

Lecture 6: Interfacial Crystallography II

In the previous lecture the emphasis was on various geometrical and crystallographic aspects of grain boundaries in simple cubic materials. In this lecture we will consider further aspects of the geometry of coincidence site lattices in cubic lattices before considering boundaries between c.c.p. and b.c.c. materials and finally the crystallography of twin boundaries.

The Displacement-Shift-Complete (DSC) lattice

At the end of the previous lecture Bollmann's 0-lattice theory was reviewed and examples discussed of coincidence site lattices (CSLs). In a cubic material (i.e., materials with simple cubic, body-centred cubic and face-centred cubic lattices), a CSL is the lattice of points with a common origin common to lattices 1 and 2, such as for example the CSL formed by a rotation of 53.1° about $[001]$ (or, equivalently, 36.9° about $[00\bar{1}]$) where Σ , the ratio of the volumes of the primitive coincidence cell and the primitive crystal lattice unit cell, is 5.

For a particular CSL, the DSC lattice is the coarsest lattice that contains both lattices 1 and 2 as sub-lattices. The relevance of this DSC lattice is that for angular deviations away from exact CSL orientations, the dislocations in any boundary plane between lattices 1 and 2 accommodating this angular deviation are DSC dislocations.

Thus, for example, for $\Sigma = 5$, described as a rotation of 36.9° about $[001]$, the vectors $[2\bar{1}0]$, $[120]$ and $[001]$ define a right-hand set of vectors which specify the primitive coincidence cell when the lattice is a simple cubic lattice. Expressed as a single 3×3 matrix where the columns represent these three vectors, it is evident that the primitive coincidence cell can be represented by the matrix

$$C = \begin{bmatrix} 2 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The determinant of this matrix is 5, i.e., the value of Σ .

For simple cubic lattices the primitive vectors defining the DSC lattice, expressed a matrix of column vectors, D , are such that for simple cubic lattices,

$$CD = I$$

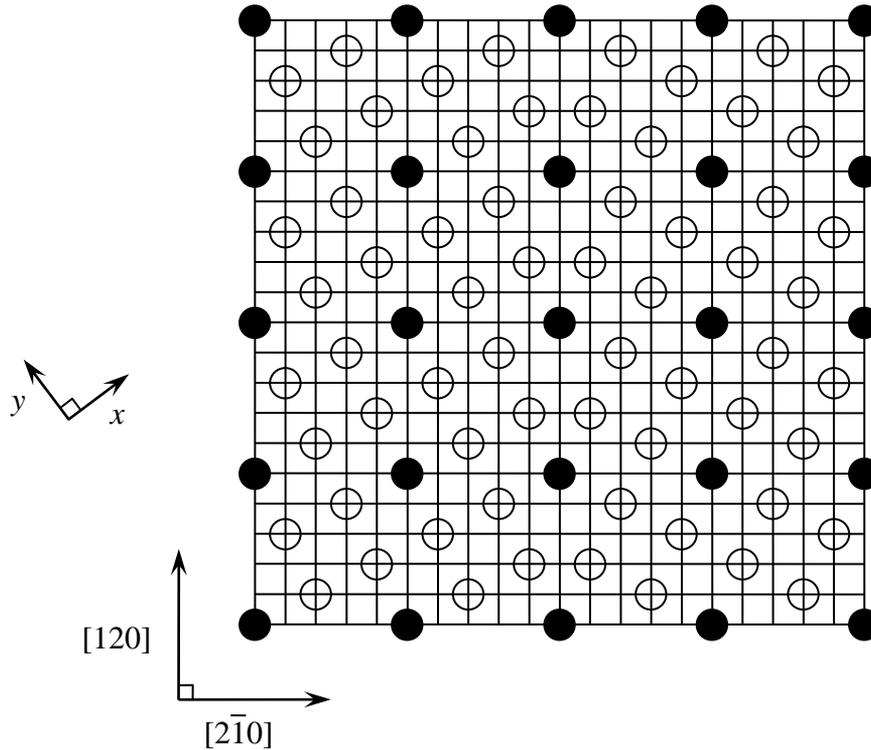
where I is the unit 3×3 matrix. For $\Sigma = 5$,

$$D = \frac{1}{5} \begin{bmatrix} 2 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

so that

$$C\tilde{D} = \frac{1}{5} \begin{bmatrix} 2 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & \bar{1} & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I$$

This relationship between the CSL lattice and the DSC lattice demonstrates that as Σ increases, the magnitudes of the DSC vectors will, in general, decrease.



For high-angle tilt grain boundaries in cubic metals, atomistic simulations have established the principle that some coincidence site lattice orientations are more ‘special’ than others. Thus, for example, in copper, symmetrical tilt $\Sigma = 5$ 36.9° grain boundaries of the type considered in the previous lecture are favoured relative to symmetrical tilt $\Sigma = 41$, 12.7° , $\Sigma = 37$, 18.92° and $\Sigma = 17$, 28.1° grain boundary orientations when their structures are relaxed using a suitable interatomic potential.

Hence, while CSL and DSC lattices are helpful in the understanding of certain aspects of the geometry of grain boundaries in cubic crystals, it must be recognised that these are often a first step in understanding and defining grain boundary crystallography. All too often, experimental studies demonstrate that in ‘real’ polycrystalline cubic metals, the crystallography of an individual grain boundary is not amenable to a CSL description likely to be meaningful in any physical context.

While it can be argued that minimization of the energy of grain boundaries is a reasonable target to achieve for a particular geometry, that geometry may not be close to a ‘reasonable’ CSL, and it must always be remembered that attainment of a minimum energy configuration is an ideal, rather than necessarily what a given system, or part of a system, is able to achieve kinetically.

