

CHAPTER 20

Deformation Twinning

85. CRYSTALLOGRAPHY OF TWINNING

An outline description of the crystallography of deformation twinning was given in Section 8, where the twinning elements K_1 , K_2 , η_1 and η_2 , together with the plane of shear, S , and the shear magnitude, s , were defined. These elements define a *twinning mode* and this section will be concerned mainly with the factors which determine the modes observed in particular crystal structures. In the formal theory, no restriction will be placed on the twinning elements, and the criteria used to select the operative modes, such as reasonably small values of s , are partly intuitive and have to be justified by comparison with experiment. This approach is best for most twins, but there are some special examples in which the twin boundary may be regarded as a particular case of a high angle grain boundary. K_2 and η_2 must then be operative slip elements of the original (or parent)[†] structure.

The theory to be developed will include a more rigorous treatment of the two types of deformation twin discussed on p. 54 and of the orientation relations between parent and twin crystals. In the classical theory, two twinned structures are related by reflection in a plane (the twinning plane) or by a rotation of 180° about a direction (the twinning direction) and this leads to four different relative orientations in the most general case. As discussed on p. 54, a sufficient condition for a simple shear to reproduce the original lattice, or some superlattice of the original lattice, is that a unit cell of the structure, defined by three non-coplanar vectors in K_1 and K_2 , is sheared into an equivalent cell. The orientation of the new (twin) lattice relative to the original lattice may then be described either as a reflection in K_1 or as a rotation of 180° about η_1 . However, the important feature of deformation twinning is the shape change resulting from the simple shear, and it thus seems logical to consider the possibility of a more general definition which rests only

[†] Twinning is a mutual condition and each crystal of a twin pair may be regarded as the twin of the other. In deformation twinning, this reciprocity means that equal but oppositely directed shears will convert region 1 into region 2 and vice versa. In some experimental conditions, such as twin arrays produced by martensitic transformation, the twin boundaries may readily be induced to move in opposite directions by opposite external stresses. Often, however, deformation twins nucleate and grow from an original single crystal matrix which is then conventionally described as the parent structure. The nomenclature is a little unfortunate, inasmuch as the parent of a given twin is also a twin of that twin.

on the requirement that a simple shear deformation of the parent lattice will reproduce this lattice in another orientation. This more general definition, proposed by Crocker (1959) and Bilby and Crocker (1965), leads to the prediction of additional possible modes, in which either three or four of the twinning elements may be irrational, and to non-classical orientation relations between twin and parent.

As already noted on p. 54, there are only two classical orientation relations for lattices and for centrosymmetric structures, and these are often described simply as "reflection" and "rotation" twins respectively, it being understood that the type I reflection is in K_1 and the type II rotation is about η_1 . The division into type I and type II twins is most conveniently made on the basis of rational K_1 and η_2 or rational K_2 and η_1 respectively, but many structures form compound twins in which all four elements are rational. For compound twins, the plane of shear must be rational and, if it is a mirror plane of the structure, orientations I and II become identical (see below). However, there is no general requirement of this type so that, even with compound twins, it may be necessary to distinguish between two possible orientation relations which may be called type I compound and type II compound twins respectively (Rowlands *et al.*, 1968). For clarity, Christian and Laughlin (1988) have suggested that when the type I and type II orientations of a compound mode are equivalent, it should be described as having a "combined" orientation.

The simple crystallography of compound twins in structures of high symmetry led to a method of deducing the twinning elements by choosing a plane of symmetry normal to K_1 as the plane of shear, thus defining η_1 . A procedure of this kind has no obvious physical significance and also has the disadvantage of resting on an experimental determination of K_1 , whereas the aim of a theory should be to predict all of the twinning elements. The method does give the correct twinning elements for many of the twins observed in metals (Hall, 1954), but becomes unwieldy or incorrect in cases where some of the elements are irrational. A more systematic theory was developed by Jaswon and Dove (1956, 1957, 1960), who assumed that the twinning elements may be selected by minimizing the magnitude of the shear. They considered first a type I twin in a simple Bravais lattice, so that parent and twin are mirror images in K_1 . If the twinning shear is to move all the parent lattice sites to their correct twin positions, the possible η_1 directions are readily found by projecting parent sites onto the common K_1 plane.

Consider a set of parallel lattice planes of spacing d and label them consecutively as ... $\bar{3}\bar{2}\bar{1}0123\dots$, etc. A homogeneous shear s of the lattice on the positive side of plane 0 is now specified by translating planes $123\dots$ parallel to themselves through distances sd , $2sd$, $3sd$, etc. in the direction of the unit vector \mathbf{l} parallel to η_1 . For a type I twin in which *all* lattice points are moved to their final positions by the shear, the new positions of the lattice points must be mirror images in K_1 of their original positions. Thus if the lattice sites of plane $\bar{1}$ are projected onto plane 1, the possible η_1 directions are given by the set of vectors connecting any site of plane 1 to any site projected from plane $\bar{1}$.

We have seen previously in Fig. 8.12 that the assumption that the shear moves all the lattice points to their final positions is not necessarily correct, as the structure of the interface may require in addition a relative translation of the parent and sheared lattices.

However, any such translation \mathbf{t} [see eqn. (9.1)] cannot be detected macroscopically or by X-ray diffraction, so that the classical descriptions of the orientation relations remain valid. For the purpose of deducing the crystallographic elements of a particular twinning mode, only the shear components of the total relative displacements need be considered and neither non-zero values of \mathbf{t} nor any inhomogeneous displacements in the interface region will affect the calculation of the mode of minimum shear. At the atomic level, however, such a translation destroys the pseudosymmetry (or "antisymmetry") operations (Pond, 1985, 1988; Pond and Vlachavas, 1983) which relate parent and twin structures; in Fig. 8.12, for example, the reflection symmetry of configuration (a) is destroyed in (b). There are further complications in the descriptions of the orientation relations in non-symmorphic structures which exhibit mirror glide planes or screw rotation axes connecting identical atoms in non-equivalent lattice positions. For example, if the plane of shear is a mirror glide plane in such a structure, the classical type I and type II twinning orientations are in principle distinct but differ from each other only by a rigid translation, so that they are equivalent if the only measurements are of the relative orientations of twin and parent. A further discussion of \mathbf{t} will be given in relation to interface structures and defects. Of course it is quite likely that the operative mode is determined by the interface energy and hence by its atomic structure rather than simply by the value of s , but that was not Jaswon and Dove's hypothesis.

Any plane of the parent lattice which is not itself a mirror plane could serve as the K_1 plane, but it is easy to select the plane which minimizes the lattice shear. Figure 20.1 shows two lattice sites, P and R , in planes 1 and $\bar{1}$, together with the projection R' of R in 1 and it follows that

$$s^2 = (u^2/d^2) - 4 \quad (85.1)$$

where \mathbf{u} is the vector displacement $P \rightarrow R$. Thus a small shear requires a large interplanar spacing and a small vector \mathbf{u} connecting sites in planes 1 and $\bar{1}$. Equation (85.1) may be used directly to find the minimum shear by inspection, but Jaswon and Dove found it convenient to write $u \geq b$, where \mathbf{b} is the smallest possible lattice vector. The resulting inequality

$$d^2 \geq b^2/(s^2 + 4) \quad (85.2)$$

may be regarded as a condition restricting the possible values of d for any chosen maximum value of s . Thus by setting $s=1$, for example, the planes for which the shear is

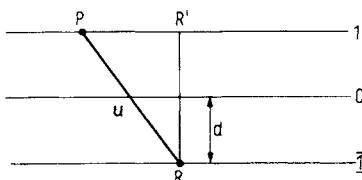


FIG. 20.1. Determination of the shear in type I twinning (after Jaswon and Dove, 1956).

less than unity may readily be enumerated and tested. Jaswon and Dove assumed that the actual K_1 plane will be that plane, which is not a mirror plane, for which the shear is least. Clearly, if there are no planes satisfying the inequality within the chosen maximum value of s , a higher value must be selected. An equivalent procedure is to calculate s for the closest-packed planes (largest d) which are not mirror planes. Substitution of this value of s in the inequality (85.2) will then show which other planes, if any, need to be considered.

Jaswon and Dove's procedure easily leads to the prediction of the actual twinning modes of almost all of the metallic structures in which the atoms occupy the sites of a single Bravais lattice. For example, in the b.c.c. structure, $b^2 = 3a^2/4$ and, for a shear of less than unity, d^2 must be greater than $3a^2/20$. The only planes satisfying the inequality are $\{110\}$, $\{100\}$ and $\{112\}$. The first two planes are mirror planes so that the $\{112\}$ planes are the only possible K_1 planes if the shear is to be less than unity. The shear then has magnitude $s = 2^{-1/2}$ and the η_1 and η_2 directions are $\langle\bar{1}\bar{1}1\rangle$ and $\langle111\rangle$ respectively. Similarly, for the f.c.c. structure, $b^2 = a^2/2$ and, if s is less than unity, d^2 must be greater than $a^2/10$. The planes satisfying the inequality are now $\{111\}$, $\{100\}$ and $\{110\}$ and thus only the $\{111\}$ planes are possible K_1 planes within this restricted range of s . In contrast to the b.c.c. structure, the K_1 planes are thus the closest-packed planes of the f.c.c. structure. In this case s is again $2^{-1/2}$ whilst η_1 and η_2 are $\langle11\bar{2}\rangle$ and $\langle112\rangle$ respectively.

For tetragonal structures, the inequality theorem indicates that the K_1 plane is $\{101\}$ and the η_1 direction is $\langle10\bar{1}\rangle$ for all axial ratios $\gamma = c/a$ which are near to unity. This corresponds to the observed twinning mode in indium which has a face-centred tetragonal (f.c.t.) structure with $\gamma \cong 1.08$. The mode has $s = \gamma - \gamma^{-1}$ and has an interesting relationship with the two cubic twinning modes. The f.c.t. structure may equivalently be regarded as body-centred tetragonal (b.c.t.) and it reduces to f.c.c. when $\gamma_{\text{fct}} = 1$ ($\gamma_{\text{bct}} = 2^{-1/2}$) and to b.c.c. when $\gamma_{\text{fct}} = 2^{-1/2}$ ($\gamma_{\text{bct}} = 1$). The f.c.t. $\{101\}$ twinning mode has $s = 0$ (and thus vanishes) at the first limit, and it becomes equivalent to the b.c.c. $\{112\}$ mode with $s = 2^{-1/2}$ at the second limit. In contrast, the b.c.t. $\{101\}$ mode has $s = 0$ at the second limit and becomes equivalent to the f.c.c. $\{111\}$ mode with $s = 2^{-1/2}$ at the first limit.

Some alloys, and especially many steel martensites, are known to have tetragonal structures for which γ_{bct} is close to unity. Transformation twinning of $\{101\}$ type has been observed in b.c.t. gold manganese alloys (Smith and Gaunt, 1962) but both transformation and deformation twins in steel martensites usually have $K_1 = \{112\}$ of the b.c.t. lattice, so that in this case the dominant twinning mode is derived from the b.c.c. mode and the predictions of the minimum shear hypothesis are not fulfilled. Another example of the failure of this hypothesis in single lattice structures is provided by crystalline mercury. If the structure is referred to a face-centred rhombohedral lattice, the mode of lowest shear is compound with conjugate K_1 planes of type $\{110\}$ and $\{001\}$, but early work in which $\{110\}$ twins were identified now seems to have been incorrect and the operative mode is actually a type II twin with a larger shear.

The Jaswon-Dove approach can also be used for type I twins in structures containing two atoms per primitive unit cell (so-called double lattice structures). The simplest assumption in this case is that the shear moves each lattice point into its mirror image

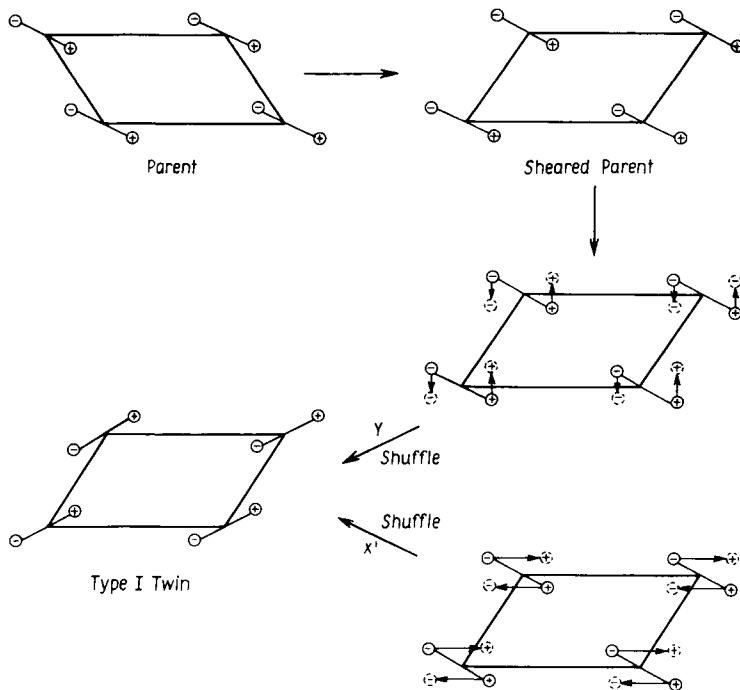


FIG. 20.2. Diagram illustrating possible twinning mechanisms in a double lattice structure. Circles marked + and - represent atoms at equal distances above and below the plane of projection. The sheared parent shows the structure after applying a homogeneous simple shear to all the lattice points, and the shuffles marked X' and Y represent the X and Y mechanisms respectively of Jaswon and Dove (1956). In the Y mechanism, the atom displacements are normal to K_1 whereas in the X' mechanism the atom movements must be in this plane but not necessarily parallel to η_1 .

position in the interface, but that the motif unit of two atoms associated with the lattice point is treated as a rigid unit during the shear. Additional displacements of the atoms are then generally necessary, and these are described as "shuffles" because, unlike the shear, they produce no macroscopic effects. For a double lattice structure, there are two simple shuffles leading to a type I twin, as illustrated in Fig. 20.2, and, following Jaswon and Dove, these are described as the X' and Y mechanisms respectively. (X' is used rather than X in order to distinguish it from another mechanism, shown in Fig. 20.3, which Jaswon and Dove also called X .) Note that if the K_1 lattice planes are regarded as corrugated atomic planes, the shuffles reverse the asymmetric corrugations.

This assumption about the division of the net atomic displacements into shear and shuffle components is clearly somewhat arbitrary and it might alternatively be assumed that the shuffles precede the shear. Moreover, in the description given by Jaswon and Dove and later followed by Bilby and Crocker, the motif units are treated as rigid during the shear, so that each atom of a double lattice structure is given the shear displacement appropriate to the midpoint of the motif pair. An equally valid factorization of the net

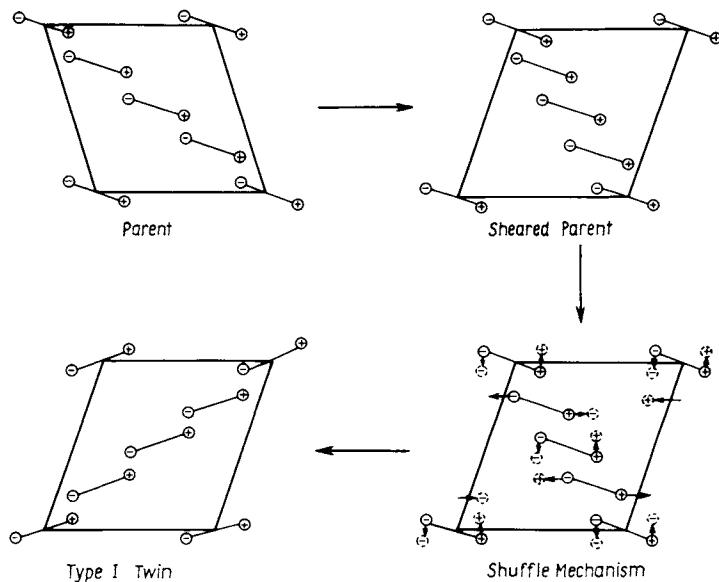


FIG. 20.3. Diagram illustrating the X shuffling mechanism of Jaswon and Dove (1957). Circles marked + and - represent atoms at equal distances above and below the plane of projection. The sheared parent shows the structure after a shear which moves one-half of the lattice points to their new positions; this arises because a primitive lattice vector in the η_2 direction crosses four lattice planes ($q=4$). The atom displacements in successive K_1 planes are alternately normal and parallel to K_1 .

movements would be first to give each atom the displacement of the homogeneous shear (i.e. to treat the atoms as embedded in a homogeneously sheared continuum) and then to define the shuffles as the remaining atomic displacements. Whether or not the alternative descriptions have any physical significance depends on the models used for interface structure and migration. There may also be a difference in the formal criteria for multiple lattice structures to be able to form twins without shuffles (see p. 865).

The previous notation is now extended so that successive *atomic* planes are denoted ... $2\bar{a} \bar{2}\bar{b} \bar{1}\bar{a} \bar{1}\bar{b} 0a 0b 1a 1b 2a 2b \dots$, and the Jaswon and Dove treatment requires that the shear gives planes $1a$ and $1b$ an identical parallel displacement which brings the atoms in these planes immediately over the atoms in $1\bar{a}$ and $\bar{1}\bar{b}$ respectively. In the Y mechanism, the atoms are also given further shuffle displacements normal to K_1 which effectively interchange the $1a$ and $1b$ planes so that they become mirror images of the $\bar{1}\bar{b}$ and $\bar{1}\bar{a}$ planes, thus producing the twin. (If the motif unit is not regarded as rigid during the shear, the shuffle displacements in the Y mechanism will be parallel to the final η_2 direction [i.e. η'_2 of Fig. 2.4] if the shuffles are supposed to follow the shear and to the original η_2 direction if the shuffles precede the shear.) In the X' mechanism, the atoms are given shuffle displacements within the K_1 planes to give the same result. Note that the shear alone cannot describe the twinning because the crystal structure produced by the

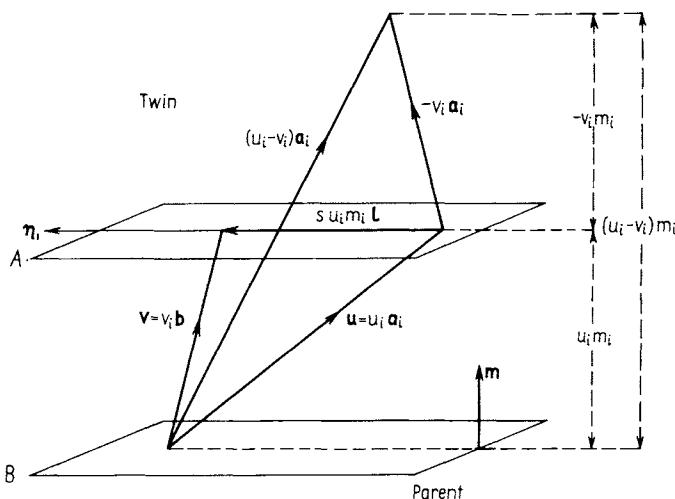


FIG. 20.4. Crystallographic relations in type I twinning (after Crocker, 1959). When the interface moves from position *A* to *B*, the vector \mathbf{u} in the parent becomes \mathbf{v} in the twin. The components of \mathbf{u} are u_i in the parent basis \mathbf{a}_i and those of \mathbf{v} are v_i in the twin basis \mathbf{b}_i . The Figure shows that the projections of the vectors $u_i \mathbf{a}_i$ and $v_i \mathbf{b}_i$ on to the normal to the K_1 plane are both equal to one-half of the projection of $(u_i - v_i) \mathbf{a}_i$ on to \mathbf{m} .

shear (Fig. 20.2) is different from that of the original (parent) phase. No reference has been made to the structure of the interface region (i.e. to the atoms originally in planes $0a$ and $0b$) in describing either the shear or the shuffles. One obvious possibility is that these atoms are given half the displacements of the Y mechanism to produce a flat atomic interface midway between the opposite corrugations in the lattice planes of parent and twin, and this is believed to be a good model for some h.c.p. twin interfaces. However, the macroscopic effects of the twinning are independent of the atomic configuration at the interface, although this structure is of considerable importance in growth mechanisms and is discussed further in Section 87.

The two types of shuffle shown in Fig. 20.2 are the only possibilities for double lattice structures in which all lattice sites are translated to their correct positions by the macroscopic shear. If the double lattice structure is regarded as a set of motif units situated at the points of a lattice, neither shuffle disrupts the motif pairs. However, the necessity for atomic shuffles lessens the significance of shearing all lattice sites to their correct positions and, in metallic structures at least, the selected motif units are usually without appreciable physical significance (i.e. they do not represent molecules). Thus it seems reasonable to examine the possibility of twinning modes in which the macroscopic shear carries only a fraction of the sites to their correct twinned positions, even if the subsequent atomic shuffles involve disruption of the motif units.

Jaswon and Dove extended their theory in this way to include cases in which only half of the parent lattice sites are moved to their final positions by the twinning shear. This led them in particular to consider the X shuffle mechanism shown in Fig. 20.3, in which the

atomic shuffles in successive planes are alternately parallel and normal to K_1 , those parallel to K_1 involving disruption of motif units.

The mechanisms of either Fig. 20.2 or Fig. 20.3 require that planes $2a2b$ are carried over planes $\bar{2} \bar{a} \bar{2} \bar{b}$ by the macroscopic shear. To investigate the possible twinning planes for this type of structure, it is thus only necessary to apply the previous projection technique to this pair of planes. An inequality analogous to (85.2) is obtained,

$$d^2 \geq b^2/4(s^2 + 4) \quad (85.3)$$

giving a necessary condition on the spacing of the K_1 planes for any prescribed value of s . Clearly the condition on d^2 can be still further relaxed by allowing smaller fractions of the parent sites to be sheared directly to the twin sites, at the expense of more complex shuffles, but consideration of this is deferred until later in this chapter.

In applying the theory to predict operative twinning modes in double lattice structures, it is now assumed that the mode selected will be that giving the smallest shear, irrespective of whether this involves an X or Y type shuffle. If the shears are comparable for alternative modes involving X or Y shuffles, however, the relative probability of the two types of shuffle may be taken into consideration. For example, if the vector joining the two atoms of the motif unit is nearly parallel to K_1 , Y shuffles will require only very small atomic displacements and hence may be considered more probable than X shuffles.

Although the Jaswon and Dove theory has been described only for type I reflection twins, essentially similar procedures may also be used for type II rotation twins (Jaswon and Dove, 1960). Instead of considering the displacements parallel to K_1 , those parallel to the rational K_2 plane are now examined. The theory as a whole is very successful in predicting the operative twinning modes in single lattice structures and in most double lattice structures, including the most common h.c.p. mode, the modes observed in bismuth, arsenic and antimony, the mode usually observed in diamond structures, and both type I and type II twins in α -uranium. However, the theory does not explain why several modes are observed in some structures, nor does it predict correctly their relative frequency, and some observations (e.g. "anomalous" h.c.p. modes) are unexplained. A description based entirely on the twinning shear cannot distinguish between a mode and its conjugate, but when the K_1 and K_2 planes are not crystallographically equivalent, it is frequently found that only one of these modes is observed. Finally, the theory does not consider non-centrosymmetric structures where there may be four different orientation relations.

The suggestion that the magnitude of the twinning shear is an important factor in determining the operative twinning mode or modes was also made by Kiho (1954, 1958), whose first paper predated that of Jaswon and Dove. He considered specifically the atom movements at an idealized parent-twin interface, and assumed that each atom moves to the nearest available twin site, and that the vector sum of the shuffles is zero. The shuffles which he described included the X and Y mechanisms, together with another mechanism to explain the anomalous twins in titanium, but he did not give a full treatment of the uranium modes. Kiho also suggested that in choosing between a twinning mode and its conjugate, the mode for which the Burgers vector of a twinning dislocation in the interface is least

should be preferred. This is equivalent to a statement that the preferred mode of a conjugate pair should be that for which the spacing of the lattice K_1 planes is smaller.

The available experimental results undoubtedly show that, in some cases, the magnitude of the shear is not the only factor which controls the operative twinning modes. The theory of Bilby and Crocker (1965), which includes a more rigorous treatment of the orientation relations and shuffle mechanisms, will now be described.

As a parent crystal and its twin remain in contact at the interface plane during the formation of the twin, it is clear that the relation between the structures must be such that this plane is invariant in any deformation relating the two lattices. This is automatically accomplished in the shear description but, in specifying the orientation relations, consideration is given to proper or improper rotations which will carry one lattice into the other. Consideration of the operations of this type which will leave the K_1 plane unaltered leads at once to the four orientation relations mentioned on p. 51, namely:

- (I) reflection in K_1 ;
- (II) rotation of 180° about η_1 ;
- (III) reflection in the plane normal to η_1 ; and
- (IV) rotation of 180° about the direction normal to K_1 .

It is also possible to have two orientations of a structure which do not correspond to any of the relations I–IV, but in which the lattices (or suitable superlattices) are connected by a simple shear. If such a shear is regarded as a form of deformation twinning, as in the Bilby Crocker formulation mentioned on p. 860, the classical definition of twinning in terms of symmetry operations is inadequate. In fact, new non-classical twinning modes were first considered to arise from the combination of two twinning operations of the classical kind, a process which has been termed "double twinning" (Crocker, 1962). A more systematic theory of twinning as a shear process was subsequently developed by Bevis and Crocker (1968, 1969), and this enables the possible classical and non-classical modes with shear magnitudes smaller than any fixed value to be enumerated. However, there is currently no very convincing experimental evidence for the occurrence of non-classical twinning, so that the assumption will first be made that the classical orientation relations are valid and a discussion of the general theory is deferred to the end of this section. The orientation relations I–IV, and the associated division into type I and type II twins, follow necessarily from the more general shear definition if the assumption is made (as on p. 54) that there exists a cell of the parent which shears into an equivalent cell of the twin.

Let the parent lattice be defined by the three non-coplanar vectors \mathbf{a}_i forming the basis A, and the twin lattice by the vectors \mathbf{b}_i forming the basis B. These bases are chosen so that each set of vectors defines a similarly shaped *primitive* unit cell. One of the above four operations generates B from A, so that the four orientation relations may be written

$$\mathbf{b}_i^{(I)} = \mathbf{a}_i - 2(\mathbf{a}_i \cdot \mathbf{m})\mathbf{m},$$

$$\mathbf{b}_i^{(II)} = 2(\mathbf{a}_i \cdot \mathbf{l})\mathbf{l} - \mathbf{a}_i,$$

$$\begin{aligned}\mathbf{b}_i^{(III)} &= \mathbf{a}_i - 2(\mathbf{a}_i \cdot \mathbf{l})\mathbf{l}, \\ \mathbf{b}_i^{(IV)} &= 2(\mathbf{a}_i \cdot \mathbf{m})\mathbf{m} - \mathbf{a}_i\end{aligned}\quad (85.4)$$

where \mathbf{m} and \mathbf{l} are unit vectors normal to the K_1 plane and in the η_1 direction respectively. As $\mathbf{b}_i^{(I)} = -\mathbf{b}_i^{(IV)}$ and $\mathbf{b}_i^{(II)} = -\mathbf{b}_i^{(III)}$, the lattices given by orientations I and IV are identical, as are those given by II and III. When the atomic positions are considered, however, the two orientations in each pair are seen to be equivalent only for structures which have a centre of symmetry. It is thus sufficient to consider only $\mathbf{b}_i^{(I)}$ and $\mathbf{b}_i^{(II)}$ when there are no more than two (identical) atoms per primitive unit cell (single or double lattice structures), but the other two relations may be needed for more complex structures. Although these do not occur in most metals known to twin, the theory will be developed in general form as far as is practicable.

Twin orientations I and II are readily seen to be related to each other by a reflection in the plane of shear. Let any parent vector have components x_i in an orthonormal basis defined by \mathbf{l}, \mathbf{m} and the unit normal to the plane of shear, $\mathbf{l} \wedge \mathbf{m}$. Then for orientation I, its twin vector has components $[x_1, -x_2, x_3]$ and for orientation II, it has components $[x_1, -x_2, -x_3]$. It follows that there is no distinction between orientations I and II if the two twin vectors are crystallographically equivalent, i.e. if the plane of shear is a mirror plane.

Consider a lattice point of the parent lying within the twin interface and identified with respect to an arbitrary origin by the parent vector \mathbf{u} . Let the interface move into the parent until it contains the origin, so that the lattice point is displaced through a distance $s(\mathbf{u} \cdot \mathbf{m})$ in the η_1 direction. The vector \mathbf{u} thus becomes a new vector \mathbf{v} , where $\mathbf{v} = \mathbf{u} + s(\mathbf{u} \cdot \mathbf{m})\mathbf{l}$. We now let u_i be the (rational) components of \mathbf{u} in the basis A and v_i be the (rational) components of \mathbf{v} in the basis B.[†] The vector $u_i \mathbf{a}_i$ in the parent thus becomes $v_i \mathbf{b}_i$ in the twin, where

$$u_i \mathbf{a}_i + s u_i m_i \mathbf{l} = v_i \mathbf{b}_i. \quad (85.5)$$

Any of the relations (85.4) may now be substituted for \mathbf{b}_i in this equation. At present the concern is only with lattices, and use of $\mathbf{b}_i^{(I)}$ and $\mathbf{b}_i^{(II)}$ gives respectively

$$(u_i - v_i) \mathbf{a}_i = -s u_i m_i \mathbf{l} - 2 v_i m_i \mathbf{m} \quad (85.6a)$$

and

$$(u_i + v_i) \mathbf{a}_i = -s u_i m_i \mathbf{l} + 2 v_i l \mathbf{l} \quad (85.6b)$$

Taking the scalar product of both sides of these equations with $\mathbf{m} = m_i \mathbf{a}_i^*$ gives

$$(u_i + v_i) \mathbf{m}_i = 0, \quad (85.7)$$

[†]The vector \mathbf{u} may have irrational components in the basis B, as may \mathbf{v} in the basis A. In this section, it will not be necessary to refer a single vector to the two different bases A and B, but use will be made of different vectors such as $u_i^A \mathbf{a}_i$ and $u_i^B \mathbf{b}_i$ which have the same rational components in A and B respectively. For this reason, the identifying superscripts will be omitted from the symbols u_i^A , v_i^B , etc. In the following description, combined rational indices $[u_i \pm v_i]$ correspond to indices $[x' - y']$ of Bilby and Crocker because of a change of sign in eqn. (85.5).

in both cases. Hence for both orientations I and II, the rational lattice vector $(u_i + v_i)\mathbf{a}_i$ must lie in the K_1 plane. This development proves that the twinning plane must contain at least one rational lattice vector. Equation (85.6b) shows, moreover, that for orientation II this rational lattice vector is parallel to \mathbf{l} , i.e. to \mathbf{n}_1 . For orientation I, eqn. (85.7) may be used to rewrite eqn. (85.6a) in the form

$$(u_i + v_i)\mathbf{a}_i = su_i m_i \mathbf{l} + 2(u_i \mathbf{a}_i - u_i m_i m_j \mathbf{a}_j). \quad (85.8)$$

The right-hand side of eqn. (85.8) consists of the sum of a vector parallel to \mathbf{l} and the projection of the vector $2\mathbf{u}$ on the K_1 plane. Thus the rational lattice vector $(u_i + v_i)\mathbf{a}_i$ will vary as \mathbf{u} varies, and the K_1 plane contains an infinite number of rational directions. This proves that, for orientation I, K_1 is rational.

The above analysis can be repeated for orientations III and IV, in which case the rational vector in the interface is $(u_i - v_i)\mathbf{a}_i$ and is parallel to \mathbf{l} for orientation III and represents an infinite set of vectors in K_1 for orientation IV. Hence it has been shown that for orientations I and IV, K_1 must be rational (type I twinning), and for orientations II and III, \mathbf{n}_1 must be rational (type II twinning). Consider type I twinning first. Then from eqn. (85.7)

$$2u_i m_i = -2v_i m_i = (u_i - v_i)m_i. \quad (85.9)$$

This relation is illustrated in Fig. 20.4. The rational vector $(u_i - v_i)\mathbf{a}_i$ of the parent lies in the plane containing \mathbf{n}_1 and \mathbf{m} , and the projections of the vectors $u_i \mathbf{a}_i$ and $-v_i \mathbf{a}_i$ on \mathbf{m} are both equal to one-half of the projection of $(u_i - v_i)\mathbf{a}_i$ on \mathbf{m} . Substituting into eqn. (85.6a) and using eqn. (85.4) now gives

$$(u_i - v_i)\mathbf{a}_i + s(u_i - v_i)m_i \mathbf{l} = -(u_i - v_i)\mathbf{b}_i \quad (85.10)$$

This equation shows that the twinning operation converts the lattice vector $(u_i - v_i)\mathbf{a}_i$ into its own twin $-(u_i - v_i)\mathbf{b}_i$. It is easy to prove that no other vectors have this property, so that $(u_i - v_i)\mathbf{a}_i$ defines a unique direction (the \mathbf{n}_2 direction). From eqns. (85.6a) and (85.9), the twinning shear is given by the vector

$$s\mathbf{l} = -2 \frac{(u_i - v_i)\mathbf{a}_i}{(u_i - v_i)m_i} - \mathbf{m}. \quad (85.11)$$

The meaning of this equation is shown in Fig. 20.5. Let \mathbf{g} be a unit vector in the direction of \mathbf{n}_2 , i.e. of $(u_i - v_i)\mathbf{a}_i$. Then eqn. (85.11) may be written

$$s\mathbf{l} = -2 \frac{\mathbf{g}}{\mathbf{g} \cdot \mathbf{m}} - \mathbf{m}. \quad (85.12)$$

and the magnitude of the shear is

$$s^2 = 4[(1/\mathbf{g} \cdot \mathbf{m})^2 - 1] \quad (85.13)$$

or, in terms of the angle 2ϕ shown in Figs. 2.4 and 20.5,

$$s = 2 \cot 2\phi$$

which is eqn. (8.2).

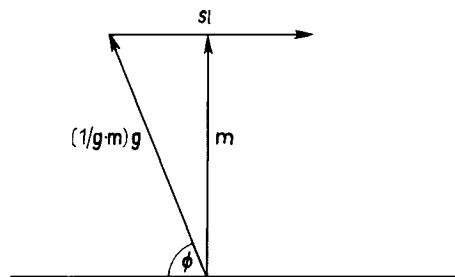


FIG. 20.5. The magnitude of the twinning shear. Unit vectors in the η_1 direction, the direction normal to the K_1 plane and the η_2 direction are \mathbf{l} , \mathbf{m} and \mathbf{g} respectively.

It has thus been proved that in type I twinning the K_1 plane is rational, and there is a unique rational direction (the η_2 direction) which is sheared into its own twin. The result has been deduced without making the assumption given on p. 54 that a unit cell of the parent is sheared into an equivalent cell of the twin. The elements K_1 and η_2 enable the amount of shear to be calculated, so that these two elements define the twin mode completely.

Next consider whether or not all the parent lattice points are carried to twin lattice sites by the shear. Let $\mathbf{w} = w_i \mathbf{a}_i$ be a primitive lattice vector in the η_2 direction, and let its projection along the normal to the K_1 plane have magnitude

$$w_i m_i = qd \quad (85.14)$$

where q is a positive integer giving the number of lattice K_1 planes traversed by this vector. The above discussion shows that all the lattice sites of the parent structure on the K_1 plane defined by \mathbf{w} will become correctly positioned lattice sites of the twin structure as a result of the shear, but it is necessary ($q > 2$) to consider further the lattice sites on the $(q - 1)$ intermediate planes. Note that whatever the structure of the interface, it reaches an equivalent position after moving forward a distance qd , so that the atom displacements are repeated in each successive group of q planes, and only one such group need be considered.

Let any lattice point in the nearest K_1 plane to that through the origin be $c_i \mathbf{a}_i$ (i.e. $c_i m_i = d$). Bilby and Crocker assumed that, in type I twinning, all the lattice points on a given K_1 plane shuffle in the same way, so that it is necessary to consider only one lattice point on each plane. Thus all the parent sites within the $(q - 1)$ planes of interest are represented by $p c_i \mathbf{a}_i$, where p is a positive integer which is smaller than q . After the homogeneous shear, the positions of these sites will become $p c_i \mathbf{a}_i + s p d \mathbf{l}$ and, using eqns. (85.6a) and (85.9) with the above definitions of \mathbf{w} and p , this becomes

$$[p c_i - (2p/q) w_i] \mathbf{a}_i + 2pd \mathbf{l} \quad (85.15)$$

Now consider the twin sites. Any site in the q th K_1 plane (defined by \mathbf{w}) may be written as $z_i \mathbf{b}_i$, where from eqns. (85.10) and (85.14)

$$-z_i m_i = qd. \quad (85.16)$$

As the bases A and B define similar unit cells, all the twin lattice sites in the $q - 1$ planes of interest are represented by the vectors

$$(z_i + rc_i)\mathbf{b}_i \quad (85.17)$$

where r (like p) is a positive integer smaller than q . (Note that it is not necessary to consider $p = q$ as we have shown that sites on this plane do not shuffle.)

