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Application of the statistical dynamical theory to γ-ray diffraction experiments on low-dislocation quartz single crystals

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Abstract

Highly monochromatic ($\Delta\lambda/\lambda = 10^{-6}$) short-wavelength ($\lambda = 0.03$ Å) γ radiation has been used in the study of the diffraction processes in real single crystals. Dislocation-free silicon crystals and quartz crystals with small concentrations of chaotically distributed dislocations were investigated. The experimental results were processed with use of statistical dynamical theories of diffraction, both fundamental and advanced. It is shown that the advanced version is more reliable in both cases. However, the values of the average lattice phase E, describing the long-range distortions of the lattice, can differ markedly from the value of 1 for quartz crystals, and parameter $L = -\ln(E)$ has a square dependence on the extinction length.

1. Introduction

In recent years, a main direction in the development of the theory of X-ray diffraction has been connected to the fundamental problem of the description of the diffraction processes in single crystals when the structures of such crystals are not known beforehand and the whole range of real structures has to be considered, with every deviation possible from the ideal structure. The successes of such theories are based on the creation of the statistical dynamical theory of diffraction (SDTD). Directed experimental research will allow the removal of the current discrepancies in the results of the various theoretical approaches within the framework of the SDTD, and will provide extensive new experimental material to researchers on the subject of diffraction theory.

The present work is one of the first teleological experimental works in this direction. Recent γ-ray (Schneider *et al.*, 1992) and X-ray diffractometry (Takama & Harima, 1994) experimental tests of the SDTD were conducted by measurement of the period of the dynamic oscillations of the intensity and the values of the integrated intensity as functions of the crystal thickness or the wavelength of the incident radiation. These methods can be used in the case of 'perfect' (*i.e.* near perfect) crystals only. We have carried out experiments on the diffraction of highly monochromatic short-wavelength γ radiation in quartz single crystals in the complex (from the viewpoint of interpreting the experimental results) intermediate case. The dislocations, because of their small concentration, cannot be considered as first class defects [as defined by Krivoglaz (1996)] in the purely kinematical case of diffraction, but also, because of the large extinction length of the radiation used, it is not always possible to attribute the dislocations as second class defects within the framework of dynamical diffraction by the renormalization of the static Debye–Waller factor (Datsenko *et al.*, 1988).

2. Theoretical and experimental background

The theory of the diffraction of X-radiation in single crystals was created for two boundary cases: the dynamical theory for ideal crystals (transmitted and diffracted waves inside a crystal are completely coherent between themselves), and the kinematical theory for highly distorted crystals (complete incoherence of the beams inside a crystal). The dynamical theory for real crystals with defects (*i.e.* with partial incoherence of the waves) has so far mainly been applied to particular cases only: an elastic uniform deformation, certain types of defects. Efforts to create a general theory of X-ray diffraction in real single crystals, containing distortions of the crystal lattice of every possible kind, have been undertaken only in recent years. First of all, we note the initial studies by Kato (1976*a*,*b*, 1979, 1980*a*,*b*,*c*) and the studies of Al Haddad & Becker (1988), Becker & Al Haddad (1989, 1990, 1992), Guigay (1989), Guigay & Chukhovskii (1992, 1995) and Chukhovskii & Guigay (1993). The SDTD is based on the solution of the averaged Takagi–Taupin wave equations.

The influence of the various kinds of distortions on the diffraction process is included in the lattice phase:

$$G = 2\pi \mathbf{q}_H \mathbf{u}(\mathbf{r}), \tag{1}$$

where $\mathbf{q}_H$ is the scattering vector, $\mathbf{u}(\mathbf{r})$ is the vector of the atom displacement in the real crystal from the position in the ideal lattice, and $\mathbf{r}$ is the radius vector in the real crystal.

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

$$f(Z) = \langle \Phi(0)\Phi^*(Z)\rangle \equiv \langle \Phi(Z)\Phi^*(0)\rangle = \langle\Phi\rangle\langle\Phi^*\rangle + \langle\delta\Phi\delta\Phi^*\rangle, \quad (2)$$

where Z is the distance between two points in the crystal. The designation $\delta\Phi = \Phi - \langle\Phi\rangle$ is applied here.

$$\Phi = \exp(\pm iG) \quad (3)$$

is the lattice phase factor,

$$\langle\Phi\rangle = \langle\exp(\pm ig)\rangle \equiv E \quad (4)$$

is the average lattice phase (in conventional theories it is the static Debye–Waller factor). Then the correlation function can be presented as

$$f(Z) = E^2 + (1 - E^2)g(Z), \quad (5)$$

where $g(Z)$ is the intrinsic correlation function.