Epitaxial (111) c.c.p. – (110) b.c.c interfaces

In experimental investigations of the deposition of c.c.p. metals on (110) b.c.c. metal substrates and of b.c.c. metals deposited on (111) c.c.p. metal substrates, it is often found that the metals deposit in such a way that either the Nishiyama–Wassermann (N–W) or the Kurdjumov–Sachs (K–S) orientation relationships, i.e.,

$$\begin{aligned} [11\bar{2}]_F &\parallel [\bar{1}10]_B \\ [\bar{1}10]_F &\parallel [001]_B \\ [111]_F &\parallel [110]_B \end{aligned} \quad (\text{N–W})$$

or

$$\begin{aligned} [\bar{1}01]_F &\parallel [1\bar{1}1]_B \\ [1\bar{2}1]_F &\parallel [1\bar{1}\bar{2}]_B \\ [111]_F &\parallel [110]_B \end{aligned} \quad (\text{K–S})$$

where the subscripts F and B denote c.c.p. and b.c.c. crystal structures (or the Face-centred and Body-centred Bravais lattices with one atom per lattice point), respectively.

In the N–W orientation relationship, two bisectors of close-packed directions within the $(111)_F$ and $(110)_B$ planes are parallel; in the K–S orientation relationship two close-packed directions within these planes are parallel. A rotation of 5.26° about the common $[111]_F \parallel [110]_B$ plane normal is required to move from the N–W to the K–S orientation relationship.

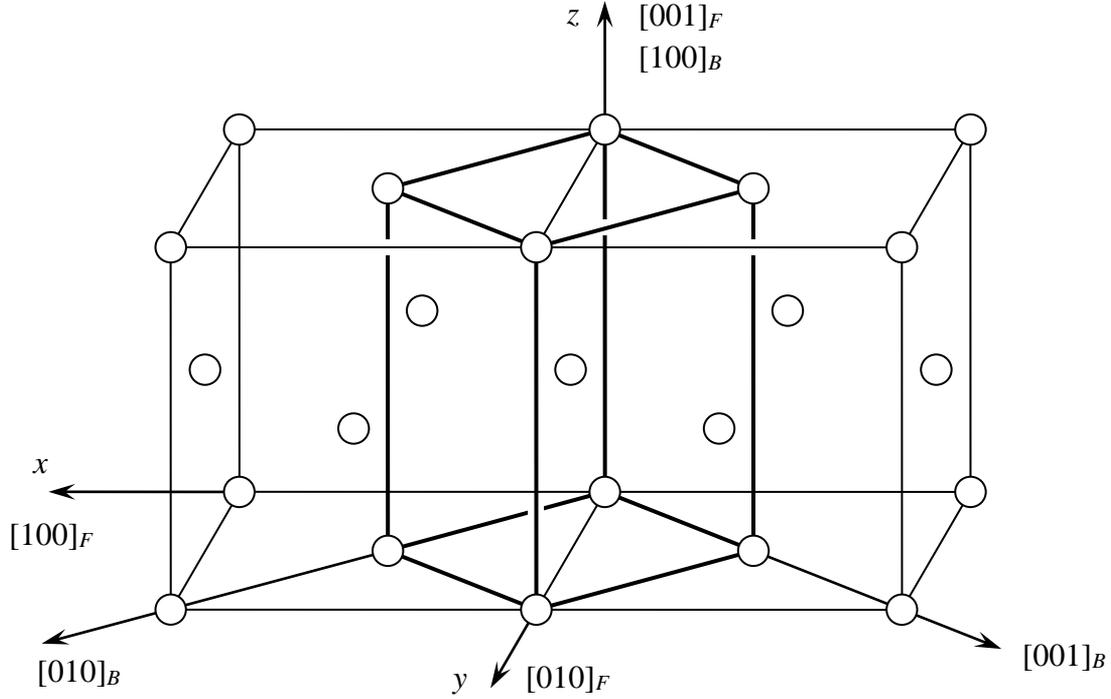
To use the O-lattice or surface dislocation formalism to describe these epitaxial interfaces, a *correspondence* has to be introduced to identify multiples of unit cells in the c.c.p. and b.c.c. crystal structures which, when suitably deformed, carry one lattice into the other. Here, we will use the Bain correspondence commonly used in the phenomenological theory of martensitic transformations:

$$(BCF) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ -1 & 1 & 0 \end{bmatrix}$$

where C here denotes correspondence. Hence, the primitive unit vectors of the F crystal structure, $\frac{1}{2}[10\bar{1}]_F$, $\frac{1}{2}[01\bar{1}]_F$ and $\frac{1}{2}[110]_F$ correspond to the primitive unit vectors $\frac{1}{2}[\bar{1}1\bar{1}]_B$, $\frac{1}{2}[\bar{1}11]_B$ and $[010]_B$, respectively, of the B crystal structure, so that $[001]_F$, $\frac{1}{2}[110]_F$ and $\frac{1}{2}[\bar{1}10]_F$ correspond to $[100]_B$, $[010]_B$ and $[001]_B$, respectively.

If we then choose an orthonormal axis system within which we define the Burgers vector content of the epitaxial interface in the N–W orientation so that

$$\begin{aligned} x_O &\parallel [11\bar{2}]_F \parallel [\bar{1}10]_B \\ y_O &\parallel [\bar{1}10]_F \parallel [001]_B \\ z_O &\parallel [111]_F \parallel [110]_B \end{aligned}$$



Example of a Bain correspondence between c.c.p. and b.c.c. unit cells. Here, a b.c.t. lattice is identified in bold within the c.c.p. crystal structure. Suitable deformation of this b.c.t. unit cell produces the b.c.c. unit cell.

the \mathbf{S} matrix in this orthonormal basis system, (oS_o) defining the deformation which formally carries the c.c.p. lattice into the b.c.c. lattice is

$$(oS_o) = \frac{a_B}{a_F} \begin{bmatrix} 2/\sqrt{3} & 0 & 1/\sqrt{6} \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{6}/2 \end{bmatrix}$$

where a_B and a_F are the lattice parameters of the b.c.c. and c.c.p. phases respectively. The Burgers vector content \mathbf{B}_O crossing a vector \mathbf{p}_O in this interface, both defined in the orthonormal system, is defined by the equation

$$\mathbf{B}_O = [\mathbf{I} - (oS_o)^{-1}] \mathbf{p}_O$$

Hence, in the N–W orientation along $[100]_O$, the total Burgers content, $\mathbf{B}_{1,O}$, is

