Mechanical twinning in crystals

J. P. Stark
Center for Materials Science, University of Texas at Austin, Austin, Texas 78712
(Received 22 February 1988)

In mechanical twinning of crystals, compound twins are examined for symmetry and found that by necessity the plane of shear is a mirror plane to enable the twins of the first and second kind to exist simultaneously.

In mechanical twinning, shear stress acts along a shear direction η_1 which lies in an invariant plane referred to as the twin plane with Miller indices K_1, see Fig. 1. Due to the action of the mechanical deformation, the envelope of planes and directions of the parent crystal are deformed from a reference sphere to an ellipsoid of revolution and a twin crystal is formed. In this modified reference system, two planes remain invariant as follows: the twin plane referred to above and the invariant plane which carries the Miller indices K_2. Additionally, the fact that two planes remain invariant prescribes that a set of vectors in those two planes remain invariant. The two invariant vectors of experimental interest are the shear direction referred to above and a second invariant direction η_2 which lies as the intersection of the second invariant plane K_2 and this plane's intersection with still a third plane often referred to as the plane of shear. The plane of shear is perpendicular to the twin plane, contains the shear direction vector η_1, and will be referred to as having Miller indices A below. Since the plane of shear contains both invariant directions η_1 and η_2, and since the plane of shear is perpendicular to both invariant planes, the plane of shear also contains the vectors normal to each of the invariant planes. In what follows, these two vectors are the vectors in reciprocal space with the same indices as K_1 and K_2. Reciprocal-space vectors for directions will be denoted by the addition of an asterisk; hence $\mathbf{K}_1^*$ and $\mathbf{K}_2^*$ refer to planes K_1 and K_2. In the same sense, the normal to the plane of shear A is a vector $\mathbf{A}^*$.

Cahn[1] has made a detailed study of the deformation of α-uranium including the twinning modes. Based upon his assessment of uranium being a low-symmetry material, he found that twins of both the first and second kinds were present. He also found that he could identify a compound twin and named the phenomena. His identification is based upon the Miller indices of both invariant planes to have rational indices. This basis automatically assures that the two invariant twinning directions are also rational. Briefly stated, in a twin of type 1, the twin plane with Miller indices K_1 and the direction η_2; which lies as the line of intersection of the invariant plane, with Miller indices K_2, and the plane of shear; both have rational indices. In a twin of type 2, the invariant plane, Miller indices K_2, and the shear direction η_1 have rational indices.

In a twin of type 1, the parent and twin crystals are related to one another by a mirror image of the unit cells across the twin plane. A suitable point-group operator which accomplishes the generation of the twin along with its interface is a mirror operator on the twin plane m_{k_1}. Note that the subscript denotes the plane or direction upon which the operator is based. In a twin of type 2, the parent and twin crystals are related by a twofold rotation along the shear direction. The point-group operator for this twin type is 2_{η_1}. Thus, the four vectors $\mathbf{K}_1^*$, $\mathbf{K}_2^*$, η_1, and η_2 which all lie in the plane of shear are related to each other geometrically by the fact that the shear direction η_1 must lie in the shear plane, K_1, and the second invariant direction η_2 must lie in the second invariant plane K_2.

Data on various deformation twinning observations are compiled in Refs. 2 and 3. One may identify the various operators which carry the parent crystal in to its twin following the Seitz notation for space groups.[4] For a twin of type 1, Cahn suggests that the two crystals are related by a mirror across the twin plane. This would imply that the operator for a type-1 twin is the following:

