Deformation and Fatigue of Hexagonal Close Packed Metals

A thesis submitted to the University of Surrey in partial fulfilment of the requirements for the degree of Doctor of Philosophy on a collaborative basis

by

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If a man love the labour of any trade, apart from any question of success or fame, the gods have called him.

R. L. Stevenson
Summary

Early metallographic studies of the deformation of h.c.p. metals were confined to cadmium and zinc. More recently magnesium, titanium, zirconium and beryllium have been required for the nuclear and aircraft industries and this has led to increased demand for a more fundamental understanding of the plastic deformation in h.c.p. metals.

These metals differ in two important respects from the cubic metals. Firstly only three coplanar shear vectors are normally available for slip and secondly mechanical twinning is a dominant deformation mode.

The results of a metallographic study of deformation in h.c.p. metals is presented in this thesis. Particular attention has been paid to the behaviour of deformation twins, because there is a dearth of information on this aspect in the literature.

The thesis may be divided roughly into four parts. In the first part the crystallography and deformation modes in h.c.p. metals is reviewed. Certain errors and confusions in the literature are discussed and where appropriate, particular emphasis is placed on magnesium and titanium, since they are typical of the technologically important h.c.p. metals.

The second part describes the behaviour of twins in these metals. It is shown that twin growth and contraction differs from the ideal depicted by crystallographic models of twinning. The third part is concerned with the effect of cyclic stresses. The first evidence for slip band extrusions in fatigued h.c.p. metals is presented. The distribution of the extrusions is related to the dislocation structure observed and the results are compared with those obtained in cubic metals. The fragmentation of twins under cyclic stresses and fatigue crack nucleation at twin boundaries is also demonstrated.

Finally the role of twinning in the deformation of h.c.p. metals is considered. A Schmid factor criterion is used to compare the ease of slip before and after twinning on \{\mathbf{10\bar{7}2}\} and \{\mathbf{11\bar{2}1}\} systems. Basal and prism slip systems are considered in parent and twinned crystal. It is found that pre-existing \{\mathbf{10\bar{7}2}\} twins greatly enhance prism slip compared with basal, while \{\mathbf{11\bar{2}1}\} twins also favour basal slip. When dislocation twin interactions are considered however, \(<c+a>\) slip can be nucleated more readily by \{\mathbf{10\bar{7}2}\} twins when prism slip occurs. Similarly for \{\mathbf{11\bar{2}1}\} twinning, only prism slip can give rise to \(<c+a>\) slip. These results may explain the relationship between ductility and slip and twinning modes in h.c.p. metals.
Acknowledgements

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6.3 Slip Systems
  6.3.1 Schmid Factors for Basal Slip in Parent and Twin
  6.3.2 Ratio of Maximum Schmid Factors for Basal Slip in Parent and Twin
  6.3.3 Schmid Factors for Prism Slip in Parent and Twin
  6.3.4 Ratio of Maximum Schmid Factors for Prism Slip in Parent and Twin
The crystallography and deformation modes of hexagonal close-packed metals

The extensive data on the metallography and crystallography of face-centred cubic and body-centred cubic metals have been the subject of several reviews in recent years, but in comparison the data for hexagonal close-packed metals remain dispersed in the literature. This is unfortunate, since the h.c.p. structure presents a number of confusing features not encountered in cubic structures. With the increasing technological application of h.c.p. metals, there does appear to be a need for a summary of the structure of these metals, with particular emphasis on the fundamentals of plastic deformation. It was considered appropriate in this review to mention electron diffraction and dislocation image contrast in thin foils of hexagonal metals, as future research on these materials will undoubtedly make use of the transmission electron-microscopy technique.

The paper is divided roughly into two parts. In the first part the crystallography of h.c.p. metals is described. The position of the atoms in the h.c.p. structure is illustrated and the locations of first, second, and third nearest-neighbour atoms are identified; a comparison is made between the interstitial positions in the h.c.p. and f.c.c. lattices. The reciprocal lattice is then introduced and used later in the discussion on electron diffraction. The choice of axes to define the indices of directions and planes is described. The Miller and Miller–Bravais notation is discussed in detail and the types of crystal planes and their spacings are examined.

In the second part the information in the preceding paragraphs is used to define the dislocations in hexagonal metals. The conditions necessary for electron diffraction from h.c.p. structures are then established and the data required for the determination of dislocation Burgers vectors in thin films are presented.

Finally, factors affecting the selection of a deformation mode and the rate-controlling processes during slip are described. The experimental observations of slip and twinning in magnesium and titanium are considered in detail, for these metals show many of the features characteristic of hexagonal metals, as well as being of some technological importance.

I. Crystal structure

1. Direct lattice

The atoms of a crystal are situated at the points of the direct lattice. In a lattice, each lattice point has identical surroundings and the locations of these points can be described by a primitive unit cell in which the lattice points lie only at the corners. The primitive hexagonal unit cell (heavy lines in Fig. 1) has axes $a_1 = a_2 \neq c$ and corresponding angles $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$.

1 Hexagonal prism.
The hexagonal symmetry in this lattice is usually illustrated by means of the hexagonal prism (full lines in Fig. 1). This prism contains three primitive unit cells in different orientations; it is not a true cell, as repetition in three dimensions of a hexagonal prism will not build up a hexagonal lattice. The full and broken lines in Fig. 1 compose 4 unit cells.

The atom positions in the hexagonal close-packed structure are shown in Fig. 2 and 3: the atoms are situated at the lattice points and at coordinates \( \frac{a}{2} \frac{a}{2} \frac{a}{2} \) or, alternatively, \( \frac{a}{2} \frac{a}{2} \frac{1}{2} \). The surroundings of the interior atoms are different from the atoms at the corners and so the atom positions in this example do not constitute a true space lattice. The actual space lattice remains hexagonal, however, with two atoms associated with each lattice point, e.g. at coordinates 000, \( \frac{a}{2} \frac{a}{2} \frac{a}{2} \). This arrangement is known as a double lattice structure and has 2 atoms in the primitive unit cell. Other metallic double-lattice structures are antimony, arsenic, bismuth (all rhombohedral), and \( \beta \)-tin (tetragonal).

If atoms are assumed to be hard spheres, the closest packing in a plane produces a series of regular hexagons. The stacking of close-packed planes of atoms one upon another can produce a f.c.c. crystal structure when the stacking sequence is \( \text{ABCABC...} \) and a hexagonal structure when the stacking is \( \text{ABAB...} \) (Fig. 2). In an ideal close-packed structure the coordination number (i.e. the number of nearest-neighbour atoms) for both f.c.c. and h.c.p. is 12. The shortest distances between atom centres along the \( \mathbf{a} \) and \( \mathbf{a} \times \mathbf{c} \) axes is usually taken as \( a \) and along the \( \mathbf{c} \)-axis as \( c/a \) (Fig. 2). The dimensions of the structure in terms of the lattice parameters are shown in Fig. 2: it follows that the axial ratio \( \gamma = c/a = \sqrt{8/3} = 1.633 \).

No pure metal has this ideal \( c/a \) ratio, although cobalt and magnesium are very near (Table I); recently hexagonal intermetallic phases having the ideal \( c/a \) ratio have been produced. In the pure metals, cadmium and zinc (\( c/a > 1.633 \)) have 6 nearest neighbours in the basal plane and 3 nearest neighbours above and below the basal plane at slightly greater distances; the other metals (\( c/a < 1.633 \)) have the 3 atoms above and below at slightly closer distances than those in the basal plane.

An atom and its 6 nearest neighbours in the basal plane are at distances \( a \) apart along the six \( \langle 1120 \rangle \) directions, while the remaining 6 atoms are at distances \( a(4 + 3\gamma^3)/2\sqrt{3} \) along 6 of the 12 \( \langle 2023 \rangle \) directions, i.e. atoms at \( \frac{a}{2} \frac{a}{2} \frac{1}{2} \) (Fig. 3); when \( c/a = 1.633 \), the latter equals \( a \), and the 12 nearest neighbours are equidistant as in f.c.c. metals. All the second-nearest neighbours are situated in adjacent close-packed planes at distances \( a(16 + 3\gamma^3)/2\sqrt{3} \) along 6 of the 12 \( \langle 4043 \rangle \) directions, i.e. atoms at \( \frac{a}{2} \frac{a}{2} \frac{1}{2} \) (Fig. 3); when \( c/a = 1.633 \) the second-nearest neighbour spacing becomes \( a/\sqrt{3} \). There are 2 third-nearest neighbours at distances \( c = \gamma a \) along \( \langle 0001 \rangle \), and at distances \( a\gamma/3 \) along \( \langle 1010 \rangle \), and 12 at distances \( a(28 + 3\gamma^3)/2\sqrt{3} \) in \( \langle 24\overline{6}3 \rangle \) directions (Fig. 3); when \( c/a = 1.633 \), the latter distance also equals \( a\gamma/3 \).

Christian has described the rule for selecting directions for nearest and second-nearest neighbours, namely, that in the notation \( \langle 1010 \rangle \), \( u \) and \( v \) may not be inter-

### Table I. Lattice parameters and melting points of some h.c.p. metals

<table>
<thead>
<tr>
<th>Metal</th>
<th>( a, \AA )</th>
<th>( c, \AA )</th>
<th>( c/a ) (room temp.)</th>
<th>Melting point, °C</th>
<th>( T_{\text{mf}}/T_{\text{mp}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd</td>
<td>2.972</td>
<td>5.695</td>
<td>1.8859</td>
<td>321</td>
<td>0.46</td>
</tr>
<tr>
<td>Zn</td>
<td>2.859</td>
<td>4.936</td>
<td>1.8563</td>
<td>410</td>
<td>0.99</td>
</tr>
<tr>
<td>Co</td>
<td>2.502</td>
<td>4.061</td>
<td>1.633</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Mg</td>
<td>3.203</td>
<td>5.200</td>
<td>1.623</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Re</td>
<td>2.760</td>
<td>4.458</td>
<td>1.615</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Zr</td>
<td>3.233</td>
<td>5.147</td>
<td>1.593</td>
<td>1860</td>
<td>0.13</td>
</tr>
<tr>
<td>Ti</td>
<td>2.905</td>
<td>4.683</td>
<td>1.5873</td>
<td>1800</td>
<td>0.13</td>
</tr>
<tr>
<td>Hf</td>
<td>3.194</td>
<td>5.051</td>
<td>1.581</td>
<td>2220</td>
<td>0.12</td>
</tr>
<tr>
<td>Be</td>
<td>2.281</td>
<td>3.576</td>
<td>1.560</td>
<td>1300</td>
<td>0.17</td>
</tr>
</tbody>
</table>

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*METALLURGICAL REVIEWS*
changed, e.g. if there is a nearest neighbour in [2023],
there will be no nearest neighbour in [0223], and the
second-nearest neighbours are in directions [0443],
&c.t.

The interstitial holes in f.c.c. and h.c.p.7,8 structures
are similar. For the ideal structure the octahedral
interstices (Fig. 4a) are surrounded by atoms arranged
on a regular octahedron; these interstitial holes have
coordinates $\frac{1}{2} \frac{1}{2} \frac{1}{2}$, which is equivalent to a vector
$\frac{1}{2}[0443]$ of magnitude $a/\sqrt{2}$ from the origin. There
are also four tetrahedral interstices (Fig. 4b) per unit
cell at coordinates $\frac{1}{4} \frac{1}{4} \frac{1}{4}$, $\frac{1}{4} \frac{1}{4} \frac{1}{4}$, 003, 006$. There are
thus 1 octahedral and 2 tetrahedral holes/atom, as
in f.c.c. structures.

If the atoms in a h.c.p. structure are assumed to be
rigid spheres of radius $r$ in contact along close-packed
directions, the maximum radius of sphere that can be
accommodated in an octahedral or tetrahedral site
is 0.41$r$ or 0.22$r$, respectively. The fraction of the
space occupied in f.c.c. and h.c.p. is the same, 0.74,
compared with 0.68 for b.c.c. and 0.52 for primitive
cubic packing.

2. Reciprocal lattice

It will be convenient at this point to introduce the
reciprocal lattice; this geometrical concept will be
particularly useful in the subsequent discussion on
indexing diffraction patterns and crystal planes.

A reciprocal lattice is composed of reciprocal lattice
points, each point lying on the normal (through the
origin) to a set of parallel and equidistant planes $(hkl)$
in the direct lattice and its distance from the origin is
inversely proportional to the spacing of the planes.

i.e.

$$r^{*}_{hkl} = \frac{K}{d_{hkl}}$$

where $K$ is a constant and $r^{*}_{hkl}$ is the distance from the
origin to the reciprocal lattice point corresponding
to the family of planes having the spacing $d_{hkl}$ in the
direct lattice.

If the vectors describing the reciprocal lattice and the
direct lattice are $a_{1}^*$, $a_{2}^*$, $a_{3}^*$ and $a_{1}$, $a_{2}$, $a_{3}$, respectively,
the reciprocal lattice is constructed by drawing $a_{i}^*$
normal to both $a_{2}$ and $a_{3}$ such that the scalar products become

$$a_{1}^* . a_{2} = a_{1}^* . a_{3} = 0 \quad \ldots [1]$$

and

$$a_{1}^* . a_{1} = a_{2}^* . a_{2} = 1 \quad \ldots [2]$$

the general case being $a_{i}^* . a_{j} = \delta_{ij}$, where $\delta_{ij} = 1$
when $i = j$ and otherwise is zero.

The reciprocal lattice for h.c.p. structures is a primi-
tive hexagonal lattice. The axes $c$ and $e^*$ are parallel
but $a_{1}^*$ and $a_{3}^*$ are at 60°, instead of 120° as in the
direct lattice (Fig. 1). Also $|a_{1}^*| = |a_{3}^*| = 2a/\sqrt{3}$
and $|e^*| = 1/c$.

The direct lattice in Fig. 3 should be compared
with the reciprocal lattice in Fig. 5. The (001) reciprocal
lattice plane is indexed in terms of Miller indices in Fig. 5a. A three-dimensional model of the reciprocal lattice of magnesium is shown in Fig. 5b; these models are particularly useful when indexing Laue zones in electron-diffraction patterns. In this lattice a vector
\[ \mathbf{r}_{hkil} = n_1 a_1^* + n_2 a_2^* + n_3 c^* \]
drawn from the origin to any point having coordinates \( hkl \) is perpendicular to the plane in the crystal lattice whose Miller indices are \( hkl \). Since the planes of a zone are all parallel to their line of intersection, the zone axis, their normals must be coplanar. The planes of a zone will then be represented in the reciprocal lattice by a set of points lying in a plane passing through the origin of the reciprocal lattice. Thus, the reciprocal lattice array of points describes completely the angular relationships and spacings of crystal planes in the direct lattice.

### Table II. Indices of directions and planes

<table>
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<tr>
<th>Directions</th>
<th>Miller indices (3 axes)</th>
<th>Miller-Bravais indices (4 axes)</th>
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<tr>
<td>([UVW])</td>
<td>([uvtw])</td>
<td>([uv.w])</td>
</tr>
<tr>
<td>(* [001]</td>
<td>0001</td>
<td>001</td>
</tr>
<tr>
<td>330</td>
<td>1120</td>
<td>120</td>
</tr>
<tr>
<td>300</td>
<td>2110</td>
<td>210</td>
</tr>
<tr>
<td>021</td>
<td>2023</td>
<td>243</td>
</tr>
<tr>
<td>210</td>
<td>1010</td>
<td>100</td>
</tr>
<tr>
<td>010</td>
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<td>011</td>
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<td>423</td>
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<td>203</td>
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<td>212</td>
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<td>120</td>
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<td>510</td>
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<td>540</td>
</tr>
<tr>
<td>311</td>
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<td>513</td>
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<td>5413</td>
<td>543</td>
</tr>
<tr>
<td>411</td>
<td>7253</td>
<td>723</td>
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**Indices of Burgers vectors**

<table>
<thead>
<tr>
<th>(hkl) Miller-Bravais indices</th>
<th>(HKL) Miller indices</th>
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</thead>
<tbody>
<tr>
<td>(* [hkl] )</td>
<td></td>
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</table>

### II. Crystallographic indices

Three different axial systems can be used to define the indices of directions and planes in the h.c.p. structure, i.e. rhombohedral, orthorhombic, and hexagonal.\(^1\,5,\,13-15\) Ott and Crocker\(^1\) suggest that the orthorhombic is worthy of much wider use, but since there exists a strong preference in the metallurgical literature for the hexagonal system of axes, only the latter is considered in this review. A number of recent texts discuss Miller-Bravais notation for planes, but omit\(^1\,15,\,17\) or deal very briefly\(^5,\,18\) with the indexing of directions.

#### 1. Indices of directions

Figure 1 shows the hexagonal prism: the 3-axis system is based on the 3 vectors \( a_1, a_2, c \), which define the primitive unit cell. Any direction \( d_3 \) will have 3 indices, \( U, V, W \), given by

\[ d_3 = Ua_1 + Va_2 + Wc \]

Crystallographically equivalent directions do not have the same mathematical form, e.g. the close-packed directions in the basal plane have indices \([100], [110], [010]\) (Fig. 3).

The 4-axis system is based on the vectors \( a_1, a_2, a_3, c \) (Fig. 1); \( a_3 \) is redundant since \( a_3 = - (a_1 + a_2) \). In this system a direction \( d_4 \) will have 4 indices \( uvtw \) such that

\[ d_4 = Ua_1 + Va_2 + Wa_3 + wc \]

The condition that \( U + V + T = 0 \) is now imposed and the crystallographically equivalent directions then have similar indices, e.g. the close-packed directions become \([210], [110], [010]\) (Fig. 3).

The redundant digit is sometimes omitted to produce the 4-axis 3-index notation, i.e. \( uv.w \). The similarity between equivalent directions is again obscured, and it is most important to avoid confusing the two 3-index notations based on 3 and 4 axes, because they produce different indices for a given direction. It is therefore recommended that indices based on the 4-axis hexagonal system be known as Miller-Bravais indices, while indices based on any 3-axis system, including hexagonal, be known as Miller indices.\(^1\)

Directional Miller indices \( UVVW \) may be converted to Miller-Bravais indices \( uvtw \) by the following equations.

\[ U = u - t, \quad V = v - t, \quad W = w \]

or

\[ U = \frac{1}{3}(2U - V), \quad V = \frac{1}{3}(2V - U), \quad t = -(u + v), \quad w = W \]

Important directions are listed in Table II in the Miller and Miller-Bravais notation.\(^20\)

#### 2. Indices of planes

There are two methods for deriving indices of a plane. The usual method is to determine the intercepts of the plane on the respective axes of the direct lattice in...
multiples of fractions of the unit distances along each axis. The reciprocals of these values, reduced to the
smallest integers having the same ratio, are the indices
of the plane (Fig. 6a).
An alternative and more elegant method is to define
the indices of planes as the components of vectors in
reciprocal space. This is particularly useful when
dealing with electron-diffraction patterns. Then a
plane with Miller indices \((HKL)\) making intercepts
\(a_1/H, a_2/K, c/L\) on the axes of the direct lattice, will
have a vector, \(\mathbf{r}^*\) normal to the plane, of the type
\[
\mathbf{r}^* = H\mathbf{a}_1^* + K\mathbf{a}_2^* + L\mathbf{c}^*
\]
where \(\mathbf{r}^*\) is referred to the reciprocal lattice basis
(Fig. 6b). Thus, the Miller indices of a plane are pro-
portional to the reciprocals of the intercepts which the
plane makes on the basic vectors of the direct lattice and
are also the components referred to the reciprocal
lattice basis of the vector normal to the plane. Miller
and Miller-Bravais indices of planes are readily inter-
changed, since a plane with \((hkil)\) or \((hk.l)\) Miller-
Bravais indices has Miller indices
\[
(HKL) = (hk.l) \quad \ldots \quad [5]
\]
Indices of planes are listed in Table II for the two
axial systems. It should be noted that a direction is
not normal to a plane of the same indices except for
directions of the type \(\langle 0001 \rangle\) and \(\langle hkl \rangle\). The indices
of the normal to a plane \((hkil)\) are \([hk.l]3(\frac{1}{c})^2\) \(l\)\).\(^{20}\)

† Note error in Refs. (15) and (19).