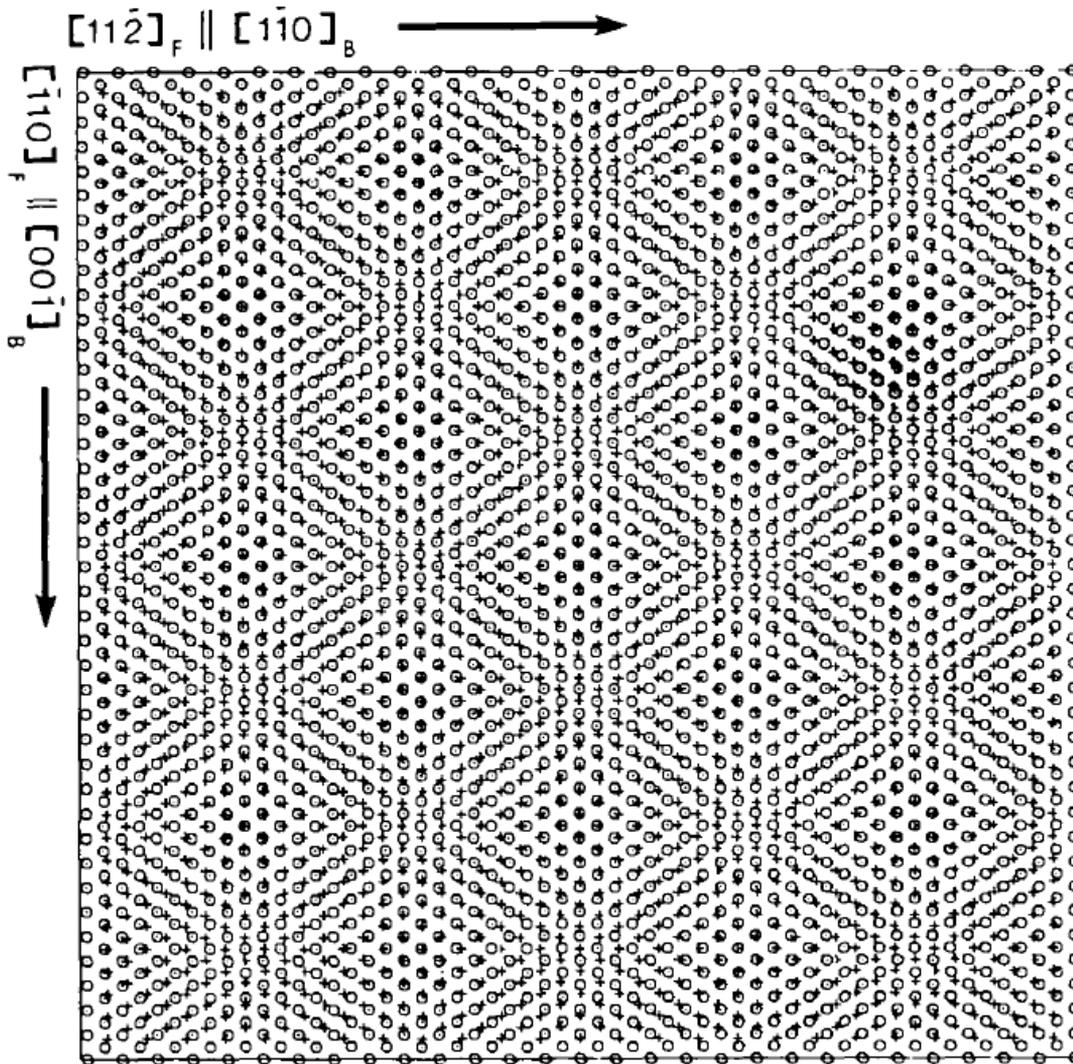
$$\mathbf{B}_{1,O} = \left[1 - \frac{\sqrt{3}}{2} \frac{a_F}{a_B}, 0, 0 \right]$$

while along $[010]_O$ the total Burgers content, $\mathbf{B}_{2,O}$, is

$$\mathbf{B}_{2,0} = [0, 1 - \frac{1}{\sqrt{2}} \frac{a_F}{a_B}, 0]$$

and so the misfit between the c.c.p. and b.c.c. lattices can be fully relieved in a purely formal sense by a rectangular array of edge dislocations with Burgers vectors $[11\bar{2}]_F$ and $[\bar{1}10]_F$. Other interpretations are of course possible – there is no requirement for purely edge dislocations to relieve this misfit.

Another way of visualising this misfit is to use nets representing atom positions in unrelaxed (111) c.c.p. and (110) b.c.c., such as in the example below in which $a_F/a_B = 1.291$ taken from K.M. Knowles and D.A. Smith, *Acta Crystallographica A* **38**, 34–40 (1982). Here, atoms in the b.c.c. plane are represented by circles and atoms in the parallel c.c.p. plane are represented by crosses. Regions where there are low degrees of misfit can be identified, in which the crosses and circles superimpose, separated by lines of poor misfit where the crosses and circles are in registry.



Twin boundaries

When a crystal is composed of parts that are oriented with respect to one another according to some symmetry rule, the crystal is said to be twinned. The most frequently occurring symmetry rule of twinning, but not the only one, is that the crystal structure of one of the parts is the mirror image of the crystal structure of the other part, in a certain crystallographic plane called the *twinning plane*. Often the plane of contact between the two parts, called the *composition plane*, coincides with the twinning plane.

Twinned crystals are often produced during growth, from the vapour, liquid or solid. Alternatively, a single crystal may be made to become twinned by mechanically deforming it.

Twinning can also arise as a result of a phase transformation from one crystal structure to another within a material: martensite phases produced as a result of martensitic transformations often have twinning as their lattice invariant shear.

It is also usual for ferroelectric phases to exhibit twinning as a result of phase transitions on cooling from a higher temperature phase which may, or may not, be ferroelectric.

Twinned crystals of minerals are often found in nature; in such cases, it is not always clear whether the twins were produced by growth or by deformation.

In this part of the lecture we shall be dealing mainly with deformation twins, but it is important to realize that this represents only a fraction of the general phenomenon of twinning.