$$\alpha_1=(m_{k_1} \mid t_1) \ . \tag{1}$$

For a type-2 twin, Cahn suggests that the twin operator is

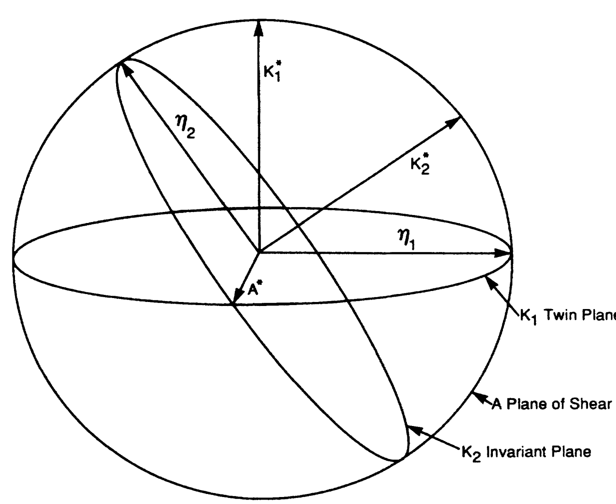

FIG. 1. Geometry of parent crystal.

TABLE I. Summary of compound twins.

Crystal	Group	Plane of shear as a mirror
Cubic metals	$Im3m, Fm3m$	$(1\bar{1}0)$
Si,Ge	$Fd3m$	$(1\bar{1}0)$
GaSb,InSb,ZnS	$F\bar{4}3m$	$(1\bar{1}0)$
PbS	$F\bar{4}3m$	$(1\bar{1}0)$
Hexagonal-trigonal		
As,Sb,Bi	$R\bar{3}C$	$(\bar{1}2\bar{1}0)$[a]
Hg	$R\bar{3}m$	$(\bar{1}2\bar{1}0)$
α-Zr,Zn,Mg	$P6_{3/m}mc$	$(\bar{1}2\bar{1}0)$
$CaCO_3$,$NaNO_3$,$FeCO_3$	$R\bar{3}c$	$(\bar{1}2\bar{1}0)$[a]
Tetragonal		
$KAlSi_2O_6$	$I4_1/a$	(001)[a]
BSn	$I4/a\ md$	(010)
In	$I4/m\ mm$	(010)
Mn_3O_4	$I4_1/a\ md$	(010)
TiO_2,SnO_2	$P4_2/m\ nm$	(010)[a]
Orthorhombic		
α-U	$Cmcm$	(001)
KNO_3	$Pbnm$	(001)[a]
$CaSO_4$	$Pbnm$	(010)[a]
$BaSO_4$	$Pnma$	(001)[a]
Monoclinic		
$Pb_4As_2S_7$	$P2_1/m$	(010)[a]
$CaMgSi_2O_6$	$C2/c$	(001)[a]
$(NH_4)_3H(SO_4)_2$	$C2/c$	(001)[a]

[a]Glide or displaced mirror.

a 180° rotation about the shear direction as follows:

$$\alpha_2=(2_{\eta_1}\,|\,t_2)\ . \tag{2}$$

In these equations, the subscript on the point-group operator denotes the plane or direction upon which the operator is based.

To have a compound twin, both of these operators should be altering the symmetry of the parent crystal simultaneously. That is, the homologous points r_2 and r_1 between the two twinned crystals for a type-1 twin are related by

$$r_2=(m_{k_1}\,|\,t_1)r_1 \tag{3}$$

and the analogous relation for twins of type 2 is as follows:

$$r_2=(2_{\eta_1}\,|\,t_2)r_1\ . \tag{4}$$

With the compound twin, both of these operators must be restricting the symmetry of the twin.

Now point-group operators generally require an orthogonal coordinate system for easy expression. It is indeed fortunate that a natural orthogonal coordinate system is available herein. Namely, the vector $\mathbf{K}_1^*$ associated with the twin plane is perpendicular with a vector describing the shear direction $\boldsymbol{\eta}_1$. The cross product of those two vectors defines the third direction of a logical

TABLE II. Glide or displacement vectors, $(m_A\,|\,\tau)\in G_1$.