3. Stereographic projection\(^{1,7}\)

The angles between planes are dependent on the \(c/a\)
ratio and so each h.c.p. metal requires a separate
stereographic projection. The angles between planes
for magnesium and titanium are given in Refs. (25)-(31).
Computer-programmed tables are available in which
angles between planes are given for values of \(c/a\) ranging
from 1.5 to 3.0.\(^{19,28,29}\) Hu\(^{30}\) has published stereo-
graphic projections of the \((1010)\) and \((10\bar{1}2)\) planes for
titanium.

It should be noted that the standard projections for
h.c.p. metals contain planar indices, although the
points on the projection correspond to the position
of the plane normals. For example, the \([10\overline{1}\overline{1}]\) direction

\[\begin{align*}
\text{6 Miller indices (230) of a plane.} & \\
\text{7 Double stereogram for titanium. The [10\overline{1}1] twin-} & \\
\text{ning shear direction lies at the intersection of the (12\overline{1}0) plane} & \\
\text{of shear and the (10\overline{1}2) twinning plane.} & \\
\end{align*}\]

\[\begin{align*}
\bullet & \text{plane normals; } \\
\circ & \text{directions; } \\
\diamond & \text{direction and plane} \\
\end{align*}\]
lies at the intersection of (1012) and (1210) great circles and there is no pole at this position in the usual basal plane-projection (Fig. 7). It is therefore often convenient to plot a 'double stereogram' which contains projections of both plane normals and rational directions. Angles between directions (not normally tabulated) have also been computed. Fig. 7 shows a double stereogram for titanium in which the positions of important directions are compared with plane normals having the same indices. The double stereogram is especially useful when considering extinction in thin foils of dislocations having Burgers vectors not in the basal plane, e.g., <1123>. (See Section VI.3.)

It must be emphasised that the general crystallographic equations involving directional indices that are given in text-books are applicable to h.c.p. structures only when Miller indices are used; equivalent equations for Miller–Bravais indices are given by Otte and Crocker, Rarey et al., and Neumann.

III. Crystal planes and spacings

Important planes and directions in the hexagonal lattice are illustrated in Fig. 8. There are three important zone axes (directions of intersection of planes), namely, <0001>, <1010>, <1120>. The <0001> zone contains planes of the type (hk0) which intercept the basal plane at 90°. The <1120> zone contains planes of the type (110n), the (1100) being known as prism planes of type I. The <1010> zone contains planes of the type (1210n), the (1210) being known as prism planes of type II. Planes of the type (hkln), n ≠ 0, are known as pyramidal planes.

The intrinsic Peierls–Nabarro stress for slip is expected to be smaller for planes having the largest interplanar spacings (i.e. low-index planes containing the greatest density of atoms) and containing the shortest lattice translation vectors. The interplanar spacing is given by

\[ a \left[ \frac{4}{3} (h^2 + k^2) + \left( \frac{2}{a} \right)^2 \right]^{-\frac{1}{2}} \]

where \( hkl \) are the Miller or Miller–Bravais indices of the planes. The interplanar spacing along the c-axis is \( \frac{c}{2} \) and the planar density is \( \frac{2}{a^2} \sqrt{3} \).

However, a difficulty arises when non-basal planes are considered, since these planes are not uniformly spaced. Thus, although for diffraction purposes \( d_{1010} \) and \( d_{1210} \) are given by \( a\sqrt{3}/2 \) and \( a/2 \), respectively, when discussing slip on these planes, the slip surface is considered to be corrugated to include atoms in A and B layers in (0001) planes and the density of atoms in the (1010) slip planes is doubled, becoming \( 2/ac \). Using ball models, Nicholas has demonstrated clearly the atom positions and geometry in crystal planes of hexagonal structures. The variation in planar spacing and atomic density for (1010) and (0001) planes in several hexagonal metals is shown in Table III. On the basis of the Peierls–Nabarro model, prism slip is expected to replace basal slip as the predominant slip mode when the \( c/a \) ratio becomes \( \frac{1}{\sqrt{3}} \) (1.73), since then both the (1010) spacing and density are greater than corresponding values for the basal plane. Although this concept apparently accounts for prism slip in titanium and zirconium, it fails to explain the predominance of basal slip in cobalt, magnesium, and beryllium. (See further discussion in Section VIII.4.)

IV. Crystallography of twinning in h.c.p. metals

A detailed analysis of the crystallography of twinning in hexagonal structures has been carried out by Crocker and reported by Christian. The twinning elements of the most frequently occurring twins are given in Table IV.

### Table III. Relative density of atoms and interplanar spacing in (1010) and (0001) planes

<table>
<thead>
<tr>
<th>Metal</th>
<th>( c/a ) ratio</th>
<th>Ratio of atom densities, ( \frac{(1010)}{(0001)} = \frac{2/ac}{2/a^2\sqrt{3}} )</th>
<th>Ratio of interplanar spacings, ( \frac{(1010)}{(0001)} = \frac{a{\sqrt{3}/2}}{c/2} )</th>
<th>Stacking-fault energy (basal plane), ergs/cm²</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd</td>
<td>1.886</td>
<td>0.92</td>
<td></td>
<td>~150</td>
<td>117</td>
</tr>
<tr>
<td>Zn</td>
<td>1.866</td>
<td>0.94</td>
<td></td>
<td>~300</td>
<td>58, 115, 117, 118</td>
</tr>
<tr>
<td>Co</td>
<td>1.823</td>
<td>1.00</td>
<td></td>
<td>~26</td>
<td>115</td>
</tr>
<tr>
<td>Mg</td>
<td>1.823</td>
<td>1.07</td>
<td></td>
<td>~300</td>
<td>58</td>
</tr>
<tr>
<td>Ti</td>
<td>1.877</td>
<td>1.09</td>
<td></td>
<td>~300</td>
<td>54, 116</td>
</tr>
<tr>
<td>Be</td>
<td>1.868</td>
<td>1.10</td>
<td></td>
<td>~180</td>
<td>116</td>
</tr>
</tbody>
</table>
1. Shape change produced by twinning

Twining causes a sphere to become an ellipsoid and this shape change can be conveniently illustrated by sections parallel to a plane of shear.1,4,6 Such a section is shown schematically in Fig. 10. The plane of shear, the twinning plane, and the shear direction are projected on a stereogram in Fig. 7.

There are two planes that remain undistorted by the twinning shear, i.e. the magnitude of all angles and directions in these planes are unchanged. The planes lie normal to the plane of shear and are designated \( K_1 \) and \( K_2 \). While the twinning plane \( K_1 \), containing the twinning shear direction \( \eta_1 \), does not change its position, \( K_2 \) is displaced to \( K_2' \) by the twinning shear. The lines of intersection of the plane of shear with \( K_2 \) and \( K_2' \) are \( \eta_2 \) and \( \eta_2' \), respectively.

The shape changes associated with \{1012\}, \{1121\}, and \{1122\} twinning are illustrated in Fig. 11. The twinning shear \( S \) varies with \( c/a \) ratio; the acute angle \( 2\phi \) between \( K_1 \) and \( K_2 \) is related to the shear \( S \) (Fig. 10) by

\[
S = 2 \cot 2\phi
\]

Figure 11 shows that a free surface parallel to (0001) plane would be tilted \( \approx 4^\circ, 7^\circ, \) and \( 35^\circ \) by \{1012\} twinning in magnesium and \{1120\} and \{1121\} twins in titanium, respectively.

When a crystal is completely converted to a twin, all directions lying in the initially acute sector between \( K_1 \) and \( K_2 \) (Fig. 10) are shortened, while all directions lying in the obtuse sector are lengthened. The standard stereographic projection can be divided into regions indicating the sense of the length-change of specimens after twinning on any twin system.

Alternatively, a change in length can be calculated using the expression:

\[
\frac{l}{l_0} = (1 + 2s \sin \chi \cos \lambda + s^2 \sin^2 \chi)^{1/2} \quad \ldots [6]
\]

where \( l_0 = \) length before twinning,
\( l = \) length after twinning,
\( \chi = \) angle between direction of \( l_0 \) and \( K_1 \),
\( \lambda = \) angle between direction of \( l_0 \) and \( \eta_1 \),
\( s = \) twinning shear.


Table IV. Twinning elements

<table>
<thead>
<tr>
<th>Metal</th>
<th>Twinning plane (1st undeformed plane) ((K_1))</th>
<th>Twinning shear direction ((\eta_1))</th>
<th>Second undeformed plane ((K_2))</th>
<th>Direction of intersection of plane of shear with (K_1) ((\eta_2))</th>
<th>Plane of shear perpendicular to (K_1) and (K_2)</th>
<th>Magnitude of twinning shear</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd</td>
<td>{1012}</td>
<td>{1012}</td>
<td>{1012}</td>
<td>{1012}</td>
<td>{1010}</td>
<td>0.17</td>
</tr>
<tr>
<td>Zn</td>
<td>{1012}</td>
<td>{1012}</td>
<td>{1012}</td>
<td>{1012}</td>
<td>{1010}</td>
<td>0.139</td>
</tr>
<tr>
<td>Mg</td>
<td>{1121}</td>
<td>{1121}</td>
<td>{1121}</td>
<td>{1121}</td>
<td>{1120}</td>
<td>0.131</td>
</tr>
<tr>
<td>Ti</td>
<td>{1122}</td>
<td>{1122}</td>
<td>{1122}</td>
<td>{1122}</td>
<td>{1100}</td>
<td>0.167</td>
</tr>
<tr>
<td>Ti</td>
<td>{1121}</td>
<td>{1121}</td>
<td>{1121}</td>
<td>{1121}</td>
<td>{1100}</td>
<td>0.199</td>
</tr>
</tbody>
</table>

Mg Be

Ti

Be

0.638

0.229

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- 15 -
There is no change in length, \( l/l_0 = 1 \), for directions in \( K_1 \) and \( K_2 \).

The above discussion applies to changes in length of directions lying within the twinned volume. When twinning is incomplete, and for distances large compared with the twin lamella, the dimensional changes may be modified for directions lying in the quadrant bounded by \( K_2 \) and the plane normal to \( K_1 \) and \( \eta_1 \) (\( OX \) in Fig. 10). This effect is important when the twinning shear is large.\(^{39}\)

2. Stereographic projection of twin poles

Greninger and Troiano\(^{40}\) first showed how deformations involving homogeneous shear, such as twinning and martensitic transformations, can be described using stereographic projection. The relative positions of planes and directions before and after twinning can be readily determined geometrically by this method if the twinning elements are known.

All the twinning elements listed in Table IV have rational indices and the twins are known as rational or compound twins. It follows from the definition of a twin that the position of poles after twinning on these systems can be obtained by:\(^{1,4,5}\)

(a) Reflections across \( K_1 \), equivalent to a rotation of 180° about the normal to \( K_1 \).

(b) Reflection across a plane perpendicular to \( K_1 \) and \( \eta_1 \), equivalent to a 180° rotation about \( \eta_1 \).

The poles in the (0001) matrix projection have been moved to their position after twinning on (1012) in Fig. 12. The position of the basal pole in twin and matrix, the twin elements, and the \( <1130> \) zones are also shown. The positions of the poles after twinning can be found by simply rotating the poles in the (0001) projection about one axis through an angle equal to 20, where \( \theta \) is the acute angle between the plane \( K_1 \) and the (0001) pole; the sense of rotation is such as to initially reduce \( \theta \). For example, in titanium the following data are applicable.

11 Shape changes produced by twinning. Sections parallel to the plane of shear for a (1012) twin in zinc, b (1012) twin in magnesium, c (1122) twin in titanium, d (1121) twin in titanium.
A rational plane in the matrix will in general become an irrational plane in the twin, e.g. in Fig. 12 the basal plane in titanium after (1012) twinning becomes a plane inclined 4° 52' to the (1010) in the twin about the [1012] axis. Directions in $K_1$ are unchanged in position and have similar-type indices after twinning, e.g. [1011] and [1012] for the (1012) twin. Planes in $\eta_1$ zones are also unchanged in position and have similar-type indices after twinning (Table V), although relative to the parent matrix these planes are rotated about their normals, i.e. the positions of the atoms in these planes are changed. Although indices of directions in $K_2$ and planes in the $\eta_2$ zone are of the same type after twinning, their positions are changed from those occupied in the matrix.

The above data can be deduced from Fig. 12, which shows the position of $\eta_1$ and $\eta_2$ zones. The great circle corresponding to the $\eta_1$ zone is in the same position on the stereographic projection for both twin and matrix, whereas the $\eta_2$ zone in the matrix moves to $\eta_2$ in the twin.

The indices of planes and directions after twinning can be deduced analytically. The following set of expressions avoids fractional indices.

If $K_1 = [HKL]$ and $\eta_0 = [UVW]$ (or alternatively $K_2$ and $\eta_1$, respectively), then the directional Miller indices $[uvw]$ in the parent matrix transform to $[u'v'w']$ in the twin according to:

\[
\begin{align*}
  u' &= u(HU + KV + LW) - 2U(Hu + Kv + Lw) \\
  v' &= v(HU + KV + LW) - 2V(Hu + Kv + Lw) \\
  w' &= w(HU + KV + LW) - 2W(Hu + Kv + Lw)
\end{align*}
\]

... [7]

Planar indices $(hkl)$ in the parent matrix transform to $(h'k'l')$ in the twin according to:

\[
\begin{align*}
  h' &= h(HU + KV + LW) - 2U(Hh + Kh + Ll) \\
  k' &= k(HU + KV + LW) - 2V(Hk + Kh + Ll) \\
  l' &= l(HU + KV + LW) - 2W(Hl + Kl + Ll)
\end{align*}
\]

... [8]

Planar indices $(hkl)$ in the parent matrix transform to $(h'k'l')$ in the twin according to:

\[
\begin{align*}
  k' &= k(HU + KV + LW) - 2K(Uk + Vl + Wl) \\
  l' &= l(HU + KV + LW) - 2L(Ul +Vk + Wl)
\end{align*}
\]

It is apparent from these equations that directions in $K_1$ and $K_2$ retain their indices (i.e. $Hu + Kv + Lw = 0$) as do planes in the $\eta_1$ and $\eta_2$ zones (i.e. $Oh + Vk + Wl = 0$).

---

Table V. Planes parallel in twin and parent matrix

<table>
<thead>
<tr>
<th>Twin plane $K_1$</th>
<th>Zone axis $[0\bar{1}2]$</th>
<th>Rotation axis $[\bar{2}10]$</th>
<th>Angle of rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1012)</td>
<td>(1011)</td>
<td>[1210]</td>
<td>94° 52'</td>
</tr>
<tr>
<td>(1122)</td>
<td>(1100)</td>
<td>[1100]</td>
<td>63° 58'</td>
</tr>
<tr>
<td>(1011)</td>
<td>(1100)</td>
<td>[1100]</td>
<td>34° 54'</td>
</tr>
</tbody>
</table>

A rational plane in the matrix will in general become an irrational plane in the twin. Plane normals in parent matrix; plane normals coincident in matrix and twin; and φ poles are indexed relative to twin.

---

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12 Basal plane projection for titanium, showing (1012) twinning elements.

+ Plane normals in parent matrix;

• Plane normals in (1012) twin; § Plane normals coincident in matrix and twin;

• and φ poles are indexed relative to twin.
V. Dislocations in h.c.p. metals

Read and Frank and Nicholas have enumerated the possible dislocations in h.c.p. structures and compared their energies, assuming them to be proportional to the square of the Burgers vector; more recently Yoo and Wei have applied anisotropic elasticity theory to dislocations in zinc. Subsequent reviews of dislocations in h.c.p. metals are presented by Nabarro et al. and Christian. A convenient notation, analogous to the Thompson tetrahedron for f.c.c. metals, has been used by Berghezan et al. and Damiano to describe the Burgers vectors in h.c.p. structures (Fig. 13). Some possible Burgers vectors and their relative energies are listed in Table VI. Both Miller and Miller-Bravais indices are used to describe the vectors and the notations should be clearly distinguished to avoid confusion. Both types of index are included in Table VI. In Table II, for directions corresponding to possible Burgers vectors, the Miller indices have not been reduced to the smallest integer and are equal in magnitude to the equivalent Miller-Bravais direction vector; thus Burgers vectors can be readily converted from one axial system to the other.

The following points are worth emphasising at this stage. The magnitude of a vector in terms of the lattice parameters is given by

$$a[U^2 - UV + V^2 + \left(\frac{c}{a}\right)^2 W^2]$$

and

$$a[3(u^2 + w^2 + v^2) + \left(\frac{c}{a}\right)^2 W^2]$$

where $[UVW]$ and $[uvw]$ are Miller and Miller-Bravais indices, respectively.

The Burgers vector, $\mathbf{a}$, can be represented in magnitude and direction by $\langle 110 \rangle$, $\langle 010 \rangle$, and $\langle 100 \rangle$ (Miller notation) and $a/3 \langle 1120 \rangle$ (Miller-Bravais notation); the latter is stated incorrectly in Refs. (19), (37), (52), (53).

Confusion is best avoided by simply referring vectors to unit distances $(a,a,a,c)$ along the respective axes, i.e. $\langle 11120 \rangle$, $\langle 1123 \rangle$.

Three glide directions are coplanar and are associated with the shortest Burgers vectors, $\mathbf{a}$, (Table VI (1)) lying in the close-packed directions in the basal plane. The other important Burgers vectors $\mathbf{c}$ (Table VI (2)) and $\mathbf{c} + \mathbf{a}$ (Table VI (3)) do not lie in a close-packed direction. The largest vector, $\langle \mathbf{c} + \mathbf{a} \rangle$, may be represented by

$$AB + ST = \left[AB + ST\right] \cdots [9]$$

When Burgers vectors have components along the c-axis, e.g. $\langle \mathbf{c} + \mathbf{a} \rangle$-type Burgers vectors, the vector should be in the form $\langle a a 2a \rangle$ or $\langle 1123 \rangle$, the modulus of the vector being $(a^2 + c^2)^{1/2}$; the forms $a/3 \langle 1123 \rangle$, $(a^2 + c^2)/3 \langle 1123 \rangle$, &c., are incorrect in Refs. (19), (37), (52), (53).

