Twinning and symmetry

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Twins of the first and second kind are found to be indistinguishable in crystals of high symmetry. A basis for the symmetry dependence is found which will delineate some situations where this is expected. Namely, when the space group of the twinned crystals is the same and contains the transformation operator which relates the two crystals, and when the twinning operator contains no translation, such compound twins are expected. Furthermore, the two invariant planes and directions are members of the same families of planes and directions, respectively. Otherwise, either compound twins are found where the invariant planes are not members of the same family or the compound twin transforms into the two separate kinds.

INTRODUCTION

Cahn[1] has made a detailed study of the deformation of α-uranium including the twinning modes. Since uranium is a crystal of low symmetry, he found that twins of both the first and second kinds were present in the material. Briefly stated, in type 1, the twin plane with reciprocal lattice vector K_1, and the direction η_2, which lies as the line of intersection of the invariant plane, with reciprocal lattice vector K_2, and the plane of shear are both rational. In type 2 the invariant plane with reciprocal lattice vector K_2 and the shear direction η_1 are rational. Herein, the lattice vector Q_1 is perpendicular to the twin plane (K_1) while the Q_2 is perpendicular to the invariant plane (K_2).

Cahn states that compound twins with rational indices for K_1, K_2, η_1, and η_2 are found in cubic, hexagonal, and trigonal metals. His basis for the statement was the experimental observations made by others as well as the work he undertook with uranium. It is the purpose of this Brief Report to rationalize Cahn's statement and show that such an observation is based on the symmetry of the crystal involved and the twinning operation, α.

Examples of the relation between symmetry and the twin domains of crystals where the domains are related to the coset of the space group of the parent crystal have been worked out recently by Jancovec[2] and Chuiko.[3] The group symmetry can also describe the domain boundary as developed by Gratias, Portier, Fayard, and Guymont.[4] A useful summary of the status of the structural relationships is also given in Wyckoff.[5]

The Seitz[6] notation will be used for space-group operations as needed.

DEVELOPMENT

Consider a twin of type 1. We establish a right-handed coordinate system with the z axis parallel to the [001] of the parent crystalline cell. It is assumed that the crystal direction perpendicular to the twin plane, Q_t, or K_1 in reciprocal space, makes an angle θ with the [001] and thus the z axis. It is possible to rotate the crystal an angle ϕ_z about the z axis and bring the vector Q into the x-z plane, i.e., the plane perpendicular to the y axis. A second crystal rotation of angle θ_y about the y axis would bring the twin plane perpendicular with the z axis and parallel with the x-y plane. The operation of twinning then occurs on the x-y plane by the imposition of the twin operator γ. Generally, the twin operator γ will be either a rotation of 180° about the z axis or a mirror image about the x-y plane. The inverse rotations $\theta_y^{-1}\phi_z^{-1}$ will bring the two into position in relation with the parent crystal. (See Fig. 1.)

Thus the operator which will create the twinned crystal relative to the parent is $(\alpha \mid t)$:

$$\alpha=\phi_z\theta_y\gamma\theta_y^{-1}\phi_z^{-1} . \tag{1}$$

The homologous points r_1 and r_2 between the two crystals (1) and (2) are related by

$$r_2=(\alpha \mid \underline{t})r_1 . \tag{2}$$

The two crystals are related to one another by the two space groups describing their structures. G_1 is the group of the parent crystal and G_2 is the group of the twin domain. In any twin the unit-cell shape and size are preserved; however, the group of the twin may not be identical with the group of the parent due to the relaxation of atomic positions following the shear along η_1.

Every point r_1' deduced from r_1 by any $(g \mid \Psi)$ where the latter is a member of the group of the parent crystal is equivalent to $(\alpha \mid \underline{t})$ and defines the same twin boundary;

$$r_2=(\alpha \mid \underline{t})(g \mid \Psi)r_1=(\alpha g \mid \alpha\Psi+\underline{t})r_1 \tag{3}$$

or $(\alpha \mid \underline{t})G_1$ for the whole group.

It is easy to show by direct matrix manipulation that the rotational portion of the interface operator $(\alpha \mid t)$ may be rearranged into an equivalent operator as follows:

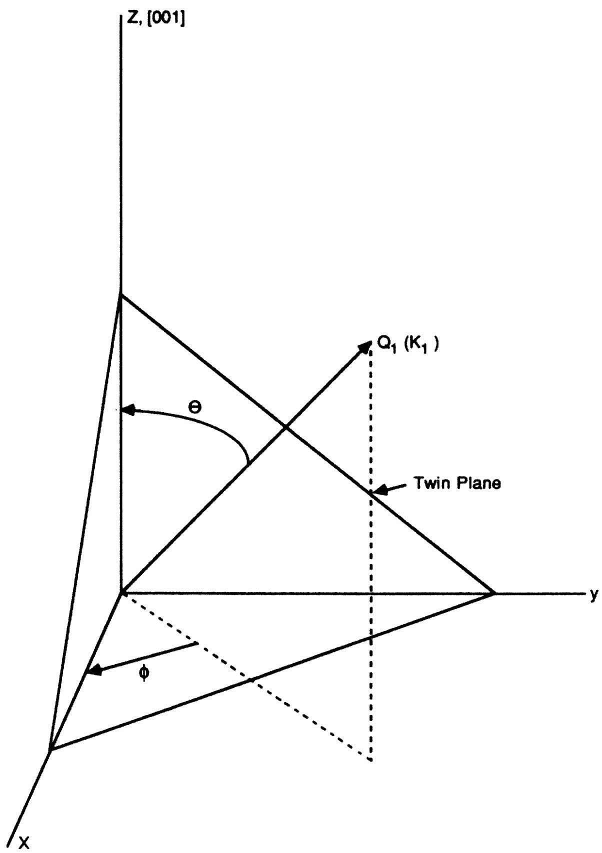

FIG. 1. Twinning geometry.

