11.2-9 HIGH RESOLUTION DIFFUSE X-RAY SCATTERING STUDY OF DEFECT STRUCTURE IN SILICON SINGLE CRYSTALS BY EXPLORING RECIPROCAL SPACE AROUND DIFFERENT LATTICE POINTS WITH A FOUR CRYSTAL X-RAY DIFFRACTOMETER. By

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Point defect aggregates in nearly perfect single crystals produce anisotropic diffuse X-ray scattering (DXS) from reciprocal space around reciprocal lattice points (relps) (Krishan Lal in Synthesis, Crystal Growth and Characterization, (Krishan Lal (ed.), North Holland, Amsterdam, (1982), p. 287). Here, we report results of measurements of diffuse X-ray scattering, made around four different reciprocal lattice points of dislocation-free silicon single crystals grown by the Czochralski method. The specimens were cut from a boule grown along [111] direction with large surfaces along (111) planes. Plane surfaces were ground, lapped and polished along the following four sets of planes: (111), ($\bar{1}$10), (001) and ($\bar{1}\bar{1}$2). A four crystal X-ray diffractometer was employed for measurement of diffuse scattering. Three dislocation-free (111) silicon plane crystal monochromators were used in the (+,−,−) setting to achieve a $K\alpha_1$ exploring beam with low values of angular and wavelength spreads. The specimen formed the fourth crystal oriented in the (+,−,−,+) configuration. A $MoK\alpha_1$ exploring beam was used. DSX measurements were made in two planes of reciprocal space which were perpendicular to each other around each of the following four reciprocal lattice points : 111, $\bar{2}$20, 004 and $\bar{2}\bar{2}$4. In both these planes measurements were made with the scattering vector $\vec{K}^*$ along four directions. Diffraction curves were recorded before each set of DXS measurements.

The half widths of the diffraction curves recorded for the 111, $\bar{2}$20, 004 and $\bar{2}\bar{2}$4 reflections were 8.5, 7.0, 4.5 and 4.0 seconds of arc, respectively. The ratios of the half widths agree well with those expected theoretically. The diffuse scattering distribution around all the reciprocal lattice points was observed to be anisotropic with DXS intensity higher on the $\theta>\theta_B$ side. Here θ is the glancing angle and θ_B is the Bragg angle. This shows that in these crystals, interstitial defects give a dominant contribution to the DXS. The DXS data were plotted on log-log scale and the values of $|\vec{K}|^*$ at knee points determined. Knee points are the points on the log DXS 1 versus log K^* plots where the slope changes value. The knee points observed with the four relps are 74 in all. The reciprocal of K^* values at knee points gives the size factor of point defect clusters. The 74 knee points cluster around four values of the scattering vector $|\vec{K}|^*$ with maximum number around K^* values in the range $1 - 3 \times 10^4$ cm^{-1}. This corresponds to defects clusters of sizes in the range $0.3 - 1 \times 10^{-4}$ cm. The other size factors are $1.6–2.5 \times 10^{-5}$ cm (11 knee points); $1–1.4\times10^{-4}$ cm (14 knee points) and $2 - 5 \times 10^{-4}$ cm (19 knee points).

11.2-10 A QUANTITATIVE STUDY OF DIFFRACTED X-RAY INTENSITIES FROM NATURAL DIAMOND CRYSTALS BY USING MULTICRYSTAL X-RAY DIFFRACTOMETERS AND COMPARISON WITH SILICON CRYSTALS. By

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Preliminary high resolution X-ray topographic and diffractometric measurements on natural diamond crystals, made in our laboratory, had shown that natural diamond crystals exhibit anomalously high peak intensities of diffraction maxima, even though their degree of perfection is rather low. Here, we report results of a systematic quantitative study of intensities of diffraction, peak as well as integrated, from a number of natural diamond crystals. A dislocation free silicon single crystal was taken as a reference and all measurements were made on this under identical conditions. A triple— and a four— crystal X-ray diffractometer were used which employ highly monochromated and collimated $K\alpha_1$ radiations. For these measurements $MoK\alpha_1$ and $CuK\alpha_1$ radiations have been used. Specimen diamond crystals are (111) platelets of about 1 mm in thickness and a few mm^2 in area. The exploring $K\alpha_1$ beam irradiated an area : 0.2 x 1.2 mm^2 on the specimen surface. The $\bar{2}$20, $\bar{4}$40, $\bar{1}$13 and $\bar{2}\bar{2}$4 reflections were studied in the Laue (transmission) geometry. Bragg (reflection) geometry was used for measurements made with 111 and 333 reflections. The reference silicon single crystal was disc-shaped (diameter = 23 mm ; thickness - 1mm) with flat surfaces along (111) planes. In most of the experiments the specimen was the third crystal of the diffractometer, aligned in the (+,-,+) configuration. Experiments were also done with the specimen at the fourth crystal position in the (+,-,+,-) setting. High resolution diffraction curves, section and traverse topographs were recorded. The curvature of the lattice planes was also measured.

Typical half widths of diffraction curves of diamond crystals were about 60 seconds of arc, showing that these had rather low degree of perfection. Diffraction curves of silicon single crystals, on the other hand, are very sharp with half widths in the range : 5-10 seconds of arc. The peak as well as the integrated intensities of all the diffraction curves of diamond crystals are substantially higher than those of silicon single crystals. For example, in the case of $\bar{4}$40 reflection (Laue geometry ; $MoK\alpha_1$ radiation), the peak intensity ratio between diamond and silicon crystals was 7 : 1 and the integrated intensity ratio was 29 : 1. The peak intensity ratio for 333 reflection (Bragg geometry ; $MoK\alpha_1$ radiation) was 11 : 1 and the integrated intensity ratio was 48 : 1. When the differences in the absorption coefficients and atomic scattering factors of carbon and silicon are taken into consideration, the anomaly further increases. Extinction does not seem to explain the observed differences. Possible reasons responsible for these results will be discussed.