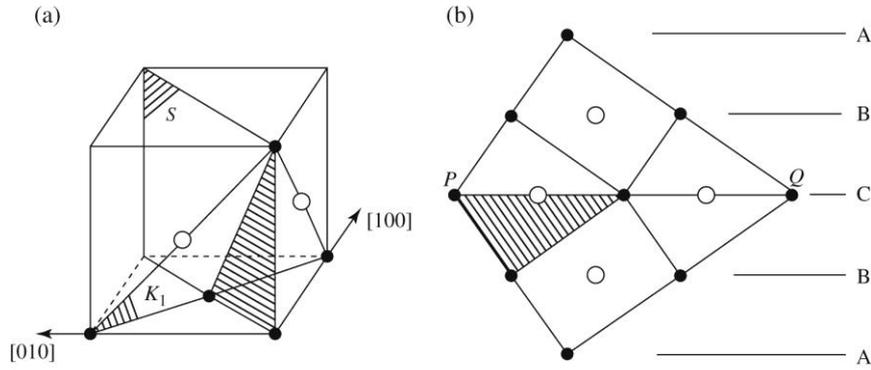
It is relevant that the formal crystallographic description of deformation twinning that will be developed here can be applied to all twinning operations irrespective of how they are produced physically.

A simple example of twinning which can be produced in a variety of ways is provided by c.c.p. metals. In this case the symmetry rule connecting the differently oriented parts is that one part is the *mirror image* of the other in a $\{111\}$ plane. Because the composition plane is usually itself a $\{111\}$ plane, the structures can be shown as being mirror images of one another in this plane, as in the figure below, in which the composition plane is (111). It can be seen that nearest neighbour relations are preserved at the boundary, but that an error in the stacking of the (111) planes occurs, so that the stacking sequence ABCABC is turned into ABCBAC, e.g., ABCABCACBAC... As a result, there is a thin layer of h.c.p. material at the twin boundary – the sequence BCB. This stacking fault will have associated with it a characteristic energy, just as in stacking faults generated between partial dislocations in c.c.p. metals.

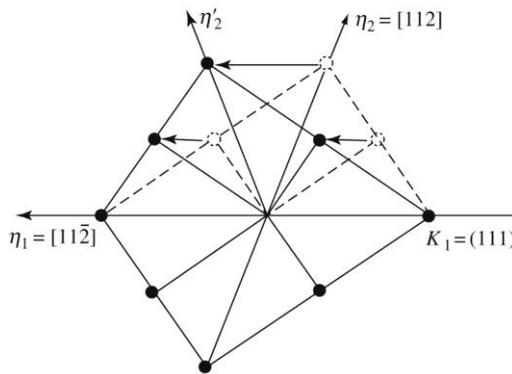
It is natural to suppose that such an error might occur during the growth of the crystal. The experimental evidence is that the formation of growth twins is quite sensitive to the conditions of growth.

Twins in c.c.p. crystals grown from the melt are not common, but gold films produced by vapour deposition contain a multitude of twins, as do layers of electro-deposited copper, and in both cases, the faster the rate of deposition, the higher the density of twins. Twinned grains are often seen in copper, α -brass and stainless steel polycrystals which have been cold-worked and then heated so as to produce recrystallisation. In a recrystallised material, a straight-sided lamella which is in a twin orientation to the rest of a grain is called an *annealing twin*; it can be regarded as a twin produced during crystal growth from the solid state. It is interesting that growth twins in aluminium are rare.

This is because the energy of a stacking fault, and therefore of a twin boundary, in aluminium is relatively high.



Structure of a twin in a c.c.p. metal. The plane S in (a) is the plane of the figure in (b), with the corresponding triangles in (a) and (b) shaded. The plane K_1 is the composition plane, PQ in (b).



Formation of a twin in a c.c.p. metal by shear. The dotted lines indicate the structure above the composition plane, K_1 , before the shear occurs.

Examination of the figure above shows that the twinned crystal could have been produced by homogeneously shearing part of a single crystal. This immediately suggests that twin formation may be a mechanism of plastic deformation. In fact, this mechanism is not very easy to observe in c.c.p. metals, because of the relative ease with which they glide. However, Cu, Ag and Au crystals all twin prolifically during the later stages of tensile tests at low temperatures, and Cu has been found to twin when shock-loaded at ordinary temperatures.

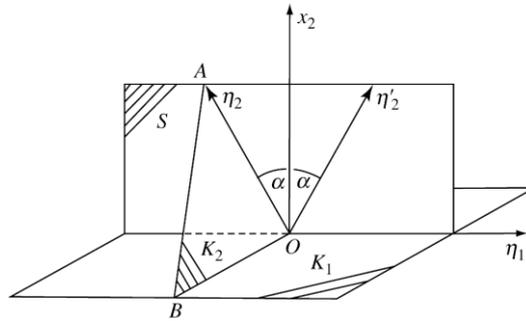
The minimum atom movements needed to accomplish twinning by shear in a c.c.p. crystal are shown in the above figure. A displacement of $\frac{1}{6}[11\bar{2}]$ applied to the upper part of an originally single crystal produces a stacking fault. The same displacement applied at successively higher (111) layers produces a twin. This could be achieved by passing a partial dislocation with the Burgers vector $\frac{1}{6}[11\bar{2}]$ over each (111) plane above the composition plane.

Description of deformation twinning

Deformation by glide preserves the crystal structure in the same orientation. Deformation by twinning reproduces the crystal structure, but in a specific new orientation. Macroscopically, it is evident that the deformed regions that have taken up a twin orientation with respect to the original crystal are lamellae that have undergone a homogeneous simple shear.

The effectiveness of the simple shear in describing the lattice reorientation has led to a general description of deformation twins in terms of a simple shear of the Bravais lattice. However, a simple shear applied to atom positions, as distinct from lattice points, is *not* always capable of producing all the atom movements that are needed to form a twin.

Confining ourselves, for the present, to the problem of shearing the Bravais lattice, we will ask the following question: can a homogeneous simple shear be applied to a Bravais lattice so as to change its orientation, but not its structure?