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Confusion is best avoided by simply referring vectors to unit distances $(a,a,a,c)$ along the respective axes, i.e. $\langle 11120 \rangle$, $\langle 1123 \rangle$.

Table VI. Burgers vectors of dislocations in h.c.p. metals

<table>
<thead>
<tr>
<th>Type of dislocation (Fig. 13)</th>
<th>Total number of dislocations (including negative)</th>
<th>Vector</th>
<th>Direction indices of vector</th>
<th>Magnitude of vector in terms of lattice parameters</th>
<th>Relative energies of dislocations $\gamma = \sqrt{\frac{8}{3}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perfect dislocations</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 AB, AC</td>
<td>6</td>
<td>$a_n, a_c$</td>
<td>$\langle 1120 \rangle$</td>
<td>$</td>
<td>a</td>
</tr>
<tr>
<td>2 ST, TS</td>
<td>2</td>
<td>$c$</td>
<td>$\langle 0001 \rangle$</td>
<td>$</td>
<td>c</td>
</tr>
<tr>
<td>3 ST + AB, AC, &amp;c.</td>
<td>12</td>
<td>$c + a$</td>
<td>$\langle 1123 \rangle$</td>
<td>$\sqrt{</td>
<td>a</td>
</tr>
<tr>
<td>Imperfect dislocations</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 AC, BC, &amp;c.</td>
<td>6</td>
<td>$\frac{1}{2}a + \frac{1}{2}c$</td>
<td>$\langle 1010 \rangle$</td>
<td>$\frac{</td>
<td>a</td>
</tr>
<tr>
<td>5 cS, cT, &amp;c.</td>
<td>4</td>
<td>$\frac{1}{2}c$</td>
<td>$\langle 0001 \rangle$</td>
<td>$\frac{</td>
<td>c</td>
</tr>
<tr>
<td>6 AS, BS, &amp;c.</td>
<td>12</td>
<td>$(4) + (5)$ above</td>
<td>$\langle 2023 \rangle$</td>
<td>$\frac{</td>
<td>c</td>
</tr>
</tbody>
</table>

13 Burgers vectors in the h.c.p. lattice (see text).
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14 Stacking faults in the h.c.p. lattice (see text).

15 Projection of atoms in (0001). Dotted lines are traces of possible (1010) slip surfaces. Slip along XY trace disturbs least bonds.

- atoms in A position; o atoms in B positions.

16 Ewald sphere construction in reciprocal lattice.

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but the $XY$ plane is favoured since the least number of bonds is disturbed.\textsuperscript{56}

Slip and twinning in non-basal planes has been analysed by Rosenbaum;\textsuperscript{55} in particular, he considered a twinning model based upon $(c+a)$ dislocations dissociating in $(1122)$ planes according to reaction [17]. Among the pyramidal planes, $(101\overline{1})$ are unique in that they contain both $a$ and $c+a$ vectors (Fig. 8c), as do all $(101\overline{1})$ planes; dissociation of $a$-type dislocations does not appear possible in any $(101\overline{1}n)$ plane where $n$ is an integer.\textsuperscript{42,57}

The only stacking faults that preserve the nearest-neighbour configuration in h.c.p. structures are faults in the basal plane;\textsuperscript{43,44} in these structures Shockley partial dislocations are always associated with intrinsic faults and Frank partials with extrinsic faults.\textsuperscript{42,57}

Stacking faults are frequently produced in hexagonal metals by precipitation of vacancies.\textsuperscript{48,56-58,61} For example, a single layer of vacancies (Fig. 14c) produces an unstable high-energy stacking sequence ABAB/ABA (Fig. 14d). It may be converted to a lower-energy fault by:

(a) Passing a pair of equal and opposite partial dislocations (dipole) over adjacent slip planes to produce

\textbf{ABA/c/ABA} (Fig. 14e)

an extrinsic fault violating 3 next-nearest neighbours bounded by Frank partials of type $aS$; thus, a high-energy fault is bounded by low-energy partials.

(b) Passing an $A\sigma$-type partial across the loop to produce

\textbf{BC/BC/AB} (Fig. 14f)

an intrinsic stacking-fault with 1 violation of next-nearest neighbours bounded by Frank–Shockley composite partials of the type $AS$; thus a low-energy fault is bounded by high-energy partials.

$$A\sigma + aS \rightarrow AS$$

$$\frac{1}{3}[10\overline{1}0] + \frac{1}{3}[0001] \rightarrow \frac{1}{3}[2023] \ldots [19]$$

$$\frac{1}{3}[210] + \frac{1}{3}[001] \rightarrow \frac{1}{3}[423]$$

The fault energy associated with (b) is $\sim \frac{1}{2}$ that produced in (a) and $\frac{1}{3}$ that produced by dissociation in equation [14].

If the vacancies precipitate in two adjacent layers an unfaulted loop is produced with an $ST$-type Burgers vector; such loops are glissile in the $c$-direction. $AS$- and $ST$-type loops have been studied in thin foils of cadmium,\textsuperscript{56} zinc,\textsuperscript{56,58} magnesium,\textsuperscript{68} and beryllium.\textsuperscript{39(b)}

17 Electron-diffraction patterns frequently obtained from h.c.p. metals. The structure factor is zero for reflections marked X. Zone axes are given in terms of Miller and Miller-Bravais indices, together with the corresponding indices of the foil plane.
VI. Electron diffraction by h.c.p. metals

1. Diffraction patterns

Electron-diffraction patterns are interpreted most readily in terms of the reciprocal lattice. The Ewald sphere construction in reciprocal space gives the condition for diffraction from a particular set of planes. Consider the sphere (Fig. 16) of radius 1/\( \lambda \) that intersects the origin of the reciprocal lattice at \( O \), where the crystal planes spaced \( d_{hkl} \) apart are inclined at an angle \( \theta \) to the incident electron beam along \( EO \). Let a reciprocal lattice vector \( r_{hkl} \) equal OP, then P will be on the sphere if

\[
\sin \theta = \frac{r_{hkl}}{2/\lambda} = \frac{\lambda K}{2d_{hkl}} \quad \text{(since } r_{hkl} = \frac{K}{d_{hkl}}) \]

This is equivalent to Bragg’s law. Thus, depending on the structure factor, a diffracted beam will arise whenever the reflecting sphere intersects a reciprocal lattice point, the direction of the diffracted beam being given by FP. The maximum reciprocal lattice spacing obtainable is given by

\[
r_{hkl} = \frac{2 \sin \theta}{\lambda} = \frac{2}{\lambda} ; \theta = 90^\circ
\]

thus a limiting sphere may be constructed, centred at \( O \), of radius 2/\( \lambda \), within which all possible reflections will lie.

Since the wavelength of electrons at 100 kV is \( \lambda \sim 0.037 \AA \), the Bragg angles are very small, i.e. \( \sim 10^{-2} \) radians or 1 degree. The radius of the reflecting sphere is therefore \( \sim 27 \AA^{-1} \), which is so large compared with the lattice spacing that the sphere can be approximated to a plane. The diffraction pattern produced by an electron beam entering a h.c.p. crystal along any zone axis can now be determined by imagining a plane normal to the electron beam and passing through the origin of the reciprocal lattice shown in Fig. 5b. Some commonly occurring diffraction patterns for h.c.p. metals are shown in Fig. 17.11

The magnitude of the reciprocal lattice vector in the diffraction pattern is determined from

\[
r_{hkl} = \frac{n\lambda}{d_{hkl}}
\]

where \( n \lambda \) is the camera constant measured in the electron microscope.

The interpretation of electron-diffraction patterns of h.c.p. metals is more complicated than in cubic metals. For example, a low-index zone axis may be normal to a plane having irrational indices. Consequently, although the diffraction pattern may represent a low-index reciprocal lattice plane, the foil plane may be irrational. The approximate indices of irrational planes normal to prominent zone axes are given in Fig. 17.

As in the case of X-ray diffraction the structure factor becomes zero and there is no diffracted beam when \( (h + 2k) \) is a multiple of 3 and \( l \) is odd, i.e. 1121, 2241, etc.; in Fig. 5b balls are missing at positions corresponding to forbidden reflections. However, these conditions may be relaxed for electron diffraction and extra spots can arise as a result of:

1. Elongation of reciprocal lattice spots (streaking) caused by lattice strain or presence of small precipitate platelets.
2. Double diffraction.
3. Twinning.

Extra spots likely to arise by double diffraction are marked by crosses in Fig. 17.

The spots in a single-crystal electron-diffraction pattern lie indices corresponding to planes in the direct lattice and all these planes lie in the same zone. Thus, to each diffraction pattern can be assigned a zone axis (parallel to the incident electron beam) that satisfies the relationship:

\[
HU + KV + LW = 0 \quad \text{for Miller indices} \ldots [20]
\]

\[
hu + kv + it + lw = 0 \quad \text{for Miller–Bravais indices} \ldots [21]
\]

where \( HKL \) and \( kkl \) are indices of the diffracted beam giving rise to the spot in the diffraction pattern, and \([UVW]\) and \([uvw]\) are the respective indices of the zone axis.

Zone axes are determined by the following equations: if two planes \( H_1 K_1 L_1, H_2 K_2 L_2 \) lie in a zone \( UVW \), then

\[
H_1 U + K_1 V + L_1 W = 0 \quad H_2 U + K_2 V + L_2 W = 0
\]

thus

\[
UVW = (K_1 L_2 - K_2 L_1) : (L_1 H_2 - L_2 H_1) : (H_1 K_2 - H_2 K_1) \ldots [22]
\]

This method may be applied to Miller–Bravais indices by omitting a redundant figure in the plane index. It should be emphasised, however, that the zone axis so derived contains three figures and constitutes in fact the Miller indices of the zone axis and not the Miller–Bravais indices with the third index omitted, as suggested by Phillips. Failure to appreciate the foregoing has resulted in the incorrect derivation of zone symbols for diffraction patterns in a number of recent texts. The correct Miller–Bravais symbol can be obtained from the Miller zone symbol using equation [4] (Table II) and can be checked by substituting in equation [21].

2. Identification of twin spots in diffraction patterns

The identification of twin spots in diffraction patterns from h.c.p. structures has received only brief mention in the literature. A simple yet useful stereo-
graphic method has therefore been described and compared with the normal analytical approach. A summary of the stereographic technique is presented here.

By making use of stereographic projections of matrix and twin poles, it is possible to predict the reflections from any known twin in a parent matrix of any orientation. Some elongation of reciprocal lattice points is assumed and is commonly observed in practice. The correct twin poles are superimposed on the (0001) projection, as described in Section IV.2. The great circle corresponding to the foil plane in the matrix is drawn relative to the (0001) projection. The twin poles nearest to this great circle will represent possible reflecting planes in the twin matrix.

An example will illustrate the technique. Consider a (1012) twin that lies in a foil whose surface, the parent matrix, is parallel to the basal plane and normal to the incident electron beam (Fig. 12). The parent matrix will therefore give rise to a diffraction pattern similar to that shown in Fig. 17c. The nearest rational plane in the twin, (1010), is inclined to (0001). The twin matrix diffraction pattern will be similar to that shown in Fig. 17b. The composite diffraction pattern will therefore appear as in Fig. 18a. The (1121) and (1122) twins produce parallel twin-boundary traces in a (0001) foil surface. However, the twins can be distinguished by comparing their diffraction patterns (Fig. 18b and c).

Note that all twin spots are displaced from the matrix spots in a direction parallel to the projection in the reciprocal lattice plane of the twin plane normal. This applies to all crystal structures. When the twin boundary is normal or parallel to the electron beam, the positions of the twin spots are readily obtained by rotating the matrix diffraction pattern 180° about a suitable axis lying in the plane of the diffraction pattern. Double diffraction spots frequently arise in the twin patterns and can be identified by the usual methods described for f.c.c. structures.

A more detailed discussion of these points is provided in Ref. (72).

3. Determination of Burgers vectors of dislocations

The contrast in transmission electron micrographs associated with crystal defects is discussed in detail in Refs. (11), (68), and (74). Feltner and Sefton have tabulated data for f.c.c. structures, but only brief reference is made in the literature to h.c.p. structures.

**Perfect dislocations.** The condition for invisibility of dislocations is generally \( g \cdot b = 0 \), where \( b \) is the Burgers vector and \( g \) is a reciprocal lattice vector normal to the reflecting planes, of magnitude equal to the reciprocal of the spacing between them. This is strictly sufficient only for screw dislocations, although in practice the very faint images under the condition \( g \cdot b = 0 \) often enable different Burgers vectors to be distinguished. The visibility of dislocations having [0001] Burgers vectors in zinc, when \( g \cdot b = 0 \), is discussed in Ref. (11).

The three types of Burgers vector for perfect dislocations in h.c.p. metals, are listed in Table VI. The planes containing these Burgers vectors are readily determined by drawing great circles with the corresponding Burgers vector as pole. This has been done for some dislocations having \( \langle 1120 \rangle \) and \( \langle 1123 \rangle \)-type Burgers vectors in Fig. 19. All the poles lying on these great circles satisfy the criterion \( g \cdot b = 0 \) (note that poles with +ve and —ve fourth index coincide in the stereogram) and electron-diffraction spots having these indices can be used to determine the types of Burgers vector in thin foils.

In practice, the low-order reflections are preferred...
Partridge: Crystallography and deformation modes of h.c.p. metals

and values of \( \mathbf{g} \cdot \mathbf{b} \) for the first seven reflections and the perfect dislocations listed in Table IV are given in Table VII.

Table VII shows that the three close-packed Burgers vectors in the basal plane can be distinguished from each other using only (10\(\bar{1}0\)) reflections, i.e. using a foil with (0001) plane parallel to the surface. When \( \langle 11\bar{2}3 \rangle \) - and \( \langle 0001 \rangle \)-type Burgers vectors are also present, additional reflections, e.g. \( \{1\bar{1}01\} \) and \( \{1\bar{1}22\} \), will enable any of the possible Burgers vectors of perfect dislocations to be identified. The (0002) reflection is frequently obtained in twinned crystal. Other possible combinations of reflections and Burgers vectors can be discovered in Table VII.

Partial dislocations. For partial dislocations the Burgers vector \( \mathbf{b}_p \) is no longer a lattice vector, and the vector product \( \mathbf{g} \cdot \mathbf{b}_p \) is therefore not necessarily an integer. A partial dislocation may be invisible for \( \mathbf{g} \cdot \mathbf{b}_p = 0 \) or \( \pm \frac{1}{2} \). Thus, when neither partial of an extended dislocation is visible, \( \mathbf{g} \cdot \mathbf{b}_p = + \frac{1}{2} \) or \( - \frac{1}{2} \) for one and \( - \frac{1}{2} \) or \( + \frac{1}{2} \) for the other, so that the dislocation if unextended would also be invisible. (This accounts for the double extinction in graphite, i.e. 2 partials with different Burgers vector are simultaneously invisible.)

However, under certain conditions, partials in mixed orientation may give rise to strong contrast and when \( \mathbf{g} \cdot \mathbf{b}_p = 0 \), e.g. dislocation loops with a \( \frac{1}{2} \langle 20\bar{2}3 \rangle \) Burgers vector. As with edge dislocation loops referred to above, the contrast is due to the displacement normal to the slip plane.\(^{11}\) The unambiguous determination of the Burgers vectors of partials thus requires a precise knowledge of the diffraction conditions and of the contrast associated with a particular partial and its stacking fault.\(^{14,74}\)

Fraction of dislocations invisible. Table VIII shows the fraction of perfect dislocations invisible (assuming all Burgers vectors are equally represented) for any one of the first seven reflections. Clearly micrographs taken with only one strong diffracting beam can give very misleading values for the dislocation density. Similar data are reported for f.c.c. structures.\(^{75}\)

VII. Deformation modes

Early data on the stress/strain curves\(^{76-83}\) were restricted to results obtained with cadmium, zinc, and magnesium; recently more detailed information has become available for metals with smaller \( c/a \) ratios.\(^{6,83-86}\)

Dislocation interactions in h.c.p. metals are discussed in Refs. (46), (52), (82), (87-91), and the mechanical properties are adequately dealt with in the above references. These topics will receive only brief mention in this review and in the following discussion particular attention will be paid to magnesium and titanium.

The stresses required to activate the deformation modes in hexagonal metals are very dependent on the orientation of the stress axis. This is apparent for twinning in Fig. 11 and is more clearly demonstrated for slip and twinning by plotting the Schmid factor for each deformation mode, e.g.

\[
\frac{\sigma_s}{\sigma_a} = \cos \varphi \cos \lambda
\]

where \( \sigma_s = \) shear stress resolved on the slip or twin plane and in the slip or twinning direction. \( \sigma_a = \) applied stress.
Partridge: Crystallography and deformation modes of h.c.p. metals

σ and λ are, respectively, the angle between the stress axis and slip or twin plane normal and slip or twinning direction.

σc must attain a critical value, called the critical resolved shear stress (c.r.s.s.), before slip will occur. Values for the critical resolved shear stress for twinning (c.r.s.s.t.) are not so easily obtained, since nucleation becomes of predominant importance (see Section V III).

1. Slip modes

Dorn and Mitchell\(^6\) have provided a comprehensive list of deformation modes in bulk and thin-film specimens of h.c.p. metals. The slip modes in magnesium, titanium, and beryllium are summarised in Table IX.

Slip in \(<1120>\) directions occurs in all the hexagonal metals, and basal slip predominates in cadmium, zinc, cobalt,\(^92\) magnesium,\(^79\) and beryllium.\(^93-95\) The \(\{1122\}\) \(\langle\overline{1}23\rangle\) slip system operates in bulk cadmium,\(^56\) and dislocations with this Burgers vector have been observed in cadmium\(^56\) and zinc\(^55\) at room temperature and in beryllium\(^99-102\) at elevated temperatures.

