Acta Cryst. (1953). **6**, 570

Some observations on the crystallography of deformation twins.

By E. O. Hall, *Physics Department, The University, Sheffield* 10, *England.*

(*Received* 5 *February* 1953 *and in revised form* 23 *March* 1953)

Although text-books on metal physics usually include some details on the crystallographic components of twins (Schmid & Boas, 1950, p. 94; Barrett, 1943), no complete table appears to have been published. The writer has had occasion to tabulate these, and during this work a number of errors in previous work were revealed. The complete data on deformation twins are therefore given in Table 1.

Twin components

In this table K_1 is the composition plane, η_1 is the direction of shear, K_2 is the second undistorted plane, and η_2 is the direction lying in K_2 and in the plane of shear. The magnitude of the shear is given by (Schmid & Boas, 1950, p. 72)

$$s = 2 \cot \theta \, ,$$

where θ is the angle between K_1 and K_2. Since θ can be expressed as a function of the sides and angles contained in the unit cell, an analytical expression for s, common to one group of metals, can often be obtained. These formulae will now be discussed in turn.

Hexagonal metals

Here the expression for the shear is given as (Schmid & Boas, 1950, p. 94)

$$s = \frac{(c/a)^2 - 3}{\sqrt{3} \, . \, c/a} \, .$$

Recent values of c/a ratios of these metals have been inserted, and values of the shear calculated. They differ slightly from those given by Schmid & Boas.

An anomalous case of twinning in magnesium has been observed by Schiebold & Siebel (1931) with $K_1 = (10\bar{1}1)$, but this result has not been confirmed by other writers (Bakarian & Mathewson, 1943; Barrett & Haller, 1947). K_2 in this mode of twinning would be the basal (0001) plane. The shear thus has the abnormally high value of 106·6 %, which, on energy grounds, might explain its comparative rarity.

Titanium, like magnesium, also has abnormal modes of twinning. Liu & Steinberg (1952) found, in addition to the normal $(10\bar{1}2)$ mode, other sets of twins with composition planes $(11\bar{2}1)$, $(11\bar{2}2)$, $(11\bar{2}3)$ and $(11\bar{2}4)$. Only the first two of these have been confirmed by Rosi, Dube & Alexander (1953). A $(1\bar{1}00)$ plane is normal to all these planes, and, since it is a plane of symmetry in both twin and matrix, it must represent the plane of shear. A study of atom positions in this plane thus enables K_2, η_2 and s to be determined.

