

$F_{hkl}$  in  $[(33)_q 32]_3$ ,  $[(33)_q 34]_3$  and  $[(44)_q 43]_3$

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

$$\begin{aligned} [(33)_q 32]_3 &: (2,4)_{q+1} (3)_q (3)_q (4,2)_{q+1} \\ [(33)_q 34]_3 &: (4,2)_{q+1} (3)_{q+1} (3)_{q+1} (2,4)_{q+1} \\ [(44)_q 43]_3 &: (4)_{q+1} (2,3)_q (2,3)_q (3,2) (3,3,2)_q (4)_{q+1} \end{aligned}$$

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

$$\begin{aligned} F_{101} &= \csc(u/2) \cdot [0.8661 + \sin(u/6) - \sin(q+1)u] \\ F_{101} &= \csc(u/2) \cdot [0.8661 - \sin(u/6) - \sin(q+1)u] \\ F_{101} &= \cos 2v [\sin(w+2v) + D \cdot \sin w \cdot \cos(2w+v) - 2\cos 3w] \end{aligned}$$

where  $u = 12\pi/n$ ,  $v = 2\pi/n$ ,  $w = 4(q+1)$  and  $D = (2\cos 3v + 1)/\cos 2v$ . Using this modified Laue method, the crystal structure of nine new polytypes of silicon carbide were determined. The crystal structure of these new polytypes can be indicated by the Z stacking sequences as the following,

$$\begin{aligned} 231R: & [(33)_{12} 32]_3, & 249R: & [(33)_{13} 32]_3, \\ 321R: & [(33)_{17} 32]_3, & 339R: & [(33)_{18} 32]_3, \\ 237R: & [(33)_{12} 34]_3, & 417R: & [(33)_{22} 34]_3, \\ 453R: & [(33)_{24} 34]_3, & 93R: & [(44)_5 43]_3, \\ 261R: & [(44)_{10} 43]_3. \end{aligned}$$

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  $\frac{1}{6}\langle 112 \rangle$

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  $(\bar{1}\bar{1}\bar{1})_t$ , 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  $(\bar{1}\bar{1}\bar{1})_t$  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, a 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  $(\bar{1}\bar{1}\bar{1})_t$  antiphase structures by the splitting of  $00\bar{1}_t$  reflection in  $[1\bar{1}\bar{1}]_t$  and  $[\bar{1}\bar{1}\bar{1}]_t$  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  $(\bar{1}\bar{1}\bar{1})_t$  which make an angle of  $74^\circ$ , and have  $22\text{\AA}$  in spacing (corresponding to ten (111) layers), which coincide 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  $n=1^{11}$  (Friedel's twinning by merohedry): twin symmetry  $4'/m'[4] 3 2'/m[\bar{1}\bar{1}]$ , 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  $F\bar{d}3m$ , 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  $1/8 1/8 1/8, \dots$ . 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.