unchanged even when the crystal lattice is slightly deformed.

Table: Lateral and angular parameters of the unit-cell of a highly pure silicon crystal at 22.50°C and vacuum.

$a = (543\ 101.915 \pm 0.049)$ fm

$b = (543\ 102.116 \pm 0.049)$ fm

$c = (543\ 102.007 \pm 0.049)$ fm

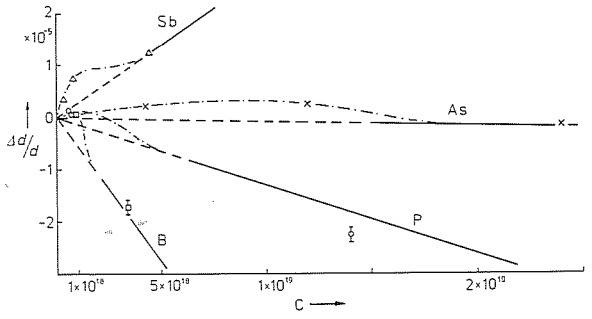
$\alpha = \pi/2 - (10 \pm 10) \times 10^{-8}$

$\beta = \pi/2 + (22 \pm 10) \times 10^{-8}$

$\gamma = \pi/2 - (5 \pm 10) \times 10^{-8}$

$V = (0.160\ 193\ 259 \pm 0.000\ 000\ 044)\ nm^3$

Figure : Lattice parameter changes $\Delta d/d$ versus (low) impurity concentration c (atoms cm^{-3}) in silicon. The individual confidential limits of each measurement are of the order of 10^{-7} $\Delta d/d$, except the two limits marked in the figure.



11.5–2 LATTICE DISTORTIONS INDUCED BY B, P, As AND Sb IN SILICON. By P. Becker and M. Scheffler, Physikalisch-Technische Bundesanstalt, Braunschweig, Federal Republic of Germany.

The lattice parameters of silicon crystals doped with B, P, As and Sb have been measured as a function of impurity concentration using a highly accurate X-ray diffraction technique (Becker, Seyfried, Siegert, Z. Physik B (1982) 48, 17). This method allows the change of lattice parameters for doping concentrations even below 10^{18} atoms cm^{-3} to be studied. Some of the results are shown in the figure. For low concentration all samples show a dilatation of the lattice if compared with a highly pure Si crystal (dotted (-·-·-) curves in the figure). For higher concentration the B, P and As doped samples show a reduced lattice parameter and only Sb gives rise to an expansion.

In order to elucidate the discrepancies between the lower and higher concentration data, parameter-free calculations of the lattice distortions at substitutional and interstitial impurities in Si are performed using the self-consistent Green's functions method (Scheffler, Vigneron and Bachelet, Phys. Rev. Lett. (1982) 49, 1965 and Phys. Rev. B to be published). In a good accordance between theory and experiment, all impurities in the sample with high doping concentrations essentially occupy substitutional sites. The amount of the lattice parameter change and the trends between different impurities quantitatively confirm the concept given by the covalent radii of the atoms (straight lines in the figure). The low concentration results, on the other hand, indicate the presence of a considerable percentage of interstitial defects.

11.5–3 MEASUREMENT OF DISORDER-DIFFUSE X-RAY SCATTERING USING A DIFFRACTOMETER. By T.R.Welberry, Research School of Chemistry, Australian National University, CANBERRA, Australia. & A.M.Glazer, Clarendon Laboratory, Parks Rd., OXFORD, England.

Substitutional or orientational disorder occurs widely throughout many branches of crystallography. But while conventional structure solution using Bragg reflections has become more or less a routine operation, the measurement and interpretation of diffuse x-ray scattering for problems involving disorder is still done largely on an ad hoc basis. Recently we have sought to develop methods, using conventional Weissenberg equipment, to make the systematic study of disorder problems in molecular crystals a more routine process. (Epstein et al, Acta Cryst.A38, 611-618 (1982);Welberry et al, Acta Cryst. B38, 1518-1525 (1982); Epstein & Welberry, Acta Cryst. A39, 882-892.(1983)). In this paper we present the results of a comparative study of these film-based methods with experiments we have recently carried out on a diffractometer, which were undertaken in order to assess the reliability of the film-based methods.

In order to make the comparison as close as possible the diffractometer (Stoe Stadii-2) was set up to correspond in resolution to the Weissenberg camera. With the detector 125mm from the sample a vertical detector slit-width of 4mm. gave comparable resolution to a 1mm. layer-screen gap on a 30mm. radius Weissenberg camera. The horizontal detector-slit width, which corresponds to resolution in theta and which has no counterpart on the Weissenberg camera, was set at 2mm. For an example run, stationary counts of 100 secs. were made at points in reciprocal space on a grid a*/10 by c*/5 for the h0l section of the chosen sample: 1,4-dibromo-2,5-diethyl-3,6-dimethylbenzene; Space Group $P2_1$, a=9.084, b=4.459, c=17.940 Å, β = 122.82. Data was collected for one half of

the layer for $2\theta < 51.2^{\circ}$ (for Cu K_{α}), resulting in about 3500 data points and a total collection time of about 1 week. Counting time was chosen after some initial tests to achieve average counting errors in the intensity measurements of better than 10%. In all, data for 6 reciprocal lattice sections have been collected, and a detailed comparison with corresponding photographic data will be described.

An example contour plot, illustrating the quality of data obtained is shown in Figure 1.