The degree of perfection of the crystal structure can be described by two parameters: the average lattice phase E, which characterizes the long-range perfection (at distances more than the extinction length Λ_0), and the intrinsic correlation length τ:

$$\tau = \int_0^\infty g(Z)\,\mathrm{d}Z, \quad (6)$$

which characterizes the short-length perfection (at distances less than Λ_0).

$$\Lambda_0 = V_0[r_0\lambda|F_{hkl}|\exp(-W_{hkl})], \quad (7)$$

where V_0 is the elementary cell volume, r_0 is the classical electron radius, λ is the wavelength of the radiation used, F_{hkl} is the structure factor for a given reflection and $\exp(-W_{hkl})$ is the thermal Debye–Waller factor.

By analogy, the generalized correlation functions of higher orders can be defined and the correlation lengths of higher orders are represented as

$$\tau_n = \int_0^\infty g^n(Z)\,\mathrm{d}Z. \quad (8)$$

The change of E from 0 to 1 covers the entire region of the long-range structural perfection of the crystal. For a given E, the diffraction phenomena depend on the intrinsic correlation length τ.

In the present paper, the integrated intensity is of particular interest. The integrated intensity $\rho^\Sigma_{g/i}$ can be presented as the sum of four terms, *e.g.*, for the diffracted wave,

$$\rho^\Sigma_g = \rho^c_g + \rho^i_g + M^{(1)}_g + M^{(2)}_g, \quad (9)$$

where ρ^c_g is the purely coherent part, ρ^i_g is the purely incoherent part and $M^{(1)}_g$ and $M^{(2)}_g$ are the mixed parts.

In the expressions for the integrated intensity, in addition to the independent parameters τ and E there is the effective correlation length of the lattice phase given by

$$\tau_e = (1 - E^2)\tau + E^2\Gamma, \quad (10)$$

where Γ is the correlation length of the incoherent part of the wave field.

The physical sense and the values of the parameter Γ have been discussed in recent theoretical and experimental works. Strict reasons for the choice of this value do not exist at present. Kato (1980*b*) assumed that

$$\Gamma = \eta\Lambda_0/E, \quad (11)$$

where $\eta \simeq 1$. In this case, $\Gamma \gg \tau$. Later, Polyakov *et al.* (1991) estimated

$$\Gamma \simeq (1 - E^2)\tau^2/E\Lambda_0 \ll \Lambda_0/E \quad (12)$$

and Bushuev (1994) postulated that

$$\Gamma = E\tau^2/\Lambda_0. \quad (13)$$

As to the parameter τ, almost all experimental tests of the applicability of the SDTD to processing the experimental data specify a very small value of τ, comparable with the sizes of microdefects. This is in accord with the original valuations by Kato. Thus, Voronkov *et al.* (1987) obtained $\tau \simeq 50$–100 Å, Schneider *et al.* (1992) found $\tau \leq 200$–1000 Å, Takama & Harima (1994) gave $\tau \simeq 50$–100 Å.

In contrast, the values of Γ produced by these experiments differ markedly from those assumed by Kato. The experimental work gave values of Γ comparable with τ: $\Gamma \simeq \tau/2$ (Schneider *et al.*, 1992) and $\Gamma \simeq (1 \text{ to } 6)\tau$ for different specimens (Takama & Harima, 1994). Such small values of Γ are in good accord with the estimates (12) and (13). It should be noted, however, that all the aforementioned experiments were conducted on 'perfect' dislocation-free single crystals of silicon, in which spherical precipitates of SiO_2 with diameter ~ 100–300 Å represent the main infringement of the ideal crystal structure; the question on the value of Γ for crystals with more distorted structures remains open. Nevertheless, the theoretical accounts of Becker & Al Haddad (1992) involving the use of the self-consistent theory have resulted in the replacement of Γ with $\tau_2 \simeq \tau/2$ [see equation (8)], *i.e.* again Γ is the order of τ.

Kato (1991, 1994) recently presented a more general form of the statistical theory of diffraction permitting inclusion of the effects of diffuse scattering in the self-consistent form. Thus, the starting wave equations are free from the Takagi–Taupin approximation. This new approach to the problem is under development at present.

With regard to the experimental tests, it should be noted that practically the first work in this direction (Olekhnovich *et al.*, 1983) was conducted using X-ray diffraction in single-crystal silicon with the relatively considerable dislocation density of 3×10^5 to 5×10^7 cm^{-2}. Unfortunately, the authors used the expressions of Kato (1980*c*) for mathematical processing

of the experimental data, in which two arithmetic errors for the mixed parts of the integrated intensity appeared. Processing these data with use of the exact mathematical expressions of Al Haddad & Becker (1988) gave rather good conformity between the theory and the experiment. Note that the value of Γ was taken as Λ_0/E, and by varying the parameter Γ a very insignificant improvement of the fitting accuracy was observed.