The elements of deformation twinning. O is an origin, K_1 is the composition plane (twin plane), η_1 is the shear direction in K_1 , and K_2 is a plane which is rotated, but undistorted as a result of the twinning operation. S is the plane of shear perpendicular to K_1 which intersects K_1 in η_1 . η_2 is a rotated, but undistorted direction common to S and K_2 . 2α is the angle between η_2 and the direction η_2' to which η_2 is rotated by the simple shear. x_2 is parallel to the normal to K_1 and bisects the angle 2α . OB defines the direction in K_1 perpendicular to η_1 .

The geometry of a simple shear is illustrated above. All points of the lattice on the upper side of the plane K_1 are displaced in the shear direction η_1 by an amount u_1 proportional to their distance above K_1 . Thus

$$u_1 = sx_2$$

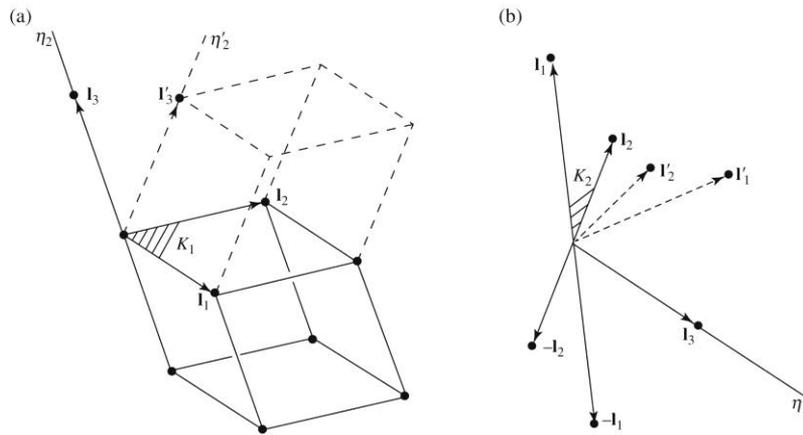
where s is the magnitude of the simple shear. The plane containing η_1 and the normal to K_1 is called the plane of shear, S . It can be seen that a vector parallel to η_2 in S will be the same length after the shear has been applied if the angle α which it makes with the normal to K_1 is given by

$$s = 2 \tan \alpha$$

The angle α is simply the angle between η_2 and the normal to K_1 . With the exception of vectors parallel to OB , which are not rotated by the simple shear, all vectors in the plane containing η_2 and OB are unchanged in length, although rotated. This plane, AOB , in the figure above, is conventionally labelled K_2 and is called the second undistorted plane. K_1 is neither rotated nor distorted; it is both the composition plane and the twin plane.

So far it has not been specified whether the elements K_1 , K_2 , η_1 and η_2 are rational or not, i.e. whether or not they pass through sets of points of the Bravais lattice. In this respect, the condition that the *lattice is to be reproduced* can be fulfilled in two ways.

In the first, K_1 is rational. Therefore, we can pick two lattice vectors \mathbf{l}_1 and \mathbf{l}_2 in K_1 (as in the figure below). These vectors are not affected by the shear. If then η_2 is rational, there is a third lattice vector \mathbf{l}_3 parallel to η_2 that is unchanged in length by being sheared to \mathbf{l}_3' . Remembering that $-\mathbf{l}_3'$ is also a lattice vector (lattices are centrosymmetric), it can be seen from (a) below that the new cell defined by the basis vectors \mathbf{l}_1 , \mathbf{l}_2 and \mathbf{l}_3' is a reflection in the twin plane K_1 of the cell defined by the basis vectors \mathbf{l}_1 , \mathbf{l}_2 , and $-\mathbf{l}_3$ in the unsheared lattice. If this cell is a possible primitive unit cell of the lattice, the whole lattice is reconstructed by the shear. If it is not a primitive unit cell, then only a superlattice made up of a fraction of the lattice points is necessarily reconstructed. Twins whose shear elements K_1 and η_2 are rational, while K_2 and η_1 are irrational, are called type I twins or reflection twins.



Further consideration of the geometry of type I twinning in (a) shows that this twinning process is equivalent to a rotation of 180° rotation about the normal to K_1 . Under these circumstances, the lattice vectors \mathbf{l}_1 , \mathbf{l}_2 and \mathbf{l}_3 parallel to the sides of the cell outlined in solid lines in (a) are rotated into vectors $-\mathbf{l}_1$, $-\mathbf{l}_2$ and \mathbf{l}_3' parallel to the sides of the cell outlined in dashed lines in (a).

A second possibility is shown in (b). In this case, η_1 and K_2 are rational, but K_1 and η_2 are not. Two lattice vectors \mathbf{l}_1 and \mathbf{l}_2 can be chosen in K_2 together with a third lattice vector, \mathbf{l}_3 , in the rational direction η_1 . These vectors define the basis vectors of a cell prior to the shearing process. After shear has taken place, this cell is defined by the basis vectors \mathbf{l}_1' , \mathbf{l}_2' and \mathbf{l}_3 . Its orientation relationship to the cell defined by the basis vectors $-\mathbf{l}_1$, $-\mathbf{l}_2$ and \mathbf{l}_3 in the unsheared lattice is a rotation of 180° rotation about η_1 . This is called a type II twin or a rotation twin.

Very commonly, all four elements K_1 , K_2 , η_1 and η_2 are rational and the two types merge. Then the twin may be called compound (or degenerate), which is the usual type in the more symmetrical crystal structures. In a cubic lattice, *only* compound twins are possible. To prove this, consider a type I twin for which K_1 and η_2 are rational. In the cubic lattice, the normal to a rational plane is itself rational, so that if K_1 is rational, then the plane of shear S is also rational because it contains two rational directions, viz. η_2 and the normal to K_1 . Therefore η_1 , being the intersection of two rational planes K_1 and S , is also rational. Finally, K_2 is rational because it contains two rational directions, η_2 and the normal to S . A similar argument can be framed for cubic crystals starting with a type II twin for which K_2 and η_1 are rational.

