obtained, the occurrence of flat accoustic modes with decreasing frequency in the phonon spectra of CeB_6, PrB_6 and NdB_6 and a decrease of the metal-boron force constant can be predicted. As a main reason for this weakening of metal-boron interactions the low compressibility of the boron framework with decreasing RE ionic size in the 3^+ valence series is proposed. Additive softening of the Einstein frequence was found for SmB_6. More sophisticated theoretical models should be elaborated to account for the observed general trend.

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SPREADING OF SDTD TO CASE OF LOW-DISLOCATION CRYSTALS

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In the last years the main direction in development of the theory of X-ray diffraction is connected to a fundamental problem of the description of diffraction processes in single crystals in the most general case, when the crystal structure of a single crystals not given beforehand, and can be considered in all real variety with every possible deviations from an ideal structure. First of all the successes of the theory are connected with creation of the bases of the statistical dynamical theory of a diffraction (SDTD). The present work is one of the first teleological experimental work in a given direction. In addition to recent gamma-ray [1] and X-ray diffractometry [2] experimental tests of SDTD results on high-perfect single crystal silicon by measurement of period of dynamical oscillations of intensity and values of integrated intensity as functions of thickness of a crystal or function of wavelength of incident radiation, that can be used in case of enough perfect crystals only, we have carried out experiments on a diffraction of high-monochromatic short-wavelength gamma-radiation ($E = 412$ keV, $\lambda = 0.03$ Å, $\leq \Delta\lambda/\lambda 10^{-6}$), on quartz single crystals with dislocation density ≤ 300 cm^{-2} in experimental conditions of complex, from the standpoint of results interpretation, intermediate case, when the dislocations because of their small concentration

cannot be considered as defects of I class in purely kinematical case of a diffraction, but because of a large extinction length of used radiation they also cannot be attributed as defects of II class (within the framework of a dynamical diffraction) by renormalization of Debye-Waller static factor.

Opportunity of measurement of absolute values of integrated reflectivity of diffracted gamma-radiation (R_i) for the several orders of reflection (hkl) in conditions of the high angular resolution was used.

The expressions for R_i, consisting from three items - purely coherent (R_{coh}), purely incoherent (R_{inc}) and mixed (R_{mix}), in our case - Laue geometry, small Bragg angles, short wavelength, sample with shape of a parallelepiped and only normal absorption will be following:

$$R_i = R_{coh} + R_{inc} + R_{mix}, \tag{1}$$

$$R_{coh} = ER_{dyn}exp(-2\tau t(1-E^2)/\Lambda_0^2), \tag{2}$$

$$R_{inc} = (1-E^2)R_{dyn}\Lambda_0/2\tau_e)[1-exp(-4\tau_e t/\Lambda_0^2)], \tag{3}$$

$$R_{mix} = E(1-E^2)R_{dyn}[(m_1+m_2)/2-n_2]. \tag{4}$$

The expressions for m_1, m_2 and n_2 are rather bulky, but do not present difficulties for account. The influence of a various kind of distortions to diffraction process is concluded in the lattice phase:

$$G = 2\pi q_H u(r), \tag{5}$$

where q_H - scattering vector, $u(r)$ - vector of atom displacement in real crystal from positions of an ideal lattice, r - radius-vector in a real crystal.

The statistical nature of distortions is described by correlation function of II order:

$$f(Z) = <\Phi(0)\Phi^*(Z)> \equiv \Phi(Z)\Phi(0) > = <\Phi><\Phi^*> + <\delta\Phi\delta\Phi^*>, \tag{6}$$

where Z - distance between two points in a crystal, for which lattice phase factors are considered. A designation $\delta\Phi = \Phi - <\Phi>$ is applied here.

$$\Phi = exp(\pm iG) \quad - \quad \text{latticephasefactor}, \tag{7}$$

$$<\Phi> = <exp(\pm i2\pi q_H u> \equiv E - \text{an average lattice phase} \tag{8}$$

(in the conventional theories it is Debye-Waller static factor).

Then the correlation function can be presented as follow:

$$f(Z) = E^2 + (1-E^2)g(Z), \tag{9}$$

where $g(Z)$ - intrinsic correlation function.

As result the degree of structural perfection of a crystal within the framework of SDTD can be described by three parameters: average lattice phase E, which characterizes long-range perfection (on distances more than extinction lengths L0), intrinsic correlation length τ:

