20.2-07 REPRESENTATION OF CUBIC CRYSTAL STRUCTURES BY A COLLECTION OF POLYHEDRA.

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The packing of Archimedean truncated octahedra fills the entire space. This Wigner-Seitz cell for an I type cubic lattice has been shown to be a useful geometric unit for all cubic crystal structures (C. Chieh, Acta Cryst. A35, 946-952 (1979)). The application of this concept has been demonstrated for structures whose geometric units possess $\bar{4}3m$ symmetry (C. Chieh, Acta Cryst. A36, 819-826 (1980)). All geometric units for structures in Im3m and Pm3m and two out of the three units in Fm3m possess m3m symmetry. Structures in these units can be represented by a set of polyhedra taken from any combination of octahedron, cube, icosahedron, truncated octahedron, truncated cube and rhombicubooctahedron. An interesting relationship between these polyhedra and the Archimedean truncated octahedron will be shown with models.

A comparison of polyhedra present in various symmorphic space groups will be made and applications of the geometric units for the representation of non-symmorphic space groups will be demonstrated. Results from further exploration of Wigner-Seitz cells as possible geometric units in hexagonal and tetragonal systems will be presented.

20.3-01 DEFECT DISTRIBUTIONS IN VARIOUS POLYTYPES OF SILICON CARBIDE.

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Since the discovery of polytypic structures in 1915 numerous theories have been proposed to explain their existence. No single theory has so far been in complete agreement with all the experimentally observed data. The screw dislocation theory by Frank (Phil. Mag.(1951) 42 p.1014) and later by Mitchell (Z. Kristallogr. Kristallgeom. (1957) 109 pt 1 p.341), Krishna and Verma (Z. Kristallogr. Kristallgeom. (1965) 121 p.36) and Pandey and Krishna (Phil. Mag. (1975) 31 p.1113, J. Crystal Growth (1975) 31 p.66, Mat. Sci. Eng. (1975) 20 p.243, Ibid. (1976) 26 p.53), correlates quite well with observation but the origin of the dislocations has remained open to question. Recently Kuhlmann-Wilsdorf, Pandey and Krishna (Phil. Mag. (1980) 42 p.527) have proposed a model in which impurity content and subsequent stress gradients could give rise to slip or buckling or both.

We are using X-ray methods, in particular X-ray topography, and electron microscopy to examine a large number of αSiC platelets which were grown from the vapour phase. In this way, we are able to assess the impurity content and defect distribution in each crystal. Work is continuing but preliminary results show that buckling is quite common with radii of curvature being in the region of 4 to 5 metres.

Many samples show evidence of the basal slip system being active in agreement with earlier observations by Posen and Bruce (Proc. 3rd Int. Conf. on SiC, Miami Beach, Florida 17-20 Sept 1973, p.238). Stacking faults parallel to the basal plane have also been found.

Defect distributions in different polytypes are compared and of particular interest are crystals containing more than one polytype. It is expected that this information will be useful in improving our understanding of the growth mechanisms operating during growth of polytypic materials.

20.3-02 X-RAY STUDIES ON POLYTYPISM AND CRYSTAL STRUCTURE OF SILICON CARBIDE.

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Silicon carbide is a typical layer compound and up to the present more than 150 polytypes of SiC are known. The author has developed a modified Laue method which is very efficient in identifying polytypes of SiC, especially when the total number of layers in a unitcell becomes quite large. Using this method in examining more than 1000 SiC crystals, we have found eighty-five new polytypes of silicon carbide.
In order to determine the crystal structure of some of these new polytypes, oscillation as well as Weissenberg methods have been tried though without success, because only diffraction spots of the basic polytypes 6H and 15R could be found in these photographs. A modified Laue method to determine the crystal structure of these polytypes is presented. The intensity of the (hkl) reflection is

$$I_{hkl}=K\lambda^4 \frac{1+\cos^2 2\theta}{\sin^2\theta} I_0(\lambda)F_{hkl}J(\lambda)Q(\theta)$$

where $I_0(\lambda)$ is the intensity of the incident beam of wavelength λ in the continuous spectra and $J(\lambda)$ the sensitivity factor of the photographic film for X-rays of this wavelength. For rhombohedral SiC polytypes,

$$F_{hkl}=3\left[f_{si}+f_c\exp\left(2\pi i\frac{3l}{4n}\right)\right]\sum_p \exp\left(2\pi ip\frac{l}{n}\right)$$

where p is the serial number of the A layers included in the summation. The calculation of