The case of α -U

Orthorhombic uranium, α -U, shows, amongst other twin modes, a type I twin mode with $K_1 = (112)$, $\eta_2 = [312]$ and a type II twin mode with $K_2 = (11\bar{2})$ and $\eta_1 = [31\bar{2}]$. In these two examples it happens that the elements of the two twins are related by interchange of K_1 and K_2 , and of η_1 and η_2 . Two twins related in this way are said to be *reciprocal* to one another. The crystallography of two such twinning modes is distinct, but they have the same shear magnitude since the angle between K_1 and K_2 is the same for each mode.

Examples of twin structures

(i) C.c.p. metals

From studies of deformation twin lamellae in Cu and in Ag–Au alloys, it has been shown that a shear of magnitude 0.707 in the $[11\bar{2}]$ direction describes both the macroscopic shear and the lattice reorientation of a twin on a (111) plane. This agreement is not entirely trivial, because the same lattice reorientation could be produced by a shear of double the magnitude, i.e. 1.414, in the reverse sense. For the shear of 0.707 the twinning elements are

$$K_1 = (111), \quad \eta_1 = [11\bar{2}], \quad K_2 = (11\bar{1}), \quad \eta_2 = [112]$$

In this example, the same simple shear describes the macroscopic shape change, the lattice reorientation and the most plausible atom movements needed to accomplish the twin.

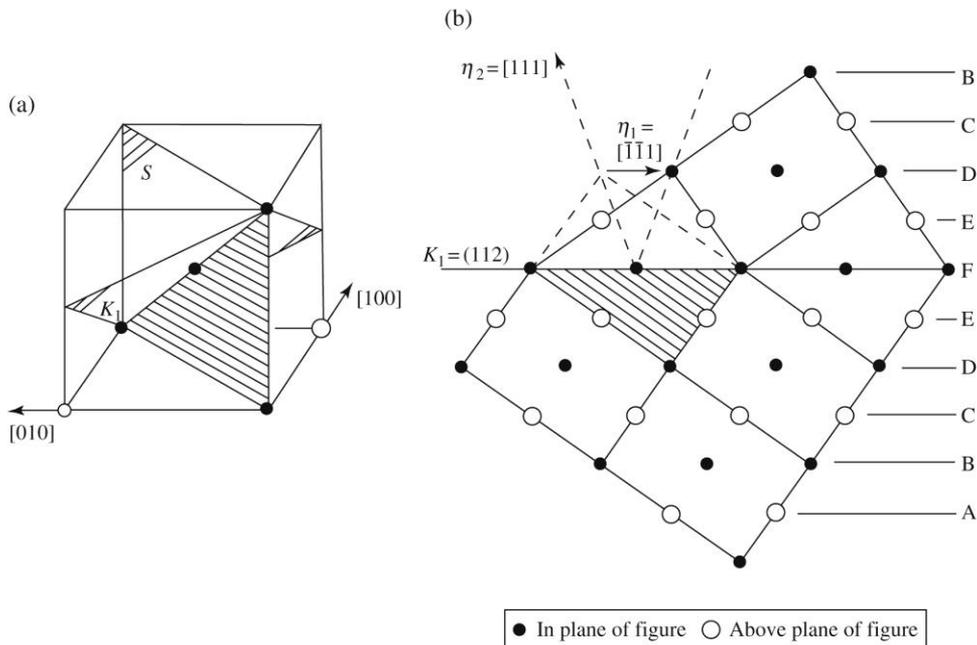
(ii) B.c.c. metals

Twinning is a relatively important mode of deformation in many b.c.c. transition metals such as Fe, V and Nb. Twinning is favoured relative to slip by a low temperature and a high strain rate. Only one type of twin is commonly found; the elements of which are

$$K_1 = (112), \quad \eta_1 = [\bar{1} \bar{1} 1], \quad K_2 = (11\bar{2}), \quad \eta_2 = [111]$$

The magnitude of the twinning shear is 0.707, the same magnitude as in $\{111\}$ twinning in c.c.p. metals. This twin is depicted in the figure overleaf. Just as for c.c.p. metals, it has been confirmed that the macroscopic shape change agrees with that predicted from the twinning elements. The atom movements described by this shear are quite plausible. They correspond to a shift of $\frac{1}{6}[\bar{1} \bar{1} 1]$ on successive (112) planes. In forming the b.c.c. structure from horizontal (112) layers, six layers are stacked before the seventh falls vertically on top of the first; the stacking sequence can be written as ...ABCDEFAB... .

The passage of a single partial dislocation with the $\frac{1}{6}[\bar{1} \bar{1} 1]$ Burgers vector produces a stacking fault of the form ABCDEFEFAB... . Little is known about the energy of such a fault, except that it is not so low as to permit extended dislocations to be readily observed in the transmission electron microscope. The passage of $\frac{1}{6}[\bar{1} \bar{1} 1]$ partials on successive planes would produce the twin sequence ABCDEFEDCB... . While such purely geometric considerations are very useful for establishing how twins might be produced it is difficult for perfect $\frac{1}{2}\langle 111 \rangle$ dislocations in b.c.c. metals to dissociate into well-defined partial dislocations and stacking faults. Therefore, if the production of twins in b.c.c. metals involves $\frac{1}{6}\langle 111 \rangle$ partials, a mechanism for their formation has to be invoked in any theory of twin formation in b.c.c. metals.



Twining elements

The twinning elements of various crystals are presented in the table below. Only some of the twinning elements need to be experimentally determined, e.g. K_1 , η_1 and the magnitude of the shear, s , or K_1 and η_2 . The remaining elements then follow from the geometry of a simple shear.

Most twins observed experimentally in systems other than cubic are either compound twins, or Type I twins, in which K_1 and η_2 are rational. Type II twinning is more rare. The table includes examples of martensitic transformation twins, as well as a number of examples of the more rare Type II twins. Rational approximations to indices of irrational planes and directions are indicated in the table by quotation marks.

Some of the twinning modes tabulated are reciprocal to one another, so that the K_1 and η_2 of one mode becomes the K_2 and η_1 of the reciprocal mode, and vice-versa; the $\{10\bar{1}1\}$ and $\{10\bar{1}3\}$ twinning modes in magnesium are an example.