The lattice shuffles must relate the twin lattice sites of eqn. (85.17) to the parent lattice sites of eqn. (85.15), and so are described by the vectors Δ^1 , obtained by subtracting eqn. (85.15) from eqn. (85.17). However, eqns. (85.4), (85.10) and (85.16) show that, for orientation I,

$$c_i\mathbf{b}_i = c_i\mathbf{a}_i - 2d\mathbf{m}$$

and

$$z_i\mathbf{b}_i = z_i\mathbf{a}_i + 2qd\mathbf{m}$$

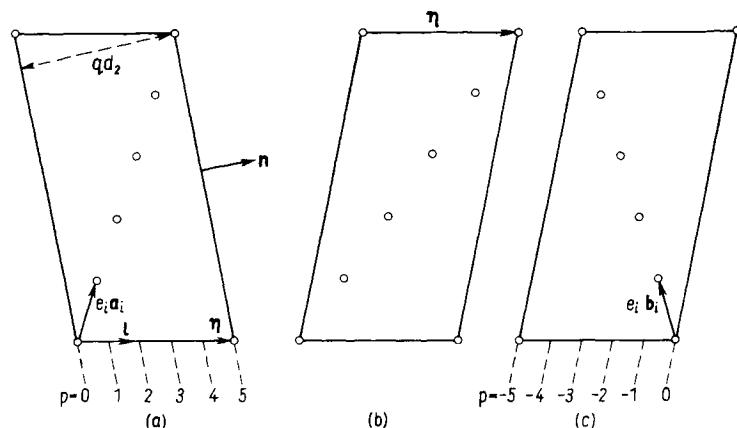
so that after subtracting,

$$\Delta^1 = [(r - p)c_i + (2p/q)w_i + z_i]\mathbf{a}_i + 2d(q - r - p)\mathbf{m}. \quad (85.18)$$

For a given parent site, the parameters z_i and r representing the twin site may be regarded as disposable; that is, which parent and twin sites are related by the vector Δ^1 may be freely chosen. From eqn. (85.18) it follows that $\Delta^1 \cdot \mathbf{m} = (q - p - r)d$. Thus the component of Δ^1 normal to K_1 is zero, i.e. the related parent and twin sites lie in the same K_1 plane if $p + r = q$. In general, the shuffles might be expected to minimize $|\Delta^1|$. Although it is not always possible to choose the parameters so that $\Delta^1 = 0$ for all sites, this can be done when $q = 1$ or 2. For $q = 1$, there are no intermediate lattice sites to be shuffled and, for $q = 2$, there are only the sites on the plane defined by $p = 1$. The shuffle vectors for this plane are all zero if $r = 1$ and $z_i = -w_i$ are chosen. More generally, if q is even, the lattice points in the plane $p = q/2$, as well as those in the plane $p = q$, are sheared directly to their twin positions, as may be seen by choosing $r = p$ and $z_i = -w_i$.

The case $q = 2$ corresponds to Fig. 20.1, where it was assumed that the η_2 direction relates lattice points on K_1 planes a distance $2d$ apart. All lattice points are then translated to their twin sites by the shear, as has just been shown analytically. When $q = 1$, there is a degenerate case of Fig. 20.1, in which the lattice vector \mathbf{RP} passes through a lattice point in plane 0.

Figure 20.6 illustrates some possible lattice shuffles for a $q = 4$ twinning mode of a single lattice structure. No shuffles are required for the plane $p = 2$, but the atoms on the planes $p = 1, 3$ undergo equal and opposite shuffles. A choice $r = p$ and $z_i = -w_i$ gives shuffles of $\Delta^1 = -\frac{1}{2}\mathbf{w} + 4d\mathbf{m} = -\frac{1}{2}w_i\mathbf{b}_i$ for $p = 1$ and an equal and opposite vector for $p = 3$. Note that these displacements are identical for any c_i , and that any other choice of z_i will give a vector Δ^1 which represents a longer and more complex displacement between the two K_1 planes. The vectors $\pm\frac{1}{2}w_i\mathbf{b}_i$ are formed by the shear from the vectors $\pm(1/2)\mathbf{w}$ and thus are parallel to $\pm\eta'_2$ in Fig. 2.4. (If the shuffles are regarded as preceding the shear, the choice $r = p$ produces displacements $\pm(1/2)\mathbf{w}$, i.e. parallel to $\pm\eta_2$.)

FIG. 20.6. Lattice sites in type II twinning for $q=5$.

The alternative choice $r=q-p$ means that the shuffles are within the K_1 plane, but not parallel to η_1 . For $p=1$, $\Delta^1 = \frac{1}{2}(4\mathbf{c} - \mathbf{w})$ if $z_i = -w_i$, and this choice of z_i thus cannot be generally valid as the shuffle would then vary with c_i . In order to minimize $|\Delta^1|$, the shuffle must relate the parent site to the nearest twin site in the same K_1 plane. If this corresponds to a particular vector $2\mathbf{c}_1 - \frac{1}{2}\mathbf{w}$ then, for any parent site specified by $\mathbf{c} = \mathbf{c}_1 + \mathbf{f}$ (where $f_i m_i = 0$), the correct shuffle is obtained by a choice $z_i = \pm(2f_i + w_i)$ for $p=3, 1$ respectively.

Consider now the atomic movements during the formation of the twin; for q or $\bar{q} > 2$, these may have smaller magnitudes than the shuffles of the Bravais lattice points. The positions of the atoms in the parent are given by $(u_i + \xi_{n,i})\mathbf{a}_i$ [see eqn. (5.8)], where $\xi_{n,i}\mathbf{a}_i$ is the position of the n th atom in the unit cell relative to some chosen origin. The twin lattice will correspondingly have sites at $(v_i + \xi_{n,i})\mathbf{b}_i$. The unit cell origins may always be chosen so that $\sum_n \xi_{n,i}\mathbf{a}_i = \sum_n \xi_{n,i}\mathbf{b}_i = 0$; if there are only two atoms in the primitive unit cell, this means that the origin is at the centre of symmetry.

After the lattice shear, the lattice sites are given by eqn. (85.15) and, for a rigid motif unit, the atom sites are given by the same expression with the addition of $\xi_{m,i}\mathbf{a}_i$. For orientation I, the twin lattice sites are given by eqn. (85.17) with $\mathbf{b}_i = \mathbf{b}_i^{(I)}$ [eqn. (85.4)] whilst, for orientation IV, the twin sites are given by the negative of eqn. (85.17) with $\mathbf{b}_i = \mathbf{b}_i^{(IV)}$. As already noted, these two expression are equivalent, and the twin lattice sites for orientations I and IV are identical. The atom sites in the twin are obtained by adding $\xi_{m,i}\mathbf{b}_i^{(I)}$ or $\xi_{m,i}\mathbf{b}_i^{(IV)}$ respectively to the vector representing the lattice sites. The sheared parent atom sites may thus be subtracted from the twin atom sites to obtain the atomic shuffle vectors \square^1 . These vectors are given by

$$\square^1 = \Delta^1 - (\xi_{n,i} \pm \xi_{m,i})\mathbf{a}_i \pm 2\xi_{m,i}m_i\mathbf{m}. \quad (85.19)$$

The vector \square^1 represents the displacement added to the homogeneous shear needed to transfer the n th atom of the parent unit cell to the m th atom site of the twin unit cell.

In order to specify it, the identifying subscripts n and m must be selected, in addition to the parameters defining Δ^1 . The alternative negative and positive signs are applicable to orientations I and IV respectively.

Now consider twinning of the second kind, in which the \mathbf{n}_1 direction, but not necessarily the K_1 plane, is rational. Because $(u_i + v_i)\mathbf{a}_i$ is parallel to \mathbf{l} for orientation II [eqn. (85.6b)], it is clear that this vector is equal to the sum of the projections of the vectors $u_i\mathbf{a}_i$ and $v_i\mathbf{a}_i$ on \mathbf{l} (see Fig. 20.4). Hence eqn. (85.6b) may be written

$$su_i m_i \mathbf{l} = -(u_i - v_i)(\mathbf{a}_i \cdot \mathbf{l}) \mathbf{l}. \quad (85.20)$$

As eqn. (85.7) is valid for orientation II, so also is eqn. (85.9) and, using this, eqn. (85.20) becomes

$$s(u_i - v_i)m_i \mathbf{l} = -2(u_i - v_i)(\mathbf{a}_i \cdot \mathbf{l}) \mathbf{l}, \quad (85.21)$$

or, using eqn. (85.4),

$$(u_i - v_i)\mathbf{a}_i + s(u_i - v_i)m_i \mathbf{l} = -(u_i - v_i)\mathbf{b}_i. \quad (85.22)$$

This equation shows that the rational lattice vector $(u_i - v_i)\mathbf{a}_i$ is sheared into its own twin $-(u_i - v_i)\mathbf{b}_i$. This vector is not a unique vector, but it follows from eqn. (85.21) that

$$(u_i - v_i)[sm_i + 2(\mathbf{a}_i \cdot \mathbf{l})] = 0. \quad (85.23)$$

The vector $(u_i - v_i)\mathbf{a}_i$ is thus confined to a plane with unit normal $\mathbf{n} = n_i \mathbf{a}_i^*$, where $Cn_i = sm_i + 2(\mathbf{a}_i \cdot \mathbf{l})$. This rational plane is the conjugate twinning plane, or K_2 plane, and all vectors in it are changed to their own twins by the lattice shear.

To discuss lattice shuffles with type II twinning, Bilby and Crocker again assumed that all lattice sites in any K_1 plane move in the same way but, as K_1 is irrational, this only includes the points lying along a single row parallel to \mathbf{n}_1 . However, as all the sites on the K_2 plane through the origin are sheared directly to their twin positions, so also are those on any other K_2 plane which passes through lattice sites lying along a vector in the \mathbf{l} (i.e. \mathbf{n}_1) direction from the origin. Shuffles may be necessary for lattice sites which do not lie on K_2 planes of this type; let \mathbf{q} be a primitive lattice vector in the \mathbf{n}_1 direction and suppose that it traverses \bar{q} lattice planes of type K_2 . Because the configuration will be repeated as the interface moves through every \bar{q} planes of type K_2 , only the lattice points in one such group need be considered. This is equivalent, for type II twinning, to the assumption that all lattice sites in any K_2 plane move in the same way. The projection of \mathbf{q} along the unit normal \mathbf{n} is

$$\mathbf{q} \cdot \mathbf{n}_i = \bar{q}d_2, \quad (85.24)$$

where d_2 is the spacing of the K_2 planes. Now let any lattice point on the K_2 plane a distance d_2 from the origin be represented by the vector $e_i\mathbf{a}_i$ (i.e. $e_i n_i = d_2$), so that all the lattice sites on the intermediate group of $(\bar{q} - 1)$ planes may be represented by $\bar{p}e_i\mathbf{a}_i$, where \bar{p} is a positive integer $< \bar{q}$.

The parent site at $\bar{p}e_i\mathbf{a}_i$ will shear to a new position

$$\bar{p}e_i\mathbf{a}_i + \bar{p}s e_i m_i \mathbf{l}. \quad (85.25)$$

Let $\bar{z} = \bar{z}_i \mathbf{a}_i$ define any lattice site of the parent structure in the K_2 plane through the origin, so that $\bar{z}_i n_i = 0$. Equation (85.22) then shows that this site is sheared into a site $-\bar{z}_i \mathbf{b}_i$ of the twin lattice. Relative to this twin site, the set of vectors $\bar{r} e_i \mathbf{b}_i$, where \bar{r} is a positive integer $< \bar{q}$, specifies all the lattice sites in a group containing \bar{q} of the K_2 planes of the twin.[†] Hence the general expression for the twin sites is $-(\bar{z}_i + \bar{r} e_i) \mathbf{b}_i$ and, substituting for $\mathbf{b}_i^{(II)}$ from eqn. (85.4), this becomes

$$(\bar{z}_i - \bar{r} e_i) \mathbf{a}_i + 2\bar{r}(\mathbf{e} \cdot \mathbf{l}) \mathbf{l} - 2(\bar{z} \cdot \mathbf{l}) \mathbf{l} \quad (85.26)$$

The relations of the lattice sites, sheared lattice sites and twin lattice sites are shown in Fig. 20.6(b) for $\bar{q} = 5$.

The vector defining the lattice shuffles is now obtained by subtracting eqn. (85.25) from eqn. (85.26) as

$$\Delta^{II} = \{\bar{z}_i - (\bar{p} + \bar{r}) e_i\} \mathbf{a}_i + 2\{\bar{r}(\mathbf{e} \cdot \mathbf{l}) - (\mathbf{z} \cdot \mathbf{l}) - \bar{p} s e_i m_i\} \mathbf{l} \quad (85.27)$$

This may be written in an alternative form by noting that the endpoint of the vector $\bar{q}\mathbf{e} = \bar{q} e_i \mathbf{a}_i$ undergoes a vector displacement of $\bar{q} s e_i m_i \mathbf{l}$ as a result of the lattice shear. From Fig. 20.6(b), it is clear that the projection of $\bar{q} e_i \mathbf{a}_i$ on \mathbf{l} is equal to \mathbf{n} minus one-half of the displacement of the endpoint of $\bar{q} e_i \mathbf{a}_i$, so that

$$\bar{q}(\mathbf{e} \cdot \mathbf{l}) \mathbf{l} = \mathbf{n} - \frac{1}{2} \bar{q} s e_i m_i \mathbf{l} \quad (85.28)$$

Substituting into eqn. (85.27) now gives

$$\Delta^{II} = \{\bar{z}_i - (\bar{p} + \bar{r}) e_i\} \mathbf{a}_i - \{(\bar{p} + \bar{r}) s e_i m_i + 2(\mathbf{z} \cdot \mathbf{l})\} \mathbf{l} + 2(\bar{r}/\bar{q}) \mathbf{n} \quad (85.29)$$

In considering the shuffles of a given lattice point in type II twinning, \bar{z}_i and \bar{r} are disposable parameters corresponding to z_i and r for type I twinning. In general $\Delta^{II} = 0$ for all points only when $\bar{q} = 1$ or 2. However, for any even value of \bar{q} , the lattice points on the plane $\bar{p} = (1/2)\bar{q}$ need not shuffle, as it is always possible to choose $\bar{r} = \bar{p} = \frac{1}{2}\bar{q}$ and $\bar{z}_i = \bar{q} e_i - \mathbf{n}_i$. If $\bar{r} = \bar{q} - \bar{p}$ for all the lattice points, eqn. (85.28) or (85.29) shows with the above choice of \bar{z}_i that the shuffle vector is always parallel to \mathbf{n}_1 . This may be compared with the condition $r = p$ for type I twinning which gives a lattice shuffle vector parallel to \mathbf{n}_2' . For $\bar{q} = 4$, the shuffle vectors are $\pm \frac{1}{2}\mathbf{n}$ but, as in the analogous case of type I twinning with $q > 4$, some of the shuffles described by this assumption look improbable for $\bar{q} > 4$. The alternative choice $\bar{r} = \bar{p}$ gives shuffle displacements which are within the final position (K'_2) of the conjugate twinning plane, but are not in general parallel to the conjugate twinning direction; these displacements are, of course, in K_2 if the shuffles are supposed to precede the shear. The origin z_i for the twin sites now has to be chosen with regard to \mathbf{e} , in exact analogy with the type I shuffles in the K_1 plane. Thus if $\bar{z}_i = \bar{q} e_i - \mathbf{n}_i$, $\Delta^{II} = (\bar{q} - 2\bar{p})(\mathbf{e} + s e_i m_i \mathbf{l} - \mathbf{n}/\bar{q})$, and for $\bar{q} = 4$ and $\bar{p} = 1, 3$ the shuffles on the K'_2 plane (following the shear) are $\pm(2\mathbf{e} - \frac{1}{2}\mathbf{n} + 2s e_i m_i \mathbf{l})$. The minimum shuffle displacement of this

[†]A different specification of the type II twin sites was used in the first edition; the present formalism follows that of Bilby and Crocker (1965).

type will have this form for some particular value \mathbf{e}_1 of \mathbf{e} and, for other representative vectors \mathbf{e} , a different choice of \bar{z}_i must be made to give the same minimum shuffle. The condition for this is most readily seen by noting that the shuffle displacement in K_2 (preceding the shear) is $2\mathbf{e}_1 - \frac{1}{2}\mathbf{\eta}$ and, writing $\mathbf{e} = \mathbf{e}_1 + \mathbf{f}$, it follows that $\mathbf{z} = z_i \mathbf{a}_i$ should be chosen as $4\mathbf{e}_1 + 2\mathbf{f} - \mathbf{\eta}$. Figure 20.6 shows the lattice sites for the parent, sheared parent and type II twin for $\bar{q} = 5$.

The structure shuffles may now be defined in the same way as those for type I twinning. The general expression is

$$\square^H = \Delta^H - (\xi_{n,i} \pm \xi_{m,i}) \mathbf{a}_i \pm (\xi_m \cdot \mathbf{l}) \mathbf{l} \quad (85.30)$$

where the alternative positive and negative signs relate to orientations II and III respectively. The vector \square^H represents the displacement added to the homogeneous shear which is needed to transfer the n th atom of the parent unit cell to the m th site of the twin cell.

Equations (85.19) and (85.30) are the general expressions for the atom shuffles in any kind of twin formation, and some properties of these expressions in particular cases of interest will now be discussed. All shuffles are zero in simple lattice structures when q or $\bar{q} = 1$ or 2, and in predicting the twinning elements of these structures the lowest shear modes for q or $\bar{q} = 2$ should thus be considered first. Higher values of q or \bar{q} , with associated shuffles, need be considered only if modes are observed experimentally which do not correspond to q or $\bar{q} = 2$ predictions. This is the procedure used by Jaswon and Dove, and described above; as already noted, it gives excellent agreement with experimental results.

Now consider double lattice structures, which cover most other pure metals known to form mechanical twins. Because these structures are centrosymmetric, there are only two possible orientation relations, and the shuffles obtained by choosing positive or negative signs in eqns. (85.19) or (85.30) must thus be equivalent. It is convenient to write $\xi_{1,i} = \xi_i$ and $\xi_{2,i} = -\xi_i$ for such structures. Then if ${}^l(n,m)$ represents the shuffle associated with the movement of the n th atom of the parent to the m th site of the twin, eqn. (85.19) shows that ${}^l(1,1)$ for orientation I is equal to ${}^l(1,2)$ for orientation IV. There are similar relations of this kind for all the double lattice shuffles.

Suppose first that the twinning elements in double lattice structures are such that q or $\bar{q} = 1$ or 2. Then the lattice shuffles are zero, and there are four possible types of structure shuffle, which are respectively

$$\begin{aligned} |\square^l(1,1)| &= |\square^l(2,2)| = 2\xi_i m_i, \\ |\square^l(1,2)| &= |\square^l(2,1)| = 2[|\xi|^2 - (\xi_i m_i)^2]^{1/2}, \\ |\square^H(1,1)| &= |\square^H(2,2)| = 2\xi \cdot \mathbf{l}, \\ |\square^H(1,2)| &= |\square^H(2,1)| = 2[|\xi|^2 - (\xi \cdot \mathbf{l})^2]^{1/2} \end{aligned} \quad (85.31)$$

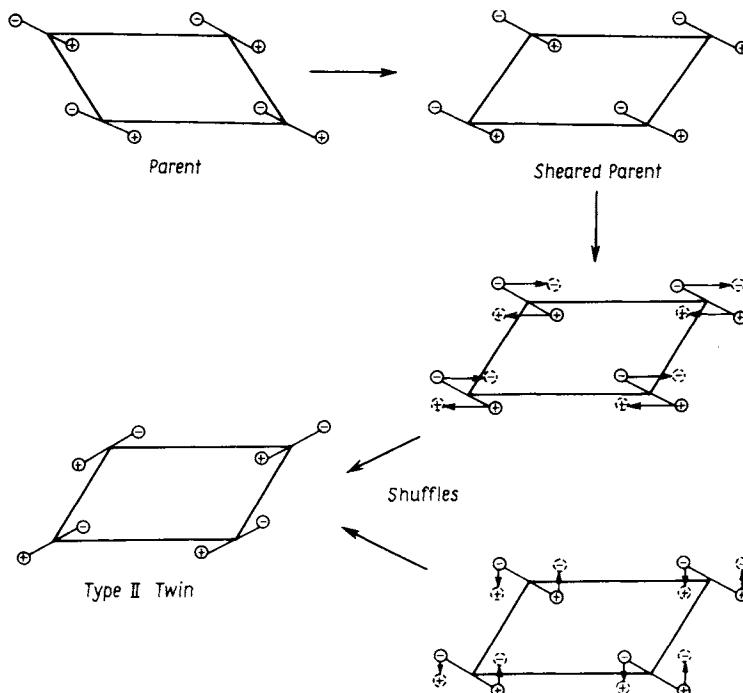


FIG. 20.7. Possible shuffles for a double lattice structure type II twin with $\bar{q}=1$ or 2. Circles marked + or - represent atoms at equal distances above and below the plane of projection. The sheared parent shows the structure after applying a homogeneous shear to the lattice points, and the two shuffle mechanisms may be compared to those in Fig. 20.2. In one mechanism, the atoms shuffle parallel to η_1 ; in the other they move normal to η_1 but not normal to K_1 .

The first two of these mechanisms, applicable to a type I twin, were described as the Y and X' mechanisms respectively earlier in this chapter, and are shown in Fig. 20.2. The second two mechanisms are correspondingly shown in Fig. 20.7.

For given twinning elements, a possible hypothesis is that the operative shuffle mechanism will be that for which $|\square|$ is smallest; this could result in either a type I or a type II orientation relation. It follows from eqn. (85.31) that, in particular cases, double lattice structures may be able to twin without atomic shuffles. Thus if $\xi \cdot m = 0$, the Y mechanism reduces to zero shuffles, whilst if $\xi \cdot I = 0$, the first of the type II shuffles similarly disappears. These two possibilities arise if the motif unit may be chosen respectively in the K_1 plane or in the plane normal to the η_1 direction, and it may be readily seen that they apply also to type I and type II twinning in centrosymmetric structures where there are more than two atoms in the motif units. On p. 863, however, it was pointed out that the division into shear plus shuffles may be made in different ways. If the motif unit is not regarded as rigid, but each atom is instead displaced individually by the twinning shear, the condition for no shuffles in type I twinning will be unchanged, but

the condition for absence of shuffles in type II twinning then becomes a motif unit lying in the K_2 plane rather than in the plane normal to η_i .

The motif unit is not uniquely defined, even for a double lattice structure, as in principle it may link an atom of one lattice to any atom of the interpenetrating lattice. However, the analysis of this section, in which the motif units are treated as rigid during the shear, implies that the separation of the atoms in a unit must be small. The analysis is purely a matter of mathematical convenience, and the only physical reality is the net displacements of the individual atoms, but it is clear that the above treatment corresponds to the natural assumption that each atom goes to the nearest available twin site. Thus it is possible to impose a restriction that $|\xi_{n,i}| \leq \frac{1}{2}$, so that unsuitable large motif units are excluded. This assumption is not adequate for large unit cells, especially if it allows atomic interchange shuffles (see p. 885), as in the formal theory of twinning of superlattices, and it is probably better then to use an alternative division into shear plus shuffles (Christian and Laughlin, 1988). It should also be noted that even the above restriction does not necessarily define the unit uniquely but, if the plane of shear is rational, the most plausible motif unit can usually be found by inspection.

In eqns. (85.31), the vector sum of the atom shuffles is zero in any mechanism, because $\square^I(1,1) = -\square^I(2,2)$, etc. From eqns. (85.19) and (85.30), we see that the vector sum of all the atom shuffles within the unit cell defined by the value of q or \bar{q} is zero for double lattice structures, provided we can ensure that the vector sum of the lattice shuffles $\sum \Delta^I$ or $\sum \Delta^{II}$ is zero. The general condition for this is readily obtained. Let $\Delta^I(p,r)$ be the type I twin lattice shuffle associated with a lattice point on the p th K_1 plane of the parent and the r th K_1 plane of the twin, and $\Delta^{II}(\bar{p},\bar{r})$ be the corresponding lattice shuffle defined with respect to K_2 planes in type I twinning. Then from eqn. (85.18), if the two sets of values of z_i which specify the shuffles $\Delta^I(p,r)$ and $\Delta^I(q-p, q-r)$ are chosen so that

$$z_i(p,r) + z_i(q-p, q-r) = -2w_i \quad (85.32)$$

it follows that

$$\Delta^I(p,r) = -\Delta^I(q-p, q-r)$$

and

$$\sum \Delta^I = 0$$

Similarly for type II twinning, the two values of \bar{z}_i corresponding to (\bar{p}, \bar{r}) and $(\bar{q}-\bar{p}, \bar{q}-\bar{r})$ shuffles respectively may be chosen so that

$$\bar{z}_i(\bar{p}, \bar{r}) + \bar{z}_i(\bar{q}-\bar{p}, -\bar{q}-\bar{r}) = 2(\bar{q}e_i - \eta_i) \quad (85.33)$$

and this gives

$$\Delta^{II}(\bar{p}, \bar{r}) = -\Delta^{II}(\bar{q}-\bar{p}, -\bar{q}-\bar{r})$$

or

$$\sum \Delta^{II} = 0.$$

Provided that pairs of values of z_i or \bar{z}_i are always chosen in this way, the net lattice shuffles are zero, and so also are the net structure shuffles in double lattice structures. For $q=1$ or 2, the result is trivial, as there are no lattice shuffles, but it is now possible to discuss the important case of $q=4$.

The restrictions on the motif unit ($|\xi_{n,i}| \leq \frac{1}{2}$) ensure that this unit is not disrupted in the $q=1, 2$ shuffles already discussed. For $q=4$, the shuffles for sites on the planes defined by $p=2, 4$ will correspond to those already discussed, as the lattice sites are sheared directly to their twin positions. For the shuffles on $p=1$ and $p=3$, assume first that the lattice shuffle vectors Δ^1 are parallel to K_1 (see p. 871). From eqns. (85.18) and (85.19), with the restriction $p+r=q$, this gives for the $p=1$ shuffles

$$\begin{aligned}\square^1(1,1) &= (2c_i + \frac{1}{2}w_i + z_i)\mathbf{a}_i - 2\xi_i m_i \mathbf{m}, \\ \square^1(2,2) &= (2c_i + \frac{1}{2}w_i + z_i)\mathbf{a}_i + 2\xi_i m_i \mathbf{m}, \\ \square^1(1,2) &= (2c_i + \frac{1}{2}w_i + z_i)\mathbf{a}_i - 2\xi + 2\xi_i m_i \mathbf{m}, \\ \square^1(2,1) &= (2c_i + \frac{1}{2}w_i + z_i)\mathbf{a}_i + 2\xi - 2\xi_i m_i \mathbf{m}.\end{aligned}\quad (85.34)$$

By choosing $z_i = -w_i$ for $\square^1(1,2)$ and $z_i = -4c_i$ for $\square^1(2,1)$, a shuffle mechanism is obtained in which

$$\square^1(1,2) = -\square^1(2,1) = (2c_i - \frac{1}{2}w_i)\mathbf{a}_i - 2\xi + 2\xi_i m_i \mathbf{m}. \quad (85.35)$$

This means that the vector sum of the shuffles associated with one lattice site of the parent is zero. This can only be achieved by using different z_i values for the $\square^1(1,2)$ and $\square^1(2,1)$ shuffles; that is, the two atoms around one parent lattice site move to different twin lattice sites, and the motif unit is disrupted. The equations for the $p=3$ plane are equal to eqn. (85.34) with $2c_i$ replaced by $-2c_i$ and $\frac{1}{2}w_i$ replaced by $3w_i/2$. The same shuffle mechanism is obtained by choosing $z_i = 4c_i - 2w_i$ for the $\square^1(2,1)$ shuffle and $z_i = -w_i$ for the $\square^1(1,2)$ shuffle.

The lattice shuffle vectors Δ^1 are not completely defined when the motif units are disrupted, as the displacement of the lattice point may be associated with that of either atom. However, if the ξ_1 atom is chosen for the site on the plane $p=1$, the ξ_2 atom must be chosen for the site on the plane $p=3$, and vice versa, and the two values of z_i then satisfy eqn. (85.32). This is necessary because $\sum \Delta^1$ must clearly be zero if the sum of \square^1 for each separate lattice point is zero. As noted above, the parameters for any double lattice structure can always be chosen so that $\sum \square^1 = \sum \Delta^1 = 0$ over the whole unit cell, whatever the value of q . When q is greater than four, however, it is not possible to make the sum of the individual shuffles at any lattice site equal to zero. This arises when $q=4$ only because each sheared parent lattice site on the planes $p=1, 3$ is midway between two twin lattice sites. For this reason, the $q=4$ shuffles are relatively simple, and may be important in practice.

The same values of z_i for the $\square^1(1,1)$ and $\square^1(2,2)$ shuffles respectively lead to an alternative shuffle mechanism in which

$$\square^1(1,1) = -\square^1(2,2) = (2c_i - \frac{1}{2}w_i)\mathbf{a}_i - 2\xi_i m_i \mathbf{m}. \quad (85.36)$$

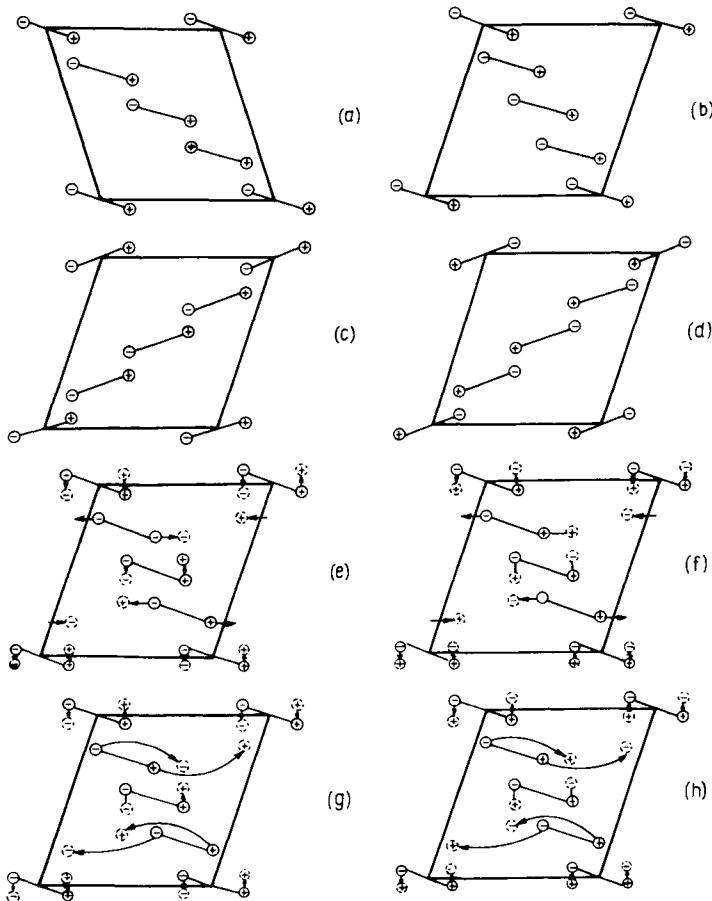


FIG. 20.8. Possible shuffling mechanisms in double lattice structure twins with $q=4$: (a) parent structure; (b) sheared parent; (c) type I twin; (d) type II twin; (e) shuffle given by eqn. (85.37) (X mechanism); (f) type II shuffle given by eqn. (85.37); (g) type I shuffle given by eqn. (85.36); (h) type II shuffle given by eqn. (85.38).

The mechanism (85.36) involves atom movements which are generally large and not parallel to the K_1 plane, in contrast to mechanism (85.35) where the movements are parallel to K_1 and may be quite small. Both mechanisms are illustrated in Fig. 20.8; that given by (85.35) is the X mechanism already described and also shown in Fig. 20.3.

The atomic shuffles for type II twins in which $\bar{q}=4$ may be investigated in a similar way. Using eqns. (85.29) and (85.30), with $\bar{z}_i = 2c_i - \mathbf{n}_i$ for $\square^{II}(1,1)$ and $\square^{II}(1,2)$ and $\bar{z}_i = 0$ for $\square^{II}(2,2)$ and $\square^{II}(2,1)$, we find that the two shuffle mechanisms for the $\bar{p}=1$ plane are

$$\square^{II}(1,1) = -\square^{II}(2,2) = -\frac{1}{2}\mathbf{n} + 2(\xi \cdot \mathbf{l})\mathbf{l}, \quad (85.37)$$

and

$$\square^{\text{II}}(1, 2) = -\square^{\text{II}}(2, 1) = -\frac{1}{2} \mathbf{\eta} + 2\mathbf{\xi} + 2(\mathbf{\xi} \cdot \mathbf{l})\mathbf{l}. \quad (85.38)$$

The same two mechanisms are obtained for the plane $\bar{p}=3$ with the choices $\bar{z}_i = \bar{q}e_i - \mathbf{\eta}$ for $\square^{\text{II}}(2, 1)$ and $\square^{\text{II}}(2, 2)$ and $\bar{z}_i = 2\bar{q}_i - 2\mathbf{\eta}_i$ for $\square^{\text{II}}(1, 1)$ and $\square^{\text{II}}(1, 2)$. These values of \bar{z}_i satisfy eqn. (85.33) to ensure that $\sum \Delta^{\text{II}} = 0$, provided that, as in the type I shuffles, different atoms of a motif pair are used to define the motion of the lattice points on $\bar{p}=1$ and 3. The two shuffle mechanisms are also shown in Fig. 20.8; that given by eqn. (85.37) represents atom movements which are parallel to $\mathbf{\eta}_1$ and may be quite small.

Now consider the problem of compound twins. A given set of twinning elements can give a type I twin if K_1 and $\mathbf{\eta}_2$ are rational and a type II twin if K_2 and $\mathbf{\eta}_1$ are rational. When all four elements are rational, we have a compound twin, and there is the possibility of two different orientation relations existing for one set of twinning elements (four if the structure is not centrosymmetric). There will then correspondingly be two different shuffle mechanisms, and the preferred orientation may be decided by the easier shuffle mechanism. However, the conditions for the formation of compound twins are rather restrictive and, in all crystal systems except rhombohedral and cubic,[†] the plane of shear must be a plane of symmetry (Crocker, 1959). In fact, the plane of shear is found to be a mirror plane in most of the operative modes of rhombohedral and cubic crystals also. Hence it follows (see p. 867) that in most single lattice structures all four orientation relations are identical in compound twins. For double lattice structures, orientations I and II will not be equivalent unless the plane of shear is a symmetry plane of the atomic arrangement, i.e. unless the motif unit may be chosen to lie in or normal to the plane of shear. In other cases of compound twins in double lattice structures, there will be two orientation relations to consider. This may be seen in Fig. 20.8, where the distinction between (e) and (f) and between (g) and (h) disappears if the motif unit is in, or normal to, the plane of shear.

Now consider briefly the phenomenon of double twinning, mentioned on p. 867. Consider the application of two successive twinning shears to a region of crystal. If a macroscopic twin is produced by the first deformation, the re-twinning represented by the second shear will not generally be possible unless there is considerable additional deformation in either the parent or the primary twin. Assuming the re-oriented region to be plate-shaped, its macroscopic habit plane will be determined by the K_1 plane of the first twin and by the amount of additional deformation which has occurred in the parent. If such situations arise, they are clearly of interest in producing a set of pseudotwinning elements, but they introduce no new principles in the crystallography of twinning. A different type of double twinning, however, results from the assumption that two twinning shears are applied simultaneously rather than successively to a region of parent. This might arise physically, for example, if a small twin nucleus retwins, and the re-oriented nucleus then grows into a macroscopic twin by the combined action of the two shears. The final product may then possess twin elements different from those of the

[†]Compound twins cannot be formed in triclinic crystals.

constituent twins, and in a sense the resolution into components has only formal significance as far as the macroscopic growth is concerned. A discussion of both these types of double twinning was given by Crocker (1962), following suggestions by Couling *et al.* (1959) and by Reed-Hill (1960) that certain anomalous twinning modes observed in magnesium are in fact due to double twinning.

From the more general result proved in Section 9 for invariant plane strains, it follows that the resultant of two simple shears will not itself be a simple shear unless either the K_1 plane or the η_1 direction is common to the two components. This is possible in a formal sense in cubic structures, for example, but the net result is to restore the original parent orientation, so that a simple combination of two twinning shears does not give physically significant results. If the above condition on the K_1 plane or η_1 direction is relaxed, the resultant deformation will not contain an invariant plane, but may contain an undistorted plane. There is thus the additional possibility of combining two twinning shears and a pure rotation to give an equivalent simple shear. In analysing this type of double twinning operation, Crocker points out the close similarity to the theory of martensite crystallography.

The two component shears and the resultant deformation must all have a principal strain equal to zero (p. 59), and this restricts the combinations to be considered to those in which the two twinning directions and the normals to the two K_1 planes are all coplanar. The two planes of shear are thus coincident, and the problem is essentially two-dimensional. Consideration of the various possible combinations of type I and type II twins then shows that the plane of shear must be rational and, furthermore, all eight twinning elements of the two component twinning modes must also be rational, so that only compound modes may be combined in this way.

The combined effect of the three component deformations is to produce an equivalent simple shear with the same rational plane of shear, so that this also represents a compound twinning mode if it satisfies one of the usual types of twin orientation relation. The general solution, however, is one in which all four elements of the equivalent shear mode are irrational, and this is thus an example of the more general type of twin which has to be defined in the way indicated on p. 860. The possible existence of "twins" with four irrational twinning elements is a remarkable result of the theory of double twinning. The assumptions of this theory nevertheless appear to be rather artificial and it seems preferable to generalize the classical theory of deformation twinning by beginning directly with the proposed definition (Bilby and Crocker, 1965) that a twinning shear is any shear which restores the lattice or a superlattice in a new orientation. The relevant theory for lattices (i.e. excluding detailed consideration of atomic shuffles) was first given by Bevis and Crocker (1968, 1969) and we follow their treatment but use matrix rather than tensor notation (Christian, 1970).

