis of energy dependences of integral reflectivity (method 2)	200	0.067 ± 0.003	18 ± 3	0.085 ± 0.0005	10 ± 2
	600	0.07 ± 0.005	–	0.088 ± 0.003	–
	400	0.006 ± 0.0007	–	0.0082 ± 0.0005	–

Note: The values of the nonstoichiometry parameter Δ for sample 4 obtained by methods 1 and 2 are 0.0003 ± 0.00005 and 0.00032 ± 0.00005, respectively (200 reflection). In sample 5, the Δ values obtained by methods 1 and 2 are 0.002 ± 0.00004 and 0.007 ± 0.00006, respectively (200 reflection).

binary crystals showed that the intensity jump $S = i_2/i_1$, where i_2 and i_1 are the intensities measured in the vicinity of the K-edges of the *A* and *B* components in the long (λ_2) and short (λ_1) wavelength ranges, is independent of the structural perfection of the sample [28]. This fact allowed us to establish the presence of the cadmium and tellurium inclusions in CdTe crystals with an excess of Cd (curves *3* and *4*) and Te (curves *5* and *6*) from the consideration of the dependences of the intensity jumps in the vicinity of the K absorption edges of Te and Cd (Fig. 9) [29]. An excess in Cd (line *3*) results in a dramatic increase in the slope of the function $\ln S = f(t)$ measured in the wavelength range in the vicinity of λ_K Cd in comparison with its slope in the stoichiometric state (line *1*). At the same time, the influence of the slope of initial line *2* corresponding to the stoichiometric composition (a jump of Te absorption) is reduced (curve *4*). The effective concentration of the components in the sample with cadmium inclusions is C_N^{Cd} = 0.67 and C_N^{Te} = 0.61, which is close to the concentration determined by X-ray spectral analysis.

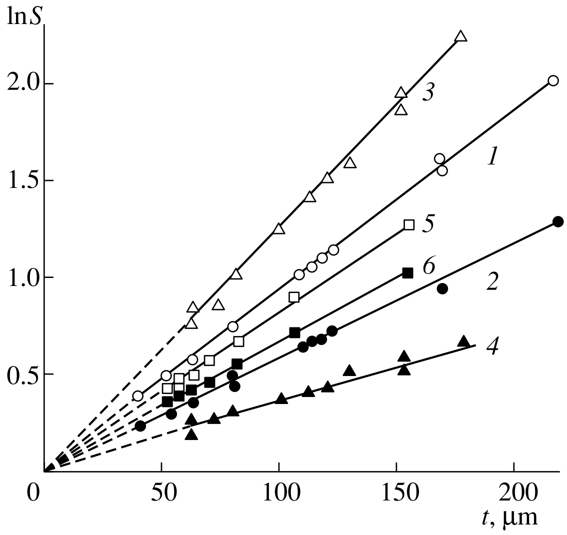

Fig. 9. $\ln S = f(t)$ dependences for CdTe crystals measured in the vicinity of the K absorption edges of Cd (curves *1*, *3*, *5*) and Te (curves *2*, *4*, *6*). (*1*, *2*) stoichiometric composition, (*3*, *4*) compositions with inclusions of the Cd phase, (*5*, *6*) compositions with inclusions of the Te phase.

It should also be indicated that the use of intensity jumps measured in the nonstoichiometric and stoichiometric crystals, S_N^{Cd}, S_N^{Te} and S_0^{Cd}, S_0^{Te}, respectively, (Fig. 9) provides the unique possibility for determining the component concentrations C_N^{Cd} and $C_N^{\mathrm{Te}} = 1 - C_N^{\mathrm{Te}}$ without the preliminary knowledge of the crystal density ρ_{CdTe}. In [29], this was made using the following relationship

$$\frac{\ln S_N^{\mathrm{Cd}}/\ln S_0^{\mathrm{Cd}}}{\ln S_N^{\mathrm{Te}}/\ln S_N^{\mathrm{Te}}} = \frac{C_N^{\mathrm{Cd}}/C_0^{\mathrm{Cd}}}{C_N^{\mathrm{Te}}/C_0^{\mathrm{Te}}}. \tag{12}$$

The dependence of intensity on the thickness $\ln S = f(t)$ was first measured for the quasi-forbidden 200 and 400 reflections in a dislocation-free InSb crystal [30]. It was shown that the displacement of the curve $\ln S_{200} = f(t)$ along the ordinate axis with respect to the line $\ln S_{400} = f(t)$ is associated with the deviation of the crystal composition from the stoichiometry at the level $\Delta = \mathrm{C_{In} - C_{Sb}} = 0.027$.

CONCLUSIONS

Summarizing the results obtained, we should like to note that the measurements of the thickness and energy dependences of integral reflectivity in the region of anomalous X-ray dispersion and analysis of the intensity jumps in the vicinity of *K* absorption edges of the components for quasi-forbidden reflections allow one to determine the composition of binary crystals not only at the qualitative but also at the quantitative level. Assuming that, in a real crystal, the multiple X-ray scattering takes place (the second Born approximation), it is also possible to determine parameters of the defect structure. Therefore, such an approximation based on the dynamical X-ray scattering is more advantageous than the concepts of considering a crystal as a mosaics.

All the results discussed above were obtained using Bremsstrahlung radiation of industrially manufactured X-ray tubes whose emission intensity does not allow one to sufficiently approach the K absorption edges and make reliable measurements in the vicinity of the point at which the scattering is determined only by the imaginary part of the coefficient of the Fourier polarizability. Such an approach would allow one to measure slight deviations from the stoichiometry and establish the relation of this phenomenon to the defect structure. The use of the synchrotron radiation should provide new scientific information and allow one to study experimentally the effect of the ordering processes in alloys on the dynamical Pendellösung oscillations of intensity predicted several decades ago. A number of results obtained with the aid of the standard radiation sources may also be used in the experiments with the use of the synchrotron radiation. Among these results is the possibility of performing standard-free measurements of dynamical X-ray scattering parameters in real crystals with the aid of a single-crystal spectrometer.

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