$$\tau = \int_0^\infty g(Z)dZ, \tag{10}$$

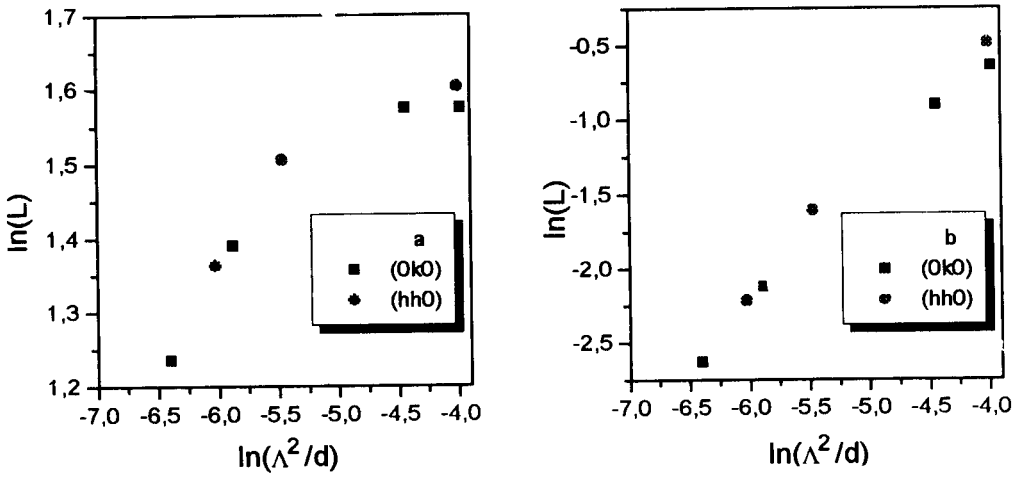

Fig. Debye-Waller static factor for reflections (0k0) and (hh0), determined for quartz crystals with dislocation density $\sim$ 70 cm^{-2}: a) calculation by initial variant of SDTD, b) calculation by advanced variant of SDTD

which characterizes short-length perfection (on distances less than Λ_0) and effective correlation length of a lattice phase τ_e:

$$\tau_e = (1 - E^2) + E\Gamma, \tag{11}$$

where Γ - correlation length of incoherent part of wave fields.

There are discussions concerning physical sense and the values of parameter Γ in the last theoretical and experimental works. The strict substantation of account of this value does not exist at present.

The data of a gamma-ray diffractometry were analysed within the framework of SDTD in two ways. Initial variant of theory, offered by Kato [3], with corrections by Haddad-Becker [4] was used, where the value of Γ is represented as $\Gamma = \Lambda_0/E$, and from here one can make a basic conclusion, that the value of $\Gamma \gg \tau$. Other approach consists of using the advanced version of the theory, offered by Becker-Haddad [5], where $\Gamma = \tau/2$, i.e. value of G has order of τ.

Typical results of experiments designed within the framework of both approaches are presented in Fig.

The choice of coordinates is basic and is connected firstly to necessity of renormalization of $L = -ln(E)$ for dislocations [6], and secondly with a fact, experimentally obtained in given work, that significance of renormalized value of L for reflections of a various type $\sim q_H \Lambda_0^2$, i.e. speed of growth of L for dislocations is more, than for Coulomb-type defects.

From linear character of dependence presented in Fig. b) it is possible to make unequivocal conclusions, that in case of low-dislocation crystals with dislocation density up to 300 cm^{-2} by use of a diffraction of short-wavelength gamma-radiation the description of diffraction processes reasonably to carry out within the framework of SDTD. Thus the assumptions on ratio between values of intrinsic correlation length τ, correlation length of

incoherent parts of wave fields Γ and extinction length Λ_0 are analogous to received earlier for high-perfect dislocation-free silicon [1,2]: $\tau/\Lambda_0 \to 0$ and $\Gamma/\Lambda_0 \to 0$, thus however the significances of E, describing long-range distortions of a lattice, change in a wider range and can strongly differ from 1. Significance of E appear considerably more, than at account with application of the assumption, that $\Gamma \sim \Lambda_0/E$.

The application of approaches of SDTD to dislocation crystals permits to remove all problems, connected to fact, that the dislocations are defects of II class ($\Lambda_0 \gg 1$), effective susceptibility turn into 0, owing to that as kinematical coherent scattering as dynamical one should disappeare [6,7].

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CHARACTERIZATION OF VACANCY-RELATED DEFECTS INTRODUCED DURING SILICON HEAT TREATMENT BY DLTS AND GAMMA-RAY DIFFRACTION TECHNIQUES

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The concentration of defects introduced by heat treatment into Si is low and usually does not exceed 10^{13} cm^{-3}. Therefore, such highly informative techniques as electron paramagnetic resonance, PTIS, TEM, etc. can not be used for the defect characterization.

To study the vacancy-related defects introduced into n-Si during annealing or aluminium diffusion at high temperatures (1000-1250°C) for $t = 0.5 - 16$ h gamma-ray diffraction techniques and capacitance deep level transient spectroscopy (DLTS) have been used. These techniques were used since they have an advantage in sensitivity over other methods for the investigation of electrically active and structural defects.

Detailed description of the techniques and set-ups is given in [1,2].

Float zone (FZ) and Czochralski (Cz) n-Si grown in $< 111 >$ direction with resistivity 10-1000Ω·cm was studied.

Different nonoxidizing ambients (argon, nitrogen, vacuum and chlorine-containing atmosphere) were used to create a vacancy supersaturation during Si heat treatments.