The theory is developed in terms of certain properties of the correspondence matrix C defined in eqn. (8.4). In the case of twinning, the matrices C , S and L are all unimodular and S has the form

$$S = I + sLm' \quad (85.39)$$

in which (as before) \mathbf{l} is a unit vector in the \mathbf{n}_1 direction and \mathbf{m} the unit normal to the K_1 plane so that, in a general coordinate system with metric \mathbf{G} (see p. 34), $\mathbf{l}'\mathbf{G}\mathbf{l} = \mathbf{m}'\mathbf{G}^{-1}\mathbf{m} = 1$ and $\mathbf{m}'\mathbf{l} = 0$. It follows from the expression for the length of a vector $|\mathbf{u}|^2 = \mathbf{u}'\mathbf{G}\mathbf{u}$ and from the equivalent expression after a rigid body rotation represented by the orthogonal matrix \mathbf{L} that $\mathbf{L}'\mathbf{G}\mathbf{L} = \mathbf{G}$, so that

$$\mathbf{X} = \mathbf{S}'\mathbf{G}\mathbf{S} - \mathbf{C}'\mathbf{G}\mathbf{C} = 0 \quad (85.40)$$

is a null matrix. Combining eqns. (85.39) and (85.40) gives

$$\mathbf{X} = \mathbf{G} + s\mathbf{G}\mathbf{l}\mathbf{m}' + s\mathbf{m}\mathbf{l}'\mathbf{G} + s^2\mathbf{m}\mathbf{m}' - \mathbf{C}'\mathbf{G}\mathbf{C} \quad (85.41)$$

An expression for the magnitude of the shear which depends only on the correspondence matrix may now be obtained by taking the trace of the matrix product $\mathbf{X}\mathbf{G}^{-1}$ and equating this to zero, to give

$$s^2 = \text{tr}(\mathbf{C}'\mathbf{G}\mathbf{C}\mathbf{G}^{-1}) - 3 \quad (85.42)$$

An equivalent equation may be obtained by inverting eqn. (85.40) to form a matrix $\mathbf{S}^{-1}\mathbf{G}^{-1}(\mathbf{S}^{-1})' - \mathbf{C}^{-1}\mathbf{G}^{-1}(\mathbf{C}^{-1})'$ which is also identically equal to zero. Combination of the resultant equation for s^2 with eqn. (85.42) then leads to a restriction on the correspondence matrix

$$\text{tr}(\mathbf{C}'\mathbf{G}\mathbf{C}\mathbf{G}^{-1}) = \text{tr}\left\{(\mathbf{C} - \mathbf{I})'\mathbf{G}^{-1}\mathbf{C}^{-1}\mathbf{G}\right\} \quad (85.43)$$

Once the correspondence is defined, it fixes not only the shear but also \mathbf{l} and \mathbf{m} . Consider, for example, the scalar combination $2m_1m_2X_{12} - m_1^2X_{22} - m_2^2X_{11}$ which is identically equal to zero from eqn. (85.40). When this expression is formed from eqn. (85.41), the terms in s and l_1 all vanish and therefore

$$Y_{11}m_2^2 - 2Y_{12}m_1m_2 + Y_{22}m_1^2 = 0 \quad (85.44)$$

where

$$\mathbf{Y} = \mathbf{G} - \mathbf{C}'\mathbf{G}\mathbf{C} \quad (85.45)$$

Equation (85.44) is a quadratic in the ratio m_2/m_1 and there are two similar equations for the ratios m_3/m_2 and m_1/m_3 ; if \mathbf{C} is known, the three equations give two possible solutions for the components of \mathbf{m} . The three components of \mathbf{l} may be determined directly from \mathbf{m} and s , or may be derived from three similar quadratic equations of the form

$$Z_{11}l_2^2 - 2Z_{12}l_1l_2 + Z_{22}l_1^2 = 0 \quad (85.46)$$

where

$$\mathbf{Z} = \mathbf{G}^{-1} - (\mathbf{C}^{-1})'\mathbf{G}^{-1}\mathbf{C}^{-1} \quad (85.47)$$

Consider now the classical theory of deformation twinning. It follows from eqn. (85.4) that, for a type I twin, the matrix \mathbf{L} of eqn. (8.4) is given by

$$\mathbf{L} = -\mathbf{I} + 2\mathbf{G}^{-1}\mathbf{m}\mathbf{m}' \quad (85.48)$$

Also, eqn. (85.12) expressed in a general coordinate system is

$$s\mathbf{l} = 2[\mathbf{G}^{-1}\mathbf{m} - (\mathbf{g}/\mathbf{m}'\mathbf{g})] \quad (85.49)$$

so that eqn. (85.39) becomes

$$\mathbf{S} = \mathbf{I} + 2\mathbf{G}^{-1}\mathbf{m}\mathbf{m}' - 2\mathbf{g}\mathbf{m}'/(\mathbf{m}'\mathbf{g}) \quad (85.51)$$

The correspondence matrix for type I twinning is thus

$$\mathbf{C} = \mathbf{L}\mathbf{S} = -\mathbf{I} + 2\mathbf{g}\mathbf{m}'/(\mathbf{m}'\mathbf{g}) \quad (85.51)$$

and the form of the equation remains unchanged if we substitute any vector parallel to \mathbf{n}_2 for \mathbf{g} and any reciprocal lattice vector normal to K_1 for \mathbf{m} . A similar development gives the correspondence matrix for type II twinning as

$$\mathbf{C} = -\mathbf{I} + 2\mathbf{l}\mathbf{n}'/(\mathbf{n}'\mathbf{l}) \quad (85.52)$$

The two correspondence matrices just derived are independent of the metric tensors \mathbf{G} and \mathbf{G}^{-1} and so give rise to classical twins in all lattices; they have the property that $\mathbf{C} = \mathbf{C}^{-1}$, so that eqn. (85.43) is automatically satisfied. They also have the property that $\text{tr } \mathbf{C} = -1$ and this is a useful necessary, although not sufficient, condition for \mathbf{C} to represent a deformation twin of classical type.

It remains to investigate the possibility of other correspondences which lead to non-classical twins. Following the Jaswon–Dove approach, it is useful to rewrite eqn. (85.42) as an inequality in order to list all chosen values of s_{\max} . In particular, this gives for the cubic system

$$\text{tr}(\mathbf{C}'\mathbf{C}) \leq s_{\max}^2 + 3 \quad (85.53)$$

As stated on p. 56, the columns of \mathbf{C} are the components of the vectors specifying the cell into which the reference cell defined by \mathbf{a}_i is deformed by \mathbf{S} . The lattice is not reproduced if any of the components of \mathbf{C} is irrational. When \mathbf{a}_i define a primitive unit cell, the point lattices of parent and twin are identical if the columns of \mathbf{C} represent lattice vectors. However, if the base vectors define a base-centred cell, it is additionally necessary that the sum of the first two columns of \mathbf{C} must be twice a lattice vector, for a body-centred cell the sum of all three columns of \mathbf{C} must be twice a lattice vector, and for a face-centred cell the sum of any two columns must be twice a lattice vector. When the elements of \mathbf{C} are rational but do not satisfy these conditions, the point lattice produced by \mathbf{S} differs from the parent lattice but has a superlattice in common, so that a twin may be produced by combining the shear with a shuffling of some fraction of the lattice sites. If some elements of \mathbf{C} are fractions, a matrix $\mathbf{W} = m\mathbf{C}$ with only integral elements may be defined, and the inequality (85.53) becomes

$$\text{tr}(\mathbf{W}'\mathbf{W}) \leq m^2(S_{\max}^2 + 3) \quad (85.54)$$

Using a trial-and-error procedure, Bevis and Crocker list 10 correspondences for cubic systems in which $m=1$, $s_{\max}^2=9$, 19 correspondences for which $m=2$, $s_{\max}^2=3.5$, and 31 correspondences for which $m=4$, $s_{\max}^2=2.5$. For primitive lattices, the fraction of the

lattice points sheared direct to twin positions is $1/m$, but it may be $2/m$, $1/m$ or $\frac{1}{2}m$ for centred lattices.

New unimodular matrices may be derived from any given C by interchanging rows or columns, or changing their signs. In the cubic system, these operations simply lead to equivalent variants of C but, in systems of lower symmetry, the numbers of non-equivalent variants which may be derived from each cubic correspondence are: tetragonal, nine; rhombohedral, 16; orthorhombic and hexagonal, 36; monoclinic, 144; triclinic, 576. However, many of these do not represent possible twins because the restriction of eqn. (85.43) involves lattice parameters in non-cubic systems.

Consider the set of planes and directions K_1 , K_2 , η_1 and η_2 which define a mode arising from a particular correspondence C . The associated conjugate mode is then obtained by interchanging K_1 and K_2 and η_1 and η_2 and also has the correspondence C . A different but closely related twinning mode is obtained by interchanging the indices of K_1 and η_1 and of K_2 and η_2 and reversing the sign of either the old or the new K_2 and η_1 . This new mode arises from the correspondence $(C^{-1})'$, i.e. the transpose of the inverse of the original correspondence, and the interchange leads strictly to an equivalent shear (of the same magnitude) in the reciprocal lattice provided that the direct and reciprocal metrics are also interchanged. However, the new shear mode is valid for all possible reciprocal lattice parameters and, as the direct and reciprocal lattices belong to the same crystal system, these parameters may be chosen to equal those of the original direct lattice. Thus the correspondences C and $(C^{-1})'$ define separate but related shear modes for a given lattice. If the lattice is centred, the fraction of the lattice points sheared directly to twin positions will normally not be the same for the two modes.

For non-conventional twinning modes, the elements derived from C are different from those derived from C^{-1} . The apparent difference conceals a close relationship; the shear matrix derived from C^{-1} represents in the twin basis an equal and opposite shear to that derived in the parent basis from C . Thus the new twinning mode would convert the twin produced by the original mode back to the original parent orientation. It follows that the indices of the K_1 plane in a non-conventional twinning mode are different when referred to parent and twin bases and are described by the correspondences C and C^{-1} respectively; the same applies to K_2 , η_1 and η_2 . Moreover, the relation between the twinning elements derived from C and $(C^{-1})'$ applies equally to those derived from C^{-1} and C' .

The correspondence matrices may be divided into seven different classes by considering the various crystallographic degeneracies which arise from relations between C , C^{-1} , C' and $(C^{-1})'$. The most general class of twinning mode arises when none of the three derived matrices is crystallographically equivalent to C and the indices K_1 , K_2 , η_1 and η_2 associated with the mode and its inverse are then all different, so that eight sets of twinning elements are associated with the four correspondences. In the other classes, there are various predicted relations between the individual twinning elements; for example, if C and C^{-1} are crystallographically equivalent, but not identical, the twinning elements given by the two correspondence matrices may be written $ABCD$ and $BADC$ respectively, whereas if C and $(C^{-1})'$ are crystallographically equivalent, the twinning elements obtained from C and C^{-1} have the forms $ABAB$ and $EFEF$ respectively. Both of these are degenerate cases of

non-conventional twinning modes, but two of the seven classes include the condition $C = C^{-1}$ which gives rise to classical twinning modes. Of the 60 correspondence matrices mentioned above, 42 represent conventional or classic modes and 18 represent non-conventional modes.

To end this section, consider the problem of defining deformation twinning in alloys. Laves (1952) and many later authors have emphasized that, in the absence of shuffles, it is impossible to twin many superlattice structures as a homogeneous shear produces a new superlattice which can be represented as a different ordering of the atoms of the various chemical species on the sites of the disordered lattice. From one point of view, a superlattice is just a particular example of a multiple lattice structure, and no new principles need be invoked in deducing the possible twinning modes which will, in general, require structure shuffles in addition to the displacements of the simple shear. However, these shuffles would usually simply effect interchanges of some of the atoms, and are thus extremely improbable during deformation twinning. In discussing the possible twin modes of superlattices, it is thus necessary to distinguish "interchange" shuffles from the lattice and structure shuffles considered above (Christian and Laughlin, 1988). In fact, some superlattice structures have been found to undergo deformation "twinning" without the necessary shuffles in a mode appropriate to the disordered structure and, following Laves, this is often referred to as "pseudotwinning". The sheared region which comprises the pseudotwin generally has a lower symmetry than the parent structure; for example, if the usual b.c.c. twinning mode is applied to the B2 (L_{20}) superlattice, the pseudotwin has a structure with orthorhombic symmetry.

The change of structure implies that the new region will have a higher free energy per atom, and the change should strictly be regarded as a particular case of a stress-induced fully coherent martensitic transformation with no change of volume. This argument may be extended to any non-ideal solid solution, to which the application of a twinning shear produces a change in the pair correlations (Laves, 1966) or traps interstitials in different positions (Magee *et al.*, 1971). In such a solid solution, "true" twinning is thus strictly not possible, although the structural and symmetry changes may be too small in practice to be detected experimentally. The extreme form of this conclusion (Cahn, 1977) is that, as there are no absolutely pure metals or perfectly random solid solutions, deformation "twinning" will always in principle be accompanied by some structural and energetic changes. Cahn suggests that, because the assignment of some limit to the permissible structure change would be arbitrary, we should not attempt to distinguish between twinning and "twinning", i.e. between true and pseudotwins, but should recognize that changes of structure and symmetry are always involved in the process which we describe as deformation twinning. However, it is convenient to retain the term pseudotwinning for structures with nearly perfect long-range order because, as explained above, the operation of a twinning mode of the disordered system may then give a relatively large change in structure and symmetry.

As the normal twinning modes of the (disordered) f.c.c. and b.c.c. structures both have $q=4$ for simple cubic lattices and $q=8$ for their reciprocal lattices (b.c.c. and f.c.c. respectively), it follows that lattice (interchange) shuffles will only be avoided for a cubic

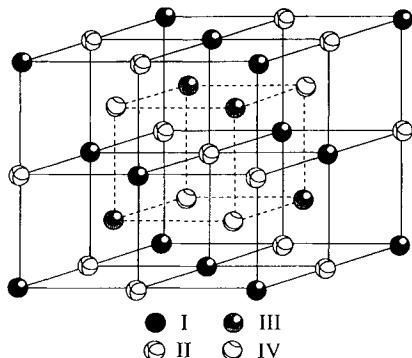


FIG. 20.9. Superlattice structures derived from b.c.c. structure (after Christian and Laughlin, 1987). The basic superlattice structures have site occupancy as follows: B2, *B* atoms occupy sites I and II and *A* atoms occupy sites III and IV; B32, *B* atoms occupy sites I and II and *A* atoms occupy sites I and IV; DO₃, *B* atoms occupy sites I and *A* atoms occupy sites II, III and IV.

superlattice which has the same Bravais lattice as the disordered structure. This is only possible for stoichiometric compositions of the form A_nB , where $n=p^3-1$ and p is an integer. Although there is some experimental evidence for the formation of compounds with the first composition in this series, A_7B , it seems unlikely that such ordering will occur in many alloy systems. The ground state diagrams of Richards and Cahn (1971) shown in Figs. 6.10 and 6.11 include one cubic superlattice of the f.c.c. structure ($L1_2$ in Strukturbericht notation) and three of the b.c.c. structure (B2, B32 and DO₃). Figure 20.9 shows the b.c.c. superlattices in terms of the occupancy of sites on four interpenetrating f.c.c. lattices, from which it is immediately obvious that a mode derived from the usual b.c.c. mode has $q=4$ for B2 and $q=8$ for B32 and DO₃. The true, no-shuffle mode of lowest shear for the B2 structure actually has the same K_1 plane as the normal disordered mode, but the direction of η_1 is reversed and the shear magnitude is twice as large. A similar "reversed f.c.c. shear" will produce a true twin in the L1₂ superlattice, but a very large shear, four times that of the disordered structure and applied in the same η_1 direction, is required to satisfy the geometrical conditions for true twins in either B32 or DO₃. The B2 and L1₂ twinning modes were discussed by Arunchalam and Sargent (1971), who pointed out that they may be deduced directly from the table of modes published by Bevis and Crocker (1969).

When the superlattice is non-cubic, the new modes derived from different variants of the disordered mode are no longer all equivalent. Some of these derived modes, applied without interchange shuffles, will again change the crystal structure and so may be described as pseudomodes. Other variants, however, will produce true twins in the ideal superlattice. In a detailed discussion based on the Bevis-Crocker theory, Christian and Laughlin (1987, 1988) have enumerated the modes for all non-equivalent variants of the non-cubic structures predicted by Richards and Cahn. Two types of true twin are discussed, namely type I/II, where the direct mode gives a type I orientation and the

conjugate mode a type II, or vice versa, and “combined”, where these two orientations are equivalent. The term “combined” is used rather than “compound” as all the modes are necessarily compound in the original sense that all the twinning elements are rational.

86. OPERATIVE TWINNING MODES IN METALLIC STRUCTURES

We may now apply the theory of the previous section to the prediction of the most likely twinning modes in any structure, assuming these modes to be governed by the magnitude of the lattice shear and the complexity and magnitude of the shuffles. Equation (85.13) may be rewritten as

$$s^2 = 4 \frac{|\mathbf{w}|^2}{(\mathbf{w} \cdot \mathbf{m})^2} - 1 \quad (86.1)$$

Now writing $s < s_{\max}$, where s_{\max} is any chosen maximum shear, and using eqn. (85.14),

$$|\mathbf{w}|^2 < q^2 d^2 \{(s_{\max}/4) + 1\} \quad (86.2)$$

which is a condition on the interplanar spacing d of a set of possible K_1 planes and the shortest lattice vector \mathbf{w} between two such planes qd apart. The inequality (86.2) reduces to (85.2) for $q=2$, and to (85.3) for $q=4$, if $|\mathbf{w}|$ is replaced by $|\mathbf{b}|$. This may sometimes be convenient but, as noted in the previous section, the inequality then becomes a necessary condition only (i.e. it may not be a sufficient condition) for the minimum shear on the planes of spacing d to be less than s_{\max} . There is no need to investigate separately the conditions for type II twinning, as the possible type I modes with K_1 rational will automatically give the type II modes with K_2 rational.

The inequality (86.2) is independent of any coordinate system but, in using it, care must be taken if a superlattice cell of higher symmetry is used instead of a primitive unit cell. Thus if \mathbf{G}, \mathbf{G}^* are the metrics of the primitive bases \mathbf{A}, \mathbf{A}^* , and we represent the K_1 planes by the vector $\mathbf{k} = k_i \mathbf{a}_i^*$, where k_i are integers with no common factor, inequality (86.2) becomes, in subscript form (see Table II),

$$(G_{ij} w_i w_j)(G_{ij}^* k_i k_j) < (w_i k_i)^2 \{(s_{\max}^2/4) + 1\}. \quad (86.3)$$

However, if we use a larger unit cell for convenience, and k_i and w_i are still given integral values, we have to introduce the cell factors I (p. 38). Using Table III, the inequality now becomes:

$$(I')^2 (G_{ij} w_i w_j)(G_{ij}^* k_i k_j) < I^2 (w_i k_i)^2 \{(s_{\max}^2/4) + 1\}. \quad (86.4)$$

It is frequently more convenient to refer the twinning elements to a centred cell, and thus to use the inequality (86.4).

The prediction of the twinning elements for the single lattice structures was discussed on p. 860 where it was found that, for most metallic structures, the normally observed twinning mode is the mode of lowest shear consistent with the absence of shuffles. In the structures for which this statement is valid, the operative mode and its conjugate are

crystallographically equivalent, and the shear is very much smaller than that of any rival “non-shuffle” mode. This is not true for mercury, which is considered separately below.

In some double lattice structures, it is commonly observed that more than one twinning mode may be active during deformation, but almost all of the many experimental observations of deformation twinning in cubic and tetragonal single lattice structures indicate that only the minimum shear modes are operative. However, there are isolated reports of additional twinning modes, for example in b.c.c. iron–beryllium alloys and in b.c.t. iron–nickel–carbon martensites, and there is also the possibility that transformation twinning in martensite (see Chapter 22) may utilize effective twinning modes different from those produced by plastic deformation. Thus, it is now appropriate to consider briefly the application of the Bevis and Crocker general theory to the prediction of other possible modes in single lattice structures, including non-conventional modes which do not satisfy the classical definition of a twin.

It follows from the description on p. 884 that a unimodular lattice correspondence C leading to twinning elements K_1 , K_2 , η_1 , η_2 and s will also have an associated conjugate mode obtained by interchanging K_1 and K_2 and η_1 and η_2 . For cubic lattices, the pair of additional modes obtained by interchanging the indices of K_1 and η_1 and of K_2 and η_2 , and reversing the sign of either the old or the new K_2 and η_1 , also have the same shear magnitude although the amount of shuffling required will be different if the lattice is centred. Bevis and Crocker (1969) used the 60 correspondence matrices mentioned on p. 884 as input data to derive the twinning elements of the corresponding modes for cubic lattices and gave examples from all seven classes of correspondence. They published a table showing a selection of their results in the form of 26 different sets of indices derived from the various matrices C and C^{-1} each giving rise, in the absence of crystallographic degeneracy, to up to four different twinning modes by applying the above permutations of indices. Of the 26 basic modes, 13 are both conventional and compound whilst the other 13 are non-conventional, and 11 of these have four irrational twinning indices of the form $x \pm y^{1/2}$, where x and y are integers. Many of the K_1 planes in the compound modes are mirror planes so that the shear would reproduce the parent lattice in the same orientation and this operation could thus not be described as twinning. However, in such cases the K_2 plane is generally not a mirror plane so that the conjugate shear represents a possible twinning mode. The plane of shear is always rational for the non-conventional modes, and this is a general feature of cubic lattices; the orientation relation may be described as a rotation about the normal to this plane of shear.

To investigate the possible twinning modes in the six non-cubic crystal systems, Bevis and Crocker first considered the modes which arise from variants of the unit correspondence matrix. The unit matrix itself leads, of course, to zero shear in all systems but nine of its variants obtained by interchanging rows, interchanging columns and changing the signs of rows and columns (see p. 884) satisfy the restriction (85.43) and so may lead to twins in some crystal systems. These nine correspondence matrices are all symmetric and three of them are diagonal; they all satisfy the condition $C = C^{-1}$ and so represent conventional twinning modes with at least two rational elements. The nine independent modes of the triclinic system reduce to four modes in the monoclinic system,

to three modes in the orthorhombic system, to a single mode (excluding shears which restore the original lattice) in the hexagonal system, to single modes in the tetragonal and rhombohedral systems, and of course to no modes in the cubic system.

The procedure was repeated for a slightly more complex correspondence which has 20 variants leading to twinning in triclinic systems, reducing to eight, six, three, two and one independent modes in the monoclinic, orthorhombic, tetragonal, hexagonal and cubic systems respectively. Most of these modes are non-conventional with four irrational elements.

The twinning modes predicted for the f.c.c. and b.c.c. structures by the no-shuffle, minimum shear hypothesis on p. 862 are both derived from the correspondence matrix

$$C = \begin{pmatrix} 0 & 1 & 1 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 1 & 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 1 \end{pmatrix} \quad (86.5)$$

which leads to the f.c.c. mode, whilst C' leads to the b.c.c. mode. Shears of magnitude $2^{-1/2}$ on the {111} plane lead to twins in the simple cubic, f.c.c. and b.c.c. structures but the fractions of parent lattice sites which are sheared directly to twin positions are respectively $\frac{1}{2}$, 1 and $\frac{1}{4}$; whereas for a twinning shear of the same magnitude on the {112} plane, these fractions are $\frac{1}{2}$, $\frac{1}{4}$ and 1. Several other examples of f.c.c. or b.c.c. modes which involve no shuffles are found among the cubic modes listed by Bevis and Crocker but these are all conventional type modes, and non-conventional modes with zero shuffles are only possible if shear magnitudes outside the limits specified on p. 883 are allowed.

All reported instances of twinning in f.c.c. structures have the expected {111} habit plane but, in an experimental study of twinning in iron–beryllium alloys and iron–nickel–carbon martensites, Richman and Conrad (1963) and Richman (1964) found evidence for b.c.c. twins with rational {013} and irrational “{089}” and “{127}” habits. However, the iron–beryllium alloys were ordered and twinned copiously on the {112} planes whilst the untempered martensites should have been b.c.t. rather than b.c.c. and, in addition, presumably contained a fine structure of {112} transformation twins. These factors, combined with the small size of most of the anomalous twins, makes the experimental determination of the anomalous modes very difficult and, in a later electron microscopic study, it was concluded that the unusual twin modes observed by Richman in martensite were probably {112} deformation twins with macroscopic habits deviated from the {112} twin plane because of their interaction with the transformation twins. In a later study of iron–beryllium alloys, Green and Cohen (1979) were unable to find evidence of the anomalous modes reported by Richman. Table XVI lists all the predicted b.c.c. modes with $s \leq 2$ and the modes in which one-half of the lattice points shuffle with $s \leq 1$. The {013} habit is seen to be a possible no-shuffle mode, albeit with a rather large shear, but the other two of Richman’s reported modes are not among those predicted.

TABLE XVI. PREDICTED AND OBSERVED TWINNING MODES IN SINGLE LATTICE STRUCTURE
(CHRISTIAN AND MAHAJAN, 1995)

Structure	K_1 { }	K_2 { }	η_1 ()	η_2 ()	s	P { }	References to some supporting experimental studies
f.c.c	111	111	112	112	$2^{-1/2}$	110	Cu, ^{1,2} Ag and Cu alloys, ^{3,7} Ni, ^{9,10} Al alloys ^{11,12} and Co Fe alloys ^{13,16}
b.c.c	112	112	111	111	$2^{-1/2}$	110	Fe and its alloys ¹⁷⁻³¹ ; Nb and its alloys ³²⁻³⁴ ; Mo-Realloys ^{35,36} Mo ⁴⁰
(no shuffle)	147	101	311	111	$3^{1/2}/2^{1/2}$	121	
	112	110	111	001	$2^{1/2}$	110	
	013	415	531	111	$7^{1/2}/2^{1/2}$	231	Fe-Be alloys ⁴¹⁻⁴²
b.c.c	112	332	111	113	$2^{1/2}/4$	110	
($\frac{1}{2}$ atoms shuffle)	5,8,11	101	513	111	$6^{1/2}/4$	121	Fe-Ni and Fe-Ni-C martensites ⁴³ Fe-Ni alloy ⁴⁴
	145	341	111	139	$7/58^{1/2}$	321	
	013	011	031	011	1	100	
f.c.t.	011	011	011	011	$\gamma^1 - \gamma$	100	
	111	111	112	112	$(2\gamma^2 - 1)/2^{1/2}\gamma$	110	
b.c.t	011	011	011	011	$\gamma^1 - \gamma$	110	
(no shuffle)	112	112	111	111	$(2 - \gamma^2)/2^{1/2}\gamma c^*$	110	
	121	a	b	111	$(2 - 5\gamma^2 + 5\gamma^4)^{1/2}2\gamma$	d	
b.c.t	e	101	513	f	$(26 - 29\gamma^2 + 9\gamma^4)^{1/2}4\gamma$	g	
($\frac{1}{2}$ atoms shuffle)	h	110	531	111	$(4 + 2\gamma^2)^{1/2}4$	112	
f.c.rhombohedral	011	100	100	011	$8^{1/2}c/(1 + 2c)^{1/2}(1 + c)^{1/2}$	011	
	j	111	121	k	$\frac{(2 + 8c + 22c^2)^{1/2}}{2(l - c)^{1/2}(1 + 2c)^{1/2}}$	m	Hg ⁴⁵⁻⁴⁷

Notes: The two f.c.t. modes are linked to their equivalent b.c.t modes. All b.c.c no shuffle modes with $s \leq 2$ and half-shuffle modes with $s \leq 1$ are included, but not all the derived b.c.t modes are listed. γ is the axial ratio of the appropriate tetragonal lattice (≈ 1.035 for b.c.t. martensite), and c ($\approx -1/7$ for Hg) is the cosine of the rhombohedral interaxial angle. The irrational indices a, b and d-m are:

a = $\gamma^2 - 2$, $3\gamma^2$, $2 - 3\gamma^2$; b = $-1 - \gamma^2$, $3\gamma^2 - 1$, $3 - 5\gamma^2$; d = $2\gamma^2 - 1$, $1 - \gamma^2$, $-\gamma^2$; e = $14 - 9\gamma^2$, $8, 26 - 15\gamma^2$; f = $5 - 3\gamma^2$, $1 + \gamma^2$, $5 - 3\gamma^2$; g = $-1.5 - 3\gamma^2 - 1$; h = $6 - \gamma^2, 10 + \gamma^2, 8\gamma^2$; j = $-1 - 5c$, $-1 - c$, $1 - 3c$; k = $-1 - 7c$, $-2 - 6c$, $1 - c$; m = $1 + c$, $-2c$, $1 + 5c$.

* Predicted minimum shear, no-shuffle modes which have not been observed.

Key to references

- 1) Blewitt, Coltman and Redman (1957)
- 2) Mahajan, Barry and Eyre (1970)
- 3) Suzuki and Barrett (1958)
- 4) Venables (1961)
- 5) Narita and Takamura (1974)
- 6) Mori and Fujita (1977)
- 7) Mori and Fujita (1980)
- 8) Haasen (1958)
- 9) Robertson (1986)
- 10) Haasen and King (1960)
- 11) Gray (1988)
- 12) Pond and Garcia-Garcia (1981)
- 13) Chin, Hosford and Mendorf (1969)
- 14) Mahajan and Chin (1973a)

Key to references (*continued*)

- 15) Mahajan and Chin (1974)
- 16) Mahajan and Chin (1973b)
- 17) Priestner and Leslie (1965)
- 18) Le, Bernstein and Mahajan (1993)
- 19) Paxton (1953)
- 20) Leslie, Hornbogen and Dieter (1962)
- 21) Mahajan (1969)
- 22) Altshuler and Christian (1966)
- 23) Zukas and Fowler (1961)
- 24) Mahajan (1970)
- 25) Rosenfield, Averbach and Cohen (1963)
- 26) Hull (1961)
- 27) Hull (1963a)
- 28) Hull (1963b)
- 29) Honda (1961)
- 30) Terasaki (1967)
- 31) Edmondson (1961)
- 32) Boucher and Christian (1972)
- 33) Wessel, France and Begley (1961)
- 34) McHargue (1964)
- 35) Hull (1963c)
- 36) Mahajan (1972a)
- 37) Mahajan (1972b)
- 38) Mahajan (1975)
- 39) Mahajan (1971)
- 40) Mahajan and Bartlett (1971)
- 41) Richman and Conrad (1963)
- 42) Richman (1963)
- 43) Rowlands, Fearon and Bevis (1968)
- 44) Rowlands, Fearon and Bevis (1970)
- 45) Guyoncourt and Crocker (1968)
- 46) Crocker, Heckscher, Bevis and Guyoncourt (1966)
- 47) Abell, Crocker and Guyoncourt (1971)

Further experiments on twinning in cubic iron–nickel and tetragonal iron–nickel–carbon martensites were reported by Rowlands *et al.* (1968). These authors found some b.c.c. deformation twins with the {5,8,11} habit of Table XVI. Although all four sets of indices are rational, so that the mode is compound, the orientation relationship is of type II, probably because of a minimum shuffle criterion. With a type II orientation relation, only one-half of the atoms have to shuffle whereas five-sixths of the atoms would have to shuffle to restore the structure in a type I relation. As the {101} plane is a mirror plane, the reciprocal mode is not a true twinning mode in b.c.c.; a shuffle of half the atoms results in an unchanged orientation of the original structure. Rowlands *et al.* (1970), in a further investigation, reported that deformation twins of other than {112} type are extremely rare, but they found some fine (possibly transformation) twins with a {145} habit, which is the conjugate mode to the {013} mode reported by Richman. In contrast, Fearon and Bevis (1974), in a later publication from the same laboratory, reported only {112} transformation twins in a cubic iron–nickel alloy.

Rowlands *et al.* (1968) also tentatively identified two tetragonal derivatives of the “{5,8,11}” mode in the carbon-containing martensite, both of which correspond to conventional type II modes. They point out, however, that non-conventional derivatives of this mode are also possible and there seems no reason why these should not occur in suitable circumstances. Although only one-half of the atoms are sheared to the correct positions, this mode has a smaller shear than the usually observed b.c.c. mode (see Table XVI). A possible reason for its occurrence in martensites is that, in the cubic structure, the {5,8,11} twin can propagate undeviated across a {112} twin boundary, and hence across the set of fine parallel {112} twins which are produced by the transformation mechanism. Bevis and Vitek (1970) suggested that a possible reason for the observation of some fine {145} twins in martensite is that a determining factor is the interfacial energy of the coherent K_1 habit plane, rather than the magnitude of the shear, as atomistic calculations indicate that the {145} habit has the next lowest interfacial energy after {112}.

The present position seems to be that the anomalous twinning modes have been identified in the b.c.t. structure with no more certainty than in b.c.c. and the overwhelming majority of observations on both deformation and transformation twins in b.c.t. martensites show only the dominant twinning mode to have the same elements as the b.c.c. {112} mode and a shear $s = 2^{1/2}(a/c) - 2^{-1/2}(c/a)$. This mode is derived from the correspondence (86.5) but, as already noted on p. 862, it is also the same mode as that deduced for the f.c.t. structure. Any b.c.t. structure may, of course, alternatively be regarded as f.c.t. with $a_{fcf} = 2^{1/2}a_{bct}$ and when this change is made the {112} plane of the b.c.t. structure becomes the {101} plane of the f.c.t. structure, with similar changes of the other twinning elements as shown in Table XVI. When face-centred indices are used, this twinning mode arises from four of the variants of the unit correspondence matrix and when the axial ratio is made equal to unity, so that the structure is f.c.c., the shear becomes zero and the twinning mode ceases to exist. When the structure becomes b.c.c., in contrast, the shear is not zero but $2^{-1/2}$ and the usual b.c.c. crystallography applies. As pointed out on p. 862, there are equivalent relations between the b.c.t. {011} mode and the f.c.c. {111} mode, and these are also shown in Table XVI. In general, it is convenient to choose the unit cell of a centred tetragonal structure so that the axial ratio differs as little as possible from unity. Thus ferrous martensites with interstitial solutes are described as b.c.t. and have twinning shears of approximately $2^{-1/2}$, as the {011} b.c.t. low shear mode apparently does not operate, whereas indium and its alloys are described as f.c.t. and have very small twinning shears.

Now consider twinning in solid mercury, which has a rhombohedral structure and is notable, as pointed out on p. 862, as the only other known example of a single lattice structure in which the no-shuffle, minimum shear mode is not the operative twinning mode. In contrast to the other single lattice structures, the predicted lowest shear mode and its conjugate are not crystallographically equivalent for the rhombohedral structure, so that there are two possible K_1 planes, namely (001) and (110) for shears of lowest magnitude. Early observations (Andrade and Hutchings, 1935) suggested that only the (110) plane is operative, but it now appears that these results were incorrect and that the true mode is of type II with an irrational habit plane close to (135) (Crocker *et al.*, 1966; Guyoncourt and Crocker, 1968; Abell *et al.*, 1971). The elements of this mode are given in Table XVI; it involves no shuffles and has the second smallest shear, which is nevertheless appreciably larger than the shear of the (001) (110) conjugate pair (0.63 and 0.46 respectively for mercury). The conjugate type I mode is seen from Table XVI to have a (111) K_1 plane, but apparently does not occur. Crocker speculates that this may be because the slip plane is also (111) and points out that the same reason was previously advanced for the non-appearance of the (001) mode at a time when both the slip plane and the twinning plane had been incorrectly determined. It is also interesting to note that the observed mode has the same correspondence (86.5) as the f.c.c. and b.c.c. modes, whilst the unobserved minimum shear modes are derived from variants of the unit correspondence matrix.

The twinning modes of the pure components which have single lattice structures are normally also found for essentially disordered solid solutions based on these single lattice

TABLE XVII. POSSIBLE TRUE TWINNING MODES IN CUBIC SUPERLATTICES AFTER CHRISTIAN AND LAUGHLIN (1988)

Mode No.	S	K_1	K_2	η_1	η_2	s^2	True twin in	Some supporting experimental results
<i>(a) Modes without shuffles</i>								
1.3	(110)	(1̄1̄1)	(001)	[1̄12]	[1̄10]	2	L1 ₂	Cu ₃ Au ^{1,2} and Ni ₃ (Al, Ti) ^{3,4}
1.3 ^T	(110)	(1̄12)	(1̄10)	[1̄1̄1]	[001]	2	B2	Ti-Ni and Ti-Fe-Ni alloys ⁵
1.9	(110)	(1̄12)	(001)	[1̄1̄1]	[1̄10]	8	B2, B32, DO ₃ , L1 ₂	Fe ₃ Al(Do ₃) ⁶
1.9 ^T	(110)	(1̄11)	(1̄10)	[1̄12]	[001]	8	B2, B32, DO ₃ , L1 ₂	
<i>(b) Modes with 50% (non-interchange) shuffles</i>								
2.3 ^T	(110)	(1̄1̄4)	(1̄10)	[2̄21]	[001̄]	$\frac{1}{2}$	B2	Ti-Ni and Ti-Fe-Ni alloys ⁵
1.2	(001)	(1̄20)	(100)	[210]	[01̄0]	1	B2, L1 ₂	
2.5	(001)	(1̄30)	(110)	[310]	[1̄10]	1	B2, B32, DO ₃	
1.3	(110)	(1̄11)	(001)	[1̄12]	[1̄10]	2	B2, B32, DO ₃	
1.3 ^T	(110)	(1̄12)	(1̄10)	[1̄1̄1]	[001]	2	L1 ₂	

Key to references

- 1) Mikkola and Cohen (1966)
- 2) Chakraborty and Starke (1975)
- 3) Guimier and Strudén (1970)
- 4) Kear and Oblak (1974)
- 5) Goo, Duerig, Melton and Sinclair (1985)
- 6) Guedo and Rieu (1978)

solvents. As emphasized on p. 885, however, if sufficient long-range order develops, so that the structure may be regarded as a perfect or imperfect superlattice of the disordered structure, the ordinary twinning mode may become a pseudomode which, in the absence of interchange shuffles, will produce incorrect ordering in the sheared lattice. For superlattice structures which retain cubic symmetry, all variants of the normal mode become pseudomodes of the superlattice. The true modes are listed in Table XVII, but only the L1₂ mode seems actually to occur. The B2 mode, which is also included among the possible b.c.c. modes of Table XVI, has the same shear as the L1₂ mode but has not been observed. Some B2 alloys are known to form pseudotwins in preference to the higher-shear, true mode, whilst in others an alternative twinning mode of lower shear in which 50% of the atoms undergo non-interchange shuffles has been found experimentally. Paxton (1994) has calculated using density functional theory in the local density approximation that for energetic reasons it is impossible to form a pseudotwin of a fully ordered B2 alloy of equiatomic composition.