Dislocations dissociated in the basal planes have been observed in cobalt\(^103,104\) and in the \(\alpha\)-titanium phase in a titanium alloy.\(^104(a)\) Stacking faults lying in basal planes in magnesium and beryllium and in basal and non-basal planes in titanium (Fig. 20) are frequently found within \(\{10\overline{1}2\}\) twins after deformation;\(^105\) their origin is not at present clear, but they may account for the faulting detected in titanium using X-rays.\(^107\) Basal plane faults are also found within transformation twins in quenched pure titanium.\(^108-109\) Stacking faults in the basal planes of cadmium and zinc, hitherto attributed to dissociation of glissile dislocations,\(^56\) are now believed to arise from precipitation of vacancies generated either by cold work\(^48-87-110-113\) or by surface oxidation of both thin foils\(^58-59\) and bulk material.\(^114\)

<table>
<thead>
<tr>
<th>Reflection</th>
<th>Ref 1</th>
<th>Ref 2</th>
<th>Ref 3</th>
<th>Ref 4</th>
<th>Ref 5</th>
<th>Ref 6</th>
<th>Ref 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burgers vectors of perfect dislocations (× 1/2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reflection</th>
<th>Ref 1</th>
<th>Ref 2</th>
<th>Ref 3</th>
<th>Ref 4</th>
<th>Ref 5</th>
<th>Ref 6</th>
<th>Ref 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burgers vectors of perfect dislocations (× 1/2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table VIII. The fraction of perfect dislocations invisible in a h.c.p. metal (assuming all Burgers vectors are equally represented)

<table>
<thead>
<tr>
<th>Reflection</th>
<th>Fraction of dislocations invisible</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\frac{1}{2}$ (1120) type</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
</tr>
</tbody>
</table>

Thus, values of the stacking-fault energy derived from early thin-film observations are too low. Current estimates of the stacking-fault energy for several hexagonal metals are given in Table III.

In bulk polycrystalline magnesium, (1010) and (1011) slip systems have been detected at room temperature and below in highly stressed regions, i.e. grain-boundary corners. The extent of non-basal slip increases with increasing temperature and the wavy nature of the non-basal slip traces is associated with cross-slip on basal planes. In magnesium single crystals at room temperature it is extremely difficult to operate prismatic slip and the (1122) < (1123) system could not be detected in ideally oriented crystals. The reported (1122) < (1100) slip system remains unconfirmed.

A transmission electron-microscope study of deformed magnesium single crystals at room temperature also failed to reveal glissile dislocations with non-basal slip vectors. The characteristic dislocation configuration in the easy-slip region of the stress/strain curve consisted of a high density of edge dislocation braids parallel to basal planes and dislocation multipoles. These braids are formed by the cross-slip of screws, or by the sweeping up by edge dislocations of short isolated dipoles. Dislocations in (1011) planes have been reported in polycrystalline magnesium. The dislocation distribution obtained in magnesium thin foils is expected to be reliable provided the specimen temperature is kept below $\sim 70^\circ$ C.

The preference for non-basal slip in zirconium and titanium is still not completely understood. The (1010) < (1210) system predominates with secondary slip on (1011); (0001) slip is seen occasionally in bulk polycrystalline specimens and glissile dislocations on basal planes have been observed associated with hydride precipitates in titanium and zirconium. In titanium and zirconium there is no evidence of dislocation braids, which are a feature of metals deforming by basal slip.

Dislocations in titanium and zirconium are observed to climb when thin foils are heated in the electron beam. This behaviour has been erroneously attributed to cross-slip. Specimens of titanium deformed $>16%$ in tension or by rolling exhibit a polygonized structure (Fig. 22) and a high density of dislocation loops. The polygon cells are often elongated in the direction of the tensile axis or the rolling direction.

Kink-boundary formation is an important deformation mode in hexagonal metals. In magnesium, titanium, and zirconium complex kinking occurs after large tensile strains ($\sim 10%$) or at local stress concentrations. The bend plane can be a simple (1120) tilt boundary containing dislocations with the same Burgers vector (a-type, Table VI (1)). Bend planes parallel to (1010) are also frequently

![Stacking faults within a (1012)-type twin in titanium after tensile deformation. Faults in basal planes, A, and non-basal planes, B.](image-url)
observed, often associated with twins. These accommodation kinks are composed of two different a-type Burgers vectors.

There is no experimental evidence for bulk slip in the [0001] direction, but plastic deformation in the c-direction in indented zinc and magnesium has been accounted for in terms of kink-band formation.

2. Twinning modes

Possible dislocation models for twinning in these metals have been described by Westlake, Rosenbaum, and Chyung and Wei.

In a single-lattice structure (b.c.c. and f.c.c.) parent and twin structures are related by a homogeneous shear. This is not so in double-lattice structures (h.c.p.) and additional small atom displacements are required in a direction different from the lattice shear. These atom movements are called shuffles.

Twinning in (1012) planes occurs in all h.c.p. metals; this twinning mode has the lowest shear and involves simple shuffles in the plane of shear. In magnesium twinning occurs on other planes in the (1120) zone, e.g. (1101), (1103), (1105), (3304). To account for the observations of (1103) and (3304) twinning Crocker has proposed a double-twining mechanism involving retwinning of the primary twin. Unfortunately, it is difficult to obtain quantitative information on these modes because of the large amount of plastic deformation associated with the twins. Some discussions of atom movements in (1011) twinning are given by Westlake and Thornton.

In titanium, in addition to (1012), other twinning planes lying in the (1010) zone occur, e.g. (1211), (1212), (1213), (1214). The (1212) and (1214) are less common and their shuffles are complex. Shuffles in (1213) twinning are also exceptionally complex and this mode may also involve double twinning.

The magnitudes of the twinning shears are compared in Table IV. A value of 0.6 for the (1211) twin has been measured for zirconium and rhenium and seems more likely theoretically than the value of 0.2 reported previously. For (1012)-type twins the shear is a maximum in beryllium, but still small compared with other types of twin in h.c.p. metals.

The shape of a deformation twin is influenced by the twinning shear. When the shear is small the twin has a wide lenticular shape in section, since the twin interface can deviate considerably from the twinning plane without greatly increasing the twin-interface energy. (1012)-type twins are typical of this kind. In titanium the twins decrease in size in the order (1012), (1122), (1121), the last two types being much narrower than the first.

The mechanism of nucleation and growth of twins in hexagonal metals remains obscure, especially for the high-index twinning planes. There is considerable scatter in the values for the critical resolved shear stress for twinning in single crystals, e.g. 25-16,500 g/mm² in zinc. Twins may nucleate in perfect crystal at stress concentrations that raise the stress locally to the theoretical value for twin nucleation, i.e. 50 kg/mm² in zinc. Dislocation nucleation mechanisms are also invoked to explain the presence of twins having a high shear and the absence of twins with a low shear. For example, in single crystals of rhenium (c/a = 1.61), although the Schmid factor may favour (1012) twins, only (1121) twins with a large shear (s ~ 0.6) are detected, whereas in deformed polycrystalline rhenium (1012) twins are also produced. It is concluded that it is easier for slip to nucleate (1121) twins than (1012), since the latter are nucleated only by the complex slip required to maintain compatibility at grain boundaries in the polycrystal. The stress required to cause a pre-existing twin to grow is normally much
lower than the nucleation stress, although this does not appear to be the case in zinc at low temperatures. The behaviour during twin growth is sensitive to surface films, inclusions, and local high dislocation densities. Very irregular twin growth is possible when these obstacles are present.

An important factor influencing twin nucleation and morphology is the plastic accommodation necessary in the lattice adjacent to the twin interface. This has not been studied adequately as yet. A general discussion is provided by Christian and some experimental results have been reported for magnesium, zirconium, and h.c.p. intermetallics. More recently, the general problem of whether or not slip precedes twin nucleation has been discussed and related to the significance of a critical resolved shear stress for twinning. The fraction of tensile strain due to a single twin is given by

\[ l = \frac{v}{s} \]

where \( l \) = tensile strain; \( v \) = volume fraction of twin; \( s \) = twinning shear; \( m \) = Schmid factor (cos \( \phi \) cos \( \lambda \)).

The shape change in \( \{1012\} \) twinning is shown in Fig. 11a and \( b \). Twinning in \( \{1012\} \) is not possible when \( \epsilon/\sigma = \sqrt{3}/3 \). When \( \epsilon/\sigma > \sqrt{3} \) twinning is favoured by compression parallel and tension normal to the c-axis, but for \( \epsilon/\sigma < \sqrt{3} \) compression normal and tension parallel to the e-axis causes twinning. Similar considerations can be applied to \( \{1121\} \) and \( \{1122\} \) twinning found in titanium and the shape changes are depicted in Fig. 11c and d. Thus, unlike slip, twinning is very dependent on the sense of the applied stress. This can be clearly demonstrated by observing the displacements of twin interfaces produced by microhardness indentations.

VIII. Factors affecting the deformation modes

1. Von Mises criterion

A polycrystal requires five independent shear systems to undergo homogeneous strain without change in volume. A slip system is independent of others provided its operation produces a change in crystal shape that cannot be produced by a suitable combination of amounts of slip on other systems. The 6 types of slip system available in hexagonal metals are listed in Table X. Types 1 and 2, acting simultaneously but independently, will provide a total of 4 independent slip modes. This number assumes absence of cross-slip, which according to Kocks may increase the number of independent modes. The shape change produced by types 1 and 2 together is precisely equivalent to 3 acting alone. No extension parallel to the e-axis is possible using any of the systems 1–3, as they all involve \{1120\} slip directions. Since only \{1120\}-type slip directions have been reported in magnesium and titanium, the von Mises criterion cannot be satisfied.

Nevertheless, these metals are ductile, e.g., within the temperature range –196° to 20° C magnesium and titanium exhibit ductilities of \( \sim 5\% \) and \( \sim 10\% \) respectively. Alloyning magnesium with up to 14 at.-% lithium increased the ductility to \( \sim 12\% \), although the only change in deformation modes was a greatly increased amount of prism slip in \{1120\} directions.

Consequently, it was suggested that grain-boundary sliding and the twinning shear must contribute to the overall strain. However, this contribution was not considered sufficient to explain the observed ductilities, particularly at low temperatures, e.g., the complete conversion of a magnesium crystal to twin orientation will produce only \( \sim 7\% \) elongation. Tegart has therefore suggested that other non-basal slip systems must operate in h.c.p. metals. (Dislocations with \( \langle e + a \rangle \) Burgers vectors are expected to be particularly useful for increased ductility, Table V.) It is well known that alternative deformation modes may occur near grain boundaries and from the analysis of textures in titanium it was concluded that \( \{0001\} \) slip, \( \{1012\} \) and \{1122\} twinning occur with approximately equal critical resolved shear stresses, with slip on \{1100\} and \{1011\} at higher critical stresses. Furthermore, rolling textures in titanium and zirconium are readily accounted for if \{1123\} slip is allowed. Martin and Reed-Hill also found basal slip to be an important deformation mode in polycrystalline zirconium, whereas this mode is absent in single crystals. Further support for Tegart's hypothesis is provided by Baldwin and Reed-Hill, who observed \{1122\} slip traces in polycrystalline hafnium and zirconium deformed at –196° C.

Nevertheless, twinning can certainly play an important role. One effect of twinning is that in grains unfavourably oriented for slip the crystal is reoriented into a more favourable position. In magnesium single crystals, fracture in \{3034\} twins is preceded by very large plastic strains within the twins, and in certain polycrystalline magnesium alloys increased rollability is attributed to this double twinning mode.

### Table X: Independent slip systems in h.c.p. metals

<table>
<thead>
<tr>
<th>Slip system</th>
<th>Burgers vector</th>
<th>Slip direction</th>
<th>Slip plane</th>
<th>No. of slip systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>( \langle11\overline{2}0\rangle )</td>
<td>basal ( {0001} )</td>
<td>3 2</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>( \langle11\overline{2}0\rangle )</td>
<td>prism type I ( {10\overline{1}0} )</td>
<td>3 2</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>( \langle11\overline{2}0\rangle )</td>
<td>1st-order pyramidal type I ( {10\overline{1}1} )</td>
<td>6 4</td>
</tr>
<tr>
<td>4</td>
<td>c+a</td>
<td>( \langle11\overline{2}3\rangle )</td>
<td>2nd-order pyramidal type II ( {11\overline{2}2} )</td>
<td>6 5</td>
</tr>
<tr>
<td>5</td>
<td>c</td>
<td>( \langle0001\rangle )</td>
<td>prism type I ( {10\overline{1}0} )</td>
<td>3 2</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>( \langle0001\rangle )</td>
<td>prism type II ( {11\overline{2}0} )</td>
<td>3 2</td>
</tr>
</tbody>
</table>
Similarly, at room temperature and 77° K, (1012) and (1121) twinning, respectively, increase the ductility of zirconium.145,192 In a room-temperature test of textured polycrystalline zirconium,175 when the stress axis favoured twinning and for strains < 10%, the volume fraction of twins was linearly related to the total strain, although twinning contributed only < 15% to the total strain. However, at 77° K the contribution of (1121) and (1012) twinning to the total strain may reach nearly 100% at very low tensile strains192 (1–0.01%). The increase in strain-hardening rate,85 ductility, and strength186,193(a) in titanium deformed at low temperatures (–196° C) has also been attributed to twinning. Confirmation of the importance of twinning is provided by the brittleness of Cd–Mg alloy,193(b) in which twinning is eliminated by making c/a = √3.

There is general agreement that a fine grain size inhibits twinning.193(a)–195 This effect may be responsible for the reduction in ductility of titanium according to Russian workers.193(a) However Burrier et al.194 found increased ductility in fine-grain titanium (2000 grains/mm²) below – 156° C compared with coarse-grain (3–6 grains/mm²) titanium in which secondary twinning on (1122) twins caused cracking in twin interfaces. Cracks associated with twins are also found in magnesium.197 Twin-interface cracking has been observed in many hexagonal metals subjected to cyclic stresses.198 (A detailed interpretation by Armstrong196,199 of cracks associated with cyclic twinning in magnesium is open to doubt, as discussed by Partridge.198)

Although low ductilities can arise under certain conditions, Conrad14 has shown in a recent review that h.c.p. metals, e.g. titanium, zirconium, have strengths and ductilities at temperatures approaching absolute zero which indicate that these metals have a considerable potential for cryogenic applications. One must therefore conclude that Tegart’s explanation of the ductility is not unreasonable and in fact it is quite likely that twinning may activate other slip systems, either by generating locally high stresses around twins or by dislocation/twin interactions. There is some evidence for such twin interactions in h.c.p. metals.126,200,201 This is a particularly interesting possibility, since incorporation of dislocations with a-type Burgers vectors into (1012)-type twins can produce dislocations with (c + a)-type Burgers vectors,202 A stronger case has recently been made,203(b) and (c) based upon experimental data, for including twin systems as possible independent deformation modes; it is suggested that a suitable combination of twinning shears would be equivalent to (c + a) pyramidal slip. Clearly these aspects of the ductility problem deserve further study.

2. Schmid factor14,47,67,77,108

The unit stereographic triangle from the basal projection of the hexagonal lattice (Fig. 23) is formed by great circles through (0001), (1120), and (1010) poles. In Fig. 24 is plotted the variation of the Schmid factor with angle ϕ between the e-axis and the tensile-stress axis for some slip and twinning modes in titanium. Attempts have been made to derive the observed textures in magnesium and titanium by considering the Schmid factors for the various deformation modes.203

For basal slip,204 the resolved shear stress is zero for all (1120) slip vectors when the stress axis is parallel or normal to the e-axis. For other orientations in the standard triangle shown in Fig. 23 the (1120) direction is preferred, the Schmid factor becoming a maximum (0.5) when ϕ = λ = 45° (Fig. 18c). Stress axes lying in the great circle OB will cause slip equally in [1120] and [2110] directions. For prism slip205 and stress axes within the triangle, the resolved shear stress is a maximum on a single system (0110)[2110] and varies from maximum (stress axis normal to the e-axis) to zero (stress axis parallel to the e-axis). Stress axes on OB will cause duplex slip on (0110)[2110] and (1100)[1120] systems.

The range of variations of the orientation factors for all six (1012) twinning planes is depicted by the shaded region in Fig. 24; no twinning occurs when the tensile stress axis is normal to the e-axis, while many twin systems may occur when the axis is parallel to the e-axis. The most highly stressed (1121) and (1122)
twin systems are also shown for comparison in Fig. 24. When a compressive stress is applied parallel to the c-axis complex twinning takes place in magnesium,\(^{124}\) while beryllium deforms elastically before shattering\(^{76}\) at 200 kg/mm\(^2\).

During tensile deformation \(\lambda\) decreases and \(\phi\) increases; if \(\lambda > 45 > \phi\), the Schmid factor decreases initially with increasing strain, and geometrical softening can occur, i.e. for the same nominal applied stress a sudden large increase in strain is obtained.\(^{14,188}\) The phenomenon is pronounced in hexagonal metals with a limited number of slip systems. If \(\phi > 45 > \lambda\), the Schmid factor decreases with increasing strain and geometrical hardening occurs. (These effects are quite independent of any strain-hardening due to dislocation interactions.) Yield drops in magnesium\(^{206}\) and titanium\(^{421}\) have been attributed to geometrical softening. Discontinuous yielding attributed to twinning in titanium\(^{207,208}\) has not been confirmed.\(^{209}\) This type of yielding could also be due to the formation of metastable dislocation networks (in titanium\(^{216}\) and zinc\(^{211}\)).

However, it should be noted that at low temperatures serrated yielding, once attributed to dislocation avalanches or twinning, may be adequately explained in terms of adiabatic heating.\(^{212,213}\) This has been demonstrated in titanium deformed at \(-296^\circ\)C.\(^{65}\) Wein­

stein\(^{214}\) has compared the models proposed to account for the yield point in zirconium and concludes that a dynamic dislocation mechanism operating in very fine-grain material (\(< 1000\) mm) can best account for his observations.

3. Critical resolved shear stress (c.r.s.s.)

Although the orientation factor may be favourable, the resolved shear stress must exceed a certain value before the deformation mode becomes active. For example, the high resolved shear stress required to nucleate a twin may allow slip to occur having a smaller orientation factor. The macroscopic c.r.s.s. for \(\{0001\}\) \<1120\> and \(\{10\overline{1}0\}\)\<1120\> slip is known for many hexagonal metals\(^6,65\) and typical values are listed in Table IX for magnesium, titanium, and beryllium; these stresses correspond to the yield point in these materials when the strain sensitivity is \(~ 10^{-4}\).

The measured value of the c.r.s.s. depends very much on the measuring sensitivity and the imperfections present in the material tested. For example, Roberts and Brown\(^{220}\) found that a departure from elasticity in zinc occurred at \(~ 6\) g/mm\(^2\), compared with the macroscopic yield stress of \(20\) g/mm\(^2\). In recent years a microyield stress (or precision elastic limit, p.e.l.) has been determined for several metal single crystals\(^{821}\) and is defined as the stress to produce a residual plastic strain of \(~ 10^{-6}\).

In practice, a unique elastic limit is difficult to obtain in magnesium and zinc in the microstrain region, since non-linear behaviour occurs at very nearly zero stress.\(^{222}\) Two further definitions have been proposed to specify the behaviour of these materials.\(^{222}\) A specimen is loaded and unloaded at progressively increasing stresses until the linear stress/strain plot changes to a closed loop and finally to an open loop. Two microyield points, \(\tau_{\delta}\) and \(\tau_{\beta}\) are then determined. \(\tau_{\beta}\) is the resolved shear stress below which no area is detectable within the load/unload curves; this is the stress required to cause bowing of the dislocation lines in the basal planes. The anelastic limit, \(\tau_{\delta}\), is the lowest stress at which the loop is observed to be 'open' for a unidirectional stress; this is the stress required to activate dislocation sources. In magnesium, \(\tau_{\beta}\) and \(\tau_{\delta}\) have values of \(~ 5\) g/mm\(^2\) at \(~ 6\times 10^{-6}\) strain and \(~ 32\) g/mm\(^2\) at \(~ 10^{-4}\) strain, respectively. These values should be compared with the normally measured macroscopic yield points \(~ 10^{-4}\) strain sensitivity) in Table IX; these are the stresses required to move large numbers of dislocations.