Table 1. *Crystallography of twinning*

Metal	Crystal structure	Twinning indices K_1	η_1	K_2	η_2	Shear S	Theoretical shear	Remarks
α-Fe	B.-c.c.	(112)	$[11\bar{1}]$	$(11\bar{2})$	[111]	0·707	$\sqrt{2}/2$	
Be	H.c.p.	$(10\bar{1}2)$	$[\bar{1}011]$	$(10\bar{1}\bar{2})$	$[10\bar{1}1]$	0·199		$c/a = 1{\cdot}568$
Ti	H.c.p.	$(10\bar{1}2)$	$[\bar{1}011]$	$(10\bar{1}\bar{2})$	$[10\bar{1}1]$	0·189		$c/a = 1{\cdot}587$
Mg	H.c.p.	$(10\bar{1}2)$	$[\bar{1}011]$	$(10\bar{1}\bar{2})$	$[10\bar{1}1]$	0·129	$\dfrac{(c/a)^2 \sim 3}{\sqrt{3} \, . \, c/a}$	$c/a = 1{\cdot}624$
Zn	H.c.p.	$(10\bar{1}2)$	$[10\bar{1}\bar{1}]$	$(10\bar{1}\bar{2})$	$[10\bar{1}1]$	0·139		$c/a = 1{\cdot}856$
Cd	H.c.p.	$(10\bar{1}2)$	$[10\bar{1}\bar{1}]$	$(10\bar{1}\bar{2})$	$[10\bar{1}1]$	0·171		$c/a = 1{\cdot}886$
Mg	H.c.p.	$(10\bar{1}1)$	$[\bar{1}012]$	(0001)	$[10\bar{1}0]$	1·066	$\sqrt{3} \, . \, a/c$	
		$(11\bar{2}1)$	$[\bar{1}\bar{1}26]$	(0001)	$[11\bar{2}0]$	0·638	a/c	
Ti	H.c.p.	$(11\bar{2}2)$	$[\bar{1}\bar{1}23]$	(0001)	$[11\bar{2}0]$	1·276	$2a/c$	Anomalous modes
		$(11\bar{2}3)$	$[\bar{1}\bar{1}22]$	(0001)	$[11\bar{2}0]$	1·914	$3a/c$	
		$(11\bar{2}4)$	$[\bar{2}\bar{2}43]$	$(11\bar{2}\bar{4})$	$[22\bar{4}3]$	0·468	$(c^2/a^2 \sim 4)/2c/a$	
β-Sn	Tetragonal	(301)	$[\bar{1}03]$	$(\bar{1}01)$	[101]	0·119	$(c/2a)(a^2/c^2 - 3)$	$c/a = 0{\cdot}541$
In	Tetragonal	(101)	$[10\bar{1}]$	$(\bar{1}01)$	[101]	0·150	$(c/a)(1 - a^2/c^2)$	$c/a = 1{\cdot}078$
As	Rhombohedral	(110)	$[00\bar{1}]$	(001)	[110]	0·270		$\alpha = 84^\circ\, 18'$
Bi	Rhombohedral	(110)	$[00\bar{1}]$	(001)	[110]	0·118	$\dfrac{2 \cos \alpha}{\{\frac{1}{2}(1 + \cos \alpha) - \cos^2 \alpha\}^{\frac{1}{2}}}$	$\alpha = 87^\circ\, 34'$
Hg	Rhombohedral	(110)	[001]	(001)	[110]	0·447		$\alpha = 98^\circ\, 13'$
Sb	Rhombohedral	(110)	$[00\bar{1}]$	(001)	[110]	0·125	α = rhombohedral angle	$\alpha = 87^\circ\, 24'$
		(130)	$[3\bar{1}0]$	$(1\bar{1}0)$	[110]	0·299		$\theta = 81^\circ\, 30'$
α-U*	Orthorhombic	'$(1\bar{7}2)$'	[312]	(112)	'X'	0·228		$\theta = 83^\circ\, 30'$
		(112)	'X'	'$(1\bar{7}2)$'	[312]	0·228		$\theta = 83^\circ\, 30'$
		(121)	'X'	'X'	[311]	0·329		$\theta = 80^\circ\, 40'$

* Planes and directions marked X in inverted commas are irrational, but approximate values of their indices are given where possible.

Tetragonal metals

The composition plane of twinning in β-tin has recently been redetermined by Clark, Craig & Chalmers (1950) as the (301) plane. The (010) plane is normal to this, and, since it is a plane of symmetry, it must represent the plane of shear. The intersection of these two planes gives $\eta_1 = [\bar{1}03]$ and a construction of atomic positions in the twinned and untwinned state shows $K_2 = (\bar{1}01)$, $\eta_2 = [101]$.

Chalmers (1935) has studied the atom movements involved in the twinning operation, but he took the lattice as face-centred tetragonal (Clark & Craig, 1952). The unit cell is, in fact, tetragonal with four atoms in the special positions $0, 0, 0$; $0, \frac{1}{2}, \frac{1}{4}$; $\frac{1}{2}, 0, \frac{3}{4}$ and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. An analysis of the atom movements shows that very few of the atoms move into their new positions by simple homogeneous shear. However, the atoms at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ do obey the homogeneous shear rule, and their movement probably stabilizes the deformation twin and allows it to develop.

The composition plane for twinning in indium has also been recently determined (Becker, Chalmers & Garrow, 1952) as of the type (101). By considering the planes of symmetry, as in the case of β-tin, the remaining twin components and the shear can be determined.

Rhombohedral metals

The accepted components for twinning in these metals are $K_1 = (110)$, $\eta_1 = [001]$, $K_2 = (001)$, $\eta_2 = [110]$.