The pseudomode in B2 is formally a martensitic transformation from the simple cubic structure with space group $Pm\bar{3}m$ to an orthorhombic structure of space group $Cmmm$. The product structure is sometimes erroneously stated to be tetragonal because two of the axes of the orthorhombic cell are equal in the idealized case of no change of lattice parameters on ordering. Relaxation of the parameters will lead, in principle, to three unequal

axes but this may be difficult to detect. Because the pseudomode and the true mode of lowest shear have the same K_1 plane, it is thus essential to obtain experimental evidence of either the symmetry of the product or the magnitude of the shape deformation in order to establish which mode is operating. For a two-phase $\alpha + \text{B}2$ structure in alloys of approximate composition Fe_3Be , Green and Cohen (1979) showed that there is indeed the anticipated change of symmetry in the "twins" formed in the $\text{B}2$ regions, and they linked this observation with the pseudoelastic behaviour of these alloys (see Section 104). Of course, their alloys of Fe_3Be composition cannot have had fully ordered $\text{B}2$ structures.

Iron–beryllium alloys with compositions near Fe_3Be were formerly reported to form a DO_3 superlattice on ordering. Several authors have stated that deformation twinning is impossible in this structure, but Fig. 20.9 and Table XVII show that *geometric* twinning without shuffles may readily be defined. However, the very large shear makes this twinning mode very improbable in practice, and there are no reported observations of deformation twinning in either the DO_3 or the $\text{B}32$ structures. Rather similar but less complete results have been found for iron–aluminium alloys variously reported to have either the $\text{B}2$ or the DO_3 structure. Cahn and Coll (1961) found that alloys with less than 50% long-range order form pseudotwins, but that twinning was suppressed in more highly ordered alloys. Guedo and Rieu (1978) obtained evidence for twinning and detwinning in alloys with the $\text{B}2$ structure and superelastic effects in alloys with the DO_3 structure, but it is uncertain whether or not this latter effect is due to pseudotwinning.

As an alternative to a pseudomode or a high shear mode, it is possible that a twin might form in a superlattice by a mode which requires non-interchange shuffles. The first evidence for such a mode was given by Goo *et al.* (1985) for titanium–nickel and titanium–iron–nickel alloys with the $\text{B}2$ structure. The mode, which involves shuffles of half the atoms ($q=4$ in both the b.c.c. and simple cubic lattices), has the same shear magnitude as the disordered b.c.c. mode but $K_1=\{114\}$ and $\eta_1=\langle 22\bar{1} \rangle$; the full indices are shown in Table XVII. This table also gives the other possible modes with 50% shuffles, all of which have higher shear magnitudes. The shuffles involved are relatively simple and have been discussed by Goo *et al.* and by Christian and Laughlin. Assuming that all atoms are displaced by the shear (i.e. the motif units are *not* treated as rigid), the atoms which must shuffle are alternately A and B on successive planes of shear and are contained in alternate K_2 planes normal to the plane of shear. Goo *et al.* suggested that these atoms are all displaced in the same direction [Fig. 20.10(c-i)]; alternative possibilities in which the atoms move in opposite directions in successive K_2 shuffle planes or in successive rows of one shuffle plane are shown in Fig. 20.10(c-ii) and (c-iii).

In contrast to $\text{B}2$, pseudotwinning has not been reported in $\text{L}1_2$ structures, but there is evidence for the true mode of Table XVII in Cu_3Au alloys (Mikkola and Cohen, 1966; Chakraborty and Starke, 1975) and in microtwins in $\text{Ni}_3(\text{Al},\text{Ti})$ γ' phases (Guimier and Strudn, 1970; Kear and Oblak, 1974). In their work on Cu_3Au , Chakraborty and Starke found that the true mode was observed only in alloys with nearly complete long-range order, whilst disordered or partially ordered alloys formed twins with the usual f.c.c. mode. The f.c.c. type twinning was also observed in highly ordered alloys tested in compression to relatively high strains, which would have reduced the initial long-range

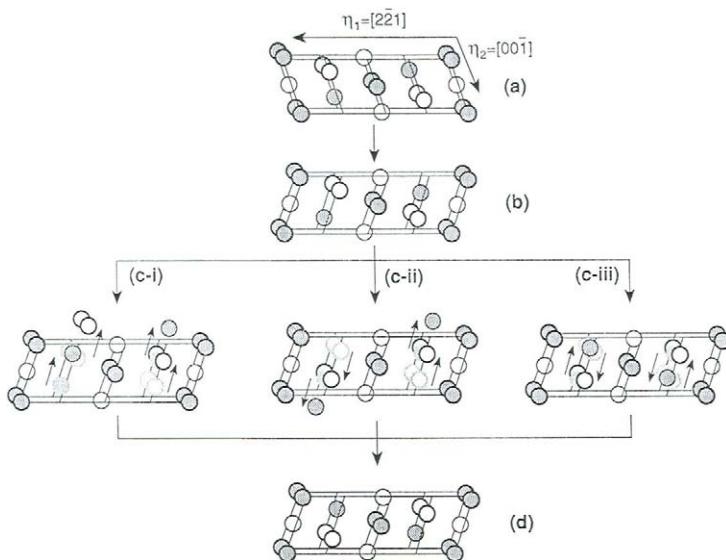


FIG. 20.10. Schematic illustration of the {114} shuffle mode in the B2 structure (after Christian and Laughlin, 1988). *B* and *A* atoms are shown by shaded and open circles respectively. (a) Parent structure; (b) sheared structure; (c-i) (c-iii) alternative shuffles; (d) combined orientation twin.

order. In this case, the twins formed only at applied shear stresses an order of magnitude larger than those required to produce true twins of the ordered structure.

For non-cubic superlattices of the f.c.c. structure, the variants of the usual f.c.c. mode may be divided into six pairs, each comprising a mode and its conjugate and having one of the six cubic {110} planes as the plane of shear. Four of the superlattices listed by Richards and Cahn (1971) were tetragonal, with either two or, in the case of Ni₄Mo, four f.c.c. mode pairs which give true twins in the superlattice. There are five, three, three and three possible true mode pairs for the orthorhombic superlattice (Pt₂Mo), the two (predicted but unobserved) monoclinic superlattices and the rhombohedral (L1₁) superlattice respectively. Experimental results have been reported for the L1₀, Pt₂Mo, DO₂₂ and D1a structures.

The most complete investigation of twinning in the tetragonal L1₀ structure is that of Shechtman *et al.* (1974) for a Ti-Al alloy. The specific variants of the {111} (112̄) cubic twin which formed during deformation were identified and shown to correspond to the true modes of the superlattice, and the shear magnitude was also measured. There are several experimental investigations of the CuAuI superlattice with the L1₀ structure, among which we may mention that of Pashley *et al.* (1969), who concluded that {111} twinning is an important deformation mechanism and speculated that the structure may be changed in some of the twins.

Hansson and Barnes (1965) and Pashley *et al.* pointed out that the structure produced by pseudotwinning of L1₀ has a single set of {111} cubic planes which are alternately occupied by atoms of each species, so that this structure is effectively that of the

$L1_1$ (CuPt) superlattice. The reverse is also true: the pseudomode of $L1_1$ yields the $L1_0$ structure. Unfortunately, there are no experimental results on twinning in $L1_1$.

Except at high temperatures, twinning is frequently the major deformation mechanism in alloys with the tetragonal DO_{22} structure, and it has been studied extensively in Ni_3V (Vanderschaeve and Sarrazin, 1977; Vanderschaeve *et al.*, 1979) and in Al_3Ti (Yamaguchi *et al.*, 1987ab.) The deformation always utilizes only the four true modes (two mode pairs) derived from disordered f.c.c. modes.

Finally, twinning has been established, but not fully investigated in the $D1a$ structure of Ni_4Mo (Nesbitt and Laughlin, 1980) and in certain nickel–molybdenum–chromium alloys with the orthorhombic Pt_2Mo structure (Tawancy, 1981). The true twins in Ni_4Mo are type I–type II in each conjugate pair whereas, in the Ni_3Pt structure, one mode pair gives true twins with combined orientations and four pairs give type I–type II orientations. In both structures, it seems probable that true twins are formed but the detailed crystallography was not established.

Now consider the double lattice structures, the most important of which is the h.c.p. structure with axial ratios differing by varying amounts from the ideal $(8/3)^{1/2}$. The metals cadmium and zinc, with the rather high axial ratios of 1.886 and 1.856, are usually considered to form a separate subgroup, the remaining metals having axial ratios ranging from slightly smaller than that for ideal close packing (cobalt and magnesium) down to 1.568 (beryllium). All the metals twin on the $\{10\bar{1}2\}$ planes, but most of the low axial ratio metals have also been reported to twin on several other planes. Additional K_1 planes reported for titanium, for example, are $\{11\bar{2}1\}$, $\{11\bar{2}2\}$, $\{11\bar{2}3\}$ and $\{11\bar{2}4\}$, and additional modes for magnesium include $\{10\bar{1}1\}$, $\{30\bar{3}4\}$, $\{10\bar{1}3\}$ and $\{10\bar{1}4\}$. Some of these “anomalous” twinning modes are well established; in others, the identification of habit plane traces as twins is open to some doubt. Note that the experimental determination of all the elements of a given mode is not possible unless the shear is measured, and this is rather difficult.

Early work showed that the full description of the $\{10\bar{1}2\}$ mode is

$$\begin{aligned} K_1 \equiv K_2 &= \{10\bar{1}2\}; & \pmb{\eta}_1 \equiv \pmb{\eta}_2 &= \langle 10\bar{1}\bar{1} \rangle; \\ \text{Plane of shear} &= \{1\bar{2}10\}; & s &= (\gamma^2 - 3)/3^{1/2}\gamma \end{aligned} \quad (86.6)$$

where γ is the axial ratio. This is one of the two hexagonal modes derived from variants of the unit correspondence matrix applied to the orthohexagonal basis. Crocker used eqn. (86.3) to make a systematic investigation of the low-shear, simple-shuffle modes and, for ideal γ , he listed 11 such modes with $s < 1$ and $q \leq 4$. In a later table published by Crocker and Bevis (1970), 15 possible modes satisfying these restrictions are given for the axial ratio of titanium. For all likely values of γ , the $\{10\bar{1}2\}$ mode gives much the lowest shear, and there can be little doubt that this is an important factor in the universal observation of this mode. There is also presumably a lower limit to the shear magnitude which can be effectively utilized in twinning; for $\{10\bar{1}2\}$ twins, for example, s becomes zero when $\gamma = 3^{1/2}$ and the shear direction reverses as γ passes through this value, as in magnesium–cadmium alloys. Experiments show that no $\{10\bar{1}2\}$ twins form near the critical composition (Stoloff and Gensamer, 1963).

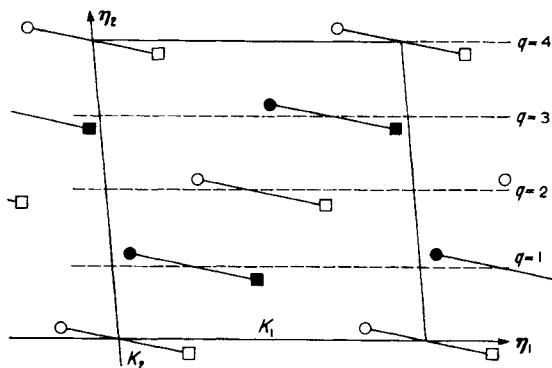


FIG. 20.11. Projection of h.c.p. structure onto plane of shear $\{1\bar{2}10\}$ of a $\{11\bar{2}0\}$ twin. Open and filled circles represent atoms of one set of lattice sites on two successive $\{1\bar{2}10\}$ planes. Squares similarly represent atoms from the second set of lattice sites on the same two $\{1\bar{2}10\}$ planes.

A projection of the h.c.p. structure onto the plane of shear is shown in Fig. 20.11, from which we see that this is a $q=4$ mode. It is obvious by inspection that there is only one reasonable choice for the motif unit. The structure is formed by the stacking of two planes of type $\{1\bar{2}10\}$ in different relative positions, half of the atoms of each lattice being contained in each plane. The motif unit thus lies in the plane of shear, which is a mirror plane of the h.c.p. structure, so that all four orientation relations of eqn. (85.4) are equivalent, and there is no distinction between a type I and a type II twin. As in the f.c.c. and b.c.c. modes, this mode is crystallographically equivalent to its own conjugate.

Comparison of Fig. 20.11 with Fig. 20.8 shows that the probable shuffle mechanism is a degenerate case of Fig. 20.8(e) or 20.8(f), these two mechanisms being identical when the motif unit lies in the plane of shear. The additional atom movements in the shuffles are thus all parallel to η_1 or normal to K_1 if the motif unit is regarded as rigid, or parallel to η_1 and η_2 if the shear is applied homogeneously to all the atom sites. The twinning mode is favoured not only by the low shear, but also by the very simple shuffle mechanism.

The predicted twinning mode with the next lowest shear for $q \leq 4$ has a K_1 plane of type $\{2\bar{2}41\}$, and has not been observed in any h.c.p. metal. The third smallest shear is a $q=4$, type I twin with $K_1 = \{10\bar{1}\}$, $\eta_2 = \langle 41\bar{5}3 \rangle$ and K_2 and η_1 irrational. This mode is important in the theory of martensite crystallography as it specifies the relationships between the two product lattices in some h.c.p. phases produced by transformation from high temperature b.c.c. phases. Such a transformation occurs, for example, in many titanium- and zirconium-based alloys and the h.c.p. plates are then often finely twinned on a single set of $\{10\bar{1}\}$ planes. As discussed in detail in Chapter 22, the reasonable assumption that the two product orientations have crystallographically equivalent correspondences with the parent lattice then fixes the η_1 direction and hence the equivalent twin mode (or its conjugate; both have been observed). It is then highly probable that one mechanism for deformation of the h.c.p. product involves the displacement of the $\{10\bar{1}\}$ transformation twin boundaries, as in other martensitic structures.

Deformation twinning on $\{10\bar{1}1\}$ has also been observed in magnesium but single twins of this type are rare and there may be confusion between genuine $\{10\bar{1}1\}$ K_1 planes and habits which have been described as $\{30\bar{3}4\}$ but which are probably associated with a double twinning process. Reed-Hill (1960) suggested a $\{10\bar{1}1\}$ low shear deformation mode, quite different from the $q=4$ transformation twinning mode. This new mode is compound, and is the reciprocal of a $\{10\bar{1}3\}$ twinning mode previously noted by Reed-Hill and Robertson (1957); it has $K_1=\{10\bar{1}1\}$, $K_2=\{10\bar{1}3\}$, $\eta_1=\langle 10\bar{1}2 \rangle$, $\eta_2=\langle 30\bar{3}2 \rangle$, $s=(4\gamma^2-9)/4(3)^{1/2}\gamma$ and $q=8$. The magnitude of the shear is 0.138 for magnesium, which is appreciably smaller than that for the $q=4$ mode. Although only one-quarter of the lattice points are carried to their correct twin positions by the shear, the atomic shuffles are simplified as the plane of shear $\{1\bar{2}10\}$ is a mirror plane which contains the motif unit, as in the $\{10\bar{1}2\}$ twins already discussed. An alternative compound mode was suggested by Hall (1954), using the plane of shear projection method, but the shear ($s \sim 1.07$) is improbably large.

The observed $\{10\bar{1}3\}$ twins in magnesium could in principle represent a type I twin with two irrational elements and $q=4$ but, although the shear for this mode is reasonably small, a more probable mode, as just discussed, is the reciprocal of the $\{10\bar{1}1\}$, $q=8$ mode. (A $q=11$ mode, which has also been suggested, has improbably complex shears.) Experimental observations on magnesium indicate, however, that both $\{10\bar{1}3\}$ and $\{10\bar{1}1\}$ twins are often components of double twins rather than single twins. Reed-Hill (1960) found that a twin plate or band appeared to form by double twinning on $\{10\bar{1}3\}$ and $\{10\bar{1}2\}$ over most of its length, except at the tips where there was single $\{10\bar{1}3\}$ twinning. The tips are thus separated from the rest of the twin by internal $\{10\bar{1}2\}$ interfaces, which presumably move outwards as the twin grows. Similar observations were made for (smaller) double twins with habits near $\{10\bar{1}1\}$, in agreement with a suggestion by Couling *et al.* (1959) that observed $\{30\bar{3}4\}$ twins in magnesium are actually double twins of $\{10\bar{1}1\} + \{10\bar{1}2\}$ type.

The predicted twinning elements of the equivalent simple shear mode for the $\{10\bar{1}3\} + \{10\bar{1}2\}$ double twinning are all irrational, but experimental results fit theoretical predictions (Crocker, 1962) quite well. The measured angle between the basal plane and the habit plane, for example, is 29° compared with predicted values of 32° for the $\{10\bar{1}3\}$ twin alone and $26.34'$ for the double twin, on the assumption that the latter has a simple shear relation to the matrix produced by simultaneous operation of the two twinning shears. (The alternative possibility [see p. 880] of retwinning a previously formed $\{10\bar{1}3\}$ twin would require plastic accommodation in the matrix which would slightly rotate the habit to $32.17'$ from the basal plane.) The small discrepancy of $2\frac{1}{2}'$ was attributed by Crocker to accommodation effects and he also showed that the expected orientation relations and shear (0.258) of the double twinned region are in good agreement with experiment. However, this is not true for the suggested $\{30\bar{3}4\}$ double twins.

Two sets of indices were originally suggested tentatively for single $\{30\bar{3}4\}$ twins; those given by Reed-Hill and Robertson (1957) have $q=10$, and those by Couling and Roberts (1956) have $q=4$, but also have a very large shear. As there is no mode with $q \leq 6$ and

$s < 1$, it seems highly probable that these bands are actually double twins and the combination $\{10\bar{1}\} + \{10\bar{1}\}$ is clearly indicated. However, although the experimental orientations are reasonably consistent with the theory, the measured habit planes deviate by about 15° from those predicted. (This discrepancy is reduced to $\sim 6^\circ$ if a $\{10\bar{1}\}$ twin is assumed to form first and then to retwin.) The results may indicate that the $\{30\bar{3}4\}$ twins form by a more complex double twinning mechanism, or may simply reflect the experimental difficulties with such small twins; no further work to resolve the discrepancy appears to have been published.

The remaining observed h.c.p. modes are $\{11\bar{2}1\}$ and $\{10\bar{1}4\}$, which both have $q \leq 4$ and $s \leq 1$, and $\{11\bar{2}2\}$, $\{11\bar{2}4\}$ and $\{11\bar{2}3\}$, which are all unpredicted within these ranges of q and s . The $\{10\bar{1}4\}$ observations are rather doubtful, but the other modes, and especially $\{11\bar{2}1\}$, are important in the deformation of several h.c.p. metals. We note that $\{11\bar{2}1\}$ is the only mode listed in Table XVIII with $q = 2$, i.e. it is the only h.c.p. mode in which all the lattice points are carried to their correct positions by the shear so that *lattice shuffles* are not required. Experimental values for the shear in rhenium (Smith, 1960) and zirconium (Sokurskii and Protsenko, 1958; Reed-Hill *et al.*, 1963; Westlake, 1963) generally agree with the predicted value of ~ 0.6 , but some confusion was caused by an earlier measurement of ~ 0.2 (Rapperport, 1959), which implied a very high value for q . It now seems probable that undetected accommodation effects were responsible for the low value of s obtained by Rapperport.

The plane of shear for the $\{11\bar{2}1\}$ mode is a mirror glide plane $\{1\bar{1}00\}$, so that the two orientation relations I and II are in principle different but may be related by a simple translation of $\frac{1}{2}c$. The shuffles required to produce a type I twin all involve equal and opposite displacements of the atoms in a motif pair through a small distance ($\sim 0.2a$) perpendicular to the K_1 plane (assuming the motif unit to be translated rigidly by the shear) as in the Y mechanism of Fig. 20.2. Crocker and Bevis (1970) suggested that the simplicity and small magnitudes of the shuffles account for the dominance of this mode (together with the smaller shear $\{10\bar{1}2\}$ mode) in the observed deformation behaviour of titanium.

An interesting feature of the $\{11\bar{2}1\}$ mode is that it provides one of the few examples in which K_2 and η_2 correspond to the observed slip plane and slip direction respectively. It follows from the theory of dislocation interfaces (Chapter 8) that a twin boundary may be regarded formally as a high angle tilt boundary formed by a dense array of lattice dislocations of edge type. The boundary could thus, in principle, be created by the accumulation of a large number of slip dislocations in a local region which then rearrange to form a twin boundary with a consequent lowering of energy. Compared with the low angle case (polygonization), it is required that the dislocations must have a lattice Burgers vector in the η_2 direction and their glide plane must be K_2 . According to this model, the twinning mode would be determined by the known deformation properties in glide. A knowledge of these elements does not uniquely define the mode, but an additional assumption about the fraction of lattice sites carried directly into their correct twin positions, or equivalently about the spacing of the dislocations in the tilt boundary, is sufficient to fix all the variables.

TABLE XVIII. PREDICTED AND OBSERVED TWINNING MODES IN h.c.p. STRUCTURES

K_1 { }	K_2 { }	η_1 ()	η_2 ()	s	q	References to some supporting experimental studies
10̄12	1012	10̄1̄1	101̄1	$(\gamma^2 - 3)/3^{1/2}\gamma$	4	Mg, ¹⁻⁴ Ti, ⁴ Co, ⁵ Zr, ⁶ Zn, ^{4,7} and Be ⁴
22̄1	0001	1, 1, 2, 1̄2	11̄20	$1/2\gamma$	4	
10̄11	10̄1̄3	10̄1̄2	30̄32	$(4\gamma^2 - 9)/4(3)^{1/2}\gamma$	8	Mg ¹⁻³ and Ti ^{6,8}
10̄11	i	i	41̄53	$(4\gamma^4 - 17\gamma^2 + 21)^{1/2}/2(3)^{1/2}\gamma$	4	
20̄21	0001	10̄1̄4	10̄1̄0	$3^{1/2}/2\gamma$	4	
11̄21	0001	11̄2̄6	11̄20	γ^{-1}	2	Re ¹ , Ti ^{4,10} , Zr ¹¹⁻¹⁴ , Co ⁵ and graphite ¹⁵
10̄1̄3	10̄11	30̄32	10̄12	$(4\gamma^2 - 9)/4(3)^{1/2}\gamma$	8	Mg ¹
10̄13	i	i	21̄1̄3	$(4\gamma^4 - 17\gamma^2 + 21)^{1/2}/2(3)^{1/2}\gamma$	4	
i	i	i	i	$(4\gamma^4 - 21\gamma^2 + 36)^{1/2}/4(3)^{1/2}\gamma$		

({10̄1̄3} double twinning)

13̄40	1100	75̄20	11̄20	$3^{1/2}$	4	
13̄41	1101	i	11̄20	$(4\gamma^2 + 3)^{1/2}/2(3)^{1/2}\gamma$	4	
13̄42	1102	i	11̄20	$(4\gamma^2 + 3)^{1/2}/2(3)^{1/2}\gamma$	4	
22̄43	0001	11̄2̄4	11̄20	$3/2\gamma$	4	
10̄14	10̄1̄0	20̄21	0001	$\gamma/3^{1/2}$	4	
11̄22	11̄2̄4	11̄2̄3	22̄43	$2(\gamma^2 - 2)/3\gamma$	6	Ti ^{4,6,8} and Zr ⁶
11̄24	11̄22	22̄43	11̄23	$2(\gamma^2 - 2)/3\gamma$	6	
30̄34						
11̄23						

Notes: i denotes an irrational plane or direction. As explained in the text, some of the reported modes have not been confirmed and appear doubtful. For greater clarity, each mode and its conjugate are listed separately. The table includes the eleven predicted modes which have $s \leq 1$ and $q \leq 4$ for the ideal axial ratio, and also the more probable $q=8$ modes for {1011} and {1013} and the $q=6$ modes for {1122} and {1124}.

Key to references

- 1) Reed-Hill (1960)
- 2) Couling, Pashak and Sturkey (1959)
- 3) Couling and Roberts (1956)
- 4) Partridge (1967)
- 5) Vaidya and Mahajan (1980)
- 6) Yoo (1981)
- 7) Lavrentyev, Salita and Kazarov (1968)
- 8) Paton and Backofen (1970)
- 9) Smith and Gaunt (1961)
- 10) Odinokova (1967)
- 11) Sokurskii and Protsenko (1958)
- 12) Reed-Hill, Slippy and Buteau (1963)
- 13) Westlake (1961)
- 14) Reed-Hill and Dahlberg (1966)
- 15) Freise and Kelly (1961)

TABLE XIX. PREDICTED AND OBSERVED TWINNING MODES IN DOUBLE LATTICE STRUCTURES
(AFTER CHRISTIAN AND MAHAJAN 1995)

Structure	K_1 { }	K_2 { }	η_1 ()	η_1 ()	s	q	References to supporting experimental studies
Rhombohedral	110	001	001	110	0.27—0.125	1	As, Bi, Sb ¹
b.c. tetragonal	101	301	101	103	0.113	4	Sn ²
Diamond	111	111	112	112	$2^{-1/2}$	2	Si ³ and GaAs ⁴⁻⁷
	111	113	112	332	$8^{-1/2}$	4	
α -uranium	'176'	111	512	—	0.214	4	8
	112	'172'	312	—	0.227	4	9
	'172'	112	—	312	0.227	4	9
	130	110	310	110	0.299	2	9
	121	'141'	'321'	311	0.329	6	9

Notes: Irrational planes or directions are shown as approximately rational indices in quotation marks. Numerical values of the shear given to avoid complexity. Only observed modes are listed.

Key to references

- 1) Gough (1933)
- 2) Tu and Turnbull (1970)
- 3j) Pirouz, Chaim, Dahmen and Westmacott (1990)
- 4) Androussi, Vanderschaeve and Lefebvre (1989)
- 5) Rabier and Boivin (1990)
- 6) Boivin, Rasbier and Garem (1990a)
- 7) Boivin, Rasbier and Garem (1990b)
- 8) Lloyd and Chiswick (1955)
- 9) Cahn (1953a)

Bullough's formal theory is closely related to the theory of martensite crystallography (Chapter 22) and may also be linked to the discussion of surface dislocations on p. 365. Figure 20.12 shows hypothetical stages in the formation of a twin. The combination of the lattice-invariant deformation (see p. 322), which is a simple shear on K_2 in the direction η_2 , with the lattice deformation, which is a rotation about the direction in K_2 normal to η_2 , produces the shape deformation, which is a simple shear on K_1 in the direction of η_1 . The more complex case of martensite differs formally in having a lattice deformation which is not simply a rotation, and the dislocations needed to ensure compatibility of lattice and shape deformations are then not pure edges. In the application to twinning, however, the dislocation content of the tilt boundary is so high that it loses physical significance; if all the lattice points are related by the twinning shear, there is one lattice dislocation on each K_2 lattice plane intersecting the twin interface. This very high dislocation content may alternatively be regarded as zero, because an equally valid description of the final situation is that the shape and lattice deformations are identical and there is no lattice-invariant deformation (see p. 366). This latter description is the one used in this chapter, but Bullough's theory shows the relevance of the alternative description if the twin really does form by accumulating slip dislocations.

As K_2 and η_2 hardly ever correspond to slip modes, this approach cannot be generally valid, but it has been considered in relation to one possible mode in the diamond structure

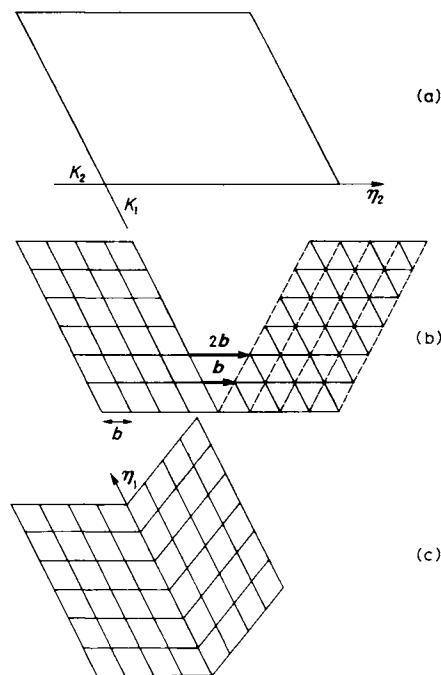


FIG. 20.12. Diagram illustrating the crystallography of Bullough's model of twinning. (a) Original lattice. (b) Part of the original lattice is given a lattice-invariant shear on the K_2 plane; this requires a dislocation of Burgers vector \mathbf{b} on each lattice K_2 plane as shown. The solid lines outline the original unit cells of the structure; the broken lines show alternative, equivalent cells in the sheared portion. (c) Combination of the lattice-invariant shear with a rotation about the normal to the plane of shear produces the twin. The total shape deformation is a simple shear on the K_1 plane in the η_1 direction.

(see below) and also in the interesting case of hexagonal graphite which forms $\{11\bar{2}1\}$ twins with a much lower theoretical shear (0.367) than titanium because of its high axial ratio ($\gamma = 2.725$). Freise and Kelly (1961) found that deformation of graphite frequently produced bend planes (tilt boundaries) of varying angle in addition to genuine twins, thus lending some support to the Bullough model. However, it does not seem possible to assign much more than formal significance to the dislocation model of the completed twin boundary, as the dislocations must lose their individual identities. Freise and Kelly used the Read-Shockley formula for grain boundary energy to deduce that the "dislocations" in the boundary will dissociate into partial dislocations, there being one partial on each atomic K_2 plane instead of one lattice dislocation on each lattice K_2 plane. It is obvious that this statement is only meaningful in a formal sense, where it may be interpreted to show that it is possible to have an interface in a twin of this type in which all the atomic positions match. Statements which are sometimes made that in this type of twinning the shear is on the K_2 plane rather than the K_1 plane focus attention on the dislocation aggregation mode, but are rather confusing because a proper distinction is not being made between the different kinds of deformation shown in Fig. 20.12.

There are no other observed h.c.p. modes for which $s < 1$ and $q \leq 4$ but it appears to be well established that $\{11\bar{2}2\}$ and $\{11\bar{2}4\}$ twins occur in some metals. In fact, if $q = 6$, these two planes are conjugate twinning planes of a single mode, as first pointed out by Kiho (1958), and the shear is only ~ 0.22 for titanium and zirconium, although it would exceed 0.5 if this mode were operative in cadmium or zinc. With $q = 6$, the shuffles are necessarily rather complex, but are considerably simplified in each case because there is a motif unit in the composition plane. Type I and type II twins are possible in principle but, as the plane of shear is the mirror glide plane $\{1\bar{1}00\}$, the two orientations differ only by a relative translation, which in this case may be regarded as parallel to η_1 . This introduces additional symmetry; for example, the atoms in a reflection twin are also related to the parent atoms by a twofold screw rotation about η_1 . The atomic structure of the various possible h.c.p. twin interfaces and the corresponding twinning dislocations are discussed in the next section; a possible set of shuffles for the $\{11\bar{2}2\}$ type I twin is shown in Fig. 20.13.

An alternative mode with a $\{11\bar{2}2\}$ habit (Hall, 1954) has $K_2 = \{11\bar{2}\bar{2}\}$, $\eta_1 = \langle 11\bar{2}\bar{3} \rangle$, $\eta_2 = \langle 11\bar{2}3 \rangle$, $s = \gamma - \gamma^{-1}$ and $q = 4$; this is, in fact, the second hexagonal mode obtained from variants of the unit correspondence matrix applied to the orthohexagonal basis and, like the $\{10\bar{1}2\}$ mode [eqns. (86.6)], it has the K_1 and K_2 planes and the η_1 and η_2 directions crystallographically equivalent. This mode is listed by Crocker and Bevis (1970) but does not appear in Crocker's original list because s slightly exceeds unity for $\gamma = 1.63$, although it is less than unity for the axial ratios of titanium and zirconium. Although fewer atoms would be required to shuffle than in the $q = 6$ mode, experimental work (see, e.g., Rapperport and Hartley, 1960) shows that the $q = 6$ mode is preferred, presumably because of the much smaller shear.

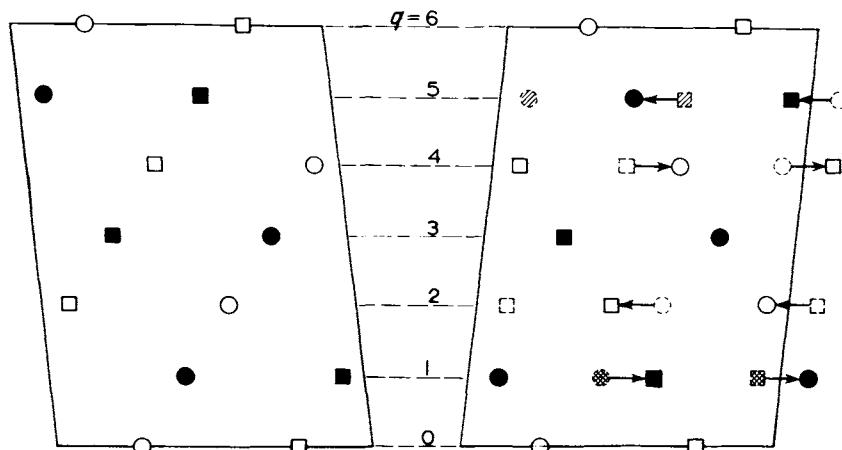


FIG. 20.13. Possible shuffling mechanism for a $\{11\bar{2}2\}$ type, $q = 6$, h.c.p. twin (after Crocker, 1959). The plane of the Figure is $\{1100\}$ and the symbols are as in Fig. 20.11 except that each $\{1100\}$ plane contains only one set of lattice sites, so that the four symbols now refer to four successive planes. The dashed and lightly hatched symbols refer to the atom positions after the shear, whilst the full symbols give the atom positions in the twin.

There remains, finally, the observation of $\{11\bar{2}3\}$ twins. Hall (1954) found a possible mode with $q=2$, but this has a very large shear of ~ 1.9 . The lowest shear for this mode with $q \leq 8$ occurs with $q=7$; another mode suggested by Kiho has $q=5$ and $s \sim 0.5$. Both of these modes would require very complex shuffles. At present there is thus no good description of $\{30\bar{3}4\}$ and $\{11\bar{2}3\}$ twinning, and it is possible that the habit plane markings of these types represent rather complex double twinning modes.

Figure 20.14 shows the suggested shuffling mechanisms for four of the operative modes in titanium and Table XVIII gives a selection of observed and predicted twinning modes for the various h.c.p. metals. It does not include the high shear $\{11\bar{2}\bar{2}\}$ mode mentioned above for which $q=4$, and three other unobserved $q=4$ modes in the Crocker and Bevis list are also omitted. These have K_1 planes of types $\{2, 8, \bar{10}, 7\}$ (a compound mode) and $\{10\bar{1}2\}$ and $\{10\bar{1}\bar{1}\}$ (type I modes).

The metals arsenic, bismuth and antimony are double lattice structures which may be compared to the face-centred rhombohedral structure of mercury as each consists of two interpenetrating face-centred rhombohedral lattices, the origin of the second being displaced along the $\langle 111 \rangle$ direction with respect to the origin of the first. The observed

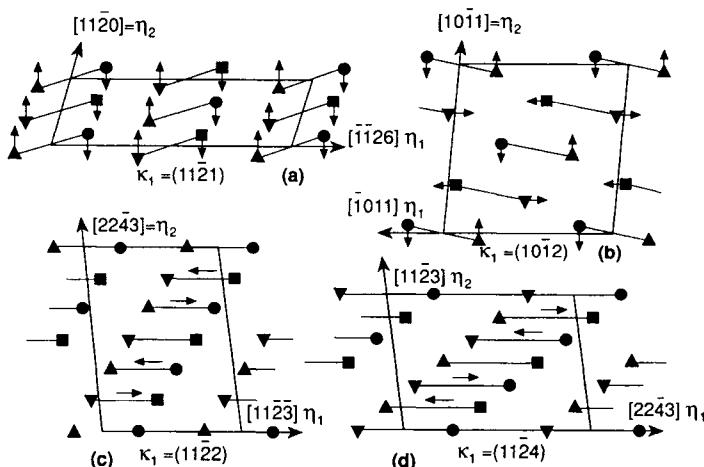


FIG. 20.14. Atomic shuffles associated with (a) $\{1121\}$; (b) $\{1012\}$; (c) $\{11\bar{2}2\}$; and (d) $\{11\bar{2}4\}$ twinning shears in titanium. The K_1 plane and the η_1 and η_2 directions are labelled in each case and the motif units at each lattice point are indicated. The atoms associated with the two interpenetrating lattices comprising the h.c.p. structure are indicated by circles and squares (first lattice) and by upright and inverted triangles (second lattice). In (a), (c) and (d) the atoms lie in four adjacent $\{1\bar{1}00\}$ planes, indicated by circles in the plane of the Figure and squares below the plane of the Figure. In (b) the atoms lie in only two adjacent $\{\bar{1}210\}$ planes, indicated by circles and upright triangles in the plane of the Figure and by squares and inverted triangles in the next plane at a distance of $a/2$ below it. The shuffles, assumed formally to precede the shear, are shown by arrows and, in (c) and (d), motif pairs of atoms move together. Shuffle components normal to the plane of the Figure are required in (c) and (d); these are not shown and depend on whether the orientation relationship is of type I or type II.

twinning mode is not, however, equivalent to the operative mercury mode but corresponds instead to the minimum shear mode predicted, but not observed, for mercury. Experimental observations show that the operative K_1 plane is always $\{110\}$ and the conjugate mode with a $\{001\}$ habit is not observed. Crocker showed that, with a proper choice of motif unit, the rotation (type II) twin involves much smaller atomic shuffles than the alternatives, and it is presumably preferred for this reason.