$$\phi_z = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \theta_y = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix},$$

$$\gamma = m_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}, \quad \text{or } \gamma = -m_z = 2_z , \tag{4}$$

$$\alpha = \phi_z \theta_y^2 \phi_z^{-1} \gamma$$
$$= \beta\gamma .$$

At this point we concentrate on those crystal systems where the twin operator γ is a member of the point group of the parent crystal. If we set

$$(\alpha \mid \underline{t}) = (\beta \mid t_1)(\gamma \mid t_2)$$
$$= (\gamma \mid \beta t_2)(\beta^{-1} \mid \gamma t_1) , \tag{5}$$

it is clear that when

$$(\gamma \mid t_2) G_1 = G_1 ,$$
$$G_2 = G_2 (\gamma \mid \beta t_2) , \tag{6}$$

we find

$$G_2 = (\beta \mid t_1)(\gamma \mid t_2) G_1 (\gamma \mid t_2)^{-1} (\beta \mid t_1)^{-1}$$
$$= (\beta \mid t_1) G_1 (\beta \mid t_1)^{-1} , \tag{7}$$

and

$$G_1 = (\beta \mid -\beta\gamma t_1)(\gamma \mid -\gamma\beta t_2) G_2 (\gamma \mid \beta t_2)(\beta^{-1} \mid \gamma t_1) ;$$

hence, for those structures, the twin may be generated by the equivalent operation

$$r_2 = (\beta \mid t_1) r_1 . \tag{8}$$

The only situations apparent to this author where Eqs. (5)–(8) will define an appropriate structure is when $\underline{t} = t_1 = t_2 = 0$ and $G_1 = G_2$.

Now the applicable structures in the above development are those where the twin plane operator $(\gamma \mid 0)$ as applied to the [001] direction of the crystal is a member of the space group of the crystal. For such structures, the equivalent twin generator $(\beta \mid 0)$ is simply a rotation of the structure by an angle of 2θ around the normal to the plane defined by the vectors [001] and Q_1; i.e., the cross product of the [001] and the twin plane normal, Q_1.

When the crystal is operated upon by $(\alpha \mid 0)$, the results is the generation of a twin where Q_1 becomes Q_1', and Q_2 becomes Q_2'; where $Q_1 = \pm Q_1'$, and Q_2 is rotated into Q_2' by the twin operator $(\alpha \mid 0)$. Here and hereafter, the plus sign refers to $\gamma = 2_z$ and the minus sign to $\gamma = m_z$.

However, when the twin operator $(\gamma \mid 0)$ is a member of the parent space group G_1 which is the same as that of the twin, the operator gives a twin which is identical with the first. Q_1 becomes Q_1'' and Q_2 becomes Q_2''. Here, however, Q_1'' is rotated from Q_1 by the angle 2θ while the same thing happens to Q_2. Now if the twin is the same crystal as described in the above, then $Q_1' = \pm Q_2''$ and $Q_2' = \pm Q_1''$. Of course, this implies that K_1 is effectively rotated into K_2, and vice versa. Similarly, the direction of shear η_1 is rotated into η_2. Because of these equivalent rotations which interchange the roles of the two planes and directions, it is obvious that if K_1 is rational, K_2 must be also, with similar relation between the shear directions η_1 and η_2. Furthermore, since effectively K_1 is replaced by K_2 in the twin, they must be members of the same family of planes. The same statement is true of two directions, η_1 and η_2.

Thus we are left with the conclusion that the twin is both a member of the first and second kind simultaneously corresponding to a type-1 twins so long as the twin generator, $(\gamma \mid 0)$, is a symmetry element of the crystal, the group of the parent and twinned crystals are the same, and there is no necessary translation in the twin operator. Furthermore, for such systems, the twin plane and invariant plane are members of the same family of planes. Also, the shear directions η_1 and η_2 are also members of the same family.

There are a large number of systems which apparently follow these restrictions; namely, the twins in cubic and hexagonal metals[7] as well as many minerals in virtually all crystal systems.[8] It is obvious that one of the important restrictions mentioned is that the space group of the parent and twinned crystal is the same; Eqs. (5)–(8) may have other solutions but they are not at all apparent to this author. The atomic relaxations after the twinning shear may not change the space group in the solution found here and this explains why one will find that the above rules apply to some twin planes but not to others associated with the same crystal.

Additionally, the subset of twins which follow the above restrictions can now be separately identified, and it has been suggested[9] that they be referred to by a terminology different from compound twin. The designation of identical twin seems meaningful to this author in view of the invariant planes belonging to the same family.

Interestingly, α-U (with a space group *Cmcm*) has the necessary symmetry of its parent crystal to have a set of twins be identical; however, its invariant planes are not from the same family. The reason is that the atomic relaxations following twinning make the space group of the twin different from the original crystal.[1]

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