After the experimental tests of the SDTD results, some questions remained unanswered. Besides the discrepancy in the physical sense and the value of the parameter Γ, the following points arise.

Schneider *et al.* (1992) and Takama & Harima (1994) found that $\tau \to 0$ and $\Gamma \to 0$ (more exactly, $\tau/\Lambda_0 \to 0$ and $\Gamma/\Lambda_0 \to 0$), and thus the value of E is always close to 1. But maybe this is true only for 'perfect' crystals with one type of lattice distortion: the conglomerates of the point defects? Also, the actual result may arise due to the use of the asymptotic formula of Becker & Al Haddad (1992), neglecting the presence of the mixed parts of the integrated intensities, which is probably only justified in the case of using short-wavelength radiation and 'perfect' crystals.

It is perplexing that the values of E obtained (0.95–0.97) are always close to 1, even for crystals of set VII described by Schneider *et al.* (1992), for which the experimentally measured values of the integrated reflectivity (R_1) differed from the values for the ideal crystal by tens of times for specimens of large thickness; the dependence of R_i on the effective thickness, being close to linear, implies that the character of the scattering is close to kinematical.

3. Choice of experimental method

In the present work, we present a continuation of the research on the experimental test of the SDTD results. The diffraction of highly monochromatic short-wavelength γ radiation is used. The reasons for the preference for γ radiation in comparison with conventional X-rays are as follows.

Firstly, the method is highly sensitive. The full width at half-maximum (FWHM) of the reflection curve for a perfect crystal (the Darwin width) obtained by the use of γ radiation is a hundredth or even a thousandth of a second of arc. The FWHM for X-rays or neutrons is about a few seconds of arc. Therefore, crystals that appear 'perfect' to X-rays and neutrons, appear far from perfect under γ radiation. γ radiation permits the investigation of the effects of rather weak distortions of the crystal lattice. In practice, it leads to the fact that the values of E can be significantly different from 1, even for 'perfect' crystals, while X-ray diffractometry produces values very close to 1. Measuring higher orders of reflection permits one to scan the full possible range of E from 1 to 0, and means that one is not confined to values of $\sim$1, which can be obtained from X-ray positions of the *Pendellösung* fringes.

Secondly, because it is technically impossible to realize the angular resolution of the diffractometer in a thousandth of second, the opportunity to measure the integrated reflectivities (R_i) in absolute units is used. This opportunity arises owing to the high penetrating ability of γ radiation (therefore it is easy to take absorption into account automatically) and the absence of the phenomenon of anomalous dispersion for such energies.

As the main material for the research, low-dislocation quartz single crystals were chosen. For comparison and a deeper analysis of the obtained results, experiments were also conducted on dislocation-free single-crystal silicon.

4. Experiment

A detailed description of the γ-ray diffractometer at Petersburg Nuclear Physics Institute (PNPI RAS) has been presented by Kurbakov *et al.* (1987) and Kurbakov & Sobolev (1994). The diffractometer is similar in structure to a standard double-crystal X-ray diffractometer; however, there are some essential differences. The first difference is the absence of a crystal monochromator. A gold plate [200 Ci ^{198}Au (1 Ci = 3.7×10^{10} Bq)] of dimensions $0.1 \times 15 \times 18$ mm activated by the thermal neutrons with a flow rate of $\sim 10^{14}$ neutrons cm^{-2} s^{-1} is used as the source of γ radiation with short wavelength ($\lambda = 0.03$ Å) and high monochromaticity ($\Delta\lambda/\lambda \leq 10^{-6}$). Because of the geometry of the source and the distance between the source and the sample and between the sample and the detector of $\sim$3 m for each and a collimator consisting of two narrow (width 0.1 mm) tungsten slits, after the source and before the sample, the diffractometer has the high angular resolution of $9''$ in the equatorial plane. The cross section of the incident γ beam is rectangular with a size of $0.1 \times h$ mm, where h can be varied from 5 to 18 mm depending on the size of the sample; thus the whole beam passes through the sample.

Because of the high penetrating ability of the γ radiation used and the smallness of the Bragg angles (*e.g.* $16'$ for the 111 reflection in Si), the specimens are investigated in the Laue geometry (note that Kato does not present the integrated intensity for the Bragg case).

