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

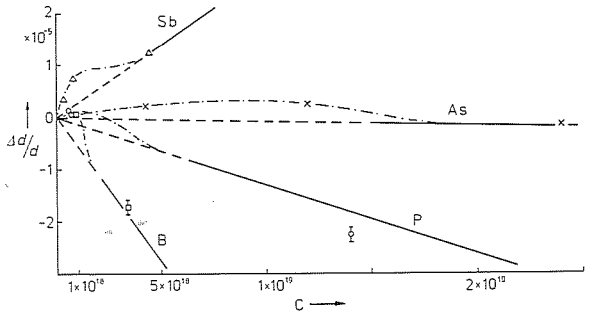
$\alpha = \pi/2 - (10 \pm 10) \times 10^{-8}$

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

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

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

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