The microyield of beryllium has been studied extensively because of its application to inertial guidance systems requiring extremely high material stability.\(^{221}\) In beryllium, \(\tau_{\beta}\) at \(5\times 10^{-5}\) strain is \(~ 10\%) of the macroyield stress (in magnesium \(~ 20\%) and \(\tau_{\delta}\) at \(~ 2\times 10^{-3}\) strain approaches the macroyield stress and after much larger strains than in magnesium.\(^{223}\)

4. Temperature-dependence of the critical resolved shear stress

In cadmium, zinc, magnesium, and beryllium basal slip is only slightly temperature-dependent below room temperature,\(^4\) unlike titanium which exhibits a much larger temperature-dependence during basal slip\(^{216}\) (Fig. 25). At similar temperatures prismatic slip in all the above metals is very strongly temperature-dependent. Magnesium and titanium are compared in Fig. 25; in magnesium there is an increase by two orders of magnitude in the c.r.s.s. for prism slip when the temperature is lowered from 300 to \(-196^\circ\)C. The weak temperature-dependence above room temperature can be accounted for in terms of the temperature-dependence of the shear modulus.

The flow stress in the basal planes of magnesium appears to be controlled mainly by the internal stress fields from excess dislocations of one sign present in the dislocation braids.\(^{125,126}\) The constriction of screws before cross-slip, the glide of jogs, and interaction with point defects will contribute to the temperature-dependent part of the flow stress at low temperatures.

The origin of the temperature-dependence of the flow stress in non-basal planes has not been resolved completely. In magnesium the easy-glide region of the
stress/strain curve, characteristic of basal slip,\textsuperscript{252, 256, 258} is absent during non-basal slip\textsuperscript{144} and a very large work-hardening rate is obtained, particularly in rhenium.\textsuperscript{252, 256} The following processes require thermal activation and may be rate-controlling during non-basal slip, depending on the temperature range and impurity levels:\textsuperscript{5, 527}

2. Overcoming the strain fields associated with impurity atoms.
3. Constriction of screw segments dissociated in the basal plane.

Using the criteria of interplanar spacing and planar atom density, the intrinsic Peierls–Nabarro stress might be expected to be smaller, and therefore non-basal slip to predominate, when $c/a < \sqrt{3}$. Clearly, these criteria do not allow a reliable prediction of the predominant slip plane in h.c.p. structures, since basal slip predominates in cobalt, magnesium, and beryllium and in the intermetallic compounds $\mathrm{Ag}_2\mathrm{Zn}$ ($c/a = 1.57$),\textsuperscript{257, 258} and $\mathrm{Cd}_2\mathrm{Ge}$ ($c/a = 1.63$).\textsuperscript{259} In beryllium the behaviour cannot be attributed entirely to impurities, since increasing purity decreased the c.r.s.s. for both prism and basal slip, but increased the ratio c.r.s.s. for prism slip/c.r.s.s. for basal slip from 5:1 to 38:1.\textsuperscript{219}

Lowering the stacking-fault energy will favour basal slip as it becomes more difficult to constrict the screw dislocations before cross-slip into prism planes; this clearly applies to cobalt. An analogous factor in intermetallic compounds is the ordering parameter, since increasing order should raise the fault energy and enhance prismatic slip.\textsuperscript{220} This agrees with the slip produced in $\mathrm{Mg}_2\mathrm{Cd}$ upon ordering.\textsuperscript{116}

The addition of lithium to magnesium raises the c.r.s.s. for basal slip,\textsuperscript{220} while the c.r.s.s. for prism slip is lowered,\textsuperscript{221, 222} but there is only a minor effect on the stacking-fault energy,\textsuperscript{223} which is large in all the hexagonal metals with the exception of cobalt (Table III). (The value of 300 ergs/cm\textsuperscript{2} for magnesium was obtained for a fault with one nearest-neighbour impurity;\textsuperscript{224} the fault energy produced by dissociation may be greater.)

Dorn and his co-workers have concluded that the Peierls–Nabarro stress is rate-controlling during prism slip in magnesium in the temperature range 23 to 177\textdegree C, while above 177\textdegree C the thermally activated cross-slip model is applicable. The reason for the reduction in the Peierls–Nabarro stress in the prism planes by lithium is not known.

In titanium containing $>100$ ppm interstitial impurity, the thermal component of the flow stress below 300\textdegree K is strongly dependent on the impurity content, and the rate-controlling process is consistent with that for overcoming impurity atoms in the prism planes.\textsuperscript{223 (a) and (b), 224} For titanium containing $<100$ ppm impurity\textsuperscript{216, 217} and in beryllium\textsuperscript{226 (a)} the rate-controlling process is supposed that for overcoming the Peierls–Nabarro stress. It remains, of course, to explain why prism slip is preferred to basal slip in titanium and it would be interesting to know the effect of purity on the c.r.s.s. for basal slip in this metal. Tyson\textsuperscript{52} has concluded that elastic anisotropy alone cannot account for the slip planes in h.c.p. metals and the stacking-fault energy must be of primary importance. This may be so in some cases, but anisotropic elasticity theory can account for slip in beryllium according to Roy.\textsuperscript{226 (b)}

A number of workers have noted the high density of dislocation loops and dislocation dipoles in h.c.p. metals after prism slip, e.g. in cadmium,\textsuperscript{56} zinc,\textsuperscript{56} titanium,\textsuperscript{130, 135} zirconium,\textsuperscript{134} and beryllium.\textsuperscript{236} The glissile screw dislocations become severely jogged and this undoubtedly contributes to the temperature-dependence of this slip mode. Furthermore, if only dislocations with $\langle110\rangle$ Burgers vectors are readily mobile, as in titanium, zirconium, and beryllium, intersecting dislocations will produce jogs in non-basal screw dislocations but not in basal screw dislocations and this may explain the different rates of work-hardening in these two planes.

**IX. Conclusions**

The incentive to improve and apply h.c.p. metals lies in the specific strength properties of alloys based on magnesium,\textsuperscript{237} titanium,\textsuperscript{238, 239} and beryllium.\textsuperscript{239}

More ductile alloys have been obtained by adding lithium to magnesium\textsuperscript{144} and either copper or aluminium to beryllium.\textsuperscript{242, 243} Titanium, while exhibiting high specific strength at elevated temperatures,\textsuperscript{238, 239, 244} is also particularly ductile at low temperatures and resistant to corrosion and is therefore especially favoured for cryogenic\textsuperscript{84, 85} and, e.g., surgical implant applications.\textsuperscript{245}

A considerable improvement in the mechanical properties of hexagonal metals may be possible but to exploit their full potential a better understanding of the interdependence of slip and twinning is required. For enhanced ductility particular attention must be paid to the factors controlling non-basal slip in the $\langle c + a \rangle$ directions. Experiments in the microstrain region, together with direct studies of the dislocation configurations in the metal tested, are making a valuable contribution to the fundamental data on the behaviour of hexagonal metals.

Recent experiments suggest several possible approaches in future research. For example, a careful control of the volume fraction and the form of dispersed phases in hexagonal metals may well enhance ductility, since Sherby\textsuperscript{246} has demonstrated increased ductility in zinc containing tungsten particles and Westlake\textsuperscript{247} has dispersion-hardened zirconium with hydride precipitates (normally considered detrimental).

It has also been suggested that cold working at very low temperatures may increase the strength at higher-temperatures to a greater extent in h.c.p. metals,\textsuperscript{44} provided the higher temperature is below the recovery temperature. Mechanical twins are known to increase the damping capacity of metals\textsuperscript{248, 249} and Reed-Hill\textsuperscript{et al.}\textsuperscript{250} have shown that controlled damping capacity can be induced in zirconium at room temperature by suitable prestrain at low temperatures. The effect is attributed to stress-induced twin-boundary movement and may have important commercial applications. The general problem of propagation of twins in work-hardened material has been considered only briefly for h.c.p. metals.\textsuperscript{251}

Finally, there is still scope for the development of preferred orientation textures\textsuperscript{253, 254, 255} and these could be significantly affected by the deliberate selection of certain twinning modes during fabrication, e.g. by shock-loading\textsuperscript{257, 258} followed by suitable heat-treatments.\textsuperscript{259}
Chapter 2
Microstructures of Magnesium and Titanium
Deformed in Tension

In this and following chapters polycrystalline specimens were made from 1/16" thick sheet. Cadmium, zinc and magnesium specimens of 99.99\% purity were annealed to give coarse grain sizes and were chemically polished in ice cold aqueous nitric acid prior to deformation and optical microscopy. Thin foils of magnesium were prepared by electropolishing in the normal methyl alcohol/nitric acid bath\(^{124}\).

Titanium specimens were made from high purity (120 VPN) polycrystalline sheet. Annealing was performed in vacuum (10\(^{-5}\) mm), first at 600°C and then at 800°C to give a grain size of \(\sim 5\) grains/\(\text{mm}^2\). Specimens were studied either after chemical or electropolishing as described in Appendix 1.

All specimens were deformed either in an Instron or a Hounsfield tensile machine at a strain rate of \(\sim 0.02\) inches/min.

In this chapter the microstructure characteristic of unidirectionally deformed material will be described, although a quantitative correlation between dislocation structure and stress/strain curves has not been attempted. In later chapters these observations will be compared with those made on specimens subjected to cyclic stresses.

2.1 Magnesium
Basal slip predominated and after 5\% strain the dislocation configurations consisted of edge dislocation braids. In foils oriented almost parallel to the basal plane the braids appeared as in fig. 2.1; similar configurations have been reported in single crystals and described in detail\(^{124,125}\). In foils oriented parallel to prism planes, non-basal dislocation segments are revealed (fig. 2.2). Large jogs on dislocations are also apparent, together with dipole loops lying in non-basal planes (fig. 2.3). These presumably arise when basal screw dislocations cross-slip on to non-basal planes. The amount of non-basal slip is generally small, as shown by the small steps in fig. 2.3, although occasional larger steps are evident in fig. 2.2.

Only \{10\(\overline{1}\)2\} twins were found in magnesium. A typical small twin is shown in fig. 2.4. An accommodation kink boundary extends from the twin tip to a grain boundary and numerous dislocations are visible within the twin.
Fig. 2.1 Böge dislocation braids in magnesium after 5% strain.

x 30,000

Fig. 2.2 (10\overline{1}0) plane in magnesium, showing long segments of dislocation lying in non-basal planes after 13% strain.

x 16,000

Fig. 2.3 (10\overline{1}0) plane of magnesium. Loops and dipoles in non-basal planes after 13% strain.

x 35,000
A larger twin in fig. 2.5 has two kinks extending from the twin tip. The dislocation structure in the twins is usually similar to that shown in fig. 2.2, with many long dislocations lying in basal planes (fig. 2.6). However, at higher strains (~10%), the twins appeared as in fig. 2.7. Short ribbons of stacking fault protrude from the twin boundary into the parent, and longer ribbons extend across the twin; all the faults lie in basal planes.

Another feature at higher strains were bands of dislocations within twinned crystal (fig. 2.8). These were formed when two twins belonging to the same system impinged; parent dislocations trapped between the twins gave rise to the dislocation bands in the twin.

When twins impinged on other twin systems or grain boundaries, extensive local slip occurred (fig. 2.9). This effect is readily apparent in optical micrographs and has been described in the literature.

2.2 Titanium

Prism slip predominated and no evidence for extensive basal slip was found. However, basal slip appeared to accommodate hydride needles that nucleated after electron beam heating (fig. A1.3). At low strains (~1500 psi), the deformation varied greatly in different grains (fig. 2.10). The dislocations lie mostly in their slip planes (figs. 1.21 and 2.11) and appear as long screws in basal plane foils (fig. 2.11). Small loops and jogs are frequently associated with these screws; in fig. 2.12 an inclined prism plane contains a large number of small loop defects. Similar observations have been made in titanium single crystals. After 10% strain, 2400 psi, interactions between two systems are apparent as short segments of dislocation lying parallel to the c-axis and having the third Burgers vector (fig. 2.13). A possible hardening effect due to this interaction has been suggested by Damiano and Herman in Be. After 15% strain, the dislocation density is generally much greater, with large numbers of dipoles and severely jogged dislocations (fig. 2.14 - 2.15).

At these strains the first evidence of sub-structure is apparent, as long low-angle boundaries parallel to the traces of the predominant prism slip planes (fig. 2.16).

In some grains extensive kink boundary networks are also present. These appear to act as barriers to dislocations, which can be seen entangled in the boundary in fig. 2.17.
Fig. 2.4 Small \{10\overline{7}2\} twin nucleated at a grain boundary in magnesium. Note accommodation kink boundary at A. x 17,000

Fig. 2.5 Larger \{10\overline{7}2\} twin and two kink boundaries (A, B) radiating from twin tip. x 14,000

Fig. 2.6 \{10\overline{7}2\} twin in magnesium. Twin boundaries at A, B, dislocations in basal planes at C. x 30,000
Fig. 2.7  
\{10\bar{1}2\} twin in magnesium. Stacking faults in basal planes cross the twin and occur in the parent adjacent to the twin interface.

x 40,000

Fig. 2.8
Dislocation debris at A where two twins on the same system impinged Parent crystal in B.

x 20,000
Fig. 2.9 Extensive local slip produced when a twin impinged on a grain boundary AB in magnesium.  

x 12,000

Fig. 2.10 Optical micrograph of titanium strained 34 showing prism slip  

x 300

Fig. 2.11 Long screw dislocations in prism planes in titanium strained 34.  

x 22,000

Fig. 2.12 Small defects and jogged dislocations behind a screw dislocation in titanium  

x 48,700
Fig. 2.13
Dislocation in titanium after 10% strain showing interactions between two slip systems is becoming more frequent. x 20,000

Fig. 2.14
Dislocations in titanium after 15% strain, showing high density of dipoles. x 28,000
Fig. 2.15 Small dislocation loops in titanium after 15% strain

x 45,000

Fig. 2.16 Initial stages of substructure formation in titanium strained 15%

x 16,000

Fig. 2.17 Kink boundary in titanium strained 15%

x 20,000
At strains of ~25%, the optical slip traces are less straight (fig. 2.18) and well developed polygon structures are developed as shown in fig. 2.19.

Only two types of twin were found in titanium, namely \{10\bar{1}2\} and \{11\bar{2}1\}. They are readily distinguished optically, the \{10\bar{1}2\} appearing wide and lenticular and \{11\bar{2}1\} forming many narrow intersecting lamellae (fig. 2.20). Some grains contained extensive twinning after 10% strain, and it became difficult to identify individual twins in thin foils (fig. 2.21). For this reason a stereographic technique was developed which facilitated the identification of twins using electron diffraction patterns from twin and parent; the technique is described in Appendix 2.

The normal appearance of twins is shown in fig. 2.22; well developed kink boundaries are often associated with the twins, and appear to traverse the twin without difficulty. However, certain twins contained bands of high dislocation density near the twin boundary. This is shown in a \{10\bar{1}2\} twin in fig. 2.23. The tip of this twin is shown at higher magnification in fig. 2.24; here the dislocation band is absent. Another twin is shown in fig. 2.25; dislocations in the bands are difficult to resolve, but appear to be composed of severely jogged dislocations and occasional stacking faults.

Stacking faults were often found within twins. In addition to basal plane faulting, non basal faults were also visible in \{10\bar{1}2\} twins (fig. 2.27 and 2.28). The faulting was also present in the parent adjacent to the twin boundary. A narrow \{11\bar{2}1\} twin is shown in fig. 2.26. Small faults are visible throughout the length of the twin, but the plane of these faults was not identified. Even in specimens strained to fracture, stacking faults were never observed except associated with twins.

Often bands of dislocations extended beyond the twin tip (fig. 2.29). This is observed in b.c.c. metals; the dislocations are considered to be slip dislocations nucleated ahead of the twin to relieve the stresses or to be emissary dislocations nucleated at the twin boundary. In the case of \{11\bar{2}1\} twinning in fig. 2.29 the dislocations ahead of the twins appear to be jogged. Their configuration suggests that these dislocations may have been produced when the twins contracted after the stress was removed. A similar configuration of dislocations is found in magnesium after untwinning and is described in Chapter 3.
Fig. 2.18
Optical micrograph of titanium strained 25%, showing wavy prism slip traces
x 330

Fig. 2.19
Substructure in titanium after 25% strain.
The cell walls lie approximately parallel to the traces of the prism slip planes
x 10,000
Fig. 2.20  Wide \{10\bar{1}2\} type twins (A) and narrow \{11\bar{2}1\} type twins (B) in titanium.

x 300

Fig. 2.21  High twin density in titanium after 10% strain

x 9000
Fig. 2.22 twin in titanium. Note parallel twin boundaries and low angle boundary traversing twin at A. x 23,000
Fig. 2.23  \{10\overline{1}2\} twin in titanium, showing band of dislocations in twin beside twin boundary (A)  
\[ \times 6000 \]

Fig. 2.24  Tip of twin in Fig. 2.23  
\[ \times 17,500 \]

Fig. 2.25  \{10\overline{1}2\} twin in titanium. Twin boundaries at A. 
Dense band of dislocations in twin  
\[ \times 20,000 \]

Fig. 2.26  Narrow \{11\overline{2}1\} twin in titanium, showing many stacking faults traversing twin.  
\[ \times 30,000 \]
Fig. 2.27 Stacking faults in \{10\bar{7}2\} twin and in parent titanium $\times 26,000$

Fig. 2.28 Basal plane and non-basal stacking faults in \{10\bar{7}2\} twin in titanium. Basal plane fault at A, \{10\bar{7}0\} fault plane at B. Unidentified fault plane at C

Fig. 2.29 Dislocation bands ahead of twins in titanium. Their configuration suggests they were produced during untwinning. $\times 13,000$
CHAPTER 3

Irregular Twin Growth and Contraction

The stages in the formation of a twin are conveniently divided into a nucleation stage, which is sometimes difficult and requires high stresses, and a growth stage which proceeds at lower stresses. The factors controlling twin nucleation in h.c.p. metals are not at present well defined; this is discussed further in chapters 5 and 6. The present chapter is concerned with twin growth and contraction by the progressive displacement of twin boundaries.

The models proposed for twin growth involve twinning dislocations gliding in planes parallel to the twinning plane. Suitable choice of Burgers vectors can provide the necessary macroscopic shear, but additional shuffles are required in the double lattice structure as discussed in Chapter 1. To minimise interfacial energy, twin interfaces tend to be planar i.e. coherent. When the twin boundary deviates from the twinning plane (incoherent twin boundary) the number of twinning dislocations and the interfacial energy increases.

