11. REAL AND IDEAL CRYSTALS


For the interpretation of experimental integrated reflecting powers of Bragg reflections Φ, obtained in the symmetrical Bragg case on parallel crystals of different perfection, is proposed to introduce the dynamical theory formulas as follows:

\[ \Phi = \frac{D}{P} R^1, \quad R^1 = R(g'), \quad g' = g_0 P, \]

where \( D \) and \( R \) are computed after W.H. Zachariasen (Theory of X-ray diffraction in crystals, N.Y., Wiley, 1945) and \( P \) — empirical parameter, being

\[ P = 1 + \left( \frac{-D}{S} \right)^2 - 0.5 \]

where \( S \) — extinction length, \( D \) — mean coherence domain dimension.

On a double-crystal spectrometer were measured the integrated reflecting powers of a series of Bragg reflections in diamond crystals of different perfection. The measurements were carried out in FeKα, CuKα, and MoKα radiations. Theoretical structure factors of W.1. Detersen (Proc. Roy. Soc. A 235, 264, 1957) were used, the coincidence of calculated \( \Phi \) with the experiment was attained by variations of parameter \( D \). The results show that in the given crystal one empirical parameter \( D \) is sufficient to describe the experiment as to the whole interval of the used wavelengths and different Bragg reflections. Assuming that the dislocation density is inversely proportional to \( D^2 \) one can estimate it in the studied crystals; the obtained values lie in the interval 5·10^{-5} – 8·10^{-4} cm^{-2} keeping with topographic data.

An analogous work done on LiF came up with the universality of the proposed approach; the values of the dislocation densities are in the interval 6·10^{-6} – 8·10^{-5} cm^{-2}.

The recalculations with the present formula of the dependence of polarization ratio on the dislocation density in Si, obtained by N.M. Glushchenko et al (in Russian: Kristallografiya 18, 6240, 1973; 22, 795, 1975) showed a good agreement between theory and experiment for all reflexes in the whole interval of dislocation densities (from dynamic to kinematic limits), where by means of traditional extinction corrections could not obtain.

The proposed approach needs a further check, especially in the region close to the kinematic limit and a concrete description of the parameter \( D \) is also necessary. But it is obvious that the given method could be useful at investigations of X-ray diffraction in sufficiently perfect crystals.

11.2–10 HIGH RESOLUTION DIFFUSE X-RAY SCATTERING STUDIES OF SILICON SINGLE CRYSTALS GROWN BY FLOAT ZONE METHOD. By Praveen Lal and S. Niranjan N. Goswami, National Physical Laboratory, Hillsdaie Road, New Delhi-110 012, India.

Diffuse X-ray scattering (DXS) measurements have been made near the 111 reciprocal lattice point (relp) of dislocation free (111) silicon single crystals grown by the float zone (FZ) method. The technique and the equipment used have been described earlier (Lal and Singh, Solid State Commun. 1977 22, 71; Lal, Singh and Verma, Acta Cryst. 1979 A35, 286; Lal in Synthesis, Growth and Characterisation, K. Lal (Ed.) 1982, North-Holland, P-207). The diffractometer was set in (1, -1, -1) configuration and MoKα was used as the exploring X-ray beam. Diffraction curves and high resolution topographs were recorded before DXS measurements. The shape of the diffraction curves shows that the specimen were nearly perfect single crystals. In some crystals the maximum value of \( \frac{D}{I_0} \) was nearly one. The top of the diffraction curve is sloping as expected on the basis of dynamical theory. A small structure is generally observed on top of the diffraction peak. The half width of these curves ranges from 3 to 10 sec of arch. The high resolution topographs showed a uniform distribution of diffused intensity.

The DXS distribution in these crystals is generally similar to that observed in CZ grown crystals. In the DKS I vs K plots (K = scattering vector) there is more than one straight line for each direction of \( \vec{K} \). The slopes of the lines for which \( \vec{K} \) are parallel to \( \vec{R} \) are greater than those of the lines for which \( \vec{K} \) is perpendicular to \( \vec{R} \). \( \vec{R} \) is the reciprocal lattice vector.

These observations support our earlier conclusions that DXS at and near the room temperature is predominantly due to point defects and their aggregates.

In finer details the DXS distribution observed for CZ crystals is significantly different from the distribution observed for CZ crystals.

The anisotropy in the DXS distribution with respect to the sense of the scattering vector for any direction in reciprocal space is smaller in these crystals as compared to that observed in the CZ crystals.

We have analysed the DXS data to find out the value of the knee points where the slopes of lines in the log DKS I vs log K plots change slopes. The knee points lie around two values of \( \vec{K} \): 1.4 ±2·10^{-5} cm^{-1} and 1.4 ±2·10^{-6} cm^{-1}. From this we can see that the size of the defect clusters is in the range of 5–7 × 10^{-4} cm and 5–7 × 10^{-5} cm. The anisotropy plots show that the defects are of vacancy type. In the CZ crystals the most prominent knee point was observed at \( \vec{K} = 10^{-4} \) cm, which corresponds to a size of around 10^{-5} cm.