In the study of the Si and quartz single crystals, the intensity distributions of the various orders of the diffraction reflection were studied. The detector is placed in the position appropriate to the chosen reflection; the crystal is turned, by step-by-step ω scan with a step of $1''$, through the whole area in which Bragg scattering occurs. Thus the detector, with a wide aperture (4 mm), registers the total scattered radiation. Then the detector is transferred to the position of the incident-beam spreading after the sample, and the intensity

Table 1. *The parameters for the various reflections hkl used for processing the experimental data*

Λ_0 is the extinction length, Q is the kinematical integrated reflection power, R_{dyn} is the dynamical limit of the integrated reflectivity.

hkl	Λ_0 (cm)	Q ($\times 10^6$ cm^{-1})	R_{dyn} ($\times 10^8$)
Silicon			
111	0.031	32.242	50.268
333	0.052	3.851	10.032
555	0.089	0.787	3.514
Quartz			
010	0.084	6.004	25.261
020	0.077	3.569	13.768
030	0.163	0.532	4.343
040	0.112	0.848	4.747
110	0.077	4.188	16.032
220	0.072	2.357	8.506
330	0.122	0.547	3.346

is registered at the non-reflecting position of the sample. The diffracted intensity is normalized to the intensity of the transmitted beam; thus it is measured in absolute units. The area under the normalized rocking curve is the integrated reflectivity R_i of the given reflection. This parameter can easily be measured with an accuracy of 2–3%. The values of some of the parameters used in processing the experimental data are listed in Table 1.

5. Technique for mathematical processing of experimental data

The experimental values of R_i in specimens of thickness greater than $\Lambda_0/2$ can lie in the range between the so-called dynamical and kinematical limits. The minimal possible value of R_i for the given reflection *hkl*, *i.e.* the dynamical limit R_{dyn}, is observed in specimens possessing the ideal crystal structure:

$$R_{dyn} = r_0\lambda|F_{hkl}|\exp(-W_{hkl})d_{hkl}/2V_0. \tag{14}$$

It should be noted that this expression is simplified for the case of γ-ray diffraction because of the small Bragg angles and only normal absorption.

The maximal possible value of R_i, *i.e.* the kinematical limit R_{kim}, is observed in specimens in which the crystal lattice is so distorted that each scattering centre radiates completely incoherently with respect to the other scattering centres. The intensities of all scattered beams are additive. R_{kin} is given by

$$R_{kin} = Qt, \tag{15}$$

where Q is the kinematical integrated reflecting power:

$$Q = r_0^2\lambda^2F_{hkl}^2\exp(-2W_{hkl})d_{hkl}/V_0^2. \tag{16}$$

The important feature of the limiting cases is that the values of the integrated reflectivity are not sensitive to the parameters that describe the defect structure of the crystal. The calculated values of R_{dyn} and Q for the reflections used in the present work are given in Table 1. Between the limiting values there is the area where the values of R_i depend on the parameters of the defect structure.

The data obtained by γ-ray diffractometry were analysed within the framework of the SDTD, with use of the initial variant of the theory, presented by Kato (1980*c*) and corrected by Al Haddad & Becker (1988) and Guigay (1989), as well as the advanced version of the theory, produced by Becker & Al Haddad (1992).

The expressions for R_i, consisting of four items, purely coherent, purely incoherent and two mixed parts, namely, in our case, the Laue geometry, the small Bragg angles, the sample in the shape of the parallelepiped and only normal absorption, are as follows:

$$R_i = R^c + R^i + M \tag{17}$$

$$R^c = ER_{dyn}W[2E(t/\Lambda_0)] \times \exp[-2(1-E^2)(\tau/\Lambda_0)(t/\Lambda_0)] \tag{18}$$

$$R^i = (1-E^2)R_{dyn}(\tau_e/\Lambda_0)^{-1}\sinh[2(\tau_e/\Lambda_0)(t/\Lambda_0)] \times \exp[-2(\tau_e/\Lambda_0)(t/\Lambda_0)] \tag{19}$$

$$M = M^{(1)} + M^{(2)} = E(1-E^2)R_{dyn}[(m_1+m_2)/2 - n_2] \tag{20}$$

where

$$W(2X) = 2\sum_{n=0}^{\infty} J_{2n+1}(2X). \tag{21}$$

Here R_i is the total integrated reflectivity, R^c is the purely coherent part, R^i is the purely incoherent part, M is the total mixed part and $J_{2n+1}(2X)$ is the Bessel function. The expressions for m_1, m_2 and n_2 are rather bulky, but do not present difficulties on that account.