The least shear hypothesis also explains the observed twinning modes in the white tin structure, which may be regarded as two interpenetrating b.c.t. lattices with the origin of the second lattice at $[\frac{1}{2} \ 0 \ \frac{1}{4}]$ with respect to the origin of the first. Because of the low axial ratio of the structure (~ 0.55) the mode previously given for martensite (and equivalently for indium) no longer gives the smallest shear. The minimum shear mode is

$$\begin{aligned} K_1 &= \{101\}, \quad K_2 = \{\bar{3}01\}, \quad \eta_1 = \langle \bar{1}01 \rangle, \quad \eta_2 = \langle 103 \rangle \\ s &= \frac{1}{2}(9\gamma^2 + \gamma^{-2} - 6)^{1/2}, \quad q = 4 \end{aligned} \quad (86.7)$$

Both $\{101\}$ and the conjugate $\{\bar{3}01\}$ are observed as K_1 planes, the latter being more frequent. Both possibilities involve quite small and simple shuffles as the motif unit may be chosen to lie in the plane of shear; these represent the degenerate case in which Fig. 20.8(e) is equivalent to Fig. 20.8(f). The preferred plane is that for which the shuffles normal to the K_1 plane are smaller than those parallel to the η_1 direction.

The elements carbon (as in diamond), silicon, germanium and grey tin all have the diamond structure in which each atom has four tetrahedrally arranged neighbours around it. The structure is equivalent to two interpenetrating face-centred rhombohedral lattices, the origin of the second being at $\frac{1}{4} \ \frac{1}{4} \ \frac{1}{4}$. By analogy with the f.c.c. structure, the twin of least shear for $q=2$ has both K_1 and K_2 planes of type $\{111\}$. Jaswon and Dove pointed out, however, that the following $q=4$ mode is possible in the diamond structure

$$\begin{aligned} K_1 &= \{111\}, \quad K_2 = \{11\bar{3}\}, \quad \eta_1 = \langle \bar{1}\bar{1}2 \rangle, \quad \eta_2 = \langle 332 \rangle \\ s &= 8^{-1/2}, \quad q = 4 \end{aligned} \quad (86.8)$$

This has quite acceptable shuffles, and one-half of the shear of the $q=2$ mode.

No observation appears to have been made of the $\{113\}$ twins which would be conjugate to the above mode, but Churchman et al. (1956) reported a $\{123\}$ twinning mode. This provided the first application of the theory described on p. 901, and Bullough (1957) showed that the mode could be predicted by using the parent slip system for K_2 and η_2 , and not allowing atomic shuffles. Unfortunately, the accompanying shear is improbably large, and later work makes it appear rather doubtful that $\{123\}$ twins do in fact exist in this structure.

The last twinning modes to be discussed in this section are those of the actinides, which include examples of metallic structures of rather low symmetry. Much work has been published on α -uranium, which is of considerable interest not only because of its industrial importance but also because it twins on several systems and provided the first known example of a metallic structure in which type II twins form with irrational K_1 planes.

Alpha-uranium has a double lattice structure made up from two interpenetrating base-centred orthorhombic cells, with origins separated by a vector $[0, -0.31, 0.5]$. The structure may be regarded as being derived from the h.c.p. structure, and the first theoretical analysis by Frank (1953) showed that one prominent mode with an irrational K_1 plane equal to " $\{172\}$ " approximately, and its conjugate with $K_1 = \{112\}$, which is also an observed mode, may be regarded as the orthorhombic equivalent of h.c.p. $\{10\bar{1}2\}$ twins. There is another possible orthorhombic mode which also degenerates into $\{10\bar{1}2\}$, but this has a larger shear and is not observed. The most frequently occurring twins in α -uranium have $K_1 = \{130\}$, and Frank pointed out that the corresponding h.c.p. plane is a $\{11\bar{2}0\}$ mirror plane. The above three modes were all discovered in a classic experimental study by Cahn (1953a), who also found another twin with $K_1 = \{121\}$. Cahn correctly identified the twinning elements of the $\{130\}$ (compound), $\{112\}$ (type I) and " $\{176\}$ " (type II) modes and also proposed that the $\{121\}$ habit represents a type I mode with $\eta_2 = (311)$.

Most of the α -uranium twinning modes were explained by Jaswon and Dove, who also predicted a minimum shear, $q = 4$, mode with $K_1 = \{111\}$ for the type I twin and $\eta_1 = (512)$ for the type II twin. This pair of modes may be regarded as the orthorhombic equivalents of the possible h.c.p. type I mode with $K_1 = \{10\bar{1}1\}$ and $\eta_2 = (41\bar{5}3)$ (see p. 897) and the conjugate type II mode. The type II twins with irrational habit plane near " $\{176\}$ " were discovered in later work by Lloyd and Chiswick (1955) who did not, however, detect the $\{112\}$ and $\{121\}$ twins found by Cahn. The Jaswon and Dove theory is unable to distinguish between the observed and unobserved predictions, but a more systematic analysis of the shuffle mechanisms (Crocker, 1965) suggests that the most frequently observed twinning mode, which is compound with $K_1 = \{130\}$, is preferred because of its simple shuffle mechanism ($q = 2$). No significance appears to be attached to the fact that the mode is compound; there are actually four possible twinning modes with a lower shear than the $\{130\}$ mode, including another compound mode, but these all have $q = 4$. It is not clear, however, why the reciprocal to the $\{130\}$ mode, which would have a $\{110\}$ composition plane, is not observed.

The type I twin of lowest shear has a $\{111\}$ composition plane, and its reciprocal type II twin an irrational, approximately " $\{176\}$ ", plane. The shuffles in both cases would be quite large, and only the type II twin has been found. The shuffles for the mode of next lowest shear are simpler, explaining the more frequent occurrence of both the type I, $\{112\}$, and the type II, approximately " $\{172\}$ ", twins. The type II twin has the simpler shuffles, and is observed more frequently than the type I twin. The other two possible modes with $q = 4$ and a shear less than that of the predominant $\{130\}$ mode, including the low shear compound mode, are not observed.

The $\{121\}$ twin found by Cahn, but apparently very rare, cannot be explained by the assumption $q \leq 4$ used in the above predictions. Crocker points out that, according to the elements assigned to it by Cahn, it is a $q = 6$ mode, and this does not seem too improbable in view of the $q = 6$ h.c.p. mode discussed on p. 903. In the uranium case, however, the shuffles would be much more complex as the motif unit cannot be chosen to lie in the K_1 plane.

The twinning modes for the metallic double lattice structures other than h.c.p. are summarized in Table XIX (p. 901).

Mechanical twinning is the major deformation mechanism in many non-metallic materials with complex crystal structures of low symmetry and many atoms to the unit cell. Although the mechanism of such twinning is not well understood, it seems logical to suppose that the operative twinning modes are determined primarily by the shuffle mechanisms, which depend on the structures of the unit cells rather than on lattice geometry. Metallic neptunium provides an interesting example of an intermediate case; it has an orthorhombic unit cell containing eight atoms which, in a (001) projection, can conveniently be represented as binary motif units of two different kinds. Rechtien *et al.* (1971) considered the possible twinning modes to be limited by the condition that the lattice must be restored by the shear, i.e. $q=1$ or 2. The two lowest shear modes are then

$$K_1 = \{110\}, \quad K_2 = \{1\bar{1}0\}, \quad \eta_1 = \langle 1\bar{1}0 \rangle, \quad \eta_2 = \langle 110 \rangle \quad s = 0.068 \quad (86.9)$$

and

$$K_1 = \{011\}, \quad K_2 = \{01\bar{1}\}, \quad \eta_1 = \langle 01\bar{1} \rangle, \quad \eta_2 = \langle 011 \rangle \quad s = 0.630 \quad (86.10)$$

The very small shear of mode (86.9) suggests that, if the shear magnitude remains an important criterion, this mode will be preferred. Experiments on polycrystalline specimens using colour metallography confirmed that deformation twins form profusely on two habit planes of each grain and an analysis of these observations, combined with a study of habit plane traces in single crystals, showed that all the twins were consistent with the above mode. From a detailed study of the possible shuffle mechanisms, the authors predict that the most likely orientation relationship is a 180° rotation about the η_1 direction.

The most complex structure for which a detailed analysis has been attempted is that of α -plutonium, which has 16 atoms in its monoclinic unit cell. There are many operative slip systems in this metal, but in a few specimens Spiet (1964) also observed deformation twins with two different habits. The habits have not been identified because of the considerable experimental difficulties, but it has been suggested that they are probably (001) and ($\bar{2}01$). In a more complete theoretical analysis Crocker (1971) considered five conjugate pairs of modes with $q=1$ or 2 and another five pairs with $q=4$. The lowest shear mode of the second group has a slightly smaller shear (0.129) than that of the first group (0.159) but its shuffles are much more complex. Crocker examined all the shuffles with the aid of a simpler pseudostructure with only two atoms in its monoclinic unit cell and deduced that only the conjugate pair of modes suggested by Sebilleau, which have minimum shear with no lattice shuffles, is likely to be acceptable. This compound mode is

$$K_1 = (001), \quad K_2 = (\bar{2}01), \quad \eta_1 = [\bar{1}00], \quad \eta_2 = [102] \quad s = 0.159 \quad (86.11)$$

There is no clear distinction between the two conjugate modes but it is suggested that considerations related to the production of twinning dislocations in the interface may favour the ($\bar{2}01$) habit.

From the comparison of theory and experiment made in this section, we can summarize the factors which seem to determine the operative twinning modes in all metallic structures. Bilby and Crocker (1965) suggested that the operative twinning mode should

- (a) have a small shear;
- (b) require only simple shuffles (i.e. have a small value of q);
- (c) require, if possible, only shuffles of small magnitude; and
- (d) have shuffle displacements parallel to η_1 if large shuffles are essential.

Criteria (a) and (b) generally enable the most likely twinning modes to be predicted, but (c) and (d) may have to be invoked in some cases, e.g. to distinguish between a mode and its conjugate.

Laves (1952, 1966) defined a "shuffle parameter" as the ratio of the average shuffle displacement to the interatomic distance, but for any given structure it is not clear that this provides an adequate description of the above considerations. In general, the shuffles might be expected to correlate either with the energy of the interface or the kinetics of its motion, or both, and thus the influence of criteria (b), (c) and (d) on the operative modes is easy to understand in a general way. It is not so clear why a small shear should be preferred as the volume of twins required to produce a given plastic strain field varies as s^{-1} and thus increases as the twinning shear decreases. However, the stress field of an enclosed lenticular twin of fixed aspect ratio varies as s^2 , so that it should be easier to produce a given strain by a large number of small-shear twins than a smaller number of large-shear twins.

87. NUCLEATION AND GROWTH OF MECHANICAL TWINS

In this section, the physical processes by which a deformation twin forms in a solid are discussed. This requires a consideration of the atomic structure of a twin interface and the properties of defects (steps or twinning dislocations) in the interface. Twinning is especially important as a deformation mechanism when there are few operative slip systems, as in the h.c.p. metals of high axial ratio, and it is also very prevalent in the deformation behaviour of b.c.c. metals at low temperatures. The b.c.c. twins are long and thin because of the high shear, and in iron they are known as Neumann lamellae. Metallographic and X-ray investigations in the 1920s (Harnecker and Rassow, 1924; Mathewson and Edmunds, 1928) demonstrated that Neumann lamellae are probably deformation twins, but conclusive proof was not obtained until the work of Kelly (1952) and the twinning elements were first confirmed experimentally by Paxton (1953).

Early evidence of mechanical twinning in f.c.c. metals was discredited, and for many years it was believed that deformation twins do not form in this structure which has identical twinning (K_1) planes and slip planes. The work of Blewitt *et al.* (1957) was a major advance as it presented incontrovertible evidence of deformation twinning in copper at 4.2 K and 77 K. Confirmation of f.c.c. twinning came almost immediately from the experiments of Suzuki and Barrett (1958) on silver-gold alloys and those of Haasen (1958)

on nickel, and these pioneering papers were soon followed by evidence that f.c.c. alloys of low stacking fault energies may twin at temperatures up to, and even above, room temperature (Christian *et al.*, 1960; Venables, 1960). Early experimental results are described in the papers from a conference held in 1963 (Reed-Hill *et al.*, 1964) and some of the more recent results were reviewed by Mahajan and Williams (1973) and by Christian and Mahajan (1995).

The understanding of twinning was greatly advanced by a series of experiments on non-metallic materials such as calcite and sodium nitrate carried out in the former Soviet Union by Garber and his co-workers and reviewed by Cahn (1953b). When a stress is applied over a localized region, e.g. with a knife edge, a thin twin wedge may form. If this disappears on removal of the stress, the twin is termed "elastic", but in some circumstances a residual twinned region may remain, and this is called a "stopped elastic twin". The change of shape within the twin wedge is opposed by the constraints of the matrix, and the shear has to be accommodated elastically or plastically within this matrix. However, if the stress is increased sufficiently, a twin may spread across the whole cross-section of a single crystal. It then acquires planar boundaries parallel to the K_1 planes, and is termed a residual twin. Residual twins may be further enlarged by application of a stress; they do not shrink again when the stress is reduced, but may shrink if the stress is reversed.

These observations are not duplicated exactly in metals, where the production of fully elastic twins is rarely observed. The difference appears to be a result only of the presence of other deformation processes acting at low stresses to accommodate the effects produced by the twin in the surrounding matrix. There is, moreover, a close analogy between the phenomenon of elastic twinning in non-metallic materials and that of thermoelastic martensite formation in some alloys (see p. 976). When an elastic twin is formed, there is an equilibrium at all stages between the externally applied stress tending to enlarge the twin, and the internal constraints of the matrix, which oppose the growth of the twin. The matrix stresses then progressively untwin the re-orientated region as the external stresses are reduced. However, if the matrix stresses reach a sufficiently high level, some form of accommodation slip or kinking may occur, and the situation will then usually not be reversible. When the external stresses are removed, the internal stresses will only be partly able to untwin the twinned region, and we obtain a stopped elastic twin. In metals, accommodation may be so complete that there is virtually no untwinning unless the applied stresses are reversed. In the limit, the accommodating deformation may be severe enough to completely destroy coherency between twin and matrix and the twin boundary will then no longer be glissile when a stress of either sign is applied.

A macroscopic twin contained entirely within a matrix crystal almost always has a lenticular shape because of the constraints just mentioned. The ratio of twin thickness to length provides a qualitative guide to the magnitude of the twinning shear, being very small in cases where the twinning shear is large. If an energy minimization principle applies, this ratio can be calculated for elastic twins, and measured values enable the surface energy of the twin interface to be estimated (Christian, 1959). There are many possible ways in which the shape change may be accommodated, depending in

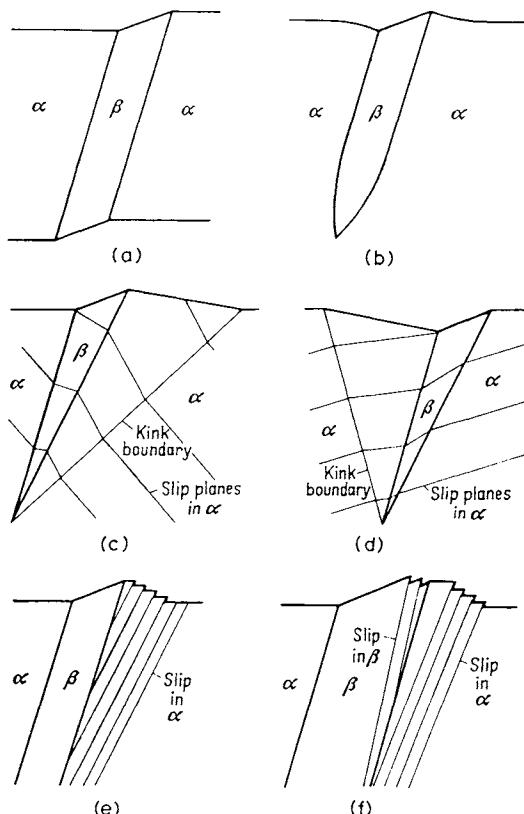


FIG. 20.15. The accommodation of the shape change of twinning: (a) unconstrained twin forming in a single crystal; (b) lenticular twin accommodated elastically in the matrix; (c, d) accommodation by kink boundaries in the matrix; (e) accommodation by slip in the matrix; (f) accommodation by slip in matrix and twin. The Figure applies equally to any displacive transformation.

detail on the crystallography of slip in the structure concerned. Some of the possibilities are illustrated in Fig. 20.15; accommodation by primary kink bands, parallel to the trace of the K_1 plane in the basal plane, is very common in h.c.p. metals and has been extensively studied (Pratt and Pugh, 1952; Moore, 1952; Holden, 1952). In some cases, there are several parallel accommodation kinks of this type, each kink corresponding to an abrupt change in the twin thickness below the surface (Moore, 1955). Secondary accommodation kinks, with traces in the basal plane normal to that of the twinning plane, are also frequently observed; whilst the primary kinks consist of assemblies of basal plane dislocations in materials like zinc, the secondary kinks have been shown to be formed from non-basal plane dislocations (Rosenbaum, 1961).

Figure 20.15 makes it obvious that in some cases the accommodation effects could mask the shape change caused by the twinning shear itself. In principle, there is always an escarpment with the ideal slope of Fig. 20.15(a), but if effects like 20.15(e) or (f) operate on

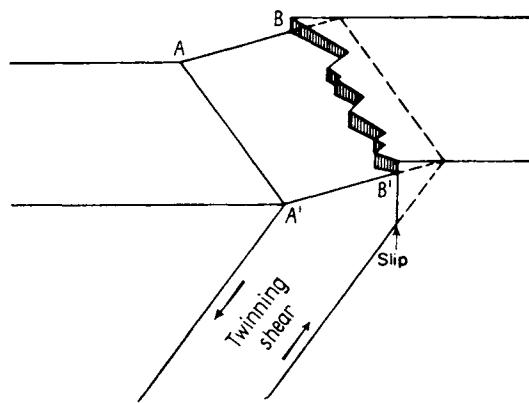


FIG. 20.16. Diagram illustrating the formation of an irregular twin edge (after Hull, 1960). The twin is held up below the surface near BB' , and the shape deformation causes slip in this region, exposing facets of slip planes.

a sufficiently fine scale, this may not readily be detectable. In the analogous situation in martensitic transformations, there is evidence that the shape change may be obscured by accommodation effects, and this may also be true of some twins.

Twins which entirely cross a single crystal (residual twins in Garber's notation) should have flat parallel boundaries, but examination of the traces in smooth polished surfaces frequently shows that one side is straight whilst the other has a characteristic zigzag marking. This effect was examined in single crystals of silicon-iron by Hull (1960), who showed that the zigzag markings correspond to slip steps on the surface. The markings result if part of the twin is held up below the surface, as illustrated in Fig. 20.16. The slip could arise from the activation of dislocation sources near the end of the stopped twin band, but the results agree better with the suggestion that the slip dislocations are formed by combination of the twinning dislocations at the end of the stopped twin.

When twinning is caused by an external stress, it is clearly necessary that the applied forces do work during the formation of the twin, i.e. that the shear stress across the twinning plane and resolved in the twinning direction should be positive. An important difference between twinning and slip deformation is that twinning is polarized, i.e. reversal of the η_1 direction will not produce a twin. This means that, for a single crystal of given orientation with respect to a uniaxially applied stress, some variants of a particular twin mode should operate only in tension, whereas others should operate only in compression. If the single crystal has completely twinned, it follows from Fig. 2.4 that all directions in the initially obtuse sector between K_1 and K_2 will have increased in length, whilst all directions in the acute sector will have decreased. However, Frank and Thompson (1955) pointed out that a slightly different rule will apply to an actual tension or compression test in a single crystal which deforms initially by forming a thin twin lamella. The average shear strain of the specimen is now f/s , where s is the twinning shear and f is the volume fraction of the twin. In the limit $f \rightarrow 0$, there will be an increase in length for a specimen

axis in the upper right quadrant formed by K_1 and the plane normal to η_1 and a decrease in length for an axis in the upper left quadrant.

By analogy with slip, it is natural to enquire whether the onset of twinning coincides with some critical value of the shear stress across the K_1 plane and resolved in the η_1 direction. Unfortunately, the scatter in measured twinning stresses is generally too large and the range of orientations available is too small to provide an adequate test of this hypothesis, especially as the incidence of twinning rather than slip as the preferred mode of deformation is itself very sensitive to orientation. It is well established, however, that the initial twin generally corresponds to the variant for which this resolved shear stress is greatest (Allen *et al.*, 1956; Cox *et al.*, 1957; Biggs and Pratt, 1958; Reid *et al.*, 1966). In b.c.c. crystals, for example, with a stress axis within the unit triangle defined by [001], [011] and $\bar{[1}11]$, the two variants in tension should be $(1\bar{1}2)[\bar{1}11]$ near [001] and $(\bar{1}\bar{1}2)[111]$ near the [001]– $\bar{[1}11]$ boundary, whilst in compression the single variant $(\bar{2}11)[111]$ should operate over the whole triangle. The different variants imply an asymmetry in the applied stress for twinning in tension and compression and this carries over to polycrystalline textured materials, as shown for iron by Richards and Reid (1968). For materials without a texture, no difference in the twinning stresses for tension and compression was found, but the twinned volume fractions and the fraction of grains containing twins were both appreciably larger in compression than in tension. The authors point out that on average the grains, even in a random aggregate, are more favourably orientated for twinning under an applied compressive stress than under a tensile stress. Similar results apply to f.c.c. metals and alloys where twins form on either the primary or the conjugate {111} slip planes (Narita and Takamura, 1974) or, in the case of constrained deformation, on the most highly stressed system (Chin *et al.*, 1969).

As already indicated, tests on b.c.c. metals give contradictory results in terms of whether or not a critical resolved shear stress law applies, but the majority of the evidence is that the orientation dependence is more complex. Body-centred cubic metals twin readily (without appreciable prior slip) only at low temperatures and/or high strain rates, and under these conditions analysis is complicated by peculiarities in the slip behaviour, which include breakdown of the Schmid law of critical resolved shear stress and large orientation dependencies and asymmetries. In very pure metals, major components of the total strain may result from slip on unpredicted (so-called “anomalous”) variants of the usual slip system. These effects are believed to be a consequence of the core structure of the screw dislocation in b.c.c. metals (Christian, 1983; Vitek, 1985) and, later in this section, evidence will be provided that twin nuclei are formed from screw dislocations. Substitutional solutes (especially rhenium) often promote twinning, whereas interstitials may sometimes prevent twinning. It is well established that twinning at low temperatures may often be inhibited by a small prestrain at a higher temperature, but very small prestrains may sometimes increase the number of twins formed upon deformation. A homogeneous distribution of dislocations is most effective in suppressing twinning, and the required prestrain also varies with testing temperature and strain rate (Boucher and Christian, 1972).

Deformation twinning is prevalent in many f.c.c. metals and in alloys of copper, silver or gold, especially at low temperatures, but is not normally encountered in f.c.c. materials of high stacking fault energy such as aluminium and its alloys. The influence of stacking fault energy has been investigated by a number of workers (Thornton and Mitchell, 1962; Peissker, 1965). However, Pond and Garcia-Garcia (1981) have reported that, even in aluminium, twins may form near the tips of cracks in thin foils where the stress concentrations are probably very high.

In normal tensile or compression tests, contrary to the behaviour of many b.c.c. metals, twins form in single crystals of f.c.c. alloys only if prior deformation by slip has so rotated the specimen axis that the primary and conjugate systems are approximately equally stressed. K_1 is then either the primary or conjugate slip plane and η_1 is the $\langle 112 \rangle$ direction of greatest resolved shear stress within that plane. Measurements of this twinning stress, however, do not support a critical resolved shear stress law, but show that twinning becomes easier as the tensile axis approaches $\langle 111 \rangle$ or the $\langle 111 \rangle$ – $\langle 110 \rangle$ zone. Narita and Takamura (1974) found that the twinning stress is not very temperature-dependent in Stage II of the stress versus strain curve, but that it decreases as the temperature is lowered if twinning occurs in stage III. Twinning is sometimes accompanied by load drops in f.c.c. alloys but, when the pretwinning slip is small, twinned regions consist of very thin plates and propagate like Luders bands (Fujita and Mori, 1975). The thickness of the plates decreases with decreasing stacking fault energy and temperature, and the onset of twinning is then signalled merely by a bend in the stress versus strain curve.

Twinning is much more common in the h.c.p. metals, largely for reasons of plastic compatibility; the five independent slip systems required for an arbitrary deformation are usually not available. In view of the confusing number of twin modes which have been reported for various h.c.p. metals, it should be re-emphasized here that the important modes are $\{10\bar{1}2\}$ for all metals and $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$ for metals like titanium. The polarization of the shear direction is dependent on the axial ratio and, in the case of $\{10\bar{1}2\}$ twinning, the shear direction changes sign at an axial ratio of $3^{1/2}$ which is within the accessible range. For alloys with axial ratios close to the critical value, no twins are formed as the twinning shear tends to zero.

Some investigations on h.c.p. metals (see, e.g., Millard and Thompson, 1952) have given results consistent with the critical resolved shear stress hypothesis, but once again the bulk of the evidence is against such a law. Values obtained by different workers on material of the same nominal purity are widely different, and this suggests, as in some forms of yielding by slip, that any critical stress is extremely sensitive to crystal purity and perfection. In addition, there are convincing reasons for believing that twinning begins from internal stress concentrations which may be produced by prior slip or microslip, and this could lead to considerable variations from sample to sample in the external stress at which twinning takes place. These ideas were strongly supported in some classical experiments by Bell and Cahn (1953) on twinning in zinc. They found that carefully prepared and handled crystals will withstand shear stresses very much higher than that normally required for twinning, but that twinning can be initiated by inducing stress concentrations, for example by pricking with a pin. In these circumstances, it seems clear

that there may be a critical resolved shear stress for growth of a twin nucleus, and that many ordinary crystals may contain such nuclei, but the stress to form a nucleus in a perfect crystal is much higher. The real stress to initiate twinning may be compared to the upper yield point in materials where dislocations are pinned by impurities; the true upper stress is rarely observed because of unavoidable stress concentrations in most mounting and testing procedures. Cahn suggested that twin nuclei should be regarded as tiny stopped elastic twins in Garber's notation.

The importance of imperfections in twin formation was confirmed by experiments on the deformation of highly perfect cadmium and zinc crystals (Price, 1960, 1961, 1962). The specimens, in the form of whiskers or thin platelets, were strained whilst under observation in an electron microscope. The stresses required for nucleation and growth of twins were an order of magnitude higher than those usually measured with macroscopic specimens.

It thus follows that, in discussing the formation of a mechanical twin, its nucleation and subsequent growth must be considered separately, as in most phase transformations. There are, moreover, two distinct growth processes, namely the lengthwise (or edgewise) growth of a lenticular twin constrained in a matrix, and the motion of the habit plane normal to itself, as in a parallel-sided twin crossing a single crystal. If a suitable nucleus exists, or is formed by the applied stress, the first process is usually catastrophic. The twin forms in a very short time, and a "load drop" may be observed in a "hard" testing machine. If the nucleation stress exceeds the growth stress, such load drops may be very large, even in comparison with those caused by sudden yielding in materials like mild steel. The growth velocity must approach the speed of sound, and energy is frequently dissipated as sound waves, giving a characteristic noise known as the twinning cry. The sudden production of a macroscopic twin may be compared to the transition stage from a stopped elastic twin to a residual twin in Garber's terminology, although the twin need not be formed in a single crystal, or extend across the whole cross-section. Many twins of this type form very rapidly (in a few microseconds) and then do not grow or shrink further on increasing or reversing the stress; they have been mechanically stabilized by losing coherency with the matrix as mentioned above. Such twins are sometimes removed by annealing at temperatures where individual atom movements can occur; in other cases, the twins grow at the expense of the matrix on annealing. After removal of the external stress, an assembly containing a constrained twin is in a state of self stress, and the strain energy presumably provides the driving force for the thermal removal or growth of the twin.

The second type of growth may also be very rapid but, under suitable conditions, slow thickening of the twin under an increasing stress can also be observed. The theory of this type of growth in a type I twin with a rational interface is analogous in many ways to that of crystal growth from the vapour. In an ideal crystal with a perfectly planar twin interface, a two-dimensional thermally activated nucleation process would be required to produce growth. Both types of growth also have analogies in the theory of martensitic transformations but, except in special cases, the semi-coherent nature of the martensitic interface makes it easier to envisage the normal growth of a martensite plate than that of the fully coherent twin interface.

In discussing the crystallography of twinning, it was noted that the composition or K_1 plane is the only invariant plane of the lattice deformation relating the two crystals. One way of avoiding high energy surfaces is for the whole twin boundary to consist of planar sections of this type, and a possible model of a tapering or lenticular twin is thus one in which there are occasional steps in the composition plane interfaces. Such steps have already been discussed; they are the twinning dislocations of Section 32. In the case of a lenticular twin, the model contains closed loops of twinning dislocation, parallel to the composition planes, and increasing in radius as the central plane of the lens (Fig. 20.17) is approached.

As discussed in Section 32, twinning dislocations have many of the properties of ordinary dislocations; in particular, they can glide in the composition plane under the action of a shear stress, enlarging or shrinking the twin by one lattice layer as they do so. From Fig. 20.17, we see that a lenticular disc may enlarge its radius simply by expansion of the twinning dislocation loops, the ratio of diameter to thickness becoming greater as it grows in this way. This process will leave increasing areas of flat twin interface near the centre of the twin and, if normal growth also takes place, new twinning dislocations must be formed on these planes. Thus the thickening of a lenticular twin, or the growth of such a twin if the length:thickness ratio is not to increase, must involve the same kind of problems as those involved in the normal growth of a parallel-sided residual twin.

The growth model which has just been described in outline is apparently restricted to compound or type I twins with rational K_1 interfaces and even then there are some complications which arise if q is greater than two or if the structure has a basis. Suppose first that d in eqn. (32.1) represents the spacing of the K_1 lattice planes so that the associated Burgers vector \mathbf{b}_T has magnitude

$$\mathbf{b}_T = d\mathbf{l} \quad (87.1)$$

where \mathbf{l} is the unit vector parallel to \mathbf{n}_1 . This step of minimum height is called an elementary twinning dislocation and, as the elastic energy is proportional to the square of the Burgers vector, it might be expected that twinning dislocations with step heights which are multiples of d will tend to dissociate spontaneously into elementary twinning dislocations. However, when the lattice correspondence does not relate primitive cells of

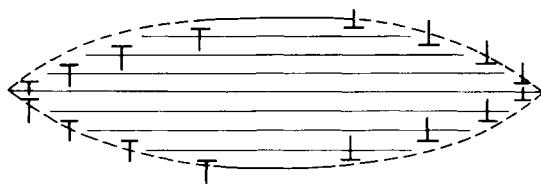


FIG. 20.17. Model of a lenticular twin. If the loops of twinning dislocation are traversed in a constant sense, elements of the loop to the left and right of the figure have the same Burgers vector but opposite line directions. As these elements are in opposition, the dislocation symbols have been reversed. If the dislocations are edges, for example, the long arm of the symbol indicates the compression side of the dislocation.

the two lattices, the two parts of the interface separated by a step of minimum height generally have different structures, and an elementary step may then be energetically unfavourable. The lattice shuffles which accompany all twinning modes with $q > 2$ imply that the interface structure repeats only at every q lattice planes parallel to K_1 if q is odd, or at every $\frac{1}{2}q$ planes if q is even, so that the Burgers vector associated with a step between two equivalent regions of coherent interface has a minimum magnitude of

$$\begin{aligned}\mathbf{b}_T &= qds \quad (q \text{ odd}) \\ \mathbf{b}_T &= \frac{1}{2}qds \quad (q \text{ even})\end{aligned}\tag{87.2}$$

This geometrical property of a particular twinning mode was first pointed out by Millard and Thompson (1952) for {1012} twins in h.c.p., and they called the step of minimum height to reproduce the interface structure a "double" twinning dislocation. More generally, such steps are now called "zonal" twinning dislocations (Kronberg, 1959, 1961; Westlake, 1961; Rosenbaum, 1964).

The dissociation of a zonal twinning dislocation into a group of q or $\frac{1}{2}q$ elementary twinning dislocations lowers the elastic energy but increases the surface energy. The elementary dislocations have parallel Burgers vectors and hence repel each other until separations are attained at which these repulsive forces are just balanced by the attractive forces due to the excess energies of the various interfaces over that of the minimum energy interface. This situation is clearly analogous to the dissociation of a lattice dislocation into partial dislocations, and the zonal dislocation which is a repeat step of the interface may be regarded as an extended dislocation comprising partial or non-repeat steps separated by "faults", i.e. by regions of higher energy interface. If the energies of these interface faults are sufficiently small, however, the separation of the elementary twinning dislocations will become large and the concept of a zonal twinning dislocation as a separate entity is no longer required.

Zonal twinning dislocations were first discussed in connection with twinning in h.c.p. structures, but the term has also been used to discuss twinning in superlattices in which the minimum step height to give an identical interface structure may be increased to some multiple of that in the disordered structure. The multiple height step is then often referred to as a zonal twinning dislocation, although this is not strictly correct, because q is now being obtained with reference to the lattice planes of the disordered structure rather than to those of the superlattice. It follows, moreover, from the discussion on pp. 885–887, that the formation of true twins by the motion of such steps would require interchange shuffles at the interface. The confusion arises because in the fully ordered structure there may be atomic planes parallel to K_1 which are equi-spaced and more numerous than the lattice planes. However, in any multiple lattice structure, it is possible to envisage interface steps between atomic planes in which the step height is smaller than that of the elementary twinning dislocation as defined above. Although it would be possible to revise the definition of the elementary twinning dislocation to make it correspond to the minimum step between atomic planes, this would cause difficulties because the twin cannot grow by motion of such a step, and the atomic planes are not necessarily equally spaced. Moreover,

as we shall see below, step defects in which the effective step height is less than the spacing of atomic planes may also arise in some structures by dissociation of elementary twinning dislocations. The definition of an elementary twinning dislocation in terms of the spacing of lattice planes will thus be retained, whilst noting the possibility that step defects of smaller Burgers vector than that given by eqn. (87.1) may be present in some interfaces. Naturally the two interface structures connected by such a step are non-equivalent for any value of q but, in the special case of superlattice structures, this difference may be confined to changes in the chemical binding, so that the extra energy of the unfavourable interface is similar to that of an antiphase boundary. The rather loose usage to be found in treatments which regard such a step as an elementary twinning dislocation may thus be compared with the way in which extended superlattice dislocations are often described as being dissociated into "lattice" dislocations, i.e. into dislocations with Burgers vectors which are repeat vectors of the *disordered* lattice.

Consider next whether the concepts of step growth can be applied to type II twins, to which the above description does not apply directly because, if K_1 is irrational, the spacing of lattice planes parallel to the interface is indefinitely small. The theory of the atomic structure and of defects in irrational (or very high index) interfaces is difficult and not well developed, and the following description is simplified and partly intuitive. On an atomic scale, an irrational interface must consist of rational facets and, in the general case, a minimum of three differently orientated facets would be required. However, as the interface of a type II twin necessarily contains one rational direction (η_1), it is possible to model it as alternate facets of two rational planes, as shown in Fig. 20.18. The most appropriate model will generally consist of facets of minimum size parallel to the two closest-packed planes in the zone axis of η_1 . If the smaller facets (P) all represent transitions between adjacent lattice planes of the larger facets (Q), and are spaced along Q either uniformly or in some regularly repeating sequence at multiples of the distance at which adjacent lattice planes of P intersect Q , the average interface will remain rational. However, as the period of the repeat pattern increases, the Miller indices of the interface become higher and higher. The larger facets will be those nearest in orientation to the mean interface plane, and the smaller facets may often be parallel to the rational K_2 plane. These smaller facets may be regarded as steps on the larger facets, and by increasing the period better and better rational approximations to an irrational plane may be obtained. For example, a first approximation to a particular interface might be produced by steps at repeated intervals of five, four and four lattice vectors along the rational Q interface, and

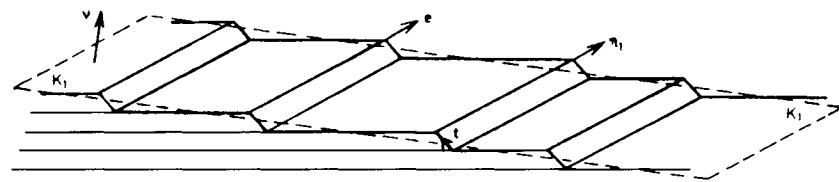


FIG. 20.18. Model of an irrational K_1 interface.

successive approximations might then consist of the following repeated step patterns: ... 544 ..., ... 5444 ..., ... 5444544 ..., ... 54445444544 ..., ... 54445445444544544 ..., etc. In the limit, when the period has become infinite, the interface is truly irrational, but the step pattern remains ordered. The interface is now an example of a one-dimensional quasi-crystal, as there is no genuine periodicity parallel to η_1 but the structure is quasi-crystalline (Levine and Steinhardt, 1986) in the interface direction normal to η_1 . (The general theory of quasi-crystals became significant after the discovery of three-dimensional quasi-crystals with fivefold symmetry [see pp. 617]). Sutton (1988) has shown that the "structural unit" model of irrational tilt boundaries with a rational tilt axis (Sutton and Vitek, 1983) may be treated as a one-dimensional quasi-crystal in which the periodic combination of *A* and *B* structural units becomes quasi-periodic in the limit. The theory has also been applied to "hidden symmetries" in generalized grain boundaries by Gratias and Thalal (1988).

Note that if the plane of the larger facets were parallel to the true K_1 plane, the steps would be twinning dislocations in screw orientation. For a matching irrational plane, however, they are an essential element in the structure of the boundary, and have been called "intrinsic twinning dislocations" (Guyoncourt and Crocker, 1968). If an irrational K_1 interface traverses a single crystal, there will be no force driving the steps in a particular direction when a stress is applied to the crystal unless a nucleating mechanism is available to supply fresh steps as required to maintain the irrationality of the interface plane. If this can be achieved, however, the steps will glide along the rational planes as the interface moves forward, and it is in this sense that they can also be regarded as twinning dislocations. This leads to the concept that steps on the rational facets could also assume edge or general orientations and local densities other than those specified by the lattice matching condition. The excess steps over the ideal model of the interface now constitute extrinsic twinning dislocations which will respond to an external stress in the same way as steps in rational K_1 interfaces. Extrinsic twinning dislocations are effectively steps in the macroscopic irrational interface, so that their motion displaces this interface.