Incoherent twin boundary regions are produced in \{10\bar{1}2\} twins in zinc and magnesium by the stresses around a microhardness impression \[^{145,176,270}\]. Some examples are shown in fig.3.1a for a \(10\bar{1}2\) twin lying in a surface parallel to \((10\bar{1}0)\). Three impressions are visible, one in the twin and two in the parent. Since twin growth causes contraction and extension normal and parallel to the \(c\)-axis respectively, the compressive stresses acting radially around an indenter cause the displacements shown diagrammatically in fig.3.2. Below the indented surface (fig.3.1b) the twin has grown locally to relieve the stress (at A) produced by the impression in the twin and two small volumes of twin are nucleated at B below the impressions in the parent. The incoherent twin interfaces are clearly unstable and degenerate into several narrow and more coherent twin interfaces. The twinning dislocations were spaced about \(4\bar{1}\) apart in the unstable interfaces \[^{145}\].

The absence of extensive elastic twinning in metals has been attributed to the occurrence of slip modes which interfere with the twinning process \[^{149}\]. This is consistent with the hysteresis effects often associated with twinning \[^{149,248}\], and the fact that untwining may be more difficult than either twin growth or twin nucleation \[^{271}\].
TWIN BOUNDARY DISPLACEMENTS IN MAGNESIUM PRODUCED BY AN INDENTER
experiments have shown that in non-metallic crystals lattice defects are generated during twin growth and contraction\textsuperscript{272,273}.

There are few experimental observations on the movement of individual interfaces in h.c.p. metals, although the reversibility of \{10\overline{1}2\} twinning has been demonstrated in zinc, magnesium and titanium for nearly coherent interfaces. In this chapter it is shown that a twin interface often becomes incoherent and that lattice imperfections in the form of dislocation debris and microtwins may be generated in the path of a moving twin boundary. The conditions favouring the formation of these microtwins are considered and compared with the effects of surface oxidation on subsequent twin growth. Secondary twinning in the parent twin may also prevent the simple reversal of the twin growth process; some secondary twinning effects in magnesium are discussed briefly.

3.1 Twin Growth

The most important factor influencing the movement of a twin boundary is the dislocation structure in the surrounding crystal. In fig.3.3 a twin in cadmium has grown and basal slip has subsequently impinged on the twin and caused the irregular interface. In magnesium (fig.3.4) twin growth followed slip in the parent and steps are present in one interface. A similar sequence is shown in titanium in fig.3.5. The \{10\overline{1}2\} twins in titanium frequently exhibit well developed facets (fig.3.6a) which lie parallel to the traces of prism slip. This has also been reported in zirconium. These incoherent facets sometimes degenerate as shown in fig.3.6b in a manner similar to that depicted in fig.3.1. Consequently small microtwins in parent orientation become embedded in the growing twin.

3.2 Twin Contraction

\{11\overline{2}1\} twins in titanium normally appear as narrow parallel lamellae (fig.2.20). When such twins are produced by bending, reversing the stress causes very irregular twin interfaces to develop (fig.3.7). However only one interface in each twin appears to have moved. This is frequently observed and many workers have concluded that one twin boundary is more mobile than the other\textsuperscript{145,274}. Similar behaviour is shown in fig.3.8; here one twin interface is irregular on a small scale (at A) whilst the other twin system has lengths of coherent interface between incoherent regions (at B) with facets again developing parallel to the prism slip traces. Two intersecting \{11\overline{2}1\} twin systems are shown in fig.3.9 after
Fig. 3.5 Irregular twin interface in $\{10\overline{1}2\}$ twin in titanium

Fig. 3.6a Facets developed in $\{10\overline{1}2\}$ twin interface in titanium. Note effect is confined to one interface.

Fig. 3.6b Breakdown of twin interface facet in titanium. Small volumes of parent oriented crystal embedded in twin at A.

Fig. 3.7 Irregular $\{11\overline{2}1\}$ twin interface produced during untwining.
Fig. 3.8 Irregular \{112\} twin interfaces in titanium after untwinning. Note small accommodation kinks near B and facets parallel to prism slip traces. \(x\ 780\)

Fig. 3.9 Untwinning on two intersecting \{112\} systems in titanium. One system almost completely untwinned except for intersecting portions e.g. at A and small twin fragments at B. \(x\ 780\)

Fig. 3.10 Twins in magnesium
(a) Chemically polished. Note absence of etched interface between secondary twins and parent matrix at A.
(b) Same area as (a) after untwinning. Normal twin contraction in twin 2. Contraction of parent twin segments at B. Note absence of surface tilt in secondary twins at A. \(x\ 620\)

Fig. 3.11 (10\bar{1}2) twin in magnesium after untwinning, showing stacking fault and dislocation debris. \(x\ 30,000\)
untw inning. The points of intersection remain, often associated with accommodation kinks (at A). One twin system has mostly untwinned completely, but small twin fragments are visible at B.

A more complex untwinning sequence may arise when secondary twinning occurs. In fig.3.10a a twin containing secondary twins produced during untwinning slightly is shown after chemical polishing. Since no interface etched up at positions marked A the secondary twins containing A must be near the matrix orientation. This is possible if the secondary twins occur on the second undeformed twinning plane e.g. if the parent twin interface is parallel to (1012) twinning plane and the secondary twin parallel to (1012) plane, the misorientation between the secondary twin and matrix is $\approx 7^\circ$. If suitable mobile kink boundaries are distributed in this region, the secondary twin/matrix interface will approximate to a low angle boundary.

To cause untwinning the stress on the specimen was reversed (fig.3.10b). Twin 2 untwinned by contracting in the normal manner, as revealed by the displaced boundaries. In twin 1 the segments of parent twin have each untwinned as shown by the displaced boundaries at B but no surface tilt is apparent in the secondary twins at A: thus the latter no longer appear to behave as twins.

The appearance of twins in thin foils taken from tensile deformed materials has been described in Chapter 2. The twin may be relatively free of dislocations or contain the normal slip dislocations. However sometimes a high dislocation density is apparent in the twin near the twin boundary. After untwinning, the majority of twins present in thin foils showed a very high dislocation density in the parent crystal adjacent to the twin boundary. This debris was often difficult to resolve, but appeared to be composed of dipole loops and severely jogged dislocations. Stacking faults were also found in these regions. Examples of basal plane faults and dipoles in magnesium are shown in figs.3.11 and 3.12. The former is similar to fig.2.29 showing dislocations extending from a twin in titanium. In fig.3.12a the foil is nearly parallel to the basal plane and the dipoles lie normal to the screw dislocation lying in the twin boundary. In fig.3.12b the foil is parallel to a prism plane and the dislocations and stacking faults lie parallel to basal plane traces; note the low dislocation density in the parent away from the twin boundary. A similar debris
Fig. 3.12a. Dislocation dipoles beside (10\overline{1}2) twin in magnesium. Twin A, parent B parallel to (0001).

$\times 40,000$

Fig. 3.12b. Dislocation debris beside (10\overline{1}2) twin in magnesium after untwinning. Twin A, parent B parallel to (1\overline{1}00).

$\times 20,000$
distribution is apparent adjacent to \{1121\} twin boundaries in titanium after twinning and untwining (fig. 3.13). The debris in these examples is believed to arise from interactions between the dislocations glissile in the twin and the moving twin boundary during untwining.

3.3 Behaviour of Incoherent Twin Interfaces

Since incoherent twin interfaces are produced during growth and contraction of twins further experiments were carried out to study the effect of the presence of such interfaces on subsequent twin boundary movement. Zinc and magnesium polycrystals were used having a basal plane texture. Incoherent regions were introduced by a Reichert Microhardness tester with a pyramidal indenter under a 5 grm load. The deformation produced in h.c.p. metals by microhardness indentations has been studied in detail. The indented twins in zinc and magnesium are shown schematically in figs. 3.14 and 3.15. The sense of the displacements can be deduced from fig. 3.2, remembering that the dimensional changes produced by \{10\overline{1}2\} twinning in zinc are in the opposite sense to those in magnesium.

In order to show the sequence of events during twin growth and contraction, the twin boundaries were repeatedly displaced and chemically polished: surface tilts produced by the boundary displacements are apparent before polishing while after polishing surface grooves mark successive boundary positions.

A zinc specimen was twinned, chemically polished and four indentations made within a twin. Fig. 3.16a shows that twin contraction occurred to produce incoherent twin boundary regions e.g. at x, in agreement with previous work. This twin was then grown further fig. 3.16b. One boundary was displaced more than the other and in this interface small boundary curvatures are present at A, B, C and D, opposite the original incoherent boundary regions; the cusps are joined to the original boundary position by straight lines corresponding to small surface tilts. These features are clearer after a slight chemical polish (fig. 3.16c), when small secondary twins are revealed within the parent twin at A. The twin was grown still further and chemically polished and successive positions of the twin boundaries can be seen in fig. 3.16d. The other boundary was also displaced and small secondary twins now appear at B' and additional twins at A. Boundary curvature is present at A, A', C' and D' but only surface tilts remain to mark the path of the boundary to B, C and D. (At T a twin on another system impinged on the twin being studied).
Fig. 3.13 Dislocation debris beside (1121) twin in titanium after untwinning. Twin A, parent B.

x 60,000
Schematic illustration of the twin interface displacements produced in a (1012) twin by the stresses around a micro-hardness indentation. Indentation made in twin lying in a (0001) surface.

Fig. 3.14 Twin in zinc. Local contraction of the twin occurs and the twin interface is displaced inwards.
(a) Section parallel to (1210)
(b) Section parallel to (0001)
When the boundary is displaced in the direction of the arrows, microtwins having the parent orientation may remain in the twin.

Fig. 3.15 Twin in magnesium. Local growth of the twin occurs and the twin interface is displaced outwards.
(a) Section parallel to (1210)
(b) Section parallel to (0001)
When the boundary is displaced in the direction of the arrows microtwins having the twin orientation may remain in the parent.
TWINNING SHEAR DIRECTION FOR CONTRACTION.

ACCOMMODATION KINK BOUNDARIES.

ZINC MATRIX (I210)

TWINNING SHEAR DIRECTION FOR GROWTH.

ACCOMMODATION KINK BOUNDARIES.

MAGNESIUM MATRIX (I210)

Fig. 3.14

Fig. 3.15
Fig. 3.16 Effect of incoherent twin interfaces on the growth of a (10\overline{7}2) twin in zinc. Parent surface approximately parallel to (0001)

(a) Surface twinned, electropolished, and twin indented. Twin boundaries displaced according to fig. 3.14b

(b) Twin grown

(c) Surface electropolished

(d) Twin grown further and surface electropolished (see text)
Twin growth and contraction was studied in magnesium. A twin was formed and indented to produce outward displacements of the twin boundary and hence incoherent regions\textsuperscript{145}. These regions persisted during small increments of twin growth because of the residual stresses remaining in the lattice after the indenter is removed\textsuperscript{147}, but eventually after large boundary displacements the boundary reverts to a normal planar interface: no microtwins were found behind these moving incoherent regions.

A sequence illustrating the behaviour of incoherent regions in magnesium during untwining is shown in fig. 3.17. The incoherent regions are produced at A, B, C and A', B', in twin 1 by indenting and similarly in twin 2: note the accommodation kinks in the parent matrix beside the boundaries AC and DE. Subsequent bending caused twins 1 and 2 to grow slightly and fresh twins on the same system to nucleate and grow at 3 and 4 in fig. 3.17b: incoherent regions are produced in twin 4 at C and B and in twin 3 at D and E, by the residual stresses. The stress was then reversed to cause untwining (fig. 3.17c): the incoherent regions at B, C and E were rejected by the contracting twins and remained in the parent lattice as microtwins associated with accommodation kinks. In addition a small twin segment from twin 5 also remained at F after an apparently perfect twin tip contracted.

3.4 Effect of Surface Oxidation on Twin Growth

Twin growth in magnesium was markedly affected by prior surface oxidation. Specimens were chemically polished and oxidised by heating in air. When during subsequent twinning a twin boundary encountered large oxide particles, local boundary displacements occurred e.g. at A, in fig. 3.18. These displacements are similar to those produced in twins by indenting the basal plane of magnesium as shown in fig. 3.2.

Fig. 3.19 shows a twin growth in a surface after oxidising to produce finer oxide particles. In the twin matrix small secondary twins are associated with oxide particles. The traces of the secondary twinning planes are parallel to the parent twin plane trace and arise from the pinning of the moving boundary by the oxide particles. The pinning points produce incoherent boundary regions which subsequently become embedded in the growing twin as microtwins of matrix orientation. The sequence is analogous to the formation of microtwins from moving incoherent twin boundaries in zinc (para. 3.3).
Fig. 3.17 Effect of incoherent twin interfaces on the growth and contraction of a (1012) twin in magnesium. Parent surface approximately parallel to (0001).

(a) Surface electropolished, twinned and twin indented. Twin boundaries displaced as in fig. 3.15b.

(b) Twin grown further

(c) Twin partially untwinned

(d) Twin untwinned further

(see text)
Effect of surface oxidation in air at 400°C on subsequent \( \{10\overline{7}2\} \) twin growth in magnesium.

**Fig. 3.18** Local twin boundary displacement due to oxide particles at A.  
\[ x \ 400 \]

**Fig. 3.19** Microtwin associated with oxide particles  
\[ x \ 225 \]

**Fig. 3.20** Twin boundary pinning and twin nucleation  
**Fig. 3.21** associated with oxide particles  
\[ x \ 225 \]
A more complex twin configuration due to oxidation is sometimes observed and an example is shown in figs. 3.20 and 3.21: the oxide particles have pinned the moving boundary and also caused twins to occur on other systems adjacent to the growing twin interface.

3.5 Discussion

The results show that slip dislocations cause irregular twin interfaces to develop and dislocation debris to be formed by interactions at moving twin interfaces. Incoherent regions in twin interfaces may give rise to microtwins during subsequent twin interface movement.

The effect of local compressive stresses produced by a microhardness indenter on deformation twins in c.p.h. metals is discussed elsewhere. In the present experiments microtwins sometimes formed during the displacement of incoherent twin boundary regions. The appearance of indented twins in the basal planes of zinc and magnesium is shown schematically in figs. 3.14 and 3.15. The twin boundaries are displaced inwards in zinc and outwards in magnesium and accommodated by suitable kink boundaries. If the twin boundaries are subsequently moved towards the centres of curvature of the incoherent regions (arrowed in figs. 3.14 and 3.15) microtwins in the twin orientation are produced in the parent magnesium and microtwins in the parent orientation in the twin in zinc: these displacements correspond to twin contraction in magnesium and twin growth in zinc. Alternatively in figs. 3.14 and 3.15 the matrix can be considered to be the twin and the twin to be the matrix: the movement of the twin boundary in the same direction to produce microtwins will then be equivalent to twin growth in magnesium and twin contraction in zinc.

Whenever a twin encounters local lattice distortions, the twin will attempt to relieve the strain by producing local boundary displacements. From the known behaviour of twins under stress (Chapter I.IV) it is possible to define approximately the conditions under which microtwin formation will be favoured: this has been done in Table 3.1 for zinc and magnesium. When the conditions are favourable, the magnitude of the stress will be the deciding factor since microtwins will tend to occur when the displaced interfaces approach the maximum degree of incoherency.

The mobility of the parent twin boundary will be increased by the rejection of the incoherent interfaces in the form of microtwins and the latter, when associated with accommodation kink boundaries are expected to be particularly stable configurations, although the microtwins may remain
**TABLE 3.1**

**EFFECT OF RESIDUAL STRESSES ON MICROTWIN-FORMATION DURING TWIN GROWTH AND CONTRACTION**

<table>
<thead>
<tr>
<th>Stress System in Parent Matrix</th>
<th>Twin in Magnesium</th>
<th>Twin in Zinc</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>growing</td>
<td>contracting</td>
</tr>
<tr>
<td>Compressive stress parallel to the a-axis</td>
<td>–</td>
<td>microtwins formed in parent matrix</td>
</tr>
<tr>
<td>Compressive stress parallel to the c-axis</td>
<td>microtwins formed in twin</td>
<td>–</td>
</tr>
<tr>
<td>Tensile stress parallel to the a-axis</td>
<td>microtwins formed in twin</td>
<td>–</td>
</tr>
<tr>
<td>Tensile stress parallel to the c-axis</td>
<td>–</td>
<td>microtwins formed in parent matrix</td>
</tr>
</tbody>
</table>
extremely incoherent. The stabilising effect of kink boundaries on incoherent twin interfaces is consistent with the rejection of the twin tip, a region of high incoherency, by the twin 5 at F in fig. 3.17d and for the greater stability of wedge shaped twins over that of parallel sided twins in bismuth \(^{148,274}\).

Oxide films are known to increase the twinning stress, but the mechanism is obscure\(^5\). The effect of oxidation on twinning in the present experiments are attributed to local surface stresses set up in the metal by the oxide film. The volume ratio of magnesium oxide is < 1 according to the Pilling-Bedworth rule, which suggests compressive stresses should be generated in the metal at the metal/oxide interface\(^{276}\). In practice there is no simple relationship between this volume ratio and the magnitude\(^{276}\) and sign\(^{277}\) of the stresses in the oxide film and it is not yet possible to predict the effect of oxide films on twin growth. However oxide particles can be responsible for the outward and inward displacements of the twin boundary and boundary pinning, depending on the surface orientation and twin system considered. These displaced regions are similar to those produced by indenting and can likewise give rise to microtwins. It is interesting to note that Kosevich et al\(^{167,278,279}\) have found similar local "bending" of twin interfaces when twins encountered inclusions or deformed regions in NaNO\(_3\), Sb, Bi, Sn and Zn.

The effects due to oxidation must be confined to a thin surface layer: similarly the observations of microtwin formation were restricted to twinning at or slightly below the free surface. Limited data on the effect of indenting on twin boundary displacements indicate a similar twinning behaviour at and below the free surface\(^{145}\); thus local stress systems around precipitates and inclusions are also expected to influence twinning within the bulk material. Some evidence for this is reported in beryllium, where intermetallic particles pinned \{10\(\overline{1}\)2\} twin boundaries\(^{169}\).

The occurrence of secondary twins within the parent twin considerably complicates the untwining process. In fact it is unlikely that such twins will be capable of completely untwining to the parent matrix orientation. Secondary twinning on the second undeformed twinning plane is a special case: in fig. 3.10, the untwining process, although leading to matrix orientation, differs from the growth process and the untwinned region may contain numerous accommodation kink boundaries.
Damage associated with kink boundaries and secondary twinning has been reported after unidirectional deformation in zinc\textsuperscript{280,281} and magnesium\textsuperscript{153}. Secondary twins and kinks associated with \{3034\} type twins in magnesium are often related to the fracture path\textsuperscript{282}. Gilman\textsuperscript{280} suggested that the markings observed in \{10\overline{7}2\} twins formed in zinc after large amounts of prior strain were due to small regions of the matrix that had not twinned with the rest of the twin band: this agrees with the observations reported in this paper and indicates the effect of glide dislocations on twin growth.