Crystal	τ
Hexagonal-Trigonal	
As,Sb,Bi	$(0,0,0,\frac{1}{2})$
$CaCO_3$,$NaNO_3$,$FaCO_3$	$(0,0,0,\frac{1}{2})$
Tetragonal	
$KAlSi_2O_6$	$(0,\frac{1}{4},\frac{1}{2})$
TiO_2,SnO_2	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
Orthorhombic	
KNO_3	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$CaSO_4$	$(0,\frac{1}{2},\frac{1}{2})$
$BaSO_4$	$(\frac{1}{2},0,\frac{1}{2})$
Monoclinic	
$Pb_4As_2S_7$	$(0,\frac{1}{2},0)$
$CaMgSi_2O_6$	$(0,0,\frac{1}{2})$
$(NH_4)_3H(SO_4)_2$	$(0,0\frac{1}{2})$

orthogonal coordinate system denoted here as $\mathbf{A}^* = \eta_1 \times \mathbf{K}_1^*$. The vector $\mathbf{A}^*$ is perpendicular to the plane of shear with Miller indices A.

Now following the operations denoted in Eqs. (3) or (4), the two crystals, the parent and twin, are related to one another by the space groups relating their structures. G_1 is the group of the parent crystal and G_2 that of the twin.

For every point deduced from r_1, in the parent crystal by the operation of the group element $(g \mid \tau) \in G_1$, an analogous point in the twin is generated by the operation of the twin operator. The relation follows:

$$\begin{aligned} r_2 &= (\alpha \mid t)(g \mid \tau) r_1 \\ &= (\alpha g \mid \alpha\tau + t) r_1 \ . \end{aligned} \tag{5}$$

If we now consider a compound twin where Eqs. (1) and (2) describe an appropriate relation between the parent and twin simultaneously, it seems obvious that a compound twin must have a twin operator where rotation about the shear direction and a mirror across the twin plane both occur. This is only possible if the plane of shear is a mirror plane. Thus, the twin operator for a compound twin should be expressible as the following:

$$\begin{aligned} (\alpha \mid t) &= (2_{\eta_1} \mid t_2) \\ &= (m_{k_1} \mid t_2 - m_{k_1} \tau)(m_A \mid \tau) \ . \end{aligned} \tag{6}$$

Now considering Eqs. (5) and (6), it is apparent that the only way in which a compound twin is possible is when the mirror associated with the plane of shear, Miller indices A, is a member of the space group of the parent crystal. That is, $(m_A \mid \tau) \in G_1$.

Such a hypothesis has been tested and the results are given in Tables I and II. The twinning data, K_1, K_2, η_1, and η_2, taken for these results appear in Refs. 2 and 3 and are summarized in Table III; the plane of shear A is deduced from these results. A necessary condition for the data to be represented is that the twin plane with reciprocal-space vector $\mathbf{K}_1^*$ is perpendicular to the shear direction η_1. The space groups of the crystals were found in Wykoff.[5] In some cases illustrated in Table I, it was immediately obvious that the plane of shear was a symmetry plane. In others, the glide mirror needed to be worked out as given in Table II.

Based upon the above, the following rule must be true: The plane of shear in compound mechanical twinning

TABLE III. Twinning results.