It can be seen that crystals of the same structure tend to twin in the same mode. The reason for the choice of mode in a given case is less well understood than might be supposed. In principle, the number of possibilities to choose from is enormous. To define a twinning shear that completely reconstructs the lattice, any three lattice vectors that form a primitive unit cell can be chosen and then from these, two must be chosen to define K_1 (for type I twins) or K_2 (for type II twins).

A common-sense criterion of selection is to make the magnitude of the shear as small as possible, so as to reduce the size of the atom movements needed to form the twin. When the possibilities for a given structure are carefully examined, it is found that a low magnitude of shear is a good point from which to start.

Further details are discussed in the book by Kelly and Knowles, as are additional aspects, such as the morphology of deformation twinning.

Friedel's classification of (growth) twinning

In X-ray diffraction work on nominally single crystals, occasions arise where the crystal under examination is composed is actually twinned, most usually as a consequence of crystal growth rather than as a consequence of deformation twinning. In the X-ray diffraction community where it is routine to examine crystals grown in the laboratory, the nomenclature used for twinning is that introduced by Georges Friedel in his 1926 textbook *Leçons de Cristallographie*. Friedel identified four ways in which twinning could arise:

- Twinning by *merohedry*
- Twinning by *reticular merohedry*
- Twinning by *pseudo-merohedry*
- Twinning by *reticular pseudo-merohedry*

We will finish this lecture by describing each of these four methods of twinning.

Table 11.1 The twinning elements of various crystals

Material	Unit cell	K_1	η_1	K_2	η_2	s	Type of twin	Ref.
Fe, V, Nb, W, Mo, Cr	b.c.c.	112	$\bar{1}\bar{1}\bar{1}$	11 $\bar{2}$	111	0.707	C	[13]
Cu, Ag, Au	c.c.p.	111	11 $\bar{2}$	11 $\bar{1}$	112	0.707	C	[9,10]
Cd	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 011	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ 1	0.171	C	[16]
Zn	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 011	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ 1	0.140	C	[16]
Co	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 011	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ 1	-0.128	C	[19]
		11 $\bar{2}$ 1	11 $\bar{2}$ $\bar{6}$	0001	11 $\bar{2}$ 0	0.614	C	[20]
Mg	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 012	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ $\bar{1}$	-0.129	C	[16]
		10 $\bar{1}$ 1	$\bar{1}$ 012	$\bar{1}$ 013	30 $\bar{3}$ 2	0.136	C	[21]
		$\bar{1}$ 013	30 $\bar{3}$ 2	10 $\bar{1}$ 1	$\bar{1}$ 012	0.136	C	[21]
Re	h.c.p.	11 $\bar{2}$ 1	11 $\bar{2}$ $\bar{6}$	0001	11 $\bar{2}$ 0	0.619	C	[22]
Zr	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 011	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ $\bar{1}$	-0.169	C	[23]
		11 $\bar{2}$ 1	11 $\bar{2}$ $\bar{6}$	0001	11 $\bar{2}$ 0	0.628	C	[24]
		11 $\bar{2}$ 2	$\bar{1}$ $\bar{1}$ 23	11 $\bar{2}$ 4	$\bar{2}$ $\bar{2}$ 4 $\bar{3}$	0.225	C	[23]
Ti	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 011	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ 1	-0.175	C	[25]
		11 $\bar{2}$ 2	$\bar{1}$ $\bar{1}$ 23	11 $\bar{2}$ 4	$\bar{2}$ $\bar{2}$ 4 $\bar{3}$	0.218	C	[25]
Be	h.c.p.	10 $\bar{1}$ 2	$\bar{1}$ 011	10 $\bar{1}$ $\bar{2}$	10 $\bar{1}$ 1	-0.199	C	[16]
Graphite	Hexagonal	11 $\bar{2}$ 1	$\bar{1}$ $\bar{1}$ 26	0001	11 $\bar{2}$ 0	0.367	C	[18]
Calcite, CaCO ₃	Hexagonal cleavage cell	1 $\bar{1}$ 02	$\bar{1}$ 101	$\bar{1}$ 101	1 $\bar{1}$ 02	0.694	C	[6,7]
	Rhombohedral cleavage cell	101	010	010	101	0.694	C	
Sapphire, Al ₂ O ₃	Rhombohedral; (Hexagonal cell)	10 $\bar{1}$ 2	$\bar{1}$ 011	$\bar{1}$ 014	20 $\bar{2}$ 1	0.202	C	[26]
	Morphological hexagonal cell	10 $\bar{1}$ 1	$\bar{1}$ 012	$\bar{1}$ 012	10 $\bar{1}$ 1	0.202	C	[26]
Bi	Rhombohedral face-centred cell	101	010	010	101	0.119	C	[16]
	Primitive rhombohedral cell	112	11 $\bar{1}$	110	001	0.119	C	

(continued)

Table 11.1 (continued)

Material	Unit cell	K_1	η_1	K_2	η_2	s	Type of twin	Ref.
Hg	Rhombohedral face-centred cell	$\bar{1}$ 35'	$\bar{1}$ 21	$\bar{1}$ 11	'0 $\bar{1}$ 1'	0.633	II	[27]
	Rhombohedral primitive cell	'12 $\bar{2}$ '	2 $\bar{1}$ 0	100	'01 $\bar{1}$ '	0.633	II	[27]
	Hexagonal unit cell	' $\bar{1}$ 431'	3 $\bar{1}$ $\bar{2}$ 1	10 $\bar{1}$ 1	' $\bar{1}$ 2 $\bar{1}$ 0'	0.633	II	[27]
β -Sn	Tetragonal I	301	$\bar{1}$ 03	$\bar{1}$ 01	101	0.119	C	[16]
In	Tetragonal F	101	10 $\bar{1}$	$\bar{1}$ 01	101	0.150	C	[16]
α -U	Orthorhombic C	130	3 $\bar{1}$ 0	1 $\bar{1}$ 0	110	0.299	C	[3]
		'1 $\bar{7}$ 2'	312	112	'3 $\bar{7}$ 2'	0.228	II	[3]
		112	'3 $\bar{7}$ 2'	'1 $\bar{7}$ 2'	312	0.228	I	[3]
		121	'32 $\bar{1}$ '	' $\bar{1}$ 4 $\bar{1}$ '	311	0.329	I	[3]
Ni-Ti	Monoclinic P	11 $\bar{1}$	'112'	'124'	21 $\bar{1}$	0.310	I	[28,29]
		'57 $\bar{7}$ '	011	011	'85 $\bar{5}$ '	0.280	II	[29]
		001	100	100	001	0.238	C	[29-31]
		100	001	001	100	0.238	C	[30,31]
Devitrite, Na ₂ Ca ₂ Si ₆ O ₁₆	Triclinic P	'010'	100	20 $\bar{1}$	'1122'	0.327	II	[32]
Albite, NaAlSi ₃ O ₈	Triclinic P	010	' $\bar{1}$ 010'	'305'	010	0.148	I	[1,2,33]
		'305'	010	010	' $\bar{1}$ 010'	0.148	II	[34]

