Comparison of the gamma-ray diffraction and DLTS data suggests that the formation of E3, E5 and E7 deep level centers during heat treatments in nonoxidizing or chlorine-containing atmosphere takes place under Si supersaturation with vacancies and excess vacancies play the major role in their formation.

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GAMMA-RAY DIFFRACTOMETRY RESEARCHES OF CHAOTICALLY DISTRIBUTED DISLOCATIONS IN QUARTZ SINGLE CRYSTALS

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Method of the non-destructive control of dislocation density in bulk single crystals, based on measurement of integrated reflectivity (R_i) high-monocromatic short-wavelength gamma-radiation is developed. The researches of a structural perfection degree of the single crystal quartz specimens were carried out by a method of a diffraction of monochromatic gamma-radiation from a source of activated by neutrons ^{198}Au ($E = 412$ keV, $\lambda = 0.03$ Å, $\Delta\lambda/\lambda \leq 10^{-6}$), at the gamma-ray diffractometer of PNPI RAS. Quartz single crystals with dislocation density, varying in a small range $0-200$ cm/cm^3 (by data of etching), were chosen as objects of research.

According to the analysis, carried out in [1], processes of a diffraction of gamma-radiation in low-dislocation quartz single crystals are well-described within the framework of assimptotic variant [2] of the statistical dynamical theory of diffraction (SDTD) [3, 4]. Taking into account a smallness of Bragg angles for gamma-radiation and having cariied out averaging on negligible small thickness oscillaiions of intensity, passing from intensity to integrated reflectivity, from the formula (7) in [5] we obtaine following rather simple expressions:

$$R_i = R_{soh} + R_{inc} ,$$

$$R_{coh} = E \cdot R_{dyn} ,$$

$$R_{inc} = 2(1 - E^2) R_{dyn} t/\Lambda_0 ,$$

$$\Lambda_0 = V_0/(\lambda r_0 F_{hkl}) ,$$

where R_{coh} – coherent part of integrated reflectivity, R_{inc} – incoherent part, E – average lattice phase (in conventional theories it is Debye-Waller static factor), R_{dyn} – dynamical limit of integrated reflectivity, Λ_0 – extinction length, V_0 – elementary cell volume, λ – wavelength of used radiation, r_0 – classical electron radius, F_{hkl} – structural factor, t – effective thickness of specimen in direction of incident radiation.

Table

Results of gamma-ray diffractometry measurements;
measurements and accounts of dislocation density (in cm/cm^3)

Sample	Sample area	t, cm	$R_i \times 10^6$	$R_d \times 10^6$	E	ρ_1	ρ_2	ρ_3	ρ_4
16	I	3.00	0.57(2)	0.32	0.991	7	2	1	0 – 2 in separate places up to 15
20	I	3.00	0.99(3)	0.74	0.979	15	10	8	4 – 5
	II		1.56(5)	1.32	0.963	27	44	63	0 – 60 average 45
15	I	3.40	1.25(4)	1.00	0.975	18	16	11	0 – 20 nonuniform clusters
	II		1.59(5)	1.35	0.967	24	48	29	0 – 30 in separate places up to 60
21	I	3.35	1.24(4)	0.99	0.975	18	50	14	0 – 30 very noniniformly
25	I	4.65	2.72(7)	2.48	0.955	33	226	96	~ 100 uniformly
	II		7.77(21)	7.55	0.854	100	258	160	~ 200
5	I	3.60	1.27(4)	1.02	0.976	18	105	46	50 – 60 uniformly
	II		2.45(7)	2.21	0.948	38	74		
	III		5.34(16)	5.12	0.874	88	138	66	90 – 100 areas sithout dislocations exist.
	IV		6.86(21)	6.65	0.832	114	286		

For determination of dislocation density the formula (20) from [6] was applied, which after transformation to form convenient for accounts is

$$\rho = \frac{R_d}{\frac{\pi}{3}(b\frac{\pi\Lambda_0}{d})^2\, Qt}$$

where ρ – dislocation density, b – Buergers vector modulus, d – interplanar distance for given reflection, Q – integrated kinematical reflecting ability, R_d – part of integrated reflectivity, stipulated by diffuse scattering. Under our assumption, R_d has the same sense, as incoherent part in SDTD. Thus, following technique of ρ calculation is accepted: from the experimental value of R_i E is determined, from the value of E R_d is calculated, and from this one ρ is determined. By accounts following values for reflection (010) were used: $\Lambda_0 = 0.084$ cm, $Q = 6.004 \times 10^{-6}$ cm^{-1}, $R_{dyn} = 0.253 \times 10^{-6}$, $b = 8.18 \times 10^{-11}$ cm.

The results of measurements and accounts are listed in table. The accounts of dislocation density, carried out on the basis of the gamma-ray diffractometry data (ρ_1), were compared to results of hydrothermal etching of crystals with subsequent counting of etching pits on a pinacoid surface (ρ_2), etching of AT-cut plates in ammonium bifluoride with subsequent counting of etching channels (ρ_3), X-ray topography of these plates (ρ_4).

On three investigated specimens from six reasonably good conformity between the data, obtained by all applicated techniques is observed. On three other specimens significant discrepancy between values of ρ, determined by methods of gamma-ray diffractometry, plates etching and X-ray topography (ρ_1, ρ_3 and ρ_4), giving the information from crystal bulk, and data of surface etching (ρ_2) has come to light. It specifies that the distribution of defects in bulk of low-dislocation quartz crystals can strongly differ from their distribution in near-surface areas. The dislocation density, determined by gamma-ray diffractometry method (ρ_1) can be considered as the integrated characteristic of the whole crystal.

The results of researches confirm very high sensitivity of chosen parameter - integrated reflectivity of short-wavelength gamma-radiation to small changes of density of linear defects. It is possible to determine dislocation density in low-dislocation crystals with accuration up to several cm/cm^3 in crystal bulk, that permits to carry out non-destructive control of large single crystals quality.

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