System	K_1	η_1	K_2	η_2
Cubic				
Cu and fcc alloys	(111)	$[11\bar{2}]$	$(11\bar{1})$	[112]
W,Cr,α-Fe,Mo,Na	(112)	$[11\bar{1}]$	$(11\bar{2})$	[111]
Gc,Si	(111)	$[11\bar{2}]$	$(11\bar{1})$	[112]
Hexagonal-Trigonal				
As,Sb,Bi,Hg	$(\bar{1}012)$	$[10\bar{1}1]$	$(10\bar{1}1)$	$[\bar{1}012]$
α-Zr,Mg,Zn	$(10\bar{1}2)$	$[\bar{1}011]$	$(10\bar{1}2)$	$[10\bar{1}1]$
$CaGO_3$,$NaNO_3$	$(\bar{1}012)$	$[10\bar{1}1]$	$(10\bar{1}1)$	$[\bar{1}012]$
$FeCO_3$				
Tetragonal				
$KAlSi_2O_6$	(110)	$[1\bar{1}0]$	$(1\bar{1}0)$	[110]
β-Sn	(301)	$[\bar{1}03]$	$(\bar{1}01)$	[101]
In	(101)	$[10\bar{1}]$	$(\bar{1}01)$	[101]
Mn_3O_4	(101)	$[\bar{1}01]$	$(\bar{1}01)$	[101]
SnO_2,TiO_2	(101)	$[\bar{1}01]$	$(\bar{1}01)$	[101]
Orthorhombic				
α-U	(130)	$[3\bar{1}0]$	$(1\bar{1}0)$	[110]
KNO_3	(110)	$[1\bar{1}0]$	$(1\bar{3}0)$	[310]
$CaSO_4$	(101)	$[\bar{1}01]$	$(\bar{1}01)$	[101]
$BaSO_4$	(110)	$[1\bar{1}0]$	$(1\bar{1}0)$	[110]
Monoclinic				
$Pb_4As_2S_7$	(101)	$[\bar{1}01]$	$(\bar{3}01)$	[301]
	(100)	[001]	(001)	[100]
$CaMgSi_2O_6$	(001)	[100]	(100)	[001]
$(NH_4)_3(HISO_4)_2$	(310)	$[1\bar{3}0]$	$(1\bar{1}0)$	[110]

crystals is a mirror plane.

Other twin generators have been suggested for mechanical twinning types 1 and 2 and are twofold rotation operators. These operators lead to erroneous conclusions as is discussed in the Appendix. Based upon that discussion, the above rule is unique in identifying compound twinning.

APPENDIX

Some authors have adopted the idea that the generators of the twin types i, γ_i, for $i=1,2$ are the following:

$$\gamma_1=2_{k_1} \, , \qquad \gamma_2=2_{\eta_1} \, . \tag{A1}$$

This approach leads to logical inconsistencies with experimental results as follows.

We take as our basis the following well-accepted idea that any crystal boundary generator $\gamma_i \notin G$ (G is the crystal point group here for brevity); otherwise, no boundary is generated and a single crystal results when $\gamma_i G=G$. That γ_i generates a twin boundary is no exception.

Hence we must have for compound twins $\gamma_1 G=\gamma_2 G\neq G$ since the action of both of the twin generators on the parent crystal must be the same. Now

$$\begin{aligned}\gamma_1 G &= 2_{\mathbf{k}_1} G = m_{\eta_1} m_A G \\ &= \gamma_2 G = 2_{\eta_1} G = m_{\mathbf{k}_1} m_A G \, .\end{aligned} \tag{A2}$$

The only way that $m_{\eta_1} m_A G = m_{\mathbf{k}_1} m_A G$ is for $m_{\eta_1}, m_{\mathbf{k}_1} \in G$. Then since $\gamma_1, \gamma_2 \notin G$, $m_A \notin G$. This is inconsistent with the data in Table I. Also, the twin plane K_1 is now a mirror, and this violates the known crystal symmetry tabulated in Table III. For example, in the fcc metals, the (111) is not a mirror plane; in Si and Ge diamond cubic, the (111) is not a mirror plane; in the bcc metals, the (112) is not a mirror plane; and so forth for all the twin planes mentioned in Table III.

[1]R. W. Cahn, Acta Metall. **1**, 49 (1953).
[2]*Deformation Twinning,* edited by R. E. Reed-Hill, J. P. Hirth, and H. C. Rogers (Gordon and Breach, New York, 1964).
[3]*Mechanical Twinning of Crystals,* edited by M. V. Klassen-Neklyudova (Consultants Bureau, New York, 1964).
[4]F. Seitz, Ann. Math. Stat. **37**, 17 (1936).
[5]R. W. G. Wykoff, *Crystal Structures* (Interscience, New York, 1963).