The present experiments suggests that twinning is not always a homogeneous plastic deformation process. It will be shown that under cyclic stress conditions the twin boundary damage may eventually lead to crack nucleation.
CHAPTER 4
Effect of Cyclic Stresses on the Microstructure of H.C.P. Metals

4.1 Previous Observations on Fatigued Crystalline Solids

The subject of fatigue has penetrated many disciplines and presents some of the most intriguing problems in the deformation of solids. Manson has quoted the number of papers published on fatigue cited by A.S.T.M. as 1000 per annum, with a 15% annual increase. Reading one report every working day one lags behind the literature at the rate of 3 years for every year read.

Fortunately there have been extensive review articles in recent years summarising the empirical data, and there have been many theoretical models proposed to account for this data. In this chapter only a brief summary of previous experiments is given sufficient to make clear the purpose and significance of the present work.

Constant strain amplitude fatigue tests show an initially rapid increase in fatigue hardening followed by saturation. The hardening is associated with regions of crystal which contain either a very high density of dislocation loops and dipoles, at low strain amplitude or a sub-grain structure, at high strain amplitudes. The saturation in fatigue hardening coincides with constant dislocation density and the residual cyclic strain \( \sim 10^{-4} - 10^{-5} \) is attributed to the flip-flop motion of the dipole loops. The high temperature dependence of the flow stress is indicative of point defects being generated during fatigue. Feltner has found equal numbers of vacancy and interstitial loops in fatigued aluminium. The dipole regions are believed to arise by cross-slip of screws. They occur in the first few per cent of the life and their distribution and density does not change thereafter.

The surface slip markings in fatigued metals are well known. After say 10% of the life, slip steps become concentrated in bands 10-50 \( \mu \) wide called striations which are softer than the slip step free regions \( \sim 0.1 \) mm wide between the striations. Saturation in the fatigue hardening coincides with striation formation. A cell structure is found in the striation regions near the free surface and these regions provide the sites for crack nucleation. Many workers have studied this stage of fatigue in f.c.c. metals and attempted to explain the formation of the striations and the nucleation of the cracks. For example it has been suggested that the
matrix is point defect hardened, with softening occurring in the striations by some unspecified mechanism which sweeps up the point defects. Sub- grain formation would then be expected in this region as observed. Some support for this model is provided by experiments on irradiated copper\textsuperscript{291}, which show that cyclic stresses produce defect free channels.

One of the characteristic features of striations in certain metals, are the formation of extrusions and intrusions\textsuperscript{290}. In this paper, slip band extrusion refers to the thin discrete ribbons of metal which grow from active slip planes during fatigue. Low\textsuperscript{292} does not distinguish between this phenomenon and the surface contours produced by clusters of slip steps i.e. striations. The two phenomena may or may not occur together, and therefore should be distinguished, as emphasised by Mine and Kuhlmann-Wilsdorf\textsuperscript{293}.

Slip band extrusion, first observed by Forsyth in Al-Cu\textsuperscript{294}, has subsequently been observed in several f.c.c. pure metals and alloys (see reviews by Parker and Begredo\textsuperscript{295}, Avery and Backofen\textsuperscript{290} and Kennedy\textsuperscript{16}). Hull\textsuperscript{296} found extrusions and intrusions in copper before 1\% of the fatigue life had elapsed and at all temperatures down to 2.4\textdegree{}K. Since thermally activated diffusion processes appeared unnecessary for extrusion, Cottrell and Hull\textsuperscript{297} proposed a mechanism involving slip on two intersecting slip systems.

Subsequent fatigue experiments with NaCl and LiF crystals oriented for intersecting slip did not produce extrusions\textsuperscript{298}; however extrusions were readily formed in Ag Cl\textsuperscript{298,299} and TlI - TlBr mixed crystals\textsuperscript{298}. The difference in behaviour in the ionic crystals was attributed to the greater ease of cross-slip in Ag Cl and TlI - TlBr.

Since the description by Mott\textsuperscript{300} of a possible cross-slip mechanism for producing extrusions several modifications have been suggested\textsuperscript{16,290}, all of which involve cross-slip of screw dislocations in some co-operative manner. But while cross-slip may be a pre-requisite for slip-band extrusion, easy cross-slip during fatigue does not necessarily give rise to extrusions. For example, in fatigued aluminium (stacking fault energy, $\gamma = 200 \text{ ergs/cm}^2$\textsuperscript{54}) cross slip is extensive but extrusions may not be produced\textsuperscript{301,302}. However, in fatigued low stacking fault energy metals e.g. Cu - 7.5 at % Al ($\gamma = 1.5 \text{ ergs/cm}^2$), Br - Brass ($\gamma = 14 \text{ ergs/cm}^2$\textsuperscript{303}), extrusions and intrusions are produced\textsuperscript{290,304}, although cross-slip is difficult, particularly at low stresses\textsuperscript{54}. Thus none of the above...
Extrusion mechanisms appear to be completely satisfactory.

There is less fatigue data available for metals having the close packed hexagonal structure; it is known however that in metals with \( c/a > \sqrt{3} \), slip is confined almost entirely to basal planes and cross-slip is difficult\(^{227,305}\).

Some observations on fatigued cadmium\(^{306}\), zinc\(^{110}\) and magnesium\(^{199,307}\) have been described, but no evidence for slip band extrusion in these metals was obtained. It will be shown in the present chapter that extrusions are found in hexagonal metals and that their distribution is consistent with a formation mechanism based upon the glide of dipole loops.

It is known that mechanical twinning can become an important mode of deformation in certain metals during high stress fatigue e.g. in antimony, bismuth\(^{308}\), cadmium\(^{249}\), zinc\(^{308,309}\), magnesium\(^{307}\), titanium\(^{311-314}\) and iron\(^{310}\). Fatigue cracks are nucleated preferentially in the twin boundary regions; this occurred within 20% of the life in magnesium\(^{307}\). The sudden nucleation of a twin in fatigued cadmium single crystals gives rise to a large increase in damping and if cycling continues at the same stress level the fatigue life after the first twin forms is very short\(^{249}\).

In a recent study of fatigue crack nucleation in annealing twin boundaries, Boettner et al\(^{315}\) showed that cracks are only produced when the primary slip plane is parallel to the twinning plane; the normal slip processes were accentuated in the vicinity of the twin interface but otherwise the fatigue process was similar to that in the parent matrix. They suggested that dislocations nucleated at steps in twin boundaries are responsible for increased slip in this region.

This model of crack nucleation is not applicable to \{10\(\overline{1}\)2\} type twin interfaces in the above c.p.h. metals: basal slip predominates during cyclic stressing and other possible slip planes (\{10\(\overline{1}\)1\}) in cadmium and magnesium and \{11\(\overline{2}\)2\} in cadmium and zinc) do not involve slip parallel to the \{10\(\overline{1}\)2\} twin plane. A fine structure, not found in annealing twins, has been reported within twins in zinc after fatigue\(^{316,317}\), but generally in fatigued specimens the appearance of deformation twin interfaces\(^{349}\) and annealing twin interfaces\(^{315,318}\) is similar. During a fatigue test the interfaces become progressively darker and apparently wider until eventually fatigue cracks are formed in the interface region.

No detailed observations of twins in fatigued metals has been made hitherto, although there is evidence that twinning may be the cause of
fatigue failure in titanium. The present experiments were therefore
designed to study in more detail the surface deformation at twin interfaces
prior to crack nucleation in h.c.p. metals. It will be shown that cyclic
stresses cause planar interfaces to become serrated, and larger twins to
be broken up into smaller twin fragments. Based on these observations
a model is proposed to account for the characteristic effects of cyclic
stresses on deformation twins.

4.2 Slip Band Extrusion in Annealed Metals

The effect of cyclic stresses on the surface topography in cadmium,
zinc, magnesium and titanium has been studied. Sheet specimens \( \frac{3}{4} \)" thick
were fatigued in reverse plane bend in an Avery machine operating at
2000 cycles/min and at stress levels to give lives between \( 10^4 \) and \( 10^5 \) cycles.
Low temperature tests were carried out by feeding liquid nitrogen on to the
surface during the test.

Only surface steps due to basal slip were detected on cadmium, zinc
and magnesium, and "hill and valley" type surface contours are well
developed in all cases (fig. 4.1-4.3). The hills can be resolved at high
magnification to be composed of basal slip steps (fig. 4.1). In zinc at
sub-zero temperatures the slip bands coarsened and their spacing increased,
extremely large height differences developing. There was a large variation
among grains of different orientation. Previous work on fatigued zinc
single crystals has shown a similar coarse slip band formation \(^{110}\).

In titanium extensive slip on \{10\(\overline{1}\)0\}<1\(\overline{2}\)0> slip systems is apparent
(fig. 4.4); the slip lines are shorter and the deformation less uniformly
distributed compared with that produced by tensile deformation (fig. 2.10).

Thin foil micrographs revealed dense patches of dislocations in
magnesium (fig. 4.5) and in titanium (fig. 4.6). The distribution of the
dense regions appeared on a finer scale in titanium.

In annealed cadmium fatigued near liquid nitrogen temperature, certain
basal slip bands showed well developed extrusions (fig. 4.2). But the
extrusions were few in number and occurred in grains favourably oriented.
Extrusions were rarely found in annealed cadmium after fatigue at room
temperature.

If twin accommodation kink boundaries and tilt boundaries are intro-
duced by slight bending prior to fatigue, a high density of slip steps and
small extrusions frequently occurred at the boundary positions (fig. 4.7a).
Fig. 4.1 Surface slip steps on annealed zinc fatigued to fracture in $10^4$ cycles at room temperature

Fig. 4.3 Surface slip steps on magnesium after fatigue. A fatigue crack lies parallel to the basal plane at A.

x 550

x 65
Fig. 4.2 The appearance of extrusions in annealed cadmium fatigued at sub-zero temperature.
Same area (a) x 240  (b) x 550
Fig. 4.4 \{10\overline{7}0\} slip traces on titanium fractured after $10^4$ stress cycles x 550

Fig. 4.5a Dense dislocation patches in magnesium after $10^5$ cycles to fracture. x 6000

Fig. 4.5b As in fig. 4.5a x 30,000
Fig. 4.6 Dense patches of dislocations in titanium after $10^4$ cycles to fracture x 40,000

Fig. 4.7 (a) Tilt boundaries in cadmium after fatigue at room temperature x 250
(b) Similar area after chemical polishing. Extruded region etched at A, normal appearance of boundary at B. x 250
During further polishing the tilt boundaries etched preferentially (fig. 4.7b): this effect is analogous to the etching of slip bands in fatigued f.c.c. metals. Fatigue damage associated with kink boundaries was recently reported in lithium fluoride.

Many extrusions were developed in magnesium at both room and sub-zero temperatures (fig. 4.8a) and at low stresses near the fatigue limit. Smaller extrusions appeared as surface debris along slip steps lying between the larger extrusions (fig. 4.8b). Extrusions were also found in magnesium fatigued in a vacuum of $10^{-7}$ torr in push-pull at room temperature. The growth of the extrusion shown in fig. 4.9 was observed during fatigue. Early in the fatigue life a small portion of this extrusion appeared first and grew rapidly to its maximum height. This was followed by steady growth along the slip band during the next few thousand cycles, when growth ceased. No further growth of the extrusion was apparent during the remainder of the test.

Slip band extrusions in titanium were much smaller (fig. 4.10) and not continuous ribbons as in cadmium and magnesium. However they exhibited specular surfaces characteristic of the extrusions in these metals, as compared with the granular, non-reflecting fretting product frequently encountered near fatigue cracks in titanium (fig. 4.11).

**4.3 Slip Band Extrusion After Untwinning**

Some specimens were twinned and untwinned by bending and subsequently polished prior to fatigue. Extrusions are then found parallel to basal slip traces in twin and parent and appear to be continuous across the twin (fig. 4.12a). There is a marked preference for extrusions to grow in the parent adjacent to the twin interface when the twin has partially untwinned (fig. 4.12b). When complete untwinning occurred, the original position of the twin was defined during subsequent fatigue by extrusions from the basal planes in the parent (fig. 4.13).

The preferential formation of extrusions in untwinned crystal is clearly shown in fig. 4.14, in which short extrusions, each parallel to the trace of the parent basal plane, are arranged in rows along traces of two sets of twin systems. The twins themselves have mostly disappeared.

In cadmium twinned and untwinned at room temperature, subsequent fatigue at room temperature produced large numbers of extrusions in regions which had twinned and untwinned (fig. 4.15a). In fig. 4.15b well developed
Fig. 4.8 Extrusions in magnesium fatigued at room temperature
(a) top of extrusion in focus \( x \times 525 \)
(b) original surface of specimen in focus \( x \times 525 \)
Fig. 4.9 Slip band extrusion in magnesium after fatigue in vacuum of $10^{-7}$ mm Hg. Extrusion formed after $2 \times 10^4$ cycles ($\sim 10\%$ life) and grew lengthwise at an average rate of $60 \mu m/cycle$.

Fig. 4.10 Slip band extrusions in titanium fatigued to failure in $10^4$ cycles.

Fig. 4.11 Fatigue crack in titanium parallel to $\{10\overline{7}0\}$ slip plane at A. Fretting damage at B. Failed in $10^4$ cycles.
Fig. 4.12a  Extrusions from basal planes in twin and matrix of fatigued magnesium  

Fig. 4.12b  Fatigued magnesium. Extrusions from parent matrix adjacent to partially untwinned twin  

x 770
Fig. 4.13 Extrusions from parent matrix at site of a completely untwinned twin. x 660

Fig. 4.14 Fatigued magnesium. Extrusions parallel to parent basal planes at sites of two twin systems after untwinning. x 300
Extrusions in cadmium fatigued at room temperature after twinning and untwining.

Fig. 4.15a Low magnification of area in cadmium showing untwinned region at A and twin at B. x 880

Fig. 4.15b Slip steps at A due to basal slip in twin during bending and before untwinning. Slip at B due to basal slip in parent after untwinning and during fatigue. Note lamellar structure of extrusion shown at C. x 1300
basal slip steps produced in a twin before untwining act as markers to reveal the surface contours across the extrusions. The lamellar structure of the extrusion is clearly visible at A in fig. 4.15c.

Slip appears to be more difficult in untwinned crystal. In fig. 4.16 the slip steps produced during fatigue do not extend into the untwinned region, although extrusions do form in this region.

The results obtained in cadmium, zinc, magnesium, and titanium, are not reproduced in zinc. After fatigue at progressively increasing stress to fracture or at various temperatures from near liquid nitrogen to 150°C, no evidence of slip band extrusion was obtained.

4.4 Discussion

The structure of fatigued metals is characterised by regions containing a high density of dislocation loops and dipoles. A similar high density of dipoles occurs adjacent to twin interfaces after untwining (Chapter 3). In previous studies the loops and dipoles are believed to arise by cross-slip.

The extent of cross slip will control the magnitude of the jog in the screw dislocation; this in turn will affect the subsequent behaviour of the screw. Small jogs are expected to glide non-conservatively to produce point defects, whilst larger jogs lead to stable dipoles. Since dislocation dipoles are found in low stacking fault energy metals after high stress fatigue sufficient cross-slip must occur to produce jogs on the glissile screw dislocations.

The stacking fault energy of cadmium, zinc and magnesium has been estimated to be 100-300 ergs/cm² (Chapter 1). Cross-slip on prismatic or pyramidal planes, although present in magnesium at room temperature (Chapter 1) is very rarely observed in bulk zinc, or cadmium. The absence of cross-slip in the latter was initially attributed to the high Peierls-Nabarro stress in the non-basal planes, but according to Friedel it is due to the difficulty in constraining the extended dislocations in the basal planes.

Thin film studies have confirmed non-basal cross-slip to be present in magnesium and absent in zinc. In addition it was shown that non-basal cross-slip can also occur in cadmium. These results are in agreement with the observations that dipoles appear in magnesium and cadmium whereas in zinc after fatigue only sessile dislocation loops are
Fig. 4.15c Displacement of 'A' type slip steps by subsequent extrusion from 'B' type slip planes. Large extrusion at A; shallow extrusion at B. x 1300

Fig. 4.16 Fatigued magnesium showing absence of fatigue slip bands in untwinned region at A compared with surrounding parent matrix at B. Note extrusions in slip free region. x 200
found in the basal planes \(^{110}\). Thus the jogs produced in zinc may be too small to produce stable dipoles; instead defects are generated which subsequently condense to form the observed basal plane loops.

It was shown in Chapter 2 that loops and dipoles are very common in tensile deformed titanium. The cross-slip of screw dislocations gliding on prism planes will produce dipole loops lying approximately in \([1\bar{1}20]\) planes and elongated parallel to the c-axis; in the case of basal slip the dipoles will tend to be elongated normal to the c-axis.*

The preference for extrusion formation to occur in crystal previously twinned and untwinned, strongly suggests that a slip band extrusion mechanism must involve the dislocation dipoles present in this region.

4.4.1 Slip Band Extrusion Model

The properties of prismatic dislocation loops has been discussed by Seitz \(^{61}\) and others and illustrated by Nabarro \(^{62}\) using fig.4.17. Let a loop lie on the surface of a cylinder which has as its axis the direction of the Burgers vector. Then the loop may glide along the surface of the cylinder; the opposite sides of the loop having opposite signs gliding in opposite directions. The only restriction on the shape of the loop produced by glide is that the projection of the loop on to a plane normal to the axis of the cylinder must remain constant. An increase or decrease in the projected area will involve climb and will be diffusion controlled. It is possible however for segments of the loop in the screw orientation to cross-slip off the glide cylinder as shown in fig.4.17: such segments may decrease the mobility of the loop.

It is here proposed that under suitable stresses the dense array of dipole loops will move together to the free surface to form an extrusion if the loops are interstitial type and intrusions if the loops are vacancy type. Fig.4.18 shows schematically the sequence of events which could give rise to either an extrusion or an intrusion, depending on the sense of the dislocation composing the dipole. This model is consistent with the experimental observations.

* In cadmium \(^{56}\) loops along \(<10\bar{7}0>\) can also arise from reactions involving dislocations with \(\frac{1}{3}\langle1\bar{1}2\bar{3}\rangle\) type Burgers vectors: in the present work dislocations of the type \(\frac{1}{3}\langle1\bar{1}2\bar{0}\rangle\) are believed to predominate and no evidence for other slip systems has been obtained. The \([1\bar{1}2\bar{2}]\) \(<\bar{7}12\bar{3}\rangle\) system will not therefore be considered further in this Chapter.
(a) Loop of dislocation \(A B C D A\), lying on a cylinder with axis parallel to the Burgers vector. The segment \(B C D\) can glide to \(E F\), leaving screw segments \(B E, D F\) which join it to \(D A B\).

(b) Projection of (a) normal to the Burgers vector.

(c) A loop \(G H J\) can spread from the screw segment \(B E\), provided that it lies on a cylindrical surface with the Burgers vector as generator.