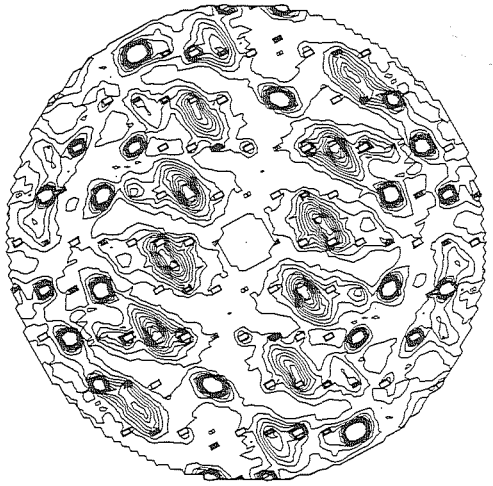


Figure 1. Contour plot of the h0l data. Contour levels are in equal increments of 250 counts. Bragg peaks appear as small quadrilaterals.

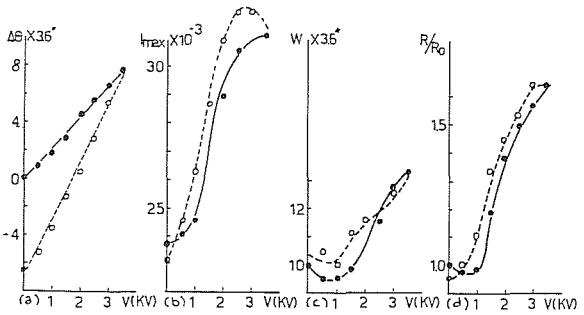


Fig. 1 Dependence of (a) peak shift, (b) maximum intensity, (c) half-width and (d) percentage integrated intensity on the applied DC voltage ((203) reflection, thickness of crystal t=0.31 mm, irradiated face at positive potential).
• increasing field; ○ decreasing field

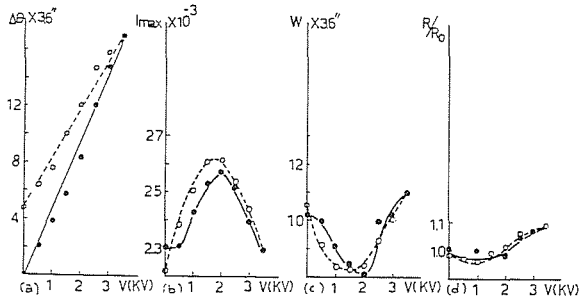


Fig. 2 Same as fig. 1 with reversed polarity.

11.5–4 EFFECTS OF ELECTROSTATIC FIELD ON THE X-RAY BRAGG DIFFRACTION OF α-QUARTZ.

By M. Calamiotou, Physics Dept., Athens Univ., E. Anastassakis, National Technical Univ., Athens, V. Psicharis and S.E. Filippakis, N.R.C. "Demokritos", Athens.

An increase of the X- and γ-ray integrated intensity of α-Quartz under the influence of an electrostatic field has been observed by Yasuda and Kato (Appl. Cryst.(1975) 8, 623) and Dousse and Kern (Acta Cryst. (1980) A36, 966) respectively, but the mechanism responsible for such an effect is not yet completely clear. We report here the results of an experimental study, in which a series of rocking curves of the (203) X-ray Bragg reflection of α-Quartz were measured in the presence of an electrostatic field up to ∿113 kV/cm. The integrated intensity at constant field was found to be time-dependent, suggesting the existence of relaxation effects. A field-dependent saturation value was reached after time intervals ranging from 20 to 45 min for field values of 16 to 113 kV/cm. Rocking curve characteristics such as peak position, peak intensity and half width were measured as a function of the field at saturation level (fig. 1a,b,c and d for percentage change of the integrated intensity). They all show hysteresis effects. It was also observed that the strength of the effect depends on the field polarity. When the negative electrode was attached to the irradiated face the effects were considerably reduced (fig. 2a,b,c,d). The measured peak shifts Δθ are typically one order of magnitude larger than those calculated on the basis of the reverse piezoelectric effect. It appears that crystal defects are largely responsible for the rather sizeable effects observed, thus preventing one from distinguishing field-dependent intrinsic contributions, such as those due to piezoelectricity and internal strains (Anastassakis, phys.stat.sol.(b) (1982) 110, 169).

11.5–5 X-RAY DIFFUSE SCATTERING IN LPE GaAlAs SOLID SOLUTIONS

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X-ray diffuse scattering (XRDS) experiments have been performed on thick (250 μm) $Ga_{1-x}Al_xAs$ ($x=0.35\pm0.05$) single crystal layers grown on (100) GaAs crystals by the liquid phase epitaxy (LPE). Using monochromatized Cu Kα radiation and small angular divergences (0.5°) of both the incident beam and the beam accepted by the counter, the I_D XRDS intensity has been accurately measured along the [100] direction in reciprocal space.
The intensity of the Compton scattering was independently measured at a few scattering angles by taking advantage of the energy resolution of a Si(Li) detector to partially separate the modified radiation. The Compton scattering data were interpolated by means of calculated incoherent scattering functions and then subtracted from the I_D. The I_{CW} intensity of the scattering due to composition waves is not dependent on the scattering vector $\vec{Q}$, while the I_{PH} intensity of the one-phonon scattering by LA and LO branches is proportional to Q^2. This made it possible to separate the two contribu-