11.2–9 THE SPECTRAL DEPENDENCE OF INTEGRATED REFLECTING POWERS OF BRAGG REFLECTIONS IN DIAMOND STRUCTURE CRYSTALS OF DIFFERENT PERFECTION. By Yu.A.Rosenberg, A.I.Kolosovsky, L.I.Kleshchinsky, I.L.Feldman, V.M.Kiselev, Inst.of Transp.Engineers, 664074 Irkutsk and N.V.Shokhirev, Inst.of Chem.Kinetics, Sib. Branch of Academy of Sciences, 630090 Novosibirsk, USSR.

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

$$\rho = \frac{\rho_{dyn.}}{P} \cdot \frac{R'}{R} \quad , \quad R' = R(g') , \quad g' = \frac{g}{P} \quad ,$$

where $\rho_{dyn.}$, R and g are computed after W.H.Zachariasen (Theory of X-ray diffraction in crystals, N.Y., Wiley, 1945) and P - empiric parameter, being

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

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 reflexes in diamond crystals of different perfection. The measurements were carried out in $FeK_{\alpha 1}$, $CuK_{\alpha 1}$ and $MoK_{\alpha 1}$ radiations. Theoretical structure factors of B.Dawson (Proc.Roy.Soc.A 298, 264, 1967) were used, the coincidence of calculated ρ with the experiment was attained by variations of parameter D. The results show that in the given crystal one empiric 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 $5 \cdot 10^5 - 8 \cdot 10^7$ 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 density are in the interval $6 \cdot 10^6 - 8 \cdot 10^8$cm^{-2}.
The recalculation with the present formula of the dependence of polarisation ratio on the dislocation density in Si, obtained by N.M. Olechnovich et al (in Russian: Kristallografia 18,1240,1973; 20,796,1975) showed a good agreement between theory and experiment for all reflexes in the whole interval of dislocation densities (from dynamic to kinematic limits), which the authors 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 Krishan Lal and S. Niranjana N. Goswami, National Phiscal Laboratory, Hillside 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 decribed earlier (Lal and Singh, Solid State Commun. (1977)22, 71; Lal, Singh and Verma, Acta Cryst.(1979) A35, 286; Lal in Synthesis,Crystal Growth and Characterization, K. Lal (Ed.) 1982, North-Holland, P-287). The diffractometer was set in (1,-1,1) configuration and $MoK_{\alpha 1}$ 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 Id/Io 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 arc. The high resolution topographs showed a uniform distribution of diffracted intensity.

The DXS distribution in these crystals is generally similar to that observed in CZ grown crystals. In the DXS I vs K^{*-2} plots ($\vec{K}^*$ = scattering vector) there is more than one straight line for each direction of $\vec{K}^*$. The slopes of the lines for which $\vec{K}^*$ is 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 predominently due to point defects and their aggregates.

In finer details the DXS distribution observed for FZ 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 DXS I vs log K^* plots change slope. The knee points lie around two values of $\vec{K}^*$: $1.4 - 2 \times 10^3$ cm^{-1} and $1.4 \sim 2 \times 10^4$ cm^{-1}. From this we can see that the size of the defect clusters is in the range of $5\text{-}7 \times 10^{-4}$cm and $5\text{-}7 \times 10^{-5}$cm. The anisotropy plots show that the defects are of vacancy type. In the CZ crystals the most prominent knee point was observed at $\vec{K}_{-4} \sim 10^4$ cm^{-1}, which corresponds to a size of $\sim 10^{-4}$cm.