In the case of diffraction of the short-wavelength radiation, having conducted averaging by the thickness oscillations of the dynamical intensity, we obtain

$$R^c = ER_{dyn}\exp[-2(1-E^2)(\tau t/\Lambda_0^2)] \tag{22}$$

$$R^i = (1/2)(1-E^2)R_{dyn}(\tau_e/\Lambda_0)^{-1} \times \{1-\exp[-4(\tau_e t/\Lambda_0^2)]\} \tag{23}$$

$$M = E(1-E^2)R_{dyn}[(m_1+m_2)/2 - n_2]. \tag{24}$$

In our case, the application of the short-wavelength radiation on the silicon and quartz crystals has shown that, in the majority of cases, the experimental value of R_i is determined only by the parameter E and does not practically depend on the value of τ up to $\tau = 10^{-5}$ m, *i.e.* in the whole range of $\tau \ll \Lambda_0$ (Alexeev *et al.*, 1989; Schneider *et al.*, 1992). Moreover, the mixed part becomes negligibly small. In the calculations with formulae (22) to (24), we used the value $\tau = 10^{-11}$ m; this actually corresponds to the condition $\tau/\Lambda_0 \to 0$.

We shall consider now two variants of the expression for τ. The first case corresponds to the condition (10). Having taken $\eta = 1$ and $\tau/\Lambda_0 \to 0$, we obtain

$$R = ER_{\rm dyn}\exp[-2(1-E^2)(t/\Lambda_0)] + (2E)^{-1}(1-E^2)R_{\rm dyn}[1-\exp(-4Et/\Lambda_0)]. \quad (25)$$

The second case corresponds to the condition $\Gamma/\Lambda_0 \to 0$; having accepted simultaneously $\tau/\Lambda_0 \to 0$, we obtain

$$R_1 = ER_{\rm dyn} + 2(1-E^2)R_{\rm dyn}t/\Lambda_0. \quad (26)$$

In our case, $R_{\rm dyn} = Q\Lambda_0/2$. Having made such a replacement, we obtain

$$R_i = ER_{\rm dyn} + (1-E^2)Qt. \quad (27)$$

We should note that formula (27) here slightly differs from the asymptotic formula (82) given by Becker & Al Haddad (1992), where, for some unclear reason, the expression for the sum of the coherent parts of the diffracted and transmitted beams was used as the coherent part of the diffracted beam.

By comparison of the above expressions and similar equations for X-ray diffraction given by Kato (1980*c*) or Al Haddad & Becker (1988) and Becker & Al Haddad (1992), it can be seen that the simpler expressions for the short-wavelength γ radiation permit easier analysis of the experimental data; moreover, the physical sense of the SDTD equations is more evident in this case.

Table 2. *The effective thickness in the direction of the incident beam t and the dislocation density (obtained by etching) N_{disl} for the investigated specimens*

	t (cm)	$N_{\rm disl}$ (cm^{-2})
Silicon specimens		
I	5	–
II	0.9	–
III	1	–
IV	2.6	–
Quartz specimens		
I	4.7	70
II	1.3	25

6. Results and discussion

6.1. *Dislocation-free silicon*

A description of all the investigated crystals of silicon and quartz is presented in Table 2. The results of the measurement of R_i for the reflections $n(111)$, where $n = 1, 3, 5$, in the silicon crystals I–IV, and the reflections $n(010)$, where $n = 1, 2, 3, 4$, and $n(110)$, where $n = 1, 2, 3$, in the quartz crystals I and II, are presented in Table 3.

The static factors $L = -\ln E$ for the silicon crystals I–IV are presented in Fig. 1 as a function of the scattering vector modulus $|\mathbf{q}_H|$ on a double logarithmic scale. The values of L were calculated from the measured values of R_i (see Table 3) by Kato's formulae and (25).

The same function is presented in Fig. 2 but with values of L calculated by the approximation formula (26).

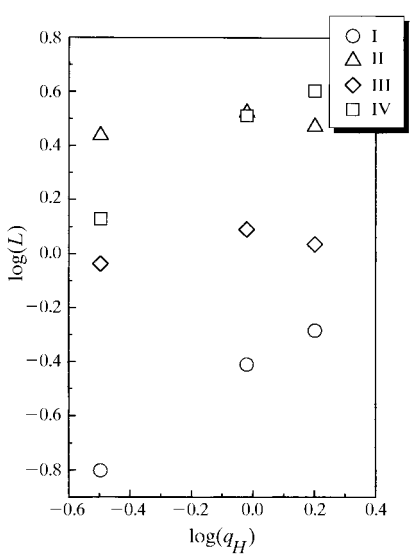

Fig. 1. The static factors $L = -\ln E$ for the silicon crystals I–IV as a function of the scattering vector modulus $|\mathbf{q}_H|$ on the double logarithmic scale. The values of L were calculated with equation (25).