The magnitude of the effective Burgers vector of such a twinning dislocation is given by the twinning shear multiplied by the height of the step in the irrational plane, i.e. by the interplanar spacing of the *Q* lattice planes resolved in the direction of the normal to the irrational K_1 plane. Hence the Burgers vector is

$$\mathbf{b}_T = u_i m_i s \mathbf{l} = \bar{d} s \mathbf{l} \quad (87.3)$$

where \mathbf{u} is any vector connecting lattice points on adjacent planes of type *Q*, and \bar{d} is the spacing of the *Q* planes resolved in the direction of the unit normal \mathbf{m} to the irrational interface. Note that the magnitude is irrational, but that the vector is parallel to the rational η_1 direction. This step in plane *Q* is the type II equivalent of an elementary twinning dislocation, but it follows from the discussion on p. 916 that the interface structure on the two sides will be identical only if a primitive lattice vector \mathbf{w} parallel to η_1 traverses not more than two lattice K_2 planes. In other cases, we must define the equivalent

of the zonal twinning dislocation by

$$\mathbf{b}_T = w_i m_i \mathbf{s} \mathbf{l} = \bar{q} \bar{d} \mathbf{s} \mathbf{l} \quad (87.4)$$

It might be considered that the intrinsic steps of the irrational interface would all have a height of $\bar{q} \bar{d}$ rather than \bar{d} , but this cannot be assumed without modelling the actual interface structure; it is conceivable, for example, that an alternating configuration at the Q facets is more favourable than a repeated configuration.

An equivalent formal treatment of a faceted interface is to use the Frank–Bilby–Bollmann equation (see Chapter 8) to calculate separately the formal dislocation content required to correct the misfit along each of the facets P and Q . This corresponds to $-\mathbf{b}_T$ for an individual step facet P , but sums to zero over a sufficient number of facets if the relative lengths of Q and P perpendicular to \mathbf{n}_I give the exact K_I interface. Various ambiguities in the dislocation descriptions of stepped and unstepped interfaces depend on how zero dislocation content is defined, and are discussed by Olson and Cohen (1979), Olson (1981), Christian and Knowles (1982) and Christian (1983).

Returning to rational twin interfaces, consider the twinning dislocations in the important metallic structures. Calculations indicate that in some twin boundaries there may exist alternative interface configurations of nearly equal energies, and the line of separation of two such regions may then be a dislocation with a Burgers vector smaller than that of an elementary twinning dislocation and a step height equal to a fraction of the spacing of atomic K_I planes. This applies specifically to the coherent {112} interface of a b.c.c. twin for which the two possible structures have been revealed by computer calculation (see p. 353). It was originally concluded that the configuration shown in Fig. 8.12(b) will have the lowest energy, except possibly for very “soft” atoms which have a pairwise potential in which the repulsive part increases relatively slowly with decreasing separation. Later work, however, indicates that the computed equilibrium structure is sensitive to the boundary conditions and method of relaxation as well as to the potential, so that it is not easy to predict what is the equilibrium interface structure for any real material. Some calculations (Bristowe and Crocker, 1975; Yamaguchi and Vitek, 1976) indicate that the lowest energy structure may not be the same in all b.c.c. metals, and also that the difference in the energies of the two structures may be very small in some materials. Bristowe and Crocker pointed out that this leads to the possible dissociation of an elementary twinning dislocation into two partial twinning dislocations separated by a strip of interface in the configuration which has the slightly higher energy.

Figure 20.19 includes the same two configurations of the b.c.c. (112) twin boundary as Fig. 8.12. By making different atomic connections, the displaced boundary (f) is seen to consist of a layer of cells which are represented in projection as interlocking isosceles triangles. Bristowe and Crocker refer to the two structures as reflection and isosceles twin boundaries respectively; note that the planar geometrical interface is coincident with a plane of atoms for the reflection (or coincidence site lattice) boundary but is midway between two atomic planes for the isosceles boundary. This diagram illustrates more clearly than did Fig. 8.12 that both boundaries appear identical when viewed from either side of the interface.

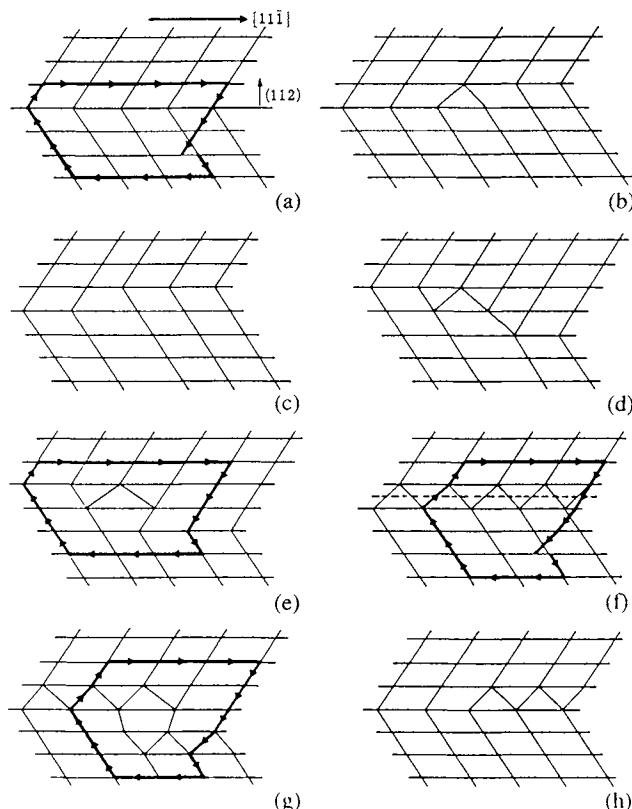


FIG. 20.19. The structures of possible twinning dislocations in b.c.c. crystals projected onto a (110) plane which has a twofold stacking sequence. A perfect reflection twin boundary is shown at (a) and this boundary contains perfect complementary, double and zonal twinning dislocations at (b), (c), (d) and (e). A perfect isosceles boundary is shown at (f) and this boundary contains an elementary dislocation at (g). A partial twinning dislocation is shown at (h).

An elementary twinning dislocation in a reflection type boundary is shown schematically in Fig. 20.19(b) and that in an isosceles boundary is shown in Fig. 20.19(g); Fig. 20.19(h) shows a reflection and an isosceles section of interface separated by a partial twinning dislocation of step height equal to one-half of the (112) plane spacing and a corresponding Burgers vector which is one-half that of the twinning dislocations of Fig. 20.19(b) and (g). In contrast to most extended lattice dislocations, there is no orientation of an applied shear stress which will tend to drive two partials from a dissociated elementary dislocation apart, as their Burgers vectors are parallel.

When a zonal twinning dislocation (or an elementary twinning dislocation if the twin mode has $q < 3$) is displaced along the K_1 interface, there is no first-order change in energy, other than the self energy of the dislocation, which may oscillate with the periodicity of the lattice in the direction of displacement. The dislocation may thus be

described as glissile, and its motion provides a mechanism for the growth or shrinkage of the twin, as described above. The lattice resistance to motion may be regarded as a friction stress arising from a kind of Peierls–Nabarro force (see pp. 273–280), and it depends on the detailed atomic structure of the step or dislocation core. In particular, if the core extends over several atomic distances along the K_1 plane, the lattice frictional resistance may be expected to be relatively small.

In early treatments of the possible nucleation and growth processes leading to the formation and subsequent spreading of new layers of the twin orientation, it was generally assumed that the core of a twinning dislocation is similar to that of a lattice dislocation and is thus quite narrow. Some justification for this assumption arises from the magnitudes of the Burgers vectors in cubic metals and especially from the close similarity between the elementary twinning dislocation in f.c.c. metals and the Shockley partial. Experimental evidence that small steps in twins are fairly sharp discontinuities has been provided by direct observation of elementary twinning dislocations which are visible when foils of f.c.c. copper (Mahajan *et al.*, 1970) or b.c.c. molybdenum–rhenium alloys (Mahajan, 1972a) containing very thin tapering twins are examined in the transmission electron microscope. However, computer calculations by Yamaguchi and Vitek (1976) and by Bristowe and Crocker (1977) indicate that twinning dislocations, at least in b.c.c. structures, are appreciably wider than lattice dislocations, and this may have important implications for the theory of twin growth. The calculations of Bristowe and Crocker (1976, 1977) have also revealed the possible existence of other step defects in b.c.c. twin boundaries, in addition to the elementary and partial twinning dislocations already described. These defects are shown in Fig. 20.19(c) and (e) and are called complementary and zonal twinning dislocations respectively.

Figure 20.19(c) shows the complementary twinning dislocation which was originally introduced by Sleeswyk (1962). It has the same step height as the elementary twinning dislocation [Fig. 20.19(b)] but, for the same sense of the step, its Burgers vector is twice as large and in the opposite direction, so that its structure is quite different. Sleeswyk introduced this defect by considering the hypothetical dissociation of a twinning dislocation in a tapering twin into a lattice dislocation and a complementary twinning dislocation according to the Burgers vector equation

$$a/6\langle 111 \rangle = a/2\langle 111 \rangle + a/3\langle \bar{1}\bar{1}\bar{1} \rangle \quad (87.5)$$

The reverse process of combination of a twinning dislocation with a lattice dislocation of antiparallel Burgers vector is clearly an equal formal possibility; in one case, the lattice dislocation is emitted from the interface, and in the other case the opposite lattice dislocation glides into the interface. In fact, however, with the pairwise potentials that were used by Bristowe and Crocker, an isolated complementary dislocation is unstable and will dissociate into elementary, partial and zonal twinning dislocations. Motion of a complementary dislocation along the K_1 plane is thus an unlikely process, but we should note that if it were to occur, the associated shear would be $2^{1/2}$ and if successive (112) planes were displaced in this way, the twinning mode produced (see Table XVI) would have $K_1 = \{112\}$, $K_2 = \{110\}$, $\eta_1 = \langle 11\bar{1} \rangle$ and $\eta_2 = \langle 001 \rangle$.

A step defect with the same Burgers vector as that of the complementary twinning dislocation but a double step height in the opposite sense is shown in Fig. 20.19(d). This simply consists of two coincident elementary twinning dislocations [each of opposite sense to that shown in (b)] and its motion produces the usual twinning shear of $2^{-1/2}$; it is, of course, unstable against dissociation into its component twinning dislocations. Consider now, however, the combination of a double step of this kind with a slip dislocation, as represented on the right-hand side of eqn. (87.3), to form a step defect of double step height but with a Burgers vector of type $a/6\langle 111 \rangle$. This is the zonal twinning dislocation shown in Fig. 20.19(e) for a reflection type boundary.

The existence of a zonal twinning dislocation in a $\{112\}$ b.c.c. twin interface was unpredicted prior to the computer simulation, and it should be emphasized that this is not a zonal twinning dislocation of the usual b.c.c. twin mode. As the Burgers vector has the same magnitude as that of the usual twinning dislocation but the step height is twice as large, it follows that propagation of such a dislocation through a series of $\{112\}$ planes will produce a shear of $2^{1/2}/4$. The corresponding twinning mode has $K_1 = \{112\}$, $K_2 = \{33\bar{2}\}$, $\eta_1 = \langle 11\bar{1} \rangle$, $\eta_2 = \langle 113 \rangle$ and $q = 4$, so that one-half of the lattice points (atoms) must shuffle as the interface moves forward. (This mode is listed in Table XVI.) The defect shown in Fig. 20.19(e) is thus correctly described as a zonal twinning dislocation of this hypothetical, smaller shear twinning mode, but the usage is rather loose when the defect is present in the boundary of a deformation twin which has formed by a different shear, or that of a non-deformation twin.

It is useful to digress here to consider the general question of steps and line defects in coherent twin boundaries. The Burgers vector specified by eqn. (32.1) is unambiguous for a given step height, but the equation is only relevant to the growth mechanism if the step has formed by a physical shear which is equivalent to the virtual process of Fig. 7.16. It is clear that, in discussing the possible defects which can arise in a coherent interface, only the positions of the atoms on the two sides of the interface are significant, and the origin of the interface is relevant only if consideration is limited to defects which may have formed in a particular way. In this sense, the possible Burgers vectors of step defects in coherent annealing twin boundaries may be found, for example, by supposing the twin and its step to have first formed by the virtual process of Fig. 7.16, followed by any rearrangement of the structure which does not remove the stepped interface. It is clear that, although such rearrangements will lead to various possible effective Burgers vectors for a step of given height, it will not generally be possible to remove the elastic discontinuity completely and so produce a pure step.

Some authors (Balluffi *et al.*, 1972; Ashby, 1972) have distinguished between grain boundary dislocations and grain boundary steps for the general grain boundary, and have suggested that there is no strain field associated with an ideal step. However, it needs to be emphasized that formation of an ideal step is rarely possible even when the step height is a multiple of the interplanar spacing; a necessary condition (Christian and Crocker, 1980) is that the plane defined by the step length and the riser is a lattice plane of a coincidence site lattice of the two crystal lattices. In the cases of coherent twin boundaries on $\{111\}$ planes of f.c.c. crystals or $\{112\}$ planes of b.c.c.

crystals, pure steps are possible when the step height is some multiple of three interplanar spacings.

It should now be clear that, if no restrictions are placed on the mechanism of formation of an interface of given structure, the set of possible Burgers vectors associated with a step of fixed height in this interface is obtained by taking any representative Burgers vector of the set [given, for example, by eqn. (32.1) or by a DSC lattice construction] and adding to it any lattice repeat vector. This procedure may be compared with that used in Section 33 to derive the possible Burgers vectors of the imperfect dislocations which may bound a given stacking fault. It should also be emphasized that, although it is possible to use different virtual lattice deformations to define the same interface, this does not lead to any ambiguities in the possible Burgers vectors of a given step; these vectors form a unique set and may be derived from any representation of the lattice relations. Pure steps may be envisaged if, and only if, this set contains a zero Burgers vector.

It is clear that the complete set of Burgers vectors of "perfect" interface dislocations (i.e. linear defects which separate two regions of identical interface structure) is identical with the set of vectors which constitute the DSC lattice of Bollmann (1970), as already discussed on pp. 373–375. These vectors link the sites of the parent lattice to those of the twin when the two lattices are in a coincident orientation and position, i.e. when $t=0$. For a single lattice structure, the DSC dislocations are the only vector translations which reproduce the interface structure. The vectors are independent of t (see p. 374) and each may be associated with a step of height d . However, in a general discussion of possible defects which reproduce the structure of an interface, Pond (1985, 1995) has shown that, in non-symmorphic crystals (i.e. crystals containing mirror-glide planes or screw rotation axes), additional dislocation type defects may in certain circumstances exist in an interface and reproduce the interface structure. Pond's theory follows on from his general treatment (Pond and Bollmann, 1979; Pond and Vlachavas, 1983) of "dichromatic colour" (or "black and white") symmetry in interface structures mentioned briefly on p. 375. He shows that, whereas defects in single crystals are characterized by the symmetry operations of translation, proper rotation or proper screw-rotation, giving rise respectively to dislocations, "disclinations" (see pp. 257–258) and "dispirations" (Harris, 1970), interface defects are characterized by combinations of symmetry operations, one from each crystal.

In Pond's formulation, the twinning dislocations considered above arise from the broken translational symmetry of the interface but, in some interfaces in non-symmorphic crystals, it is also possible to produce interface defects of translational character by combinations of point symmetry operations which are aligned but contain intrinsic glide components which are either not equal or not parallel. These "supplementary displacement dislocations", unlike the DSC dislocations, have Burgers vectors which are modified by any displacement t which breaks the translational alignment of the symmetry elements of the two crystals. Moreover, in general, such defects arise only at the junction between two differently orientated (but equivalent) interfaces and they only represent defects in a single interface when special conditions have been satisfied. The general theory of such defects (Pond, 1995) is too complex to be included here, but some special cases in connection with twinning dislocations in h.c.p. crystals will be considered.

In general, the atomic configuration at a step may be expected to adjust itself wherever possible so as to minimize the effective Burgers vector. This implies that the structures of minimum height steps in corresponding boundaries of annealing and deformation twins are likely to be identical, as the operative twinning mode of the deformation twin is likely to correspond to a minimum shear and hence to a minimum Burgers vector condition. However, in an annealing twin, there is likely to be an equal density of steps with each of the possible crystallographically equivalent directions of the Burgers vector which lie in the coherent interface (three for f.c.c. twinning) whereas, in the deformation twin, the steps will predominantly have Burgers vectors parallel to the physical η_1 direction.

For a f.c.c. twin, the structure of the fully coherent {111} interface is expected to be little relaxed from the ideal structure produced by shear without any relative translation of the two lattices. This follows from a pairwise model because, as pointed out on p. 121, differences between the various structures corresponding to ideal close-packing of spheres only appear when the computations are extended to at least third nearest neighbours. Thus the energies of an intrinsic stacking fault in the f.c.c. structure, the {111} twin boundary and the $\{111\}_c/\{00\bar{1}\}_h$ interface between the f.c.c. and h.c.p. structures are all likely to be similar and small (see pp. 122–124), and this is confirmed by the calculations of Vitek (1968) on stacking faults and those of Sutton and Christian (1982) for the cubic–hexagonal interface. The elementary twinning dislocation for f.c.c. has the same Burgers vector as a Shockley partial and a step height equal to the spacing of the {111} planes. As in the b.c.c. case, defects with other Burgers vectors of the DSC lattice are theoretically possible; for example, with the same step height and a Burgers vector in the antitwinning direction of twice the magnitude, corresponding to an elementary twinning dislocation of the 1.3 mode of Table XVII. However, these other type defects, except possibly pure steps with a height of three planes, or some integral multiple of three, seem unlikely to occur in practice. As there is probably only one stable configuration of the interface, there are unlikely to be any partial twinning dislocations in this structure.

Equivalent defects cannot form in h.c.p. twin boundaries as the basal planes of this structure are the only close-packed planes and cannot act as K_1 planes because they are already mirror planes. Simulations of the interface structures of the main h.c.p. K_1 interfaces, namely $\{10\bar{1}2\}$, $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$, have been made by Serra and Bacon (1986) using three different two-body potentials. Only one equilibrium configuration was found for the $\{10\bar{1}2\}$ interface, and the parent and twin structures are mirror images in the interface. The plane of the interface is an atomic plane formed by the coalescence of two adjacent original atomic planes which make up a corrugated lattice plane of type $\{10\bar{1}2\}$. This is the symmetrical configuration anticipated from Fig. 20.11, and discussed on p. 897, and the orientation relation is both type I and type II (i.e. “combined”) on an atomic scale. It follows that the only stable twinning dislocation expected for this mode is the zonal dislocation of double step height first discussed by Millard and Thompson. This has a Burgers vector (in the four-axis basis a, a, a, c)

$$\mathbf{b}_T = [(3 - \gamma^2)/(3 + \gamma^2)](10\bar{1}1) \quad (87.6)$$

so that

$$|\mathbf{b}_T| = [(3 - \gamma^2)/(3 + \gamma^2)^{1/2}]a \quad (87.7)$$

The Burgers vector thus has magnitude $a/(51)^{1/2} \cong a/7$ for ideal axial ratio, $\gamma = (8/3)^{1/2}$, but varies rapidly with γ . Computer simulation of the structure using two-body potentials shows that the width of the twinning dislocation is sensitive to the assumed potential.

The stable interface of a $\{11\bar{2}2\}$ twin is also an atomic plane of reflection according to the calculations of Serra and Bacon but, because the motif unit lies in the $\{11\bar{2}2\}$ planes, all the lattice planes parallel to the interface are flat in this case. The interface structure is thus that of a type I twin, but also possesses the additional symmetry discussed on p. 903. This structure was the only stable interface found by Serra and Bacon for so-called equilibrium pair potentials but, when non-equilibrium potentials were used, i.e. when the crystal was subjected to an external pressure which corresponded roughly to the Cauchy pressure, an additional stable interface was formed by relative translation of the two sets of atoms by $\mathbf{t} = [1/6(1 + \gamma^2)]\langle 11\bar{2}\bar{3} \rangle \cong (1/22)\langle 11\bar{2}3 \rangle$ parallel to the \mathbf{n}_1 direction of the $q=6$ twinning mode. This is the translation required to obtain a type II interface, but the twofold axis is midway between two atomic K_1 planes. This atomic symmetry might, however, be built into the pair potential model as the potentials used by Serra and Bacon do not well represent real materials. One of the non-equilibrium potentials also gave a third possible and less symmetrical atomic model of the interface produced by an alternative displacement parallel to \mathbf{n}_1 , but this was not stable when the other potentials were used.

As already noted, the probable twinning mode has $q=6$, so that the important twinning dislocation will be expected to be zonal, with a step height equal to three interplanar spacings of the $\{11\bar{2}2\}$ lattice planes. The core structure of this dislocation will depend on the details of the shuffle displacements, and Serra *et al.* (1988) made computations for three different possibilities. The energy and width of the step were found to be not very sensitive to the shuffle model used, but to depend on the potential. Calculations were also made for two other possible step defects in this type of boundary, having step heights of one and four interplanar spacings respectively. These steps would be twinning dislocations of other hypothetical twinning modes for which $K_1 = \{11\bar{2}2\}$; in the single step case, the mode has a high shear of ~ 1.22 and the four-layer step has more complex shuffles. Thus these dislocations are probably not important in the mechanism of deformation twinning.

Two different starting configurations were considered by Minonishi *et al.* (1982) for the atomic structure of a $\{11\bar{2}1\}$ interface, and these were called *R* and *D* respectively. Using a Lennard-Jones potential, they found two correspondingly stable relaxed structures for the interface, neither of which corresponds to mirror symmetry on an atomic scale. Similar results were obtained by Serra and Bacon, who pointed out that the lower energy (relaxed *D*) interface may be obtained from the mirror interface (unrelaxed *R*) by moving alternate basal planes in opposite senses through $(1/12)\langle 1\bar{1}00 \rangle$ to change the stacking from $\dots ABAB\dots$ to $\dots ACAC\dots$. The configuration of the higher energy (relaxed *R*) interface is similar, but it has a row of vacancies in each *B-C* transition region. The relaxed

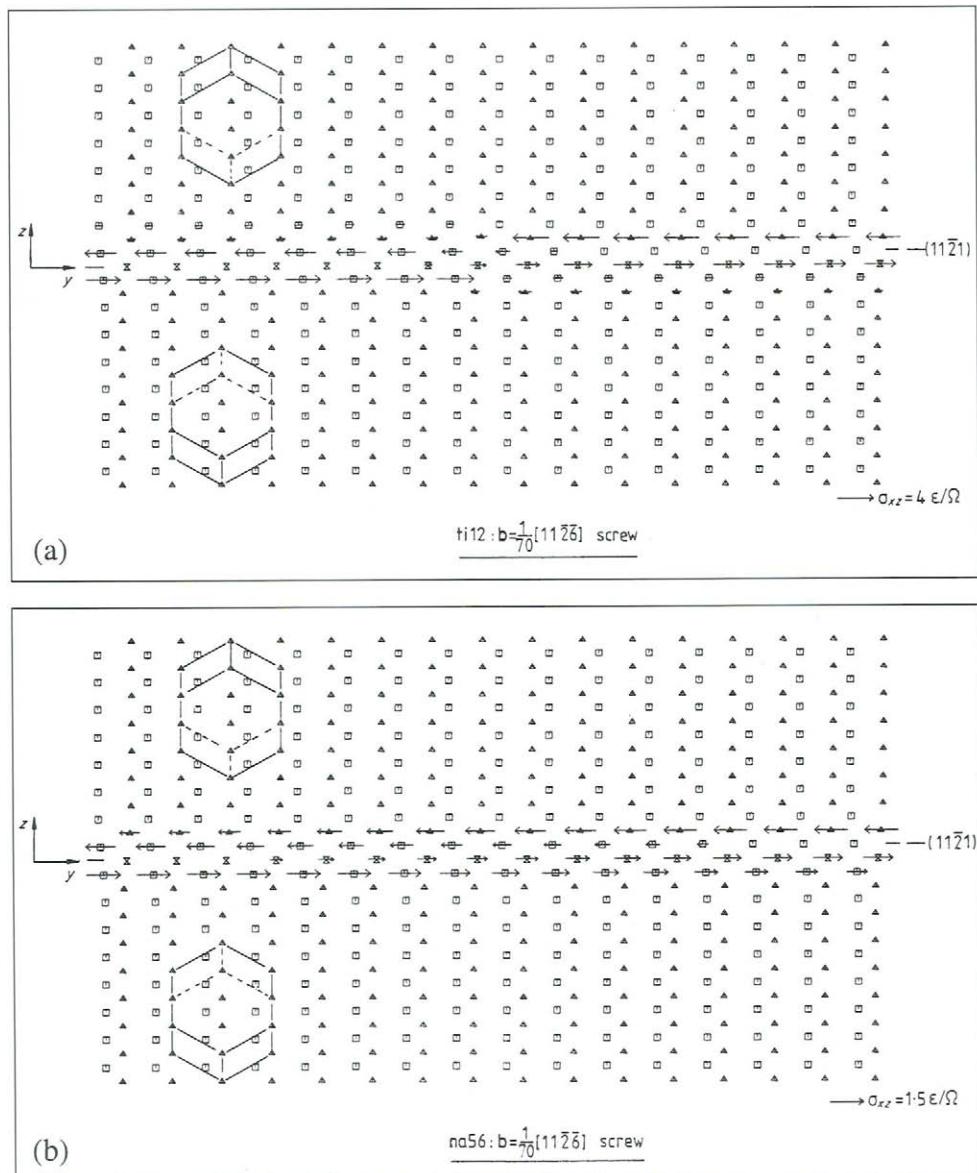


FIG. 20.20. A twinning dislocation in a $\{11\bar{2}1\}$ interface computed with two different pair potentials (after Serra *et al.*, 1988).

D interface is shown in Fig. 20.20; it again has an atomic interface plane, but in this case it is an actual atomic plane of each crystal, not a coalesced lattice plane. Serra and Bacon point out that the atom positions are connected by a twofold axis along \mathbf{n}_1 and lying at level 0 in the atomic interface of Fig. 20.20 although this symmetry was not present in the

starting configuration. As no lattice shuffles are involved in $\{11\bar{2}1\}$ twinning an elementary twinning dislocation reproduces the interface structure. This dislocation is specified by

$$\mathbf{b}_T = [1/3(4\gamma^2 + 1)](11\bar{2}\bar{6}) \quad (87.8)$$

and

$$|\mathbf{b}_T| = [2/(3 + \gamma^2)]^{1/2}a \quad (87.9)$$

For ideal axial ratios, the Burgers vector is $\mathbf{b}_T \cong (1/35)(11\bar{2}\bar{6})$. When this dislocation was simulated, however, Serra *et al.* found that it decomposed into two dislocations, each with one-half of the above Burgers vector, as first envisaged by Minonishi *et al.* These two dislocations each have a step height equal to the separation of atomic planes parallel to the interface, i.e. to one-half of the spacing of lattice K_1 planes. Although this ordinarily would not reproduce the interface structure, the non-alignment of the translational components of the mirror glide symmetry of the $\{1\bar{1}00\}$ plane of shear ensures that the two interfaces bounding such a step have equivalent structures and energies. This is an example of the "supplementary displacement dislocations" mentioned on p. 923. With two of the three potentials used, Serra *et al.* found the core width of both edge and screw twinning dislocations of this type to be very wide, implying that the steps may be very mobile.

As already noted, the edge of a twin wedge or lenticular plate in a stressed material will be a region of high stress concentration, and may be compared with a crack tip or an incomplete kink band. If the yield stress of the matrix is sufficiently high, an enclosed twin may be accommodated elastically and an adequate treatment of its stress field and of the energy of the assembly may be obtained by Eshelby's method (see pp. 466-471), which gives analytical solutions in the isotropic approximation for a twin of assumed ellipsoidal shape. Such a calculation is relevant to the possible homogeneous nucleation of a twin within a grain or in a region of stress concentration, as proposed by Orowan (1954) and discussed below. The high stress at the tip of an elastic twin will tend to produce further growth of that twin, as was shown for the analogous case of an incomplete kink band in a classical treatment by Frank and Stroh (1952).

If the twin is not completely elastic, i.e. if there has been some plastic accommodation as shown in Fig. 20.15, it becomes much more difficult to calculate the stress field and the energy, just as it does for an elastic-plastic crack. Thus it becomes important to discuss the problem of accommodation, already mentioned in connection with twin morphology, and the experimental measurement of the twinning shear in more detail. Before doing so, however, it should be mentioned that models which are not purely elastic may be used to calculate the stress field and energy of an enclosed twin. It may be regarded, for example, as a continuous distribution of infinitesimal dislocations, or attempts may be made to derive an atomistic model with some assumed interatomic potentials. A brief review of all three methods has been given by Sree Harsha (1981).

Accommodation slip at the ends of an internally terminating b.c.c. twin generally takes the form of a single slip band parallel to the K_1 plane although, in silicon-iron crystals, slip sometimes occurs also on those intersecting $\{110\}$ type planes which contain the Burgers

vector of the twinning dislocation. The slip dislocations may form directly from the twinning dislocations of the interface, as originally proposed by Sleeswyk (1962), or may be nucleated ahead of the interface.

Sleeswyk considered a dissociation of the type represented in eqn. (87.5) and supposed that this occurs in every third twinning dislocation in a tapering boundary. The lattice dislocations are then assumed to move away on their glide planes, which are of course planes parallel to the K_1 plane of the twin, and they leave behind a boundary consisting of groups of two elementary twinning dislocations and one complementary twinning dislocation. If the sequence is repeated nearly regularly, the net Burgers vector content of the new twin boundary is zero, so that its motion produces no net shear but nevertheless converts the parent structure into the twin structure. In contrast, the shape shear formerly associated with the twin is now produced in a region ahead of the twin by the glide of the regularly spaced lattice dislocations. The new twin boundary may be assumed to have a lower energy than the original boundary, but only because additional energy has been supplied to create the lattice dislocations; the dissociation in eqn. (87.5) is probably energetically very unfavourable. The postulated slip dislocations are supposed to have been emitted from the original twin interface and were called emissary dislocations by Sleeswyk.

It has been proposed that, instead of the dissociation reaction, loops of slip dislocation are created spontaneously in the high stress field near the tip of the twin. Each such loop will then expand, part of it interacting with the twin boundary to produce an $a/3[111]$ complementary dislocation in the interface, and the remainder spreading away from the twin. Clearly, if loops are nucleated on every third lattice plane, the final result will be indistinguishable from Sleeswyk's emissary slip.

The theory of emissary dislocations implies that the shape deformation associated with twin formation may be physically separated from the actual change of lattice orientation. The suggested model of the boundary and its associated emissary dislocations is shown in Fig. 20.21; the instability of an isolated complementary dislocation predicted by Bristowe and Crocker will not necessarily apply to the regularly spaced complementary dislocation of this array, which has no long-range field. In any event, if a set of emissary dislocations can be formed, the twin boundary will have some structure which produces no net shape change so that, if this boundary advances into the region already swept by the emissary dislocations, the total change is indistinguishable from the usual picture of twinning. Direct evidence for emissary slip ahead of a stopped twin in a molybdenum-rhenium alloy has been obtained by Mahajan (1975). The dislocations ahead of the twin tip were confined to a slip zone coplanar with the twin, as expected, but were of both signs, so that some modifications have to be made to the simple model.

A growing twin might have one of the two general shapes shown in Fig. 20.22 and electron microscopic observations have revealed configurations of these types (see, e.g., Votava and Sleeswyk, 1962). In some cases, parts of the twin interface may be held up by obstacles so that irregular shapes which differ appreciably from the ideal picture of Fig. 20.22 are produced. This is illustrated in Fig. 20.23. It will be seen that the separation of the lattice and shape changes allows the twin to occupy only part of the region

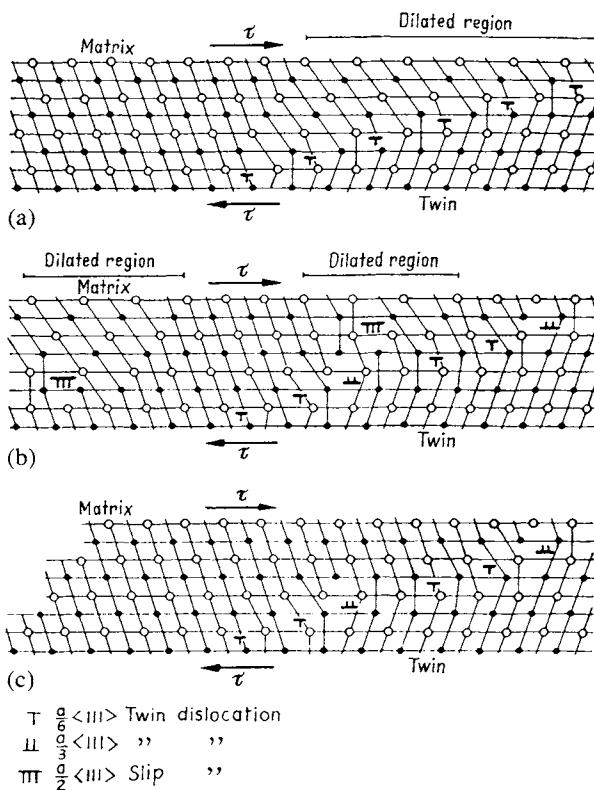


FIG. 20.21. The dissociation of a twin termination boundary in the b.c.c. structure (after Sleeswyk, 1962). Two layers of atoms are projected onto a {110} plane. In (a) the boundary between twin and matrix is represented as an array of $1/6\langle111\rangle$ twinning dislocations on successive $\{111\}$ planes. In (b) the dissociation has produced the emissary dislocations which move away from the interface under the influence of the stress, and complementary $1/3\langle111\rangle$ type twinning dislocations. The residual boundary shown in (c) has one complementary dislocation to every two twinning dislocations and produces no far-reaching strains in the lattice.

of homogeneous shear produced by the emissary dislocations, and thus to have an irregular shape.

An alternative view is that there are no emissary dislocations ahead of a moving twin interface but that, when the interface is halted for some reason, emissary slip occurs to ensure continuity of the shear and hence compatibility of the shape deformation. This would still allow the formation of twins of irregular shape, as not infrequently observed, and would avoid the difficulty that there is no driving force tending to displace the twin interface of Fig. 20.21(c).

Nearly equivalent results could be obtained in principle if the stresses at the edge of a twin merely activated dislocation sources, but the slip would then not be so homogeneous, nor confined in general to the twin plane. Even in silicon-iron, where slip on $\{110\}$ planes

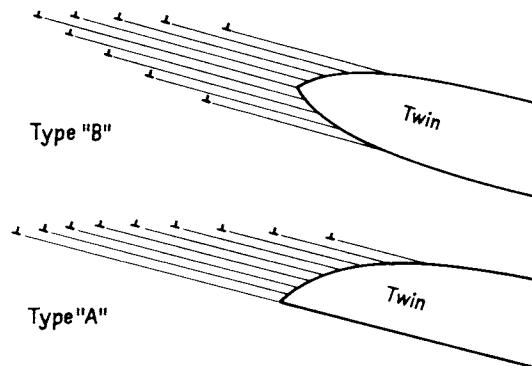


FIG. 20.22. Diagram illustrating two types of emissary dislocation array (after Votava and Sleeswyk, 1962). Associated twin fronts have been observed in molybdenum-rhenium alloys.

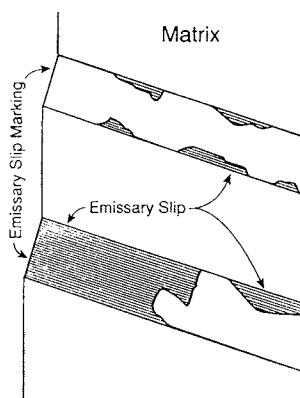


FIG. 20.23. Schematic drawing to show that twins need occupy only part of the regions of emissary slip (after Sleeswyk, 1962).

is observed to emanate from the tip or from irregularities in the side faces, there are no apparent pre-existing lattice dislocations to act as sources, and Hull suggested that, in such b.c.c. materials, $(1/2)a\langle 111 \rangle$ slip dislocations are nucleated at or near the interface but, in screw orientation, cross-slip on to $\{110\}$ planes as they move away from the region of intense stress concentration. Very approximate calculations suggest that the energetic conditions favour emissary dislocations when the thickness of the twin lamellae exceeds about 4 nm at the normal stresses at which twinning occurs in iron.

Emissary slip of the above type cannot be expected in other crystal structures as the Burgers vectors of twinning and slip dislocations are not normally parallel. Nevertheless, whenever a twin is stopped within a surrounding matrix, it should generally be possible to accommodate (i.e. reduce) the shear discontinuity at the tip by conversion of some of the twinning dislocations into "emissary" lattice dislocations. Thus, Pond and Garcia-Garcia

(1981) observed dislocation structures near twin tips in thin foils of aluminium (see p. 913) which were consistent with the formation of two "residual" Shockley partials and one "emissary" f.c.c. slip dislocation from three adjacent twinning dislocations.

Now consider the problem of growth normal to a rational K_1 plane. The twin might extend by one repeat distance (qd or $\frac{1}{2}qd$) by first forming a small island or two-dimensional nucleus, which could then spread outward under the applied stress, but a very small island will tend to collapse again because of the line tension of the peripheral twinning dislocation. A region sufficiently large to expand continuously may thus be established only by a favourable series of thermal fluctuations, so that in this idealized model there may be a nucleation difficulty at each successive equivalent position of the twin interface. Of course, there may be favoured regions of high internal stresses where steps in the interface can be more readily nucleated, for example the intersections of the coherent twin boundary with a grain boundary or a free surface.

