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 geo-
metric units possess $\overline{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, icosa-
hedron, truncated octahedron, truncated cube and rhom-
bicubooctahedron. · 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. By G.R. Fisher, Marconi Avionics Ltd.
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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 topo-
graphy, 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. By Kuo Chang-lin,
Shanghai Institute of Ceramics, Chinese Academy
of Sciences, Shanghai, China.

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 identi-
fying 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 poly-
types 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 photo-
graphic film for X-rays of this wavelength. For
rhombohedral SiC polytypes,

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

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

F_{hkl} in $[(33)_q 3\bar{2}]_3$, $[(33)_q 34]_3$ and $[(44)_q 43]_3$

structure families can be simplified. We can find that the number of layers Δp between two neighbouring A positions shows a periodic change within a unitcell as the following

$[(33)_q 32]_3$: $(2,4)_{q+1} (3)_q 3 (3)_q (4,2)_{q+1}$

$[(33)_q 34]_3$: $(4,2)_{q+1} (3)_{q+1} 3 (3)_{q+1} (2,4)_{q+1}$

$[(44)_q 43]_3$: $(4)_{q+1} (2,3,3)_q (2,3)(3,2)(3,3,2)_q (4)_{q+1}$.

Therefore, the structure factors F_{101} in $[(33)_q 32]_3$, $[(33)_q 34]_3$ and $[(44)_q 43]_3$ structure families are

$F_{101} = \csc(u/2) \cdot [0.8661 + \sin(u/6) - \sin(q+1)u]$

$F_{101} = \csc(u/2) \cdot [0.8661 - \sin(u/6) - \sin(q+1)u]$

$F_{101} = \cos 2v [\sin(w+2v) + D \cdot \sin w \cdot \cos(2w+v) - 2\cos 3w]$

where $u = 12\pi l/n$, $v = 2\pi l/n$, $w = 4(q+1)$ and $D = (2\cos 3v + 1)/\cos 2v$.

Using this modified Laue method, the crystal structure of nine new polytypes of silicon carbide were determind. The crystal structure of these new polytypes can be indicated by the Z stacking sequences as the following,

231R: $[(33)_{12} 32]_3$, 249R: $[(33)_{13} 32]_3$,

321R: $[(33)_{17} 32]_3$, 339R: $[(33)_{18} 32]_3$,

237R: $[(33)_{12} 34]_3$, 417R: $[(33)_{22} 34]_3$,

453R: $[(33)_{24} 34]_3$, 93R: $[(44)_3 43]_3$,

261R: $[(44)_{10} 43]_3$.

Some of these stacking sequences were further confirmed by high resolution TEM observation.

20.3-03 NEW ANTIPHASE STRUCTURES FORMED BY MECHANICAL TWINNING IN CuAuII ORDERED THIN FILMS. BY S. Maruyama, Department of Natural Science, Osaka Women's University, Daisen-cho, Sakai City, Osaka, Japan.

Most ordered alloys can hardly bear mechanical twins. This is because, in most cases, a simple homogeneous shear would destroy the original ordered structure, resulting in another complicated superlattice formation which does not exist in thermally equilibrium state. In CuAuI ordered lattice, however, the only one twinning shear $\frac{1}{6}[11\bar{2}]$ among three $\frac{1}{6}<112>$ on (111) planes can bring about mechanical twins without destroying the original lattice (Pashley et al. Phil. Mag. 19 (1969) 83). In CuAuII, it cannot mechanically twin without destroying the original (100) and (010) antiphase boundaries, because these would be transformed into $(1\bar{1}\bar{1})_t$ and $(\bar{1}1\bar{1})_t$, respectively, by $\frac{1}{6}[11\bar{2}]$, (111) homogeneous shear. (Here, the suffix "t" denotes that the indices refer to the twin lattice.) However, the antiphase structure CuAuII is only metastable at room temperature. Then, $(1\bar{1}\bar{1})_t$ and $(\bar{1}1\bar{1})_t$ antiphase structures might be produced after twinning shear.
The experiment was made on thin films formed by vacuum deposition. The film was made by evaporating a required amount of copper onto a gold film; 200Å in thickness, hole free, prepared by Pashley method (Phil. Mag. 4 (1959) 324). In order to give the (1/6) $[11\bar{2}]$ twinning shear on (111) planes, the film was specially prepared so that the shorter axis "c" was