Note: In the 'Type of twin' column in this table, 'C' is a compound twin, 'I' is a type I twin and 'II' is a type II twin. Rational approximations to irrational planes and directions for Type I and Type II twinning elements are denoted by quotation marks.

Twinning by merohedry

Merohedry, a word derived from Greek, implies that each component crystal has fewer faces than it would have if the crystal structure had the highest point group symmetry possible for the Bravais lattice on which it is based. The twin operation belongs to the point group of the lattice, but not the point group of the crystal.

Two examples demonstrate this principle. Pyrite, FeS_2 , has a point group $m\bar{3}$ and a primitive cubic lattice. Therefore, $\{110\}$ planes are mirror planes of the lattice, but not of the crystal structure. Such planes are candidate twin planes, and in fact both penetration and contact twins are found in pyrite with this twinning law. Zinc oxide, ZnO , has a point group $6mm$ and a primitive hexagonal lattice. Hence (0001) in ZnO can be a twin plane. This latter twinning operation is also termed inversion twinning or racemic twinning.

A particular feature of merohedral twinning important to X-ray single crystal workers is that the direct lattices and the reciprocal lattices of the different domains coincide with one another exactly, so that the twinned crystal appears to be a single crystal until the end of any single crystal X-ray diffraction procedure aimed at determining the crystal structure.

It also follows that twinning by merohedry cannot be achieved by a shear process, i.e., twinning by merohedry cannot occur in deformation twinning. Therefore, merohedral twins are twins which can only arise during crystal growth.

Twinning by reticular merohedry

Here, a multiple lattice exists which is continuous in both lattices. In the terminology introduced in Lecture 5, twinning by reticular merohedry is twinning where a coincidence site lattice (CSL) common to the two components occurs. One restriction, however, in this interpretation in terms of CSLs is that the CSL under consideration has to be amenable to a description in terms of a 180° rotation about a particular axis $[uvw]$.¹

A good example of twinning by reticular merohedry is therefore twinning on $\{111\}$ planes in c.c.p. metals, such as annealing twins in α -brass, and deformation twinning on $\{112\}$ planes in b.c.c. metals such as Fe, V and Nb, both of which have $\Sigma = 3$ CSLs.

This type of twinning mainly occurs in cubic crystals, and it is evident that the crystallography of grain boundaries in terms of CSLs when a twin description is possible is that of twinning by reticular merohedry. Obverse/reverse twinning in rhombohedral crystals is a second example. Here, the two possible settings of a rhombohedral crystal with respect to hexagonal axes, the reverse setting and the obverse setting, are related to one another by a rotation of 60° , or equivalently, 180° , about the hexagonal z -axis along which the two settings have a common three-fold axis. These are also $\Sigma = 3$ CSLs. Examples in rhombohedral crystals of such twins are obverse/reverse growth twins in calcite, iron borate and corundum.

¹ In cubic crystals, the lowest Σ value for which a twinning description is not possible is the $\Sigma = 39$ CSL for which the lowest angle/axis description is 50.13° about a $\langle 123 \rangle$ direction (H. Grimmer, *Scripta Met.* **7**, 1295–1300 (1973)).

Twinning by pseudo-merohedry

In twinning by pseudo-merohedry, the twinning is such that the symmetry possessed by the assembly of twinned crystals appears to have a symmetry higher than the symmetry of the individual crystals.

Thus, for example, a monoclinic crystal might have an angle β close to 90° . If this angle were exactly 90° , then the array of lattice points would have a point group symmetry of *mmm*, i.e., that of an orthorhombic lattice. Hence, a rotation of 180° about either the **a** axis or the **c** axis of this monoclinic crystal may produce two domain variants twinned with respect to one another. Since the assembly of twinned domains will appear to a good approximation to have the higher orthorhombic symmetry, rather than monoclinic symmetry, this type of twinning is known as *twinning by pseudo-merohedry* to differentiate it from twinning by merohedry.

Likewise, if in an orthorhombic crystal the lattice parameters *a* and *b* are very similar, then to a good approximation there is a four-fold axis parallel to [001]. Hence, the twin law in this particular case for twinning by pseudo-merohedry would be 90° about [001].

In triclinic crystals where the *b* axis is almost normal to the *a* and *c* axes, twinning by pseudo-merohedry arises by (i) reflection in (010) and (ii) rotation around [010]. In the former case this is known as *albite* twinning in feldspars; in the latter it is known as *pericline* twinning. Of course, for such twinning to be able to occur physically – the ionic interactions across the twin boundaries must be sufficiently energetically similar to those which would have formed in a single crystal, i.e., the twin boundaries must be of suitably low energy.

Twinning by reticular pseudo-merohedry

In essence, this is twinning arising in crystal growth processes which is not describable in terms of any of the other three categories. It can be considered to be related to twinning by (strict) reticular merohedry in the same way as twinning by pseudo-merohedry relates to twinning by (strict) merohedry. Thus, for example, while twinning in devitrite in the Table on page 106 can be described within the framework of deformation twinning, it is actually an example of growth twinning by reticular pseudo-merohedry.