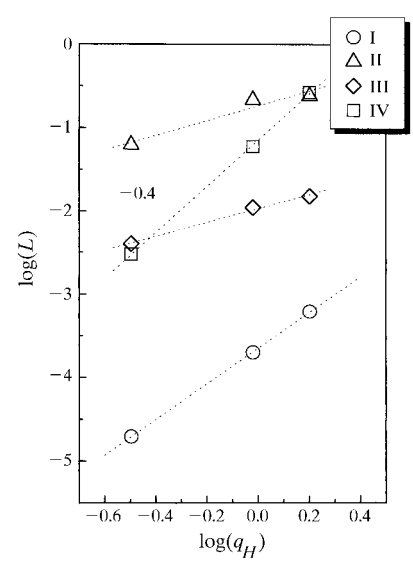

Fig. 2. The static factors $L = -\ln E$ for the silicon crystals I–IV as a function of the scattering vector modulus $|\mathbf{q}_H|$ on the double logarithmic scale. The values of L were calculated with equation (26).

Table 3. *The measured integrated R_i for the various reflections hkl for the investigated specimens*

	hkl	R_i ($\times 10^6$)
Silicon specimens		
I	111	0.509 (5)
	333	0.108 (2)
	555	0.040 (1)
II	111	3.89 (4)
	333	1.29 (2)
	555	0.298 (6)
III	111	0.732 (7)
	333	0.186 (4)
	555	0.058 (2)
IV	111	1.03 (1)
	333	1.21 (2)
	555	0.87 (3)
Quartz specimens		
I	010	4.01 (4)
	020	3.72 (4)
	030	1.65 (3)
	040	2.24 (4)
	110	3.98 (4)
	220	3.74 (4)
	330	0.86 (2)
II	010	0.721 (7)
	020	0.532 (5)
	030	0.231 (5)
	040	0.238 (5)
	110	0.567 (6)
	220	0.531 (5)
	330	0.354 (7)

It is known from the kinematical theory of diffraction presented by Krivoglaz (1996) that

$$L \simeq \int \{1 - \cos[\mathbf{q}_H \mathbf{u}(\mathbf{r})]\}\, \mathrm{d}\mathbf{r} \qquad (28)$$

when the displacements $\mathbf{u}(\mathbf{r})$ decrease rapidly with the distance. For the conglomerates of the point defects, $L \simeq (\mathbf{q}_H)^m$, where m has different values depending on the type and the shape of the conglomerates (spherical cluster, dislocation loop *etc.*), and also on the region ($|\mathbf{q}_H \mathbf{u}(\mathbf{r})| \ll 1$ or $|\mathbf{q}_H \mathbf{u}(\mathbf{r})| \gg 1$) making the principal contribution to the integral (28). Nevertheless, the linear dependence $L(q_H)$ on the double logarithmic scale must be conserved in any case.

From the comparative analysis of the data of the two approaches, one can unequivocally conclude in favour of the second approach, giving physically reasonable linear dependencies. Moreover, two characteristic inclinations of the straight lines obtained for the different silicon crystals are observed, which specify the different characters of the as-grown microdefects in the crystals.

Thus, from the measurements on the dislocation-free silicon, the main conclusion is that our γ-ray diffractometry studies conform well with the results of Schneider *et al.* (1992) and Takama & Harima (1994), pointing to better correspondence of the advanced version of the SDTD given by Becker & Al Haddad (1992) with the experimental results from the dislocation-free crystals. Such conformity of our approach to the experiments on testing the SDTD results in dislocation-free crystals with other distinguished approaches has allowed us to proceed to solving a more complex problem, namely the study of crystals with dislocations.

6.2. *Dislocation quartz*

Within the framework of the kinematical theory, Krivoglaz (1996) divided the defects of the crystal lattice into two classes based on X-ray diffraction effects.

The presence of defects of the first class [the displacements $\mathbf{u}(\mathbf{r})$ decrease rapidly with distance] does not change the δ-shaped intensity distribution, located in the reciprocal-lattice points, *i.e.* it does not result in line broadening. Such defects shift the maxima of the δ-shaped peaks and change their integrated intensity. Also, a smooth intensity distribution of the diffuse scattering occurs. In this case, the values of L are less than 1.