The nucleation of a closed loop of twinning dislocation by the combined effects of thermal agitation and applied stress may be compared to the corresponding problem of the spontaneous creation of a lattice dislocation, discussed on p. 281. For a loop of given radius, the activation energy according to a linear elastic model is proportional to the square of the Burgers vector [eqn. (31.17)], and the stress required is proportional to the Burgers vector [eqn. (31.16)]. Thus in structures with a sufficiently small twinning shear, it is possible that normal growth at finite temperatures does involve spontaneous nucleation of little islands of twin on each successive lattice plane. For example, if the Burgers vector of the twinning dislocation is about one-tenth of the interatomic distance, the assumptions made on p. 281 imply that, with a stress of $\sim 8 \times 10^{-4} \mu$, the activation energy is only $\sim 0.2 \text{ eV}$ and the critical radius is $\sim 10 \text{ nm}$. However, if the twinning dislocation has a Burgers vector greater than (say) one-third of the interatomic distance, as in cubic crystals, the probability of spontaneous nucleation will (with a linear elastic model) be almost negligible, as it is for perfect lattice dislocations.

Twinning dislocations in face-centred tetragonal or orthorhombic structures, such as those found in indium-thallium or gold-cadmium alloys, have Burgers vectors with magnitudes in the range 0.006–0.04 nm. Birnbaum and Read (1960) used eqns. (31.16) and (31.17) to show that twin boundary motion by spontaneous nucleation is quite probable in such alloys, the required activation energy being comparable to the available thermal energy at stresses corresponding to those at which the boundaries are observed to move. In these alloys, a single crystal of the high temperature cubic phase may be transformed martensitically to give a specimen consisting of a single set of parallel twins (see p. 1030). The twins are extremely mobile under small stresses and deform plastically entirely by movement of the twin boundaries, up to a limiting strain. The low stress required to move the boundaries is undoubtedly associated with the small shear, whether or not twinning dislocations are nucleated spontaneously. It should be noted that the calculation of the activation energy for nucleation using eqn. (31.17) neglects the core energy of the twinning dislocation, and this may not be justified when the elastic energy becomes small. The energy also does not include any term representing the misfit energy of the area enclosed by the loop of twinning dislocation; in other words, it is appropriate to the nucleation of a

new step on the surface of an existing twin, but not to the creation of a monolayer twin in a region of perfect lattice. However, if the calculation is correct, it seems that the normal growth of a twin which is only a few lattice spacings thick should present no difficulty, in contrast to the theory to be described below.

The conclusion that thickening of deformation twins in cubic crystals by spontaneous nucleation of successive loops of twinning dislocation is not possible rests on the assumption that the interface region possesses the elastic properties of the matrix. Several authors (see, e.g., Sumino, 1966; Delamotte and Alstetter, 1969) have pointed out that this conclusion may be erroneous and, in particular, the effective shear modulus, μ' , to be used in eqns. (31.16) and (31.17) may be appreciably lower than the modulus, μ , for bulk material. Some support for the view that the effective stress and activation energy required to nucleate a loop of twinning dislocation may be lower than the values given by the ordinary linear elastic model comes from the computer simulations of Yamaguchi and Vitek (1976) and Bristowe and Crocker (1977), which indicate that twinning dislocations have relatively wide cores and hence relatively small self energies. Yamaguchi and Vitek point out that the width of the core according to the Peierls-Nabarro model (pp. 273-276) is proportional to the shear modulus and, from the computed widths of twinning dislocations and lattice dislocations using various empirical interatomic potentials, they estimate the effective shear modulus μ' to be a factor of three to five times smaller than the modulus of the matrix. Sumino estimated the stress needed for spontaneous twinning, i.e. virtual zero activation energy [see eqn. (31.16)], as $\mu' b/2h$, and Yamaguchi and Vitek point out that, with their potentials, this is ~ 0.01 to 0.02μ . This is still rather a high stress for continuous growth of twins, but is lower than the corresponding estimate for formation of a twin nucleus from a screw dislocation, which is about 0.03μ for the same potentials. Thus growth by spontaneous nucleation of new layers is considered to be a possible mechanism, even in b.c.c. metals.

A theory for the normal growth of a twin without thermal activation was first given by Cottrell and Bilby (1951), and Millard and Thompson (1952) independently developed a similar description for the particular case of h.c.p. metals. The theory is analogous to Frank's theory of crystal growth from the vapour, and to the operation of a Frank-Read source, and is based on the topological properties of a node formed when a dislocation crosses from a parent into the twin (p. 292). This "pole dislocation" (e.g. *SNS* of Fig. 7.18) must have a Burgers vector with a component normal to the K_1 planes equal in magnitude to qd or $\frac{1}{2}qd$. As the twinning dislocation (*BN* in Fig. 7.18) moves in the interface, it rotates about the node and (together with the node) is displaced through qd for each complete revolution. Successive blocks of structure, qd in thickness, thus suffer the same vector displacement relative to each other, to give the macroscopic shear of the twinning relation. Any necessary shuffling is not, of course, described by this mechanism, but presumably occurs spontaneously as the structure grows. Single nodes, giving a spiral step of twinning dislocation, and double nodes, giving closed terraces of twinning dislocation, are both possible, as in the associated problems of crystal growth and slip.

As discussed on p. 292, the geometrical conditions necessary for the setting up of a generating node of this type can always be fulfilled, and it is possible to envisage a number

of real or virtual processes by means of which single- or double-ended sources with the requisite configuration may be achieved. Such processes include compatible slip in a matrix-twin bicrystal, as in Fig. 7.18, glide of part of an expanding dislocation loop across an existing coherent matrix-twin interface so that the twinning dislocation ends on the two crossing points, partial transformation of a previously dislocated crystal, and the welding together of separate matrix and twin crystals along the K_1 plane interfaces, through each of which an appropriate lattice dislocation emerges. A process which could be of particular physical interest is the expansion of a very thin disc-shaped twin or multilayer fault, nqd planes thick, so as to incorporate an existing lattice dislocation, or equivalently the glide of the dislocation from outside the periphery of the twin to a position where it intersects the twin disc. The limit of the twin will then be a continuous spiral of twinning dislocation running between generating nodes on the top and bottom surfaces, and rotation of the end elements in opposite directions about the pole dislocation will produce thickening of the twin upwards and downwards.

The generating node produced in this way requires the separate nucleation of at least a monolayer of twinning fault and, although the crystallographic and geometric conditions are relatively easy to satisfy, the physical operation of the source is subject to some restrictions. One of these arises from the fact that the twinning dislocations in the top and bottom surfaces have to pass each other at a separation of the fault thickness on the first revolution and this would require unrealistically high stresses if \mathbf{b}_T is appreciable and the fault is very thin. In particular, growth from a monolayer twinning fault is not likely to be feasible and estimates by Bilby (1953) indicate that, for cubic twins, a nucleus about 50 atoms thick would be required before the pole mechanism can begin to operate at experimentally observed twinning stresses. A second difficulty is that, in many lattices, the pole dislocation would not remain anchored, but would glide under the applied stress. The pole may be anchored firmly if it is a sessile partial rather than a lattice dislocation, but this is difficult to achieve. Nabarro (1952) showed that imperfect dislocations of Burgers vector $qd\mathbf{m}$ can exist only in special lattices and then are ineffective as they must lie in the composition plane. Dislocations with vectors $2qd\mathbf{m}$ can always exist, but are only useful if there is a second set of twinning planes at 60° to the first, as in b.c.c. crystals. In all other cases, the pole dislocations must be perfect dislocations in the two lattices. The stability of a node can then be due only to the difficulty which such a dislocation experiences in gliding; for example, dislocations with Burgers vectors of $c[0001]$ are suitable as pole dislocations in some h.c.p. twinning modes, and probably exist in this structure although they do not contribute to glide processes.

Direct discussion of the very early stages of growth, i.e. of twin nucleation, is difficult, although several theories of growth have obvious implications in nucleation. In general, there are three types of nucleation theory, namely (1) twin nuclei are tiny stopped twins, pre-existing in the solid as a result of growth accidents (Oliver, 1952), (2) twins form spontaneously in the elastic field of an imposed external stress and/or in the field of internal defects, and (3) twins form by some kind of dissociation of existing dislocations or other defects, utilizing, for example, the large planar stacking faults which form readily in some f.c.c. alloys or the large displacements in the core of a b.c.c. dislocation which cannot

be treated by linear elastic theory. The experiments of Bell and Cahn and of Price apparently provide evidence in support of a combination of theories (1) and (2), but many later observations strongly suggest that twin nuclei in the common metallic structures form from dislocations.

The pole theories imply that the formation of an initial planar fault or monolayer twin will be more difficult than the addition of subsequent layers as the interfacial energy is not substantially changed after the first layer. Thus Cottrell and Bilby suggested that, if the stress resisting growth is X_i , that required for nucleation will be $X_i + \sigma^f/b_T$, where b_T is the magnitude of the Burgers vector of the twinning dislocation and σ^f , the fault energy, is approximately twice the energy σ of the K_1 interface. If the fault forms by the bowing of a partial between two pinning points, an additional stress $Cb_T\mu/y$ (where C is of the order of unity and y is the source length) is needed to overcome the line tension (see p. 268). The stress X_i incorporates any intrinsic resistance to motion (lattice friction or Peierls–Nabarro force) and also the effects of specific obstacles (other dislocations, faults, impurities, etc.) through which the twinning dislocation must pass. With an assumed source length of 25 nm, and a fault energy of 40 mJ m^{-2} , the required stress is only about 2.5 times the measured twinning stress in copper, so that a fairly modest stress concentration would appear to be adequate. Venables (1961) discussed in some detail the transition from load drops and unsaulted twins to smooth stress-strain curves with highly faulted twins which occurs in f.c.c. alloys as the stacking fault energy or temperature are reduced.

The simple conclusion that the nucleation stress exceeds the growth stress by only σ^f/b is in marked contrast to a calculation based on classical nucleation theory. In this theory, as in phase transformation theory, it is assumed that macroscopic concepts may be applied so that, for a sufficiently small twin, the surface energy of the twin matrix interface will be the dominant term in the net free energy change. When a very small twin forms, the free energy of the system should thus increase, and fluctuations may be necessary to overcome the lowest "saddle point" barrier. Homogeneous nucleation theory was applied to the formation of an enclosed twin embryo by Orowan (1954) and later re-examined by Christian (1969). The calculation is most acceptable if the twin embryos are assumed to be oblate spheroids parallel to K_1 . The change in energy on forming an embryo of semi-axes R , R and y then has a negative term representing the work τ_s per unit volume of embryo done by the shear stress across K_1 resolved in the η_1 direction, a positive term of magnitude Ay/R representing the elastic energy per unit volume of the constrained twin and a further positive term representing the (non-elastic) energy of the twin interfaces. In his calculation, Orowan treated the interface energy as that of the matching K_1 planes of Fig. 20.17 plus that of the twinning dislocations assuming a uniform line tension; the constrained strain energy was treated as negligible on the assumption that the matrix stresses do not exceed the yield stress. An alternative approach is to allow this stress to approach the theoretical strength of the material on the basis that there will be no dislocation sources in the small volume around the tip of the nucleus. The strain energy must then be included, either by means of the Eshelby procedure or by treating the twinning dislocations as a pile-up, and the steps may be regarded as sections of a second interface with specific free energy σ' different from the

energy σ of the K_1 interface. The change in energy ΔG due to the formation of an embryo of volume $v = 4\pi R^2 y/3$ is

$$\Delta G/v = -\tau s + 3\sigma/2y + 3\sigma'/R + Ay/R \quad (87.10)$$

The size and shape of a critical nucleus are given by $\partial\Delta G/\partial R = \partial\Delta G/\partial y = 0$ and this defines the saddle point in ΔG . The shape of this nucleus is defined by the equations

$$\tau s R = 2Ay + 3\sigma' \quad (87.11)$$

$$\sigma R = Ay^2 + \sigma'y \quad (87.12)$$

which may be solved to give the critical thickness

$$y_c = -(p + q) \pm (p^2 + q^2 - 4pq)^{1/2} \quad (87.13)$$

where $p = -\sigma/\tau s$ and $q = \sigma'/2A$. [The minimization used by Orowan corresponds to $A = 0$, whereas some other treatments effectively have $\sigma' = 0$. The equations also depend slightly on the assumed geometry of the nucleus; that used by Orowan introduces factors of $4/3$ and $3/4$ into the second term on the right-hand side of eqn. (87.11) and the first term on the right-hand side of eqn. (87.12) respectively.]

The factor A is given in isotropic approximation by eqns. (52.26) and (52.27) and, for $\{10\bar{1}2\}$ twinning in zinc, it is about $6 \times 10^8 \text{ J m}^{-3}$. Low estimates of σ and σ' are 20 and 100 mJ m^{-2} and, with Price's measured value of $\tau = 500 \text{ MPa}$, $\tau s = 7 \times 10^7 \text{ J m}^{-3}$. The critical nucleus would thus have $y_c \approx 0.63 \text{ nm}$ (i.e. about 10 $\{10\bar{1}2\}$ lattice planes) and the corresponding values of R_c and ΔG_c are 15 nm and 75 eV respectively. This is clearly much too large an energy for homogeneous nucleation by thermal fluctuations to be feasible, and Price's original claim that the Orowan theory gives a nucleation barrier of only 1 eV seems to have been erroneous. Variations in the assumptions by setting either σ' or A equal to zero do not produce much improvement; the most favourable case is for $A = 0$, which corresponds to $\Delta G_c \approx 13 \text{ eV}$ with the above assumptions, and an appreciably larger value with the effective value of $\sigma' = 500 \text{ mJ m}^{-2}$ used by Orowan.

Homogeneous nucleation of twins is thus improbable unless there is a combination of very high stresses and very low surface and strain energies. Although the strain energy may have been reduced in the thin platelets used in Price's experiments, it is unlikely that the surface energies were substantially lower than the above estimates. It may be that the true stress concentration factor at the re-entrant nucleation sites was larger than that calculated or that the platelets contained undetected defects which aided nucleation. It is now considered probable that twinning in most metallic materials is initiated by other defects. Most nucleation models utilize the energy of one or more existing defects to make an initial single or multilayer fault which can then grow continuously or else link up with other similar faults to form a supercritical nucleus.

Continuous growth from a single-layer fault formed from the dissociation of an originally perfect dislocation in the parent lattice was originally proposed by Cottrell and Bilby (1951) for the b.c.c. structure and (independently) by Millard and Thompson for the h.c.p. structure. They suggested that a "generating node" (see p. 292) could form by the

dissociation of a single lattice dislocation, and thus avoid the need for separate nucleation. Unfortunately, there is a flaw in their analysis of this “pole mechanism” which may be best understood by considering first the general theory which was first advanced by Bilby (1953), and applied also to martensitic transformation. As already noted, Bilby and Christian (1956) considered a dislocation in the parent with Burgers vector \mathbf{b}_A which crosses the parent twin (K_1) interface and continues in the twin as a dislocation with Burgers vector \mathbf{b}_B (see Fig. 7.18). They assumed that the two Burgers vectors are related by the twinning shear, i.e. $\mathbf{b}_B = \mathbf{S}\mathbf{b}_A$, and similarly that the slip plane normal $\mathbf{m}'_B = \mathbf{m}'_A\mathbf{S}^{-1}$. The components of the Burgers vectors, referred to unit cell-based coordinate systems in the twin and parent respectively are thus related by the correspondence matrix, as might be expected also if a fixed dislocation, without dissociating, is partly engulfed by a growing deformation twin. Note also that corresponding planes in parent and twin meet edge to edge in the K_1 interface, which is a necessary geometrical condition for the propagation of slip across the interface. However, to avoid confusion, it should be noted at this point that some dissociations in which the Burgers vector of the dislocation within the twin has been given values other than $\mathbf{S}\mathbf{b}_A$ have been postulated; in general, \mathbf{b}_B is then not a lattice vector of the twin.

The passage of the dislocation leaves a step in the interface of height $h = \mathbf{b}_A \cdot \mathbf{m} = (b_A)_m$, equal to the component of \mathbf{b}_A or equivalently of \mathbf{b}_B in the direction of the unit normal \mathbf{m} to K_1 . This step is a twinning dislocation with Burgers vector $\mathbf{b}_T = \mathbf{b}_B - \mathbf{b}_A = (\mathbf{S} - \mathbf{I})\mathbf{b}_A = (\mathbf{b}_A \cdot \mathbf{m})\mathbf{s}\mathbf{l}$ and it runs between two (opposite) crossing points or from a single crossing point to the periphery of the interface. Thus each crossing point is the junction of (at least) three dislocation lines, one in each crystal and one in the interface. Bilby called this configuration in which

$$\mathbf{b}_B = \mathbf{S}\mathbf{b}_A = \mathbf{b}_A + \mathbf{b}_T \quad (87.14)$$

a generating node. As all the planes parallel to K_1 are now threaded by a “pole” dislocation with a normal component of Burgers vector, the set of parallel planes has been converted into a continuous spiral ramp leading from the parent phase to the twin. If the glissile twinning dislocation in the plane of the interface now glides along this plane whilst the other elements remain fixed, it must rotate about the node or nodes and, for each complete revolution, the K_1 interface together with the node is displaced into the matrix or twin (depending on the sense of the rotation) through a distance $h = \mathbf{b}_A \cdot \mathbf{m}$. Successive blocks of the matrix structure thus suffer the same vector displacement relative to each other in order to give the macroscopic shear of the twinning relation and any necessary shuffles are accomplished spontaneously at the step in the interface. A dislocation which both enters and leaves a twin may do so at the same K_1 interface or at the two K_1 interfaces of a twin of finite thickness. Single nodes giving spiral steps from single crossing points and double nodes giving closed terraces of twinning dislocation from opposite crossing points in one interface can both be formed as in the topologically similar models of dislocation-assisted crystal growth and Frank–Read source operation. (Note especially the similarity to a cone source.)

The dislocation configuration required for this mechanism in compound or type I twins is quite specific; the pole dislocation must have a Burgers vector component normal to the interface which is equal to either qd (for q odd) or $\frac{1}{2}qd$ (for q even) where d is the spacing of the lattice K_1 planes. Any dislocation with a lattice Burgers vector from plane 0 to plane q or $\frac{1}{2}q$ will satisfy this condition, which arises of course to ensure that \mathbf{b}_T when necessary shall be a zonal twinning dislocation and thus able to glide freely. The same condition ensures that if \mathbf{b}_A is a lattice vector of the parent crystal, \mathbf{b}_B is a lattice vector of the twin, and together with \mathbf{m}_B it defines a geometrically feasible, atomic slip system in the twin, the plane and direction of which may have relatively high indices, so that actual slip on the system may be impossible. Clearly, dislocation glide across the interface becomes a virtual rather than a physical process if the dislocation is unable to glide in the twin but, if the configuration can be formed in some other way, the resistance to slip could ensure the stability of the pole. However, in some lower symmetry crystals, there may not be any suitable pole dislocations.

It follows from this treatment that the interaction of independently formed stacking faults and dislocations may produce true generating nodes in the sense defined by Bilby and Christian (1956) and Sleeswyk (1963) at each crossing point. In particular, four variables listed by Venables (1974) are correctly disposed so that the applied stress favouring twinning continues to drive the twinning dislocation into the matrix, whereas an opposite stress reverses the motion so as to produce detwinning. These variables are:

- (i) the screw sense of the pole dislocation;
- (ii) the type of stacking fault in the parent lattice which is trailed behind the glissile partial (or twinning) dislocation;
- (iii) the side of the fault on which the glissile partial is situated; and
- (iv) the direction in which the glissile partial moves under a fixed applied stress.

It may readily be seen that, if another pole dislocation has the opposite Burgers vector (i.e. the reversed screw sense), the last two variables must also be reversed and the left-handed rotation of $-\mathbf{b}_T$ about the opposite pole will produce the same twinning shear as the right-handed rotation of the original twinning dislocation $+\mathbf{b}_T$.

The pole mechanism is usually invoked in combined nucleation and growth models of twinning which begin with the dissociation of a lattice dislocation. One simple possibility is that a glissile partial dislocation trailing a monolayer (twin type) stacking fault in the K_1 plane encounters a suitable pole dislocation threading the plane. A pole source can then be produced if the partial wraps itself around the pole. The two parts of the partial then form a dipole on adjacent K_1 planes, and between these two planes the pole dislocation is converted (formally) into the dislocation \mathbf{b}_B of eqn. (87.14). If the two opposite segments of the original partial are able to glide past each other (a very doubtful assumption with a single plane separation), they can continue to spiral upwards and downwards respectively, thus thickening the twin in both directions.

More elaborate descriptions suppose that an initial pole dislocation contains a superjog which dissociates in the K_1 plane, emitting a twinning partial into this plane and leaving a

sessile partial along the original interface. With a correct configuration, this leads to a perfect pole in which the two ends of the twinning partial spiral upwards and downwards from the sessile partial, passing it very closely on the first revolution, but never being blocked by it. Thus a twin is formed by outwardly spreading shear on what is topologically a single helicoidal K_1 interface wrapped around the pole dislocation. The sessile part of the dissociation is the vector \mathbf{b}_B referred to the parent coordinates and this becomes a lattice vector in the twin. Now suppose that the same pole dislocation dissociates into a dislocation with Burgers vector \mathbf{b}_B^* and a glissile partial $-\mathbf{b}_T$ which glides away from the superjog in the opposite direction to produce an identical intrinsic, twin type fault. This dissociation is represented by

$$\mathbf{b}_B^* = \mathbf{S}\mathbf{b}_A - 2(b_i m_i) \mathbf{l} = \mathbf{b}_A - \mathbf{b}_T \quad (87.15)$$

and variables (iii) and (iv) above have been reversed. The dislocation \mathbf{b}_T is still rotating about \mathbf{b}_A in the matrix but the vector \mathbf{b}_B^* is not a lattice vector because \mathbf{t} differs from the lattice vector $\mathbf{S}\mathbf{b}_A$ by $2\mathbf{b}_T$, which is not a lattice vector. Moreover, \mathbf{b}_B^* has the wrong screw sense as this has not changed whilst the vector of the twinning dislocation has been reversed, so that after one revolution the twinning dislocation does not advance along the pole but returns to the original sessile partial. If it recombines and then redissociates, it can continue only along its original path again, thus increasing the displacement between the same two planes and producing a high energy fault instead of a twin. This configuration, first pointed out by Cottrell and Bilby (1951) in connection with a model for f.c.c. twinning, was called an "anti-generating node" by Bilby. Twinning may in principle grow from such a node by utilizing intimate cross-slip in a manner first suggested by Venables (1961) for f.c.c. metals, and later described by Hirth and Lothe (1982) as a "ratchet" mechanism.

As mentioned above, there is a physical difficulty in the operation of a pure pole mechanism if the original twin is either a monolayer fault or has only a few layers. A generating node appears on both the top and bottom surfaces of the original fault, and the resulting twinning dislocation segments rotate in opposite senses. After one revolution, these two segments must pass one another on planes separated by the thickness of the original fault. For monolayer faults or thin twins, this would require a very large (static) stress. Bilby estimated that, for cubic twins, a nucleus about 50 atoms thick would be required before the pole mechanism began to operate at experimentally determined twinning stresses. Actually the separation of the partials is so small after the first turn that linear elastic theory may considerably overestimate the stress required; there is appreciable core overlap and atomistic calculations are needed. However, it does seem probable that the pole mechanism for growth may only be effective if a rather thick nucleus has developed in some other way, possibly by chance encounters of stacking faults with each other. In the analogous problem of the f.c.c. to h.c.p. transformation in cobalt, the situation is exactly similar except that the partials meet with a separation of two atomic layers. Seeger (1956) suggested that the partials may acquire sufficient kinetic energy to enable them to pass dynamically. This seems doubtful even for cobalt, where the effective

stress on the dislocations from the chemical driving force may be much larger than the externally imposed mechanical stress causing twinning.

Cottrell and Bilby's theory of b.c.c. twinning, although later shown to be incorrect, is instructive in clarifying the distinction between the two dissociations (87.14) and (87.15). They ingeniously utilized the fact that the twinning dislocation of type $1/6(111)$ is common to three crystallographically equivalent twin planes of type $\{112\}$. Figure 20.24 shows a length of dislocation, initially $AOBC$, lying in the K_1 plane in which it cannot glide. Part of the line OB dissociates to form an initial stacking fault in the $\{112\}$ plane, with nodes at B and O . This dissociation is

$$\frac{1}{2}[111] = \frac{1}{3}[112] + \frac{1}{6}[1\bar{1}\bar{1}] \quad (87.16)$$

Because $BDEO$ is glissile, a length EO may lie along the $[11\bar{1}]$ direction and hence is pure screw in nature. This length can then move into either the $(\bar{1}21)$ planes or the $(2\bar{1}1)$ planes which meet along the $[11\bar{1}]$ direction. As it does so it generates a new fault on the plane into which it moves and Cottrell and Bilby originally claimed that it could rotate about OB whilst moving along OB , thus generating a twin along the stacking fault. As pointed out in the original paper, the dissociation (87.16) is energetically improbable and such faults are now believed to be mechanically unstable. The energy of the fault has to be supplied by the work done by the external stress [the elastic energy of the dislocations in eqn. (87.16) just balancing] and Cottrell and Bilby estimated the stress required as σ/b , where σ is the stacking energy. This stress is only $\cong 0.001\mu$, where μ is the shear modulus, for materials of low fault energy but it has the rather large value of 0.02μ for $\sigma = 200 \text{ J m}^{-2}$, which might be an appropriate value for b.c.c. metals. Stresses of magnitude $(10^{-3} - 10^{-2})\mu$ are often applied in order to twin b.c.c. metals so that, with a modest stress concentration, the theory seemed initially attractive. However, as first pointed out by Sleeswyk (1974), the pole dislocation inside the twin does not have a lattice vector and there is a high energy fault inside the "twin". These defects were at first somewhat obscured by the initial decomposition and the utilization of the threefold symmetry around the η_1 direction.

Hirth (1963) first distinguished pure pole mechanisms from what were later called ratchet mechanisms, and Hirth and Lothe pointed out a slight modification of the Cottrell-Bilby model which shows that, in fact, it is a ratchet. The initial configuration is similar to Fig. 20.24 but OE now represents an undissociated superjog in the dislocation so that there is no stacking fault on (112) and the lines $CBOE$ and $CBDE$ are coincident and form a section of perfect dislocation. Dissociation of the superjog OE takes place as according to eqn. (87.16) and the twinning partial OFE moves into either the $(\bar{1}21)$ or the $(2\bar{1}1)$ plane but, after a single turn, the parts of this loop which rotate about O and E respectively are both blocked by the sessile partial left along OE , so that the configuration cannot act directly as a pole source. This is illustrated in Fig. 20.25 which shows in (a) the stacking sequence $\dots ABCDEF \dots$ in the matrix and the undissociated $(1/2)[11\bar{1}]$ dislocation. The dissociation (b) is such that the partial dislocation leaves along 1 to the right of Fig. 20.25(b) and the two parts return along 2 and 3 to the left of the diagram. As they are opposites and very close together at this point, they may possibly annihilate

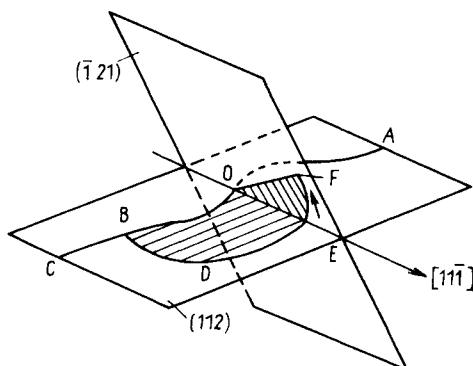


FIG. 20.24. The Cottrell-Bilby "pole" mechanism for growth of b.c.c. (after Cottrell and Bilby, 1951). AO and OC represent lengths of lattice dislocation with a Burgers vector $\frac{1}{2}[111]$. OB is a sessile partial with a Burgers vector $\frac{1}{3}[112]$ and $BDEFO$ is a glissile twinning dislocation of Burgers vector $\frac{1}{6}[111]$. There is no dislocation along OE .

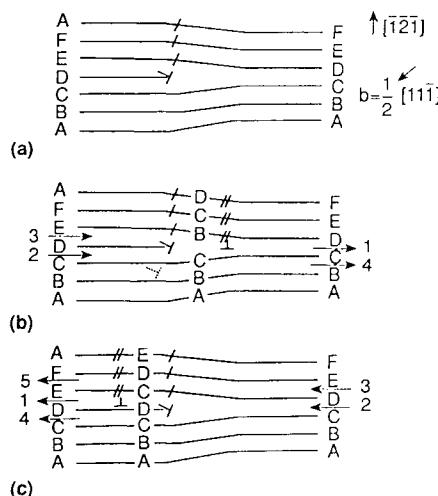


FIG. 20.25. The jog version of the Cottrell-Bilby mechanism after Hirth and Lothe (1982) (a) the undissociated $\frac{1}{2}[111]$ dislocation; (b) the configuration after dissociation into $\frac{1}{3}[112]$ and $\frac{1}{6}[111]$ dislocations; (c) the situation after the first revolution of the twinning dislocation.

over some length (formally by nucleation of a jog of unit height) leaving a closed loop to travel outwards and a residual part which is blocked by the sessile partial. Recombination with this partial will then produce the lattice Burgers vector and, if the reformed dislocation now cross-slips onto the next plane and then redissociates as before, a second loop of twinning dislocation is produced. Repeated operation of this cycle can thus (geometrically) produce a macroscopic twin. However, the mechanism requires the repeated dissociation and recombination of the lattice dislocation and this seems very improbable. Hirth and Lothe also pointed out that a dissociation into the opposite

twinning dislocation plus a larger sessile partial would give a true pole mechanism. The reaction is

$$\frac{1}{2}[111] = \frac{1}{3}[221] + \frac{1}{6}[\bar{1}\bar{1}1] \quad (87.17)$$

where $1/3[221]$ is a lattice vector of type $\langle 001 \rangle$ of the twin. Referring to Fig. 20.25(c), part of the twinning dislocation now leaves on path 1 and returns on path 3; it is not blocked but may leave again on 5 and continue to spiral upwards. The other part of the twinning dislocation leaves on path 1 and returns on path 2 and leaves again on 4 and continues to spiral in the opposite sense.

Cottrell and Bilby showed that their theory, if applied to a f.c.c. crystal, would produce only a monolayer of stacking fault, and at the time the paper was written this was in agreement with much experimental data in which twinning in f.c.c. materials was notably absent. Later, it was found that such twins are quite prevalent in alloys of low fault energy and Venables (1961) suggested a modified and ingenious mechanism for growth from a single stacking fault which was in effect the same ratchet mechanism described above for b.c.c. materials. Models involving single stacking faults seem much more reasonable for f.c.c. structures, where such faults actually occur, than for b.c.c. structures where they are never seen. Using the notation of the Thompson tetrahedron, consider the dislocation shown in Fig. 20.26 with a Burgers vector \mathbf{AC} lying in a plane except for a long jog N_1N_2 lying in a plane a . Let the part of the dislocation in a dissociate into a Frank partial and a Shockley partial

$$\mathbf{AC} = \mathbf{A}\alpha + \alpha\mathbf{C} \quad (87.18)$$

Under the action of a stress the glissile Shockley partial $\alpha\mathbf{C}$ moves away from the sessile Frank partial $\mathbf{A}\alpha$ on the plane a , leaving an intrinsic fault [Fig. 20.26(b)] and, after reaching the unstable near-semicircular configuration, winds rapidly around N_1 and N_2 to reach the position shown in Fig. 20.26(c). Two segments of the $\alpha\mathbf{C}$ dislocation delineating the fault meet along RS at a separation of only one interplanar distance, and a very large stress would be required to force these two opposite segments past each other. Note that the right-hand partial has moved downwards whilst wrapping around the pole dislocation so that it is the lower element of the dipole RS .

Venables assumed that the end element of the partial $\alpha\mathbf{C}$ combines with the sessile partial $\mathbf{A}\alpha$ along the length RN_2 and the re-formed dislocation with Burgers vector \mathbf{AC} glides to the next plane and repeats the dissociation. When the second layer of fault expands, two opposite segments of dislocation will again appear along RS , but each will be displaced by one plane from the initial pair. One of these segments on the central plane will annihilate the twinning partial left there by the first dissociation, thus turning the two layers into one continuous fault wrapped twice around the pole dislocation, and the final configuration [Fig. 20.26(e)] is now a double helical layer of fault terminated by two partials SRN_1 and SRN_2 at a separation of two atomic layers. Repetition of these operations will lead to a twin limited by a helical twinning dislocation ending in segments parallel to RS on the top and bottom surfaces. Improbable though it seems, the ratchet geometrically works by converting the pole dislocation \mathbf{b}_B^* into the dislocation \mathbf{b}_B one plane at a time.

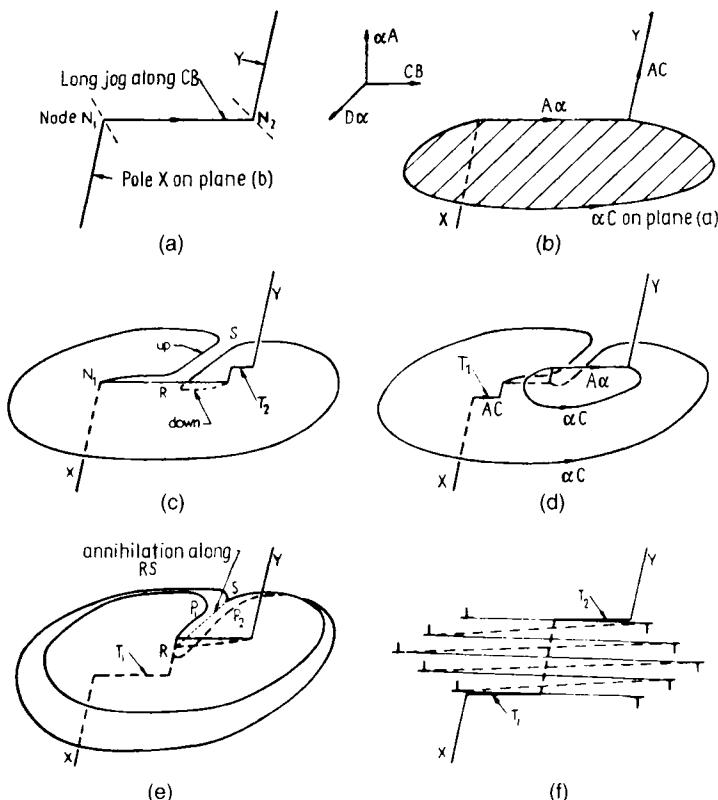


FIG. 20.26. Prismatic glide ("ratchet") mechanism for f.c.c. twin growth (after Venables, 1961). The notation is that of the Thompson tetrahedron. For details, see text.

The above discussion verifies Venables' claim, contrary to an objection by Sleeswyk (1974) that the pole dislocation in the twinned region is a perfect lattice dislocation. Venables also points out that, if only one generating node operates, a twin in the form of a planoconvex lens might be obtained. A rather similar situation is obtained when both crossing points of a given dislocation are on the same side (Fig. 20.27); once again the twin is planoconvex. Some limited experimental support for these latter models comes from the electron microscopic work of Steeds and Hazzledine (1964).

In the early discussion of Venables' theory, Hirth (1963) proposed an alternative dissociation to give a pure pole mechanism. However, Hirth's pole is not related to Venables' pole in the way that eqns. (87.14) and (87.15) are related, but involves instead dissociation of a different $\frac{1}{2}(110)$ dislocation **AB** which has a Burgers vector at 54° to the antitwinning direction, whereas that of **AC** is at 73° to the twinning direction. Hirth's dissociation

$$\mathbf{AB} = \mathbf{A}\alpha/\mathbf{BC} + \mathbf{C}\alpha \quad (87.19)$$

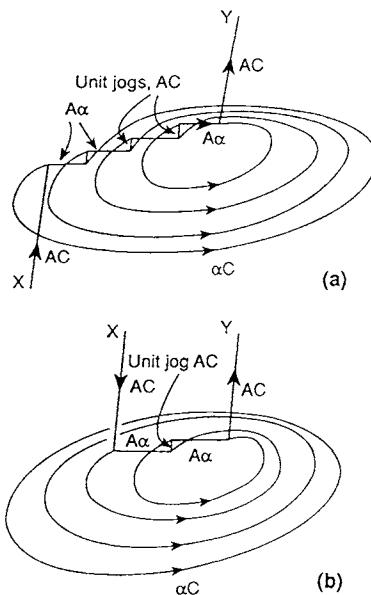


FIG. 20.27. Prismatic sources where the twinning dislocation remains in the matrix twin interface: (a) conventional prismatic source; (b) source from the end of a dipole which remains on one side of the twin to give a planoconvex shape (after Venables, 1974).

gives the opposite twinning dislocation $\mathbf{C}\alpha$ and a high energy sessile $\mathbf{A}\alpha/\mathbf{BC}$ which is of type $1/6(411)$. Another geometrically possible pure pole may be obtained by dissociating the lattice dislocation of eqn. (87.18) in the manner of eqn. (87.19) rather than that of eqn. (87.18). Suppose that the plane α is a (111) plane and that the $\alpha\mathbf{C}$ direction is $[11\bar{2}]$. Equation (87.18) is then

$$\frac{1}{2}[110] = \frac{1}{3}[111] + \frac{1}{6}[11\bar{2}] \quad (87.18a)$$

and the corresponding pure pole is

$$\frac{1}{2}[110] = \frac{1}{3}[22\bar{1}] - \frac{1}{6}[11\bar{2}] \quad (87.20)$$

Similarly eqn. (87.19), which corresponds to

$$\frac{1}{2}[011] = \frac{1}{6}[141] - \frac{1}{6}[11\bar{2}] \quad (87.19a)$$

has a ratchet version

$$\frac{1}{2}[011] = \frac{1}{6}[\bar{1}25] + \frac{1}{6}[11\bar{2}] \quad (87.21)$$

The sessile products \mathbf{b}_B with Burgers vectors $1/3[22\bar{1}]$ and $1/6[141]$ have lattice Burgers vectors $[001]_T$ and $\frac{1}{2}[101]_T$ in the twin basis whereas the products \mathbf{b}_B^* with vectors $1/3[111]$ and $1/6[\bar{1}25]$ are non-repeat vectors $1/3[111]_T$ and $1/6[521]_T$ referred to the twin lattice.