overall normal to the film plane. This was realized by rapid heating of the gold film on the substrate from room temperature to the epitaxial temperature of copper. Due to the differential dilatation between the gold film and the substrate, an uniform tensile stress was provoked in the film plane, which favoured the shorter axis "c" lying normal to the film plane, as the axis is the direction of tension after ordering process (Maruyama et al. Proc. Int. Congr. on Electron Microscopy, Toronto (1978) Vol.1 152).
The CuAuII film was stretched in [110] direction in the film plane, by a specially devised method. In detail, the film was put on a Mylar sheet using water, then the Mylar was stretched in [110] direction of the film, by 17 percent. Through the adhesive force, the film was plastically deformed in [110] direction (Maruyama et al. J. Phys. Soc. Japan 25 (1968) 1392). Mechanical twins occurred everywhere. Electron diffraction patterns revealed the existence of $(1\bar{1}\bar{1})_t$ and $(\bar{1}1\bar{1})_t$ antiphase structures by the splitting of $00\bar{1}_t$ reflection in $[1\bar{1}\bar{1}]_t$ and $[\bar{1}1\bar{1}]_t$ directions. The electron micrograph of the dark field taken from split $00\bar{1}_t$ reflections revealed two series of antiphase boundaries $(1\bar{1}\bar{1})_t$ and $(\bar{1}1\bar{1})_t$ which make an angle of 74°, and have 22Å in spacing (corresponding to ten (111) layers), which coinside well with the values calculated on the composition of the present film.

20.3-04 INTERPENETRATION TWIN IN DIAMOND. By J.D.H. Donnay and Gabrielle Donnay, Geological Sciences, McGill University, 3450 University Street, Montreal H3A 2A7.

Before 1913 this twin was a textbook example of "twinning by lattice symmetry with twin index $n=1$" (Friedel's twinning by merohedry): twin symmetry $4'/m'[\bar{4}] 3 2'/m[\bar{1}']$, where the unprimed elements give the then accepted crystal symmetry $\bar{4}3m$, and the primed elements are the additional symmetry elements of the lattice, which provide the 24 simultaneous twin operations. In 1913, with the diamond structure described in $Fd3m$, discredit befell the antihemihedral point group, and the holohedry was adopted as a matter of course, under the implicit assumption that the structure is (or should be?) the property that has the lowest symmetry of all crystal properties. But then, holohedral crystals cannot twin by merohedry! Twinning theory needs generalizing: a space-group symmetry operation may act as twin operation; the twin operation may restore the atoms of some Wyckoff position, which need not have the configuration of the lattice of the crystal, whereas other positions take on new orientations. In diamond the lattice complex D of eight carbon atoms can be fancied as made up of two representations of the F lattice complex: D = 000 F + xxx F, with $x = 1/4$, so that the second F is shifted by 1/4 the body diagonal with respect to the first F. The 16 symmetry centers lie half-way at 1/8 1/8 1/8,... . We propose twinning by inversion in 1/2 1/2 1/2, an operation that is not a symmetry operation of the whole structure, but is such an operation for 000 F, $i.e.$ half the structure. Such a twin inversion differs from a point-group operation in that the inversion point must be chosen in the structure, instead of being the fixed point, and the twin inversion operates on atoms instead of faces. Now if $\bar{4}3m$ is the correct point group, then the space group is $F\bar{4}3m$, where the 8 atoms occupy $4(a)$ and $4(c)$. Twinning restores a and inverts c: the mechanism is working. HR electron microscopy should be able to prove it.