The second class defects [when the displacements $\mathbf{u}(\mathbf{r})$ decrease slightly or do not decrease absolutely with the distance from the defects] result in the effective erosion of the δ-shaped intensity distributions (X-ray line broadening). In this case, $L \gg 1$, the effective susceptibility becomes 0, and all coherent scattering must disappear. Linear dislocations are typical second class defects.

In the dynamical approach of Datsenko *et al.* (1988), the division of the defects into two classes is preserved, as in the kinematical approach of Krivoglaz (1996); however, the X-ray diffraction effects arising from the two classes differ essentially. In the case of chaotically distributed dislocations, it appears that the numerical

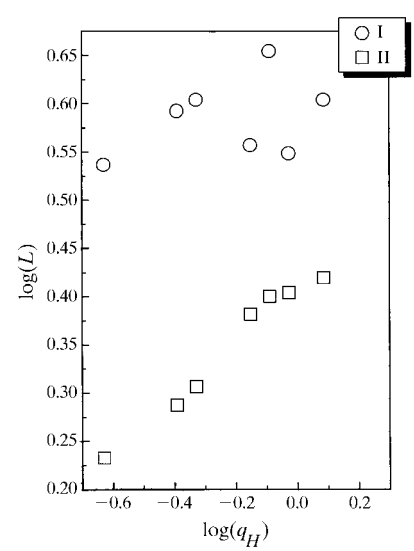

Fig. 3. The static factor $L = -\ln E$ for the quartz crystals I–II as a function of the scattering vector modulus $|\mathbf{q}_H|$ on the double logarithmic scale. The values of L were calculated with equation (25).

valuations in the qualitative analysis of the dynamical X-ray scattering in dislocation single crystals result in the effect that, at low dislocation density $N_{\rm disl}$, it is necessary to modify the expression for the index of the static factor L, appearing in the kinematical theory, in the case of dynamical diffraction by the procedure of cutting the contribution of the remote dislocations.

Thus, renormalized $L^* \simeq \Lambda_0^2 N_{\rm disl}$; hence, if $N_{\rm disl} \ll \Lambda_0^{-2}$, *i.e.* if the average distance between the dislocations is much greater than the extinction length, then $L^* \ll 1$. This means that, in single crystals, chaotically distributed dislocations with density $N_{\rm disl} \ll \Lambda_0^{-2}$ becomes first class defects because of the dynamical character of the scattering. However, if $N_{\rm disl} \gg \Lambda_0^{-2}$, the scattering becomes kinematical, and the dislocations remain second class defects; thus renormalized $L^* \gg 1$.

In the case of the application of X-ray diffraction, the critical dislocation density, at which the dislocations of the first class defects become second class defects, is of order 10^6 cm^{-2} (for the first strong reflections), and, for the γ-radiation energy, the corresponding value is of order 10^2 cm^{-2}.

Thus, the diffraction of γ radiation in the 'perfect' low-dislocation single crystals is dealt with as the complex (from the standpoint of the interpretation of the experimental results) intermediate case, when the dislocations, because of their small concentration, cannot be considered as first class defects in the purely kinematical case of diffraction, but also, because of the large extinction length of the radiation used, it is impossible within the framework of dynamical diffraction to attribute the dislocations as second class defects by the renormalization of the static Debye–Waller factor.

Quartz with dislocations was chosen as the research object because of the non-linear character of the dependence of the parameters presented in Table 1 on the value of the scattering vector, which permits more precise clarification of the dependencies of the static Debye–Waller factor; in this case, the superposition of the smoothly decreasing dependencies of the structure factors on the scattering factor is absent.

The values of L as a function of the scattering vector modulus $|\mathbf{q}_H|$ on the double logarithmic scale for the quartz crystals I and II are presented in Fig. 3. The values of L were calculated from the measured values of R_i (see Table 3) using (25). The same dependencies are presented in Fig. 4, but with values of L calculated using the approximation formula (26). It is observed that, in contrast to the results obtained for the dislocation-free silicon, here linear dependencies are not observed because (28) does not hold in this case.

Furthermore, the results of Figs. 3 and 4 were reconstructed using other abscissas. Fig. 3 was transformed into Fig. 5, and Fig. 4 into Fig. 6. Such a choice of coordinate system is connected to the aforementioned necessity of renormalizing the value of L and to the fact, experimentally obtained in the present work, that $L^*(q) \simeq q_H \Lambda_0^2$ for the reflections of the various types, *i.e.* L^* increases significantly faster than for Coulomb-type defects. The same result was experimentally established for the dislocation silicon by Khrupa (1991).