All these dissociations are, however, energetically unfavourable and the elastic part of the energy varies in the order $(87.20) > (87.21) > (87.19) > (87.18)$. The dissociations will thus take place only if there are internal stress concentrations arising from pile-ups, intersecting slip or twin bands, or other agencies.

A notable feature of the pole and ratchet mechanism is that the parent dislocation which generates the twin has a Burgers vector not in the twin plane. This is described by Venables as a prismatic source. The special configuration required might be produced if **AC** is a slip dislocation which either has a straight length along **CD** or cross-slips into *a* and then lies along **BC**, or if jogs along **BC** are produced by dislocation intersections. Other theories which are based on prismatic sources include that of Fujita and Mori (1975), which utilizes the Cottrell-Bilby dissociation into Shockley and Frank partials but does not assume a pole mechanism. In contrast to the prismatic sources there are various theories in which the dislocation αC is produced from dislocations **BC** or **DC** which lie in *a*, and these may be described as glide sources. Finally, there are theories which depend upon interactions of glide dislocations of two different systems, primary and coplanar (Mahajan and Chin, 1973a), or primary and cross-slip (Narita and Takamura, 1974). For clarity in subsequent discussion, the *a* plane will always be the twinning K_1 plane, whereas the active slip plane will be some other plane for a prismatic source and *a* for a glide source.

Several investigations (Miura *et al.*, 1968; Narita and Takamura, 1974; Fujita and Mori, 1975) have shown that, for f.c.c. metals and alloys, twinning takes place on the most active slip plane (i.e. the primary or conjugate plane, depending on the amount of slip before twinning) and twins form only after appreciable slip. The twinning stress in a tensile test decreases as the orientation of the stress axis approaches $\langle 111 \rangle$, and also as the temperature is lowered, provided the twinning occurs in stage III of the work-hardening curve, but is little affected by orientation and temperature in stage II.

Early dislocation theories for the production of f.c.c. twins from glide sources usually depended on the formation of Lomer-Cottrell locks (Suzuki and Barrett, 1958; Haasen and King, 1960; Ookawa, 1957). In principle this is not necessary because an extended dislocation lying in its slip plane with its ends pinned may be separated into component partials by the action of an external stress. This will happen if the first partial is able to bow out under the applied stress, as in a Frank-Read source, whilst the back partial is unable to follow it because of its line tension. Venables has shown that the most readily separated dislocations of this type should favour twinning when the stress axis is near $\langle 100 \rangle$, and this is contrary to observation (see p. 912). The dissociation of other glide dislocations, which would give approximately the observed dependence of twinning tendency on orientation of the stress axis, is only possible with improbably large stresses and small source lengths.

The theories mentioned above attempt to overcome difficulties of this kind by utilizing Lomer-Cottrell barriers to anchor one of the partial dislocations. In the type of barrier discussed on p. 302, the faults are of intrinsic type and the apex of the barrier is away from the dislocation pile-up. Partial dislocations are thus unable to escape from the configuration. The theories imply that this situation is reversed, the apex pointing towards the pile-up, and the faults being extrinsic. The leading partial dislocations on each

plane can now glide away under the applied stress, but examination shows that this does not agree with the observed twinning directions; the "wrong" partials escape. It seems impossible to devise a source of this type which will produce the correct twinning partials unless a high energy stair-rod dislocation of type $\alpha\mathbf{A}/\mathbf{B}\beta$ is included, and this should have little strength. More generally, Whelan (1958) has shown that the lock will have sufficient strength only if the Burgers vectors of the two interacting whole dislocations are at 120° to each other. This means that the resultant Burgers vector does not lie in the twin plane, so that the source as a whole is equivalent to the prismatic source discussed above.

Later theories are generally based on the experimental result that twinning in f.c.c. materials does not begin until slip is activated on at least two systems. The simplest description is that of Mahajan and Chin (1973a), who consider a reaction between dislocations of the primary system with Burgers vectors \mathbf{BC} and of the coplanar system with vectors \mathbf{DC} to form three Shockley partials

$$\mathbf{BC} + \mathbf{DC} = 3\alpha\mathbf{C} \quad (87.22)$$

which are then rearranged on successive planes to form a three-layer fault. A small twin is obtained when embryonic three-layer twins of this kind at different heights in a slip band grow together. Although the reaction (87.22) leads to an increase in energy (i.e. the undissociated dislocations repel each other), electron microscopic evidence on the production of extrinsic intrinsic fault pairs (Gallagher, 1966ab) suggests that it can occur by local attraction of the partials, without the stress concentration of a pile-up. More complex reactions involving slip activity on the cross-slip plane have been suggested by Narita and Takamura. Their model requires the reaction of a slip dislocation \mathbf{BC} with a Lomer dislocation \mathbf{DA} lying along the intersection of the primary and cross-slip planes to give

$$\mathbf{BC} + \mathbf{DA} = 2\alpha\mathbf{C} + \alpha\mathbf{A} \quad (87.23)$$

The Lomer dislocation \mathbf{DA} must be produced by reaction between dislocations of the cross-slip system with Burgers vector \mathbf{CA} and those of the coplanar system with Burgers vector \mathbf{DC} , and the theory has been criticized because such Lomer dislocations are seldom observed. However, the authors maintain that there is evidence of slip activity on the cross-slip plane, and that this means that the Lomer dislocations must form, even if not observed in lightly deformed material. This model was originally developed from a hypothesis that deformation twinning in f.c.c. materials may be viewed as a stress-relief process complementary to cross-slip, and it is claimed that it agrees well with the experimental results.

Yet another dislocation model (Fujita and Mori, 1975), described as stair-rod cross-slip, utilizes the same type of dissociation [eqns. (33.7) and (33.11)] as the original Cottrell-Bilby and Venables proposals, but simply assumes that a slip dislocation in (say) the primary system is held up by some obstacle along a direction \mathbf{DC} at 60° to its Burgers vector \mathbf{AC} and parallel to the intersection of the primary and conjugate slip planes, whereupon a Shockley partial $\alpha\mathbf{C}$ cross-slips into the conjugate plane, leaving behind a Frank partial $\mathbf{A}\alpha$ in place of the original lattice dislocation. This gives a wide stacking fault

on the conjugate plane, but this fault is not considered to wrap around the remaining parts of the original dislocation (as in the Venables model) but simply to extend away from this dislocation. Successive slip dislocations are then assumed to pile up behind the Frank partial and to cross-slip in the same way, thus forming an array of stacking faults on successive conjugate planes, i.e. a thin twin. Thus if the tensile axis lies in the standard unit triangle [001]–[011]–[111] the primary Burgers vector in the (111) slip plane is $a/2[\bar{1}01]$ and the dissociation is

$$a/2[\bar{1}01] = a/6[\bar{1}21] + a/3[\bar{1}\bar{1}1] \quad (87.24)$$

where the partial $a/6[\bar{1}21]$ glides away on the conjugate (111) plane. However, if the stacking fault energy is reasonably low, the original slip dislocation will be dissociated into Shockley partials $a/6[\bar{2}11]$ and $a/6[\bar{1}\bar{1}2]$, and the partial which cross-slips onto the conjugate plane will form by the further dissociation of the leading partial

$$a/6[\bar{2}11] = a/6[\bar{1}21] + a/6[\bar{1}\bar{1}0] \quad (87.25)$$

so that a low energy stair-rod is left at the junction of the two slip planes.

As previously discussed in relation to the Cottrell–Bilby theory, there is an increase in energy associated with the reactions (87.24) and (87.25) so that it is not obvious that stair-rod cross-slip will occur in practice; nevertheless, the simplicity of this proposal, which is in sharp contrast to the complexity of the Venables model, is appealing. It can be equally applied to cross-slip from the conjugate plane to give a microtwin on the primary plane, and it appears to be consistent with many of the experimental observations on f.c.c. twinning. In their original paper, Fujita and Mori (1975) pointed out that, because of conjugate or primary slip prior to stair-rod cross-slip, the twinning plane may already contain many Shockley partials with the same Burgers vector as the cross-slipped partial. If these interact strongly with the cross-slipped partials, it may be difficult for the latter to glide over large distances to create the successive faults which constitute a twin. They therefore suggested an alternative cross-slip process between coplanar slip bands on the two planes, leading to twinning partials which can easily glide. However, as found by other workers (see p. 912) and confirmed by Mori and Fujita (1977), the observed twinning direction always corresponds to the Burgers vector of the leading Shockley partial of the conjugate or primary slip direction, as predicted by the simple theory without coplanar slip.

Mori and Fujita (1980) were subsequently able to make direct electron microscopic observations (including Burgers vector analyses) of the stair-rod cross-slip of eqn. (87.25) in foils taken from single crystals of a Cu–11 at.% Al alloy deformed in tension at 77 K. The composition and test temperature were chosen to give a slow twin growth rate so that the wide overlapping stacking faults which are considered to be the initial stage of twinning could be directly observed. Observations of the progressive accumulation of stacking faults by stair-rod cross-slip on successive planes have also been made on Cu–8 at.% Ge single crystals during in-situ straining in a 3 MV electron microscope (Mori *et al.*, 1981). As the twin formed, the stair-rods and the trailing Shockley partials (or the Frank partials which represent their combined effect) accumulated at the intersections between

the primary slip bands and the twin interfaces. Other primary slip bands were found to act as obstacles to the extension of thin twin plates along the conjugate plane but, once such a band has been penetrated by the twin, its dislocations are able to contribute to thickening of the twin by the above mechanism. These results apparently confirm the Mori–Fujita growth mechanism in thin foils, but its importance in the twinning of bulk specimens remains to be established.

Now consider dislocation mechanisms which have been suggested for twin formation in b.c.c. metals and alloys. An obvious difference is that wide single-layer stacking faults have not been observed to form in any b.c.c. metal or alloy, and indeed are thought to be mechanically unstable (Vitek, 1968). Most theories of twin nucleation in this structure thus depend essentially on rearrangements within the core of a dislocation to give a multilayer twin. In particular, Sleeswyk (1963) proposed that, because of the threefold symmetry of an unstressed $a/2\langle 111 \rangle$ screw dislocation, it may be regarded as having a three-dimensional core with a $a/6\langle 111 \rangle$ partial on each of the intersecting $\{112\}$ planes. Under stress, however, this configuration will be unstable, and the partials could rearrange to form a three-layer twin on the most highly stressed of the $\{112\}$ planes. A very similar suggestion was made by Ogawa (1965), who considered that edge dislocations might spread the total Burgers vector onto three successive planes, and thus give a three-layer fault. Such speculations appear to be consistent with the early γ -surface calculations (Vitek, 1968) which indicated that very thin “twins” [strictly four-layer faults as the interfaces were of the “isosceles” type (see p. 919)] may be mechanically stable.

Interest in the core structure of the b.c.c. screw dislocation has been greatly stimulated by the important role assigned to such dislocations in the low temperature deformation behaviour (Christian, 1970, 1983; Vitek, 1985), and many computer simulations of the structure and its change when subjected to shear and/or dilatational stresses have been made. These calculations show that the core structure is quite complex and is sensitive to the (two-body) interatomic potential and to both shear and non-shear components of the stress tensor. In certain circumstances, the application of stress leads to the formation of a four-layer fault, i.e. an apparent twin embryo, rather than to deformation.

The main deformation twins in h.c.p. materials (see Table XVIII) have K_1 planes of type $\{10\bar{1}2\}$ (all metals) and $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$ (titanium group metals). In addition, $\{11\bar{2}4\}$ twins which are conjugate to $\{11\bar{2}2\}$ twins have been found in magnesium and titanium and there are several other modes, notably the conjugate $q=8$ modes $\{10\bar{1}1\}$ and $\{10\bar{1}3\}$ observed in titanium and magnesium respectively. Transformation twinning of either type I with $K_1=\{10\bar{1}1\}$, $q=4$, or its type II equivalent is frequently observed after the b.c.c.–h.c.p. martensitic transformation.

Yoo (1981) has reviewed twinning in h.c.p. materials and Fig. 20.28 shows his plot of twinning shear versus $\gamma=c/a$ ratio for various twinning modes, with the observed modes of seven h.c.p. metals superimposed. The $\{10\bar{1}2\}$ mode is found in all cases, despite the shear reversal at $\gamma=3^{1/2}$ already noted.

For a uniaxial stress applied along the c axis, twins of a particular mode may form if the mode line in Fig. 20.28 has a negative slope, whilst a compressive stress will be able to

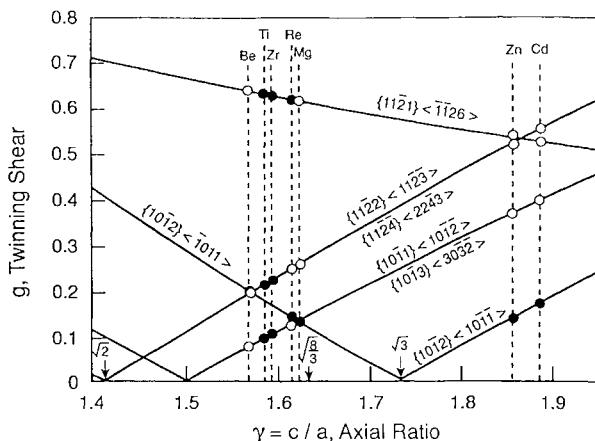


FIG. 20.28. Variation of the twinning shear with the axial ratio of the h.c.p. structure (after Yoo, 1981). The seven h.c.p. metals are indicated in the Figure by filled and open circles; a filled symbol indicates that the mode is active.

utilize only those modes on a line with a positive slope. This rule is reversed for the two conjugate modes listed on the same plot as their primary modes. Thus, with respect to the c axis, the $\{11\bar{2}1\}$, $\{11\bar{2}4\}$ and $\{10\bar{1}3\}$ twins are tension twins and the $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ twins are compression twins. The $\{10\bar{1}2\}$ twin is a compression twin for zinc and cadmium and a tension twin for all the other metals.

Millard and Thompson (1952) independently suggested a pole mechanism for the growth of $\{10\bar{1}2\}$ twins. As this is a $q=4$ mode, the expected twinning dislocation is a zonal dislocation of double step height with a Burgers vector given by eqn. (87.6), where the factor $(3-\gamma^2)/(3+\gamma^2)$ is $+(1/17)$ for ideal c/a and $-(1/13)$ for zinc which has $c/a \approx (7/2)^{1/2}$. Thompson and Millard did not explicitly consider growth from a single stacking fault, but treated the case where a separate fault and dislocation intersect; in any event, the node formed should be written

$$\mathbf{b}_B = [10\bar{1}0]_T = [0001]_P - (3 - \gamma^2)/(3 + \gamma^2)[10\bar{1}1] \quad (87.26)$$

Evidence for twinning dislocations in a $\{10\bar{1}2\}$ interface in zinc was first obtained by Antonopoulos *et al.* (1989) but the authors estimated the Burgers vector as about $\frac{1}{4}\langle 10\bar{1}1 \rangle$, which corresponds to a step of about six to eight lattice planes instead of the expected two. There is no obvious reason for this and, in other work (Lay and Nouet, 1994; Braisaz *et al.*, 1996), the correct twinning dislocations have been identified by high resolution electron microscopy. In addition, various other linear defects in the interface were identified. The defect character of these lines was determined by Pond's circuit operator and by mapping closed circuits around the defect into a reference lattice. In addition to the twinning dislocations discussed above, other dislocations with large steps (of the order of 15–17 d , where d is the spacing of the $\{10\bar{1}2\}$ planes) but with small Burgers vectors were also identified; they were all consistent with the predictions of Pond's theory (see p. 923).

Bacon and Serra (1994) have proposed a new mechanism for the thickening of a $\{10\bar{1}2\}$ twin as a result of their computer simulation. It arises from the interaction of a lattice basal plane dislocation with its $1/3\langle 11\bar{2}0 \rangle$ Burgers vector at 60° to the interface. The dislocation does not glide into the twin, propagating slip across the interface, but instead decomposes into interfacial defects. Specifically it forms m twinning dislocations plus a residual interface dislocation and the twinning dislocations can then glide in the interface, thickening or thinning the twin. Actually, the usual value of m is three, so that rather a large number of matrix dislocations would have to interact in order to get a twin of reasonable macroscopic thickness, and this is only a growth law; nevertheless, it is a mechanism which obviates the need for a pole mechanism and is thus of considerable interest.

The Burgers vector of an elementary twinning dislocation for the $\{11\bar{2}1\}$ mode in cobalt is about $(1/35)\langle 11\bar{2}\bar{6} \rangle$ and Vaidya and Mahajan (1980) suggested that the following reaction of two $\frac{1}{3}\langle \bar{2}11\bar{3} \rangle$ dislocations with a $\langle 1\bar{1}00 \rangle$ dislocation would yield a multilayer stacking fault approximating to a thin twin:

$$2(1/3)\langle \bar{2}11\bar{3} \rangle + \langle 1\bar{1}00 \rangle = 12(1/36)\langle \bar{1}\bar{1}2\bar{6} \rangle$$

It was suggested that the $\langle 1\bar{1}00 \rangle$ dislocation might arise from interactions between dislocations with **a** type Burgers vectors

$$(1/3)[2\bar{1}\bar{1}0] + (1/3)[1\bar{2}10] = [1\bar{1}00]$$

This mechanism is similar in concept to that suggested by Mahajan and Chin for f.c.c. twinning, although the $1/3\langle \bar{2}11\bar{3} \rangle$ dislocations and the spontaneous spreading of the product into 12 adjacent planes do not seem very probable. Moreover, in the case of $\{11\bar{2}1\}$ twinning it was noted above that the elementary twinning dislocations are probably split into steps of atomic height which are thus partial twinning dislocations (supplementary displacement dislocations) with Burgers vectors of about $(1/70)\langle 11\bar{2}\bar{6} \rangle$ (see p. 926).

A true pole mechanism can be envisaged in principle for $\{11\bar{2}2\}$ twinning, the pole dislocation having a Burgers vector of type $\frac{1}{3}\langle 1\bar{2}1\bar{3} \rangle$. Clearly, this appears improbable, as do specific proposals for other h.c.p. twins.

Table XX shows some results for the computed energies of the relaxed K_1 interfaces and for various structural and energetic features of steps (i.e. twinning dislocations) in these interfaces. The last column shows the applied shear strain at which the twinning dislocation was displaced along the interface. Some twinning dislocations were found to have narrow (three-dimensional) cores $\sim 1-2a$ in diameter, and these did not move until the applied shear strain reached $\sim 1-4\%$. Others have wide (planar) cores $4-6a$ in diameter and glide along the K_1 interface at much smaller applied strains. The highly glissile steps are those which correspond to the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins, and the steps of low mobility are those on the $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ interfaces. The difference in mobility of the twinning dislocations in $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ is striking in view of the apparent similarity of their interface structures; it is believed to be related to the magnitude and complexity of the atomic shuffles. In fact, the mobilities of the steps of height d in the $\{11\bar{2}1\}$ interface and $2d$ in the $\{10\bar{1}1\}$ interface, corresponding to the unobserved $\{11\bar{2}1\}$ shear mode and the

TABLE XX. COMPUTED ENERGIES AND PROPERTIES OF SOME h.c.p. TWIN INTERFACES
(after SERRA *et al.*, 1991)

K_1	γ (ε/a^2)	b_T (eq.)	s	b^2/a^2	h/d	Disl. line	Energy elast.	(ε/a) core	Core width	Critical strain
1012	1.15	38a	0.12	1/51	2	0.1	0.1	0.0	6a	0.002
1122	0.92	39a	0.27	4/33	3	3.7	1.6	2.1	a	0.014
1121	0.73	40a	0.61	3/140	$\frac{1}{2}$	0.3	0.3	0.0	11a	0.001
1011	0.64	41a	0.15	25/123	4	4.0	2.3	1.7	a	0.02
		42	0.36	37/123	2	3.6	2.4	1.2	2a	0.006

Notes: This table is adapted, with minor corrections, from Tables 1 and 2 of Serra *et al.* 1991. Only observed deformation modes plus the observed {1011} transformation twinning mode are listed. The values of s and of b^2/a^2 apply to the ideal axial ratio, $\gamma = (8/3)^{\frac{1}{2}}$. The energy unit ε is the depth of the atomic pair potential at the nearest neighbour distance.

transformation mode previously discussed, were found to be respectively very much higher and slightly higher than those of the steps in the observed modes.

Semiconductors such as silicon and germanium have relatively immobile dislocations because of high Peierls-Nabarro forces. At low temperatures, brittle fracture occurs under stress with little evidence of plastic deformation but, if deformation is obtained below the brittle ductile transition temperature of ~ 550 °C, for example by superimposing a uniform hydrostatic pressure on the specimen, deformation takes place largely by twinning. The diamond structure, as noted earlier, consists of two interpenetrating f.c.c. lattices displaced relative to each other by $(1/4)a(111)$ so, in terms of the stacking of close-packed layers, the structure is ... $A\alpha B\beta C\gamma$... A distinction has to be made between slip on a plane midway between the closely spaced α and B layers and slip on a plane midway between the widely spaced A and α layers. The two sets of dislocations are called the glide and shuffle sets respectively.

A mechanism for twinning on the {111} planes has been suggested by Pirouz (1987, 1989) and by Pirouz and Hazzledine (1991). It is an important feature of the model that, for both screw and 60° dislocations, the dissociation into partials leaves the leading partial much more mobile than the trailing partial. Consider the dissociation of part of a screw dislocation of the glide set with a Burgers vector \mathbf{BA} dissociated into partials $\delta\mathbf{A} + \mathbf{B}\delta$ on plane a between pinning points H and H' (see Fig. 20.29). The leading partial of high mobility may escape from the trailing partial and, by winding around H and H' , may eventually approach $\mathbf{B}\delta$ again from the other side. Pirouz originally assumed that, despite their mutual repulsion, the two partials could be forced together again to re-form \mathbf{BA} , which could then cross-slip onto the next plane and repeat the process. Clearly this is a ratchet mechanism very similar to those already discussed. This exact mechanism was considered for f.c.c. twinning but was rejected because it was thought that the stress needed to separate the two partials would be too high. The model clearly works better for the diamond and zinc blende structures where quite large differences in the mobilities of the partial dislocations have actually been observed, but it suffers from the inherent improbability of all ratchet mechanisms and the difficulty of fast growth. The

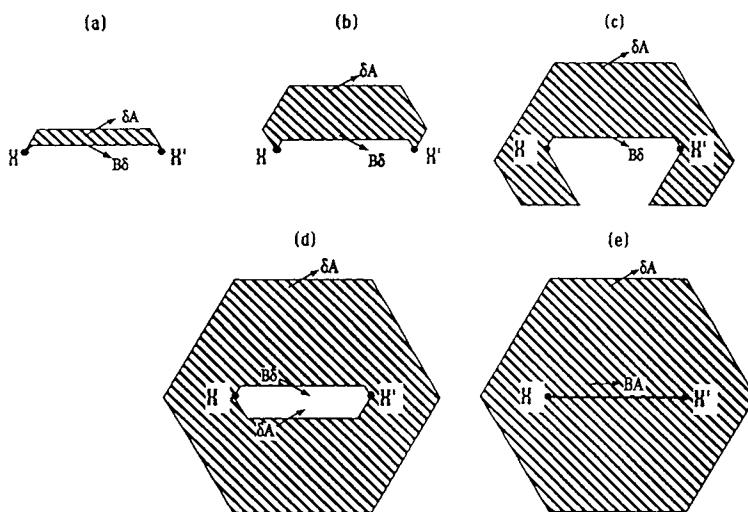


FIG. 20.29. Schematic diagram of the model proposed by Pirouz and Hazzledine (1991) for the formation of (111) twins in diamond cubic and zinc blende structures.

recombination difficulty can be avoided, at least in part, by adopting a cross-slip mechanism due to Friedel and Escaig which allows the extended configuration to cross-slip without recombining over its whole length and which can operate without any resolved shear stress on the cross-slip plane.

88. EFFECTS OF EXTERNAL VARIABLES ON TWINNING

This section examines very briefly the factors affecting twinning; for more detail, see Christian and Mahajan (1995). Many of the effects are poorly understood at present and, in such cases, the experimental results will be presented without comment.

The question of a critical resolved shear stress for twinning was discussed (inconclusively) above; the data are not accurate enough or sufficiently reproducible to decide. What is always observed is that the first twin to form is on the highest stressed plane of the particular twinning mode, thus confirming that the shear stress is important.

The effect of temperature is to increase the tendency to form twins as the temperature is reduced. In a few cases, twins will only form at liquid helium temperatures. Early, very careful work by Suzuki and Barrett (1958) on single crystals of silver-gold alloys of varying composition but fixed orientation established three regimes (see Fig. 20.30); in the high temperature region I, a localized band of twins is formed on the primary or conjugate slip planes and spreads across the specimen into two opposite quadrants. This is followed by a second band of twins which spreads into the other two quadrants. Twinning is accompanied by load drops. In region II, twin bands form on either the primary or the conjugate planes, depicting stress fields which are opposite to those given by the twin

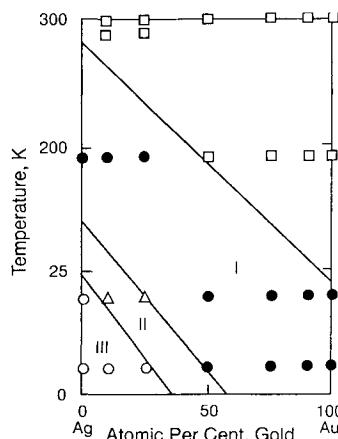


FIG. 20.30. Temperature concentration diagram showing the occurrence of twinning in silver gold alloys. In domain I, twinning occurs on the primary slip plane. In domain II, twins form on both primary and conjugate planes, but in different regions of the specimen. In domain III, the two types of twin coexist on the same planes.

bands. The twins grow until they impinge on one another. In region III, found only in silver-rich alloys at low temperatures, twins form copiously on both primary and conjugate planes.

Twin formation is also encouraged by low temperatures in b.c.c. structures, but often occurs here at the beginning of the deformation with large load drops. It is not possible, in general, to measure the stress at which twinning begins, just as it is impossible to measure a true upper yield stress.

Temperature effects are usually correlated with strain rate effects through some kind of chemical rate theory equation. But not here. The fracture toughness seems little sensitive to the strain rate at temperatures where the temperature variation is steepest. However, the strain rate can have dramatic consequences: normally ductile metals (even aluminium foil) are often brittle when shock loaded, but are perfectly ductile at more conventional strain rates.

The lower yield stress for twinning often follows a Hall-Petch relation

$$\sigma_y^T = \sigma_0 + k'd^{-1/2}$$

where d is the grain diameter, σ_y^T is the yield stress at which twinning begins and σ_0 and k' are material constants. A conventional explanation of the usual Hall-Petch equation is based on the assumption that pile-ups accumulate against a grain boundary and, at yielding or flow, the stress field at the head of the pile-up must exceed some critical value which allows a twin to form.

Not all results support the Hall-Petch equation. Vohringer (1970), for example, found a good Hall-Petch relation for Cu-5 at.% Sn alloy but, for a Cu-15 at.% Zn alloy over a similar range, the twinning stress was linear in d^{-1} rather than $d^{-1/2}$.

Twinning as a deformation mechanism is diminished and ultimately removed by interstitial solutes in b.c.c. materials. According to Magee *et al.* (1971), this may be a simple consequence of the crystallography of twinning. The disordered b.c.c. solution has interstitial atoms at random on the octahedral sites $\frac{1}{2}\langle 100 \rangle$ and $\frac{1}{2}\langle 110 \rangle$, and only one-third of these sites become octahedral sites of the product structure. The shear translates the other interstitial atoms to sites like $\langle 00\frac{1}{2} \rangle$ and $\langle \frac{1}{4}\frac{1}{4}\frac{1}{4} \rangle$, and this gives a formidably large energy which must be reduced by shuffling.

Substitutional solids generally increase the tendency to twin, although the effects vary from one solute to another. Bolling and Richman (1967) found that twinning was the main deformation mode in iron–beryllium alloys with about 25% beryllium, and many iron alloys showed a transition from slip to twinning when the solute concentration exceeded a certain value. Twinning was the initial mode of deformation at 77 K at a slightly lower stress than at room temperature. The stress versus strain curves, without load drops, were ascribed to “continual mechanical twinning”.

Several solutes apparently promote twinning in the transition metals; the outstanding example is rhenium. Substitutional solutes also have large effects on the copper group metals, largely because of the big reduction in stacking fault energy which accompanies solution in these alloys. Figure 20.31 is an old plot by Venables of twinning stress versus stacking fault energy. As cobalt alloys with higher stacking fault energies twin even more readily than the copper alloys, it has been suggested that, in f.c.c. alloys, twinning is favoured not by low fault energy but by a tendency to planar slip, as found by Gerold and Kärnthal (1989) and by Hong and Laird (1990).

A number of observations show that twinning may be suppressed by a strain previously supplied at a higher temperature. Twinning on shock loading can be prevented in this way; the amount of prestrain required increases with decreasing temperature of the test and also depends on the final strain rate. The experiments of Boucher and Christian (1972) also indicated that a homogeneous distribution of screw dislocations is more effective than a heterogeneous structure.

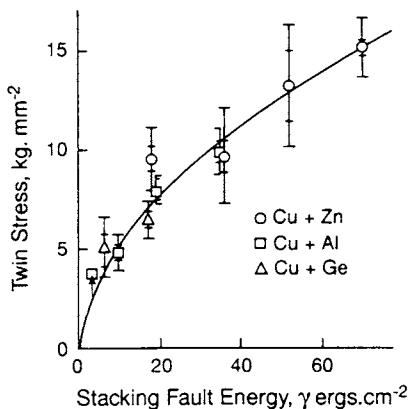


FIG. 20.31. The dependence of twinning stress on stacking fault energy for copper-based alloys (after Venables, 1974).

Precipitate particles and small inclusions generally have an inhibiting effect on twinning. In the case of partly coherent precipitates, the probable reason for this is the difficulty of forcing the twinning shear through the particle.

Some problems associated with the compatibility of slip and twinning will be examined briefly. For both cubic structures, parallel slip bands and twin lamellae are clearly geometrically possible as the K_1 plane is parallel to the usual slip plane in f.c.c. and to a frequently observed (albeit not the most favoured) slip plane in b.c.c. As noted above, this also leads to the accommodation of internally terminating twin lamellae by emissary slip, in the simplest form of which the slip is homogeneous over a band corresponding to the thickness of the twin. Mahajan (1971) has shown that in simple examples of emissary slip in molybdenum–rhenium alloys, the Burgers vectors of slip and twinning dislocations are indeed parallel.

Now consider the propagation of slip across a coherent K_1 interface of a twin. The simplest case is when the interface contains the Burgers vector of the slip dislocations, as dislocations on the intersecting slip plane must then meet the interface in screw orientation. They can thus cross-slip into the twin on any convenient slip plane of the latter without leaving a defect in the matrix–twin interface. When this condition is not satisfied, the matrix slip can still often be continued into the twin on any plane which meets the original slip plane edge to edge in the interface, but conservation of the Burgers vector then means that a linear defect must be left in the interface. If the Burgers vectors of the slip dislocations in parent and twin are corresponding vectors, \mathbf{b}_A and \mathbf{b}_B , so that they are related by

$$\mathbf{b}_B = \mathbf{S}\mathbf{b}_A = \mathbf{b}_A + \mathbf{b}_T \quad (88.1)$$

where \mathbf{S} is the twinning shear and \mathbf{b}_T the Burgers vector of the residual interface defect, their two slip planes are necessarily corresponding planes which automatically meet edge to edge. This is the case already considered in connection with the pole mechanism; if a finite length of the matrix dislocation crosses the interface, the linear defect joining the two crossing points is a twinning dislocation. Note that, if the slip is to propagate into the twin, the new Burgers vector must be a repeat vector of the twin lattice, and this requires that the step height in type I twinning must be qd or $\frac{1}{2}qd$; i.e. if $q > 2$, the defect left in the interface must be a zonal twinning dislocation (Saxl, 1968). This is the same condition as that given on p. 937 for the formation of a generating node; there is an equivalent condition for slip propagation into a type II twin.

A lattice dislocation of the parent meeting K_1 in a non-screw orientation will always have a corresponding twin vector which is either a lattice vector or an integral fraction of a lattice vector. In the latter case, the dislocation will be unable to cross the interface without leaving a stacking fault in the twin, but it will always be geometrically possible for a group of such dislocations to cross simultaneously, forming a single lattice dislocation in the twin. An example of this which has been studied experimentally is slip across a $\{10\bar{1}2\}$ twin in a h.c.p. structure. For a given twin plane, only one of the three $\langle 11\bar{2}0 \rangle$ slip vectors of the parent structure is transformed by the twinning shear into a lattice vector of the twin, and there is experimental evidence that a moving twin boundary pushes dislocations of the other two

types ahead of itself, rather than incorporating them as faults. As this twin mode has $q = 4$, pairs of dislocations of the parent lattice always transform into whole dislocations of the twin; in the case of the two $\langle 1\bar{1}20 \rangle$ close-packed vectors mentioned above, the corresponding twin vector is of type $1/3\langle 1\bar{1}\bar{2}3 \rangle$. The slip plane of the parent may be either the basal plane (0001) or a prismatic plane of type $\{1\bar{1}00\}$, and the corresponding slip planes of the twin are respectively of types $\{1\bar{1}00\}$ and $\{11\bar{2}2\}$ (Yoo and Wei, 1966). Tomsett and Bevis (1969) were actually able to observe basal plane slip in thin foils of zinc crossing a $(1\bar{1}02)$ twin boundary and continuing on the $(1\bar{1}00)$ plane of the twin, despite the unusual Burgers vector of the twin slip system (see Fig. 20.32).

Dislocations crossing a twin interface, even in non-screw orientation, are not geometrically constrained to continue on the corresponding slip plane; any plane which contains the line of intersection of the parent slip plane and the K_1 interface is a possible new slip plane and the Burgers vector of the new slip system is obtained by adding an appropriate twin lattice vector to \mathbf{b}_B to give a net vector in the new slip plane. Clearly the same addition has to be made to \mathbf{b}_T in eqn. (88.1), so that the new plane is obtained at the expense of a more complex interface dislocation and (probably) of a large slip vector. Finally, it should be emphasized that geometrical compatibility of slip across a twin interface does not imply that it will necessarily occur. The new slip system may not be a usual slip system of the crystal structure, or it may have too low a resolved shear stress acting on it.

The propagation of a deformation twin (*A*) across an existing twin (*B*) forming a secondary twin (*C*) in the crossed region may be examined by considering the compatibility of the various twinning shears, or by extending the above theory of crossing slip to the case where the crossing dislocation has a partial (i.e. twinning) Burgers

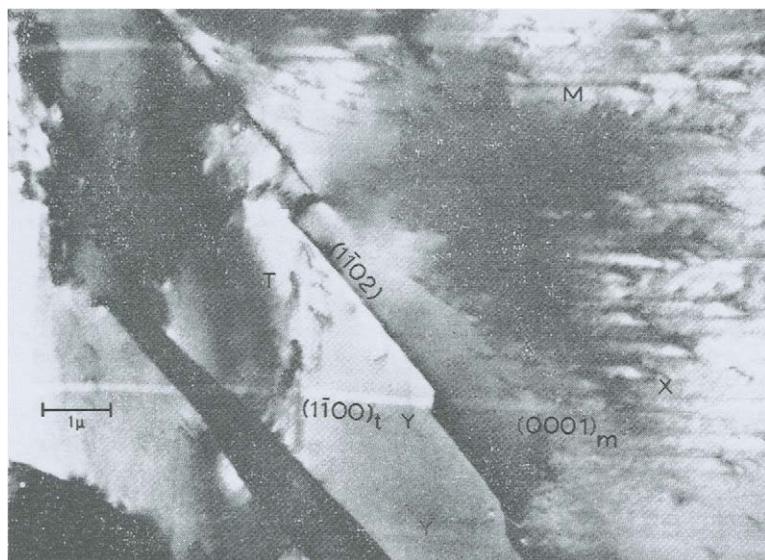


FIG. 20.32. Electron micrograph showing slip transferred from the matrix basal plane $(0001)_m$ to the $(1\bar{1}00)$ plane of a $(1\bar{1}02)$ barrier twin in zinc (courtesy of Tomsett and Bevis, 1969).

vector. General conditions were first given by Cahn (1953a) who showed that the traces of the K_1 planes matrix-*A* and *B*-*C* in that of matrix-*B* must be parallel and the direction, sense and magnitude of shear for matrix-*A* and *B*-*C* twinning must be the same. He considered specifically type I or compound twinning in which the K_1 planes of *A* and *B* intersect in the η_1 direction common to both, so that *B* undergoes no displacement normal to its K_1 plane. This means that the twinning dislocations of *A* meet the *A*-*B* interface in screw orientation and can cross-slip into *B* without leaving a defect at the interface. The K_1 planes of *A* and *C* are then mirror images in that of *B*. In an alternative geometry pointed out by Liu (1963), the K_1 planes of *A* and *C* are now parallel, so that the crossing twin *A* is undeviated but *B* is displaced. Individual twinning dislocations of the matrix-*A* interface each produce a step as they cross into *B* and the successive steps rotate the *B*-*C* interface away from the matrix-*B* interface.

Many studies have been made of the propagation of slip lines or deformation twins across existing coherent matrix-twin interfaces in f.c.c., b.c.c. and h.c.p. materials. Among more routine results is the suggestion of Rowlands *et al.* (1968) (see p. 891) that an unusual {5,8,11} twinning mode found in some b.c.c. and b.c.t. ferrous martensites arises because such twins may propagate undeviated across the closely spaced {112} transformation twin array in the martensite, at least in cubic alloys. Another interesting case arises if the deformation in a twin crossed by another is produced not by formation of a secondary twin *C* but by an equivalent slip shear. This allows relaxation of Cahn's conditions and has been studied in a f.c.c. cobalt iron alloy by Mahajan and Chin (1973a).

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