The value for s can then be obtained as

$$s = \frac{4\cos\alpha\sin\frac{1}{2}\alpha}{\{1-3\cos^2\alpha+2\cos^3\alpha\}^{\frac{1}{2}}}$$

or

$$s = \frac{2\cos\alpha}{\{\frac{1}{2}(1+\cos\alpha)-\cos^2\alpha\}^{\frac{1}{2}}},$$

where α is the rhombohedral angle. This corrects the expression given in Schmid & Boas (1950, p. 94). The redetermined values of the shear are listed.

α-Uranium

Cahn (1953) has studied the twinning modes of α-uranium. This metal is orthorhombic, and some components of the twins have irrational indices. Examples of these are more common in minerals, for, in metals of high symmetry, compound twins, with all elements rational, are usually observed. Frank (1953) has shown how these irrational modes are to be expected from a consideration of the allied structure of zinc.

References

Bakarian, P. W. & Mathewson, C. H. (1943). *Trans. Amer. Inst. Min. (Metall.) Engrs.* **152**, 226.

Barrett, C. S. (1943). *Structure of Metals*, p. 312. New York: McGraw-Hill.

Barrett, C. S. & Haller, C. T. (1947). *Trans. Amer. Inst. Min. (Metall.) Engrs.* **171**, 246.

Becker, J. H., Chalmers, B. & Garrow, E. G. (1952). *Acta Cryst.* **5**, 853.

Cahn, R. W. (1953). *Acta Metallurgica*, **1**, 49.

Chalmers, B. (1935). *Proc. Phys. Soc.* **47**, 733.

Clark, R. & Craig, G. B. (1952). *Progress in Metal Physics*, **3**, 115.

Clark, R., Craig, G. B. & Chalmers, B. (1950). *Acta Cryst.* **3**, 479.

Frank, F. C. (1953). *Acta Metallurgica*, **1**, 71.

Liu, T. S. & Steinberg, M. A. (1952). *J. Metals*, **4**, 1043.

Rosi, F. D., Dube, C. A. & Alexander, B. H. (1953). *J. Metals*, **5**, 257.

Schiebold, E. & Siebel, G. (1931). *Z. Phys.* **69**, 458.

Schmid, E. & Boas, W. (1950). *Plasticity of Crystals*. London: Hughes.

Acta Cryst. (1953). **6**, 571

Surface layer on crystalline quartz.

By O. S. Heavens, *The University, Reading, Berks., England*

(*Received* 7 *March* 1953)

In an X-ray examination of particles of crystalline quartz, Nagelschmidt, Gordon & Griffin (1952) have deduced the presence of an amorphous layer on the surface of the particles. The presence of such a layer is assumed by Clelland, Cumming & Ritchie (1952), who state that such a layer may be produced by the action of hydrochloric acid on the crystal surface. The thickness of the layer, deduced from the X-ray evidence, is of the order of 300 Å. Such a layer on a crystalline material would be readily detected by electron diffraction. In the absence of an amorphous surface layer, a rock-quartz crystal surface yields a sharp Kikuchi pattern. Fig. 1(*a*) shows the pattern obtained after treating such a crystal surface with boiling concentrated hydrochloric acid for 1 hr. The pattern is found to be very slightly *clearer* than that obtained before treatment. This may be due to the removal by etching of a strained (but still crystalline) surface layer.

It is of importance to know the minimum thickness of amorphous layer which could be detected by obscuration of the Kikuchi pattern. This will depend on the surface microtopography. If the local surface nowhere makes an appreciable angle with the mean surface, then (neglecting refraction) the depth of penetration of the beam is given by $d \sim \frac{1}{2}L\theta$, where θ is the glancing angle and L the mean free path. Putting $\theta = 0{\cdot}01$ radian and $L \sim 1000$ Å, we obtain $d \sim 5$ Å. The presence of an amorphous layer of this thickness would thus completely obliterate the Kikuchi pattern. If the local surface makes large angles with the mean surface the situation is less favourable. For the worst case, in which the beam enters and leaves a projection normally, the depth of amorphous layer