We can now unequivocally conclude that in the case of low-dislocation crystals with a dislocation density of up to 10^2 cm^{-2} by using short-wave γ-ray diffraction it is reasonable to conduct the description of the diffraction processes within the framework of the SDTD. Thus, the assumptions on the ratio between τ, Γ and Λ_0 are similar

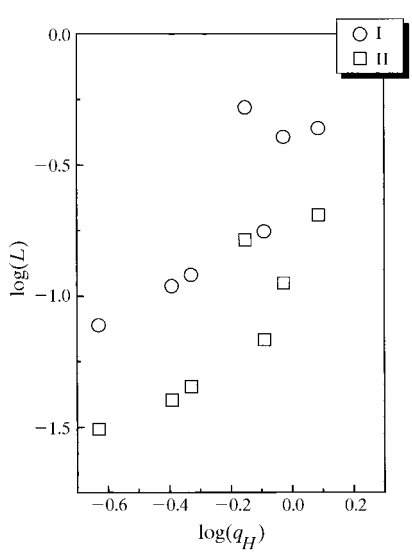

Fig. 4. The static factor $L = -\ln E$ for the quartz crystals I–II as a function of the scattering vector modulus $|\mathbf{q}_H|$ on the double logarithmic scale. The values of L were calculated with equation (26).

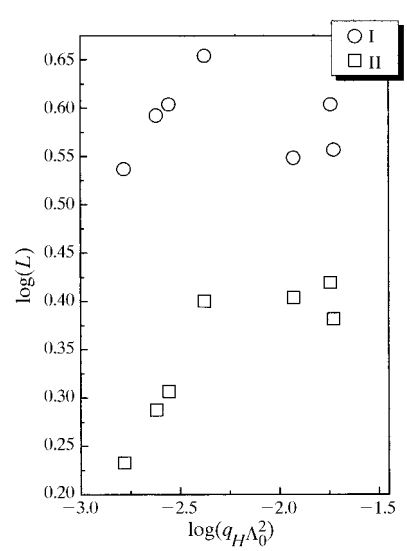

Fig. 5. The static factor $L = -\ln E$ for the quartz crystals I–II as a function of the normalized scattering vector modulus $\Lambda_0^2|\mathbf{q}_H|$ on the double logarithmic scale. The values of L were calculated with equation (25).

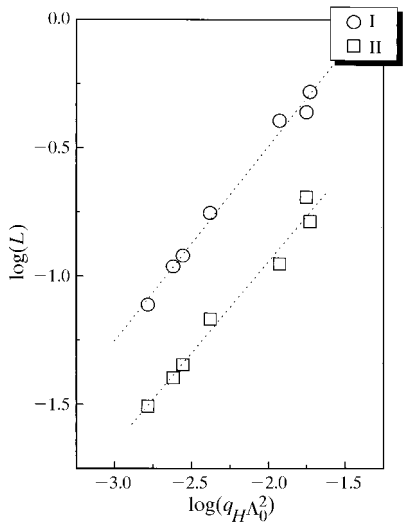

Fig. 6. The static factor $L = -\ln E$ for the quartz crystals I–II as a function of the normalized scattering vector modulus $\Lambda_0^2|\mathbf{q}_H|$ on the double logarithmic scale. The values of L were calculated with equation (26).

to those for 'perfect' dislocation-free silicon: $\tau/\Lambda_0 \to 0$ and $\Gamma/\Lambda_0 \to 0$. However, the values of E, describing the long-range lattice distortions, change in a wider range and can differ markedly from 1.

It should be noted that the application of condition (10) in our earlier works (Alexeev *et al.*, 1989; Kurbakov, 1991; Kurbakov & Sobolev, 1994), as in the studies by Olekhnovich *et al.* (1983); Voronkov *et al.* (1987) and Al Haddad & Becker (1988), resulted in underestimated values of E. Nevertheless, this fact did not influence the qualitative analysis of the defect-structure evolution during the application of various effects on the crystal lattice.

7. Conclusions

It has been shown that: (i) in the low-dislocation quartz crystals the experimentally measured values of the integrated intensities of the diffracted γ radiation are well described within the framework of the statistical dynamical theory of diffraction; thus, (ii) from the standpoint of the value of the effective correlation length, the description presented by Becker & Al Haddad (1992), and already confirmed by Schneider *et al.* (1992) and Takama & Harima (1994), is the most appropriate; (iii) the application of the approaches of the SDTD to the dislocation crystals allows removal of all the problems connected with the fact that the dislocations are second class defects according to Krivoglaz (1996); and (iv) in the low-dislocation quartz crystals, the value of the index of the static Debye–Waller factor L, obtained from the experimentally measured integrated intensities, has the dependence $\Lambda_0^2 q_H$.

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