(d) Projection of (c) normal to the Burgers vector.

Fig. 4.17 Possible glide motions of a prismatic dislocation loop.

(after Nabarro\(^62\))
FORMATION OF GLISSILE INTERSTITIAL LOOPS FROM A SCREW DISLOCATION.

Fig. 4.18a

FORMATION OF SURFACE EXTRUSIONS BY GLIDE OF INTERSTITIAL LOOPS.

Fig. 4.18b
fig. 4.19 Magnesium annealed in moist argon at 620°C and quenched into iced brine. "Punched out" loops at A produced by stresses around an inclusion x 25000
If the generation of such glissile dislocation loops during fatigue is accepted then the operation of this extrusion/intrusion model will depend on the following factors:

1. The life-time of the dipole loop i.e. before climb, cross-slip or interaction with other loops.
2. The stress to move the loop along its glide cylinder.
3. The rate of loop formation.

There is ample direct evidence (see reference 63) for the glide of loops along their slip cylinders in many crystal structures e.g. in ionic crystals (NaCl, Ag Cl), in metals having the f.c.c. (Al, Cu), c.p.h. (Cd, Mg, Zr) and b.c.c. (Fe, Nb) structures. An example of interstitial loops produced in magnesium is shown in fig. 4.19. While little is known of the behaviour of such loops during fatigue they can occur early in the fatigue life and at low temperatures (as do extrusions) and probably reach maximum density as saturation if the cyclic strain hardening rate is attained.

Taking an extrusion to be 0.1 μ thick, 10 μ high, 100 μ long and a loop diameter of 1000 μ, approximately 10^5 loops must pass along each glide cylinder and a total number of 10^8 loops will be required to produce the complete extrusion. The observed dislocation density is 10^9/ cm^2, equivalent to 10^14 loops/cm^3. Thus a volume of metal equal to that of the extrusion, when present in the matrix, would contain 10^4 loops. As expected, the loops required to produce the extrusion must come either from a volume greater than that previously occupied by the extruded material or be generated continuously as they are lost to the free surface.

The maximum dislocation velocity is ~500 metres/sec. Assuming a frequency of 60 c.p.s., in one 1/2 of a stress cycle the dislocation loop could travel ~2 metres. Thus there is ample time in one 1/2 of a stress cycle for loops to form an extrusion, if a sufficient number of loops are available and if they are not greatly impeded in their glide path.

4.4.2 Slip Band Extrusion in H.C.P. Metals

Extrusion in these metals will now be considered in terms of the above model.

The ease of slip of the dislocation loops on their glide cylinders will be controlled by the stress to move those segments of the loop in non-basal planes. This stress is likely to be high in cadmium because non-basal slip
is exceedingly difficult. Furthermore, climb processes operating simultaneously at room temperature in cadmium will further decrease the number of dislocation loops reaching the free surface. Thus few extrusions are produced in annealed cadmium compared with magnesium in which non-basal slip and dipole formation occur readily. Armstrong and Horne mistakenly identified slip band extrusions in fatigued magnesium single crystals as basal plane cracks, which appear similar under normal illumination. It is significant however that they report "cracking" is associated with untwining, which agrees with extrusion distribution in the present work. Slip band extrusions also appear likely in Figure 3 of reference 307.

The Cd - 3% Zn alloy consists of almost pure Cd matrix in which are embedded precipitates of pure zinc: the higher stresses necessary to overcome the barriers to plastic deformation in the cadmium matrix will also favour cross-slip and is presumably responsible for the greater number of extrusions produced in the alloy.

Mobile accommodation kink and tilt boundaries in hexagonal metals are composed of glissile dislocations on successive basal planes: a high dipole density giving rise to extrusions could occur in these regions by the to and fro movement of the boundaries under cyclic stressing. Similarly the high extrusion densities beside contracted twins is due to the presence of large numbers of dipoles adjacent to the twin boundaries.

The effect of prior cold work at higher stresses is to introduce large numbers of jogged dislocations which subsequently form dipoles and extrusions during fatigue.

Although the stacking fault energy in the basal plane of zinc is comparable to that of magnesium the ratio:

\[
\frac{\text{critical resolved shear stress for prismatic slip}}{\text{critical resolved shear stress for basal slip}}
\]

is very much greater for zinc than for magnesium and even in favourably oriented zinc whiskers no cross-slip is observed: thus the absence of extrusions in zinc is almost certainly associated with the absence of cross-slip in this metal; this allows only small jogs and narrow unstable dipole loops. The absence of saturation in the cyclic work hardening rate and the prolonged fatigue life of zinc is also attributed to the absence of cross-slip. The Wood mechanism.
developed formally by Kay, of crack nucleation by random reversed slip, is ideally suited to this metal, and indeed Broom and Summerton have shown that surface notches are produced in this manner; however it does not appear to be so effective in producing fatigue failure as mechanisms involving cross-slip. It may well be that the operation of the extrusion/intrusion mechanism is more effective in reducing the fatigue life because of the much greater stress concentration factor associated with small extrusions and intrusions.

4.5 Cyclic Twinning

Materials and testing technique were similar to that described in the beginning of this Chapter. A few tests were also made on cobalt, but because transformation to the h.c.p. structure was incomplete in the material examined, no further tests were made on this metal.

Twins were introduced into the metals prior to fatigue by annealing slightly bent specimens. Cadmium, magnesium and zinc were straightened at liquid nitrogen temperature to minimise deformation by slip. Titanium was straightened at room temperature to nucleate twin systems operative at this temperature. The surface strain was such that there was little evidence of slip in the twinned grains. Specimens were polished electrolytically before testing.

4.5.1 Formation of Microkink Boundaries

The twin interfaces studied were normally planar or slightly curved, approximating to coherent twin boundaries (figs. 4.20-4.21). The effect of cyclic stresses on these twins is evident early in the fatigue life as narrow bands of surface deformation at the twin/matrix interfaces: examples in magnesium and titanium are shown at A in figs. 4.20b and 4.21a,b. Note the absence of extensive slip in the adjacent lattices. The damage appears on a very fine scale, as shown in the replica of a damaged twin interface in magnesium (fig. 4.22). Damage is often greater at one twin interface of a twin (fig. 4.21-4.22); this is presumably due to differences in the mobility of the twin interfaces as mentioned in chapter 3 and discussed by Bashmakov and Soldatov and Roberts and Partridge.

The surface deformation is associated with local non-uniform twin boundary displacements which cause the trace of the twin interface to become serrated. This is clearly seen after polishing e.g. at A in figs. 4.20c and 4.21c. The surface area of the irregular twin outerface
Fig. 4.20 Magnesium, same area.
(a) as chemically polished
(b) after $2 \times 10^4$ cycles (~25% of the life)
(c) after further chemical polishing $x$ 200
Fig. 4.21 Initial stages of \{11\overline{2}1\} twin boundary fatigue damage in titanium

(a) specimen twinned, electropolished and fatigued. Fatigue damage at A after 2.6 x 10^4 cycles (~50% to life) x 925.

(b) as (a), different grain x 2400

(c) as (a) after electropolishing and further 0.5 x 10^4 cycles x 1700
is greater than the planar interface by at least 10-20%.

During subsequent polishing and near the free surface preferential etching occurs in some twin interfaces e.g. in magnesium (fig. 4.23) and titanium (fig. 4.24). This is believed to be due to the presence of small cracks.

Another characteristic of twinned regions in a fatigued specimen is the presence of small closely spaced kink boundaries. Kinks (about 0.5 μ apart) beside a twin interface in fatigued zinc are shown in fig. 4.25. Similar kinks are found in cadmium (4.26) on either side of the twin boundary, depending on which boundary is mobile. These kinks appear to accommodate the very small serrations produced in a twin interface during cyclic stressing. The kinks are analogous to the "fine structure" in twins in fatigued zinc described by Billen 316 and Barr 319. The regularity of the fine kinks in magnesium is shown in a replica in fig. 4.27.

Larger kinks (A, B, C and D in fig. 4.28a) were sometimes observed together with the finer type. An examination of this region after chemical polishing showed the coarse kinks to be attached to residual segments of twin (fig. 4.28b). The coarse kinks are similar to the accommodation kinks associated with micro twins produced during irregular twin growth and contraction, described in para 3.3.

4.5.2 Twin Fragmentation

The initial deformation shown in fig. 4.20b may be followed by further deformation which proceeds towards the centre of the twin. After polishing (fig. 4.29) it is evident that cyclic stressing has broken up twinned crystal into smaller twin fragments having irregular shapes. Note that twins 1 and 2 in fig. 4.29 are completely fragmented while the wider twin 3 remains perfect at the centre.

In certain orientations the deformation is not confined to the original twin interfaces but appears within the twin matrix at secondary twin interfaces (fig. 4.30 a-b). Twins nucleated during the fatigue test are always severely damaged e.g. at A in fig. 4.30 b-c. Twin fragmentation is apparent after polishing (e.g. compare areas outlined at X in figs 4.30 a-c): secondary twinning has converted parts of the parent twin to matrix orientation i.e. secondary twinning represents untwinning of the parent twin.

The total length of the traces of the twin interfaces and the cross sectional area of twinned crystal has been measured before and after fatigue in the area outlined at X in fig. 4.30 a-c: the twinned area
Fig. 4.22 Replica of $\{10\overline{1}2\}$ twin in magnesium after electropolishing followed by $2 \times 10^4$ cycles $(\sim 25\%$ of the life) \(x 4000\)

Fig. 4.23 Specimen as in Fig. 4.22 showing crack nuclei in twin interface revealed by electropolishing after fatigue at A. Note adjacent crack free twins at B. \(x 500\)

Fig. 4.24 Titanium specimen after $2.6 \times 10^4$ cycles followed by electropolishing. Crack nuclei in twin interfaces at A. Note crack free twins at B \(x 500\)

Fig. 4.25 Accommodation kink boundaries in zinc after $10^4$ cycles. The boundaries are spaced $\sim 0.5 \mu$ apart. \(x 1100\)

Fig. 4.26 Accommodation kinks in twinned region in cadmium after $10^4$ cycles to fracture. \(x 550\)
Fig. 4.27 Replica of fine kinks in fatigued magnesium
x 4000

Fig. 4.28 (a) Coarse kinks A - D and fine kinks on opposite side of twin in zinc.
(b) same area after polishing, showing residual twin fragments.
x 730

Fig. 4.29 Twinned magnesium after fatigue followed by polishing. Twin 1 completely fragmented.
Twin 3 partly fragmented.
x 250
Magnesium, same area.
(a) as chemically polished
(b) after $2 \times 10^4$ cycles ($\sim 25\%$ of the life)
(c) after further chemical polishing

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decreased by ~15% whilst the total length of interface increased by ~250%.

The progressive destruction of the twin fragments and crack nucleation is shown in fig. 4.31. Twins on at least three systems are severely damaged after $2 \times 10^4$ stress cycles, equivalent to ~25% of the fatigue life. The area out-lined at A is shown at higher magnification after polishing in 4.31c: the characteristic twin fragments are revealed and in addition small cracks are present at some interfaces, e.g. at A. The same area after cycling to failure in a further $6 \times 10^4$ cycles is shown in fig. 4.31d: typical fatigue damage is apparent at many twin fragment interfaces but there is little change in the crack lengths.

A similar sequence taken from the same grain is shown in fig. 4.32a-b. After polishing a crack is apparent at A and after further cycling to failure the crack has not propagated beyond that twin fragment interface, although fatigue damage has developed at other twin fragments.

The fragmentation at pre-existing twins also occurred in cadmium (fig. 4.33) and zinc (fig. 4.34) during fatigue at room temperature.

It should be noted that all the microstructures appeared in different grains of the same specimen after 25% of the fatigue life has elapsed. Clearly the manner in which the twins deform is dependent on their orientation with respect to the applied stress. In suitably oriented grains the normal slip processes also occur (para. 4.2).

4.5.3 Twin Interface Damage

The damaged area in fig 4.31b is shown at higher magnification in fig 4.35a. Filamentry growths are visible protruding from the damaged surface regions. They are best detected by focussing slightly above the specimen surface (fig 4.35b). This phenomenon is very common in all the metals studied except zinc and the filaments occur in various forms. In cadmium (fig 4.36) the filaments are small and irregular. In magnesium the filaments occurred predominantly in the needle form (fig. 4.37a) but some planar growths were occasionally observed (fig 4.37b). In the latter the plates appear transparent to light, since surface slip steps could be seen through the plate (fig 4.37b at A).

To confirm that the filaments were protruding above the surface and not lying on the surface, a microhardness indenter was placed just in contact with the surface and moved across the position of the filaments. Two twins in magnesium were selected, marked 1 and 2 in fig 4.36; the
Fig. 4.31b  Magnesium - same area
(a) as chemically polished  Mag x 122
(b) after $2 \times 10^4$ cycles (~25% of the life)  Mag x 122

- 93 -
Fig. 4.31c After further chemical polishing  x 930

Fig. 4.31d After further 6.10^4 cycles to failure  x 930
Fig. 4.32a Magnesium, twinned, fatigued $2 \times 10^4$ cycles, electropolished. Crack at A in twin interface. x 1300

Fig. 4.32b As Fig. 4.32a, after further $6 \times 10^4$ cycles to fracture. x 1300

Fig. 4.33 Twin fragmentation in fatigued cadmium x 240

Fig. 4.34 Twin fragmentation in fatigued zinc. x 670
Fig. 4.35a Region of fig. 4.31b at higher magnification, original specimen surface in focus  

x 1400

Fig. 4.35b As a) above, but focussed above specimen surface. Filamentary growths in focus at A.  

x 1400
Fig. 4.36 Filamentary growths at a twin boundary in cadmium after fatigue
x 312

Fig. 4.37a Needle shaped growths at twin boundary in magnesium after fatigue
x 1230

Fig. 4.37b Planar growths at twin boundary in magnesium after fatigue. Note slip steps visible through platelet at A.
x 550
apparent irregular twin interfaces in this figure are actually due to filamentary growths. Twin 1 is also shown at higher magnification in fig 4.39a; two filaments, A, B, are visible. The scratches made by the diamond indenter are shown at D in fig 4.39b; the filaments have disappeared.

A similar sequence is shown for twin 2 in fig 4.40 and a needle-like filament A. Only a bent piece remains after scratching (fig 4.40b).

The replica of the early stages of twin boundary fatigue damage shows some evidence of filamentary growths (fig 4.22) but this is more pronounced after larger numbers of cycles, as shown in fig 4.41. Extraction replicas from fatigued magnesium often showed evidence of oxide in electron diffraction patterns from the filaments. However some pieces of filamentary growths also gave a magnesium diffraction pattern (fig 4.42); the plate-like shape of the filament is apparent in this figure.

Filaments on titanium occurred less frequently in the needle form (fig.4.43). Well developed platelets were the most common twin boundary damage feature. A similar procedure was adopted to confirm the discrete nature of these growths. Platelets parallel to \{11\overline{2}1\} twins are shown in fig 4.44a; again a slip step is visible through the plate of A. The filaments are broken up by the diamond (fig 4.44b). Another twin behaved similarly (fig 4.45). In the latter one plate appears to have torn off at A whilst the other has broken into smaller pieces at B.

Some observations on cobalt are included because of their similarity to the previous results. For example twins introduced by bending show evidence of damage in the twin interfaces after fatigue (fig 4.46) and similar filamentary structures are apparent on two twin systems in fig 4.47.

A thin foil taken from a fatigued specimen shows a high density of dislocations in a band approximately parallel to the trace of the twin boundaries (fig 4.48). This debris was similar to that described in Chapter 3 in crystal twinned and untwinned, being composed of loops and jogged dislocations.

4.5.4 Fatigue Fracture

Fatigue cracks nucleate and grow in basal planes of cadmium, zinc and magnesium (fig.4.3) and in prism planes of titanium (fig.4.11). Cracks
Fig. 4.38 Twins in magnesium after fatigue x 280

Fig. 4.39a Twin 1 in fig. 4.38 showing filaments at A and B x 750

Fig. 4.39b As Fig. 4.39a after scratching with diamond indenter x 750

Fig. 4.40a Twin 2 in fig. 4.38 showing filament at A x 600

Fig. 4.40b As fig. 4.40a after scratching with diamond indenter x 600
Fig. 4.41 Replica of twins in magnesium after $6 \times 10^4$ cycles to failure.
(a) x 4000
(b) x 4000

Fig. 4.42 Extraction replica from twin boundary in fatigued magnesium. Diffraction pattern of magnesium metal obtained from filament shown. x 32,000
Fig. 4.43 Fatigue damage and whiskers at \{11\overline{2}1\} twin interfaces in titanium. Note damage confined to one boundary, that boundary adjacent to A is as polished.

x 2400

Fig. 4.44a Whisker growths at \{11\overline{2}1\} twin boundaries after cyclic stressing. Note slip trace visible through whiskers at A.

x 1320

Fig. 4.44b As fig. 4.44a after diamond scratching

x 1320
Fig. 4.45a Whisker growths at \{11\overline{2}1\} twin in titanium at A

x 1230

Fig. 4.45b As in fig. 4.45a after diamond scratching.
Note small fragments at B.

x 1230

Fig. 4.46 Twin boundary damage in cobalt at A.

x 1700

Fig. 4.47 Cobalt twinned by bending followed by fatigue stressing. Whisker growths at interfaces of narrow twins at A

x 550

Fig. 4.48 Dislocation debris around a \{11\overline{2}1\} twin interface in a fatigue specimen.

x 20,000
also follow twin boundaries e.g. cadmium fig 4.49 and magnesium fig 4.50. When the twin volume fraction is large an irregular fracture path develops (fig 4.51). The crack is clearly propagating along the twin fragment interfaces as shown in fig 4.52. A characteristic feature of cracks in titanium is the very local nature of the deformation associated with fatigue fractures. A twin boundary crack in titanium is shown in fig 4.53; there is no evidence for slip associated with paths 1-2 and 3-4. In fig 4.54 extensive deformation is apparent in one grain but is much less apparent at 1 and 2. Extensive slip is associated with an irregular crack path.

4.6 Discussion

Dislocation damage due to cyclic twinning is found below the surface of bulk specimens after cyclic stressing. However the behaviour of twins at a free surface is expected to differ in detail from that below the surface; it is the surface behaviour which is particularly important in fatigue.

At high stress levels fresh twins can form continuously during a fatigue test. The effect of lower stress cycling on pre-existing twins has not hitherto been considered in detail, although twin boundary damage is observed at stress levels insufficient to nucleate fresh twins. This is consistent with the fact that the stress required to grow a pre-existing twin is much less than that required to nucleate a fresh twin (Chapter 1 VII 2). During both high and low stress fatigue, twin fragments are formed either at the new twin positions or at pre-existing twin sites; the irregular shape of the fragments is in marked contrast to the normal lenticular shape of twins characteristic of unidirectional stressing. The considerable increase in twin boundary area associated with twin fragmentation may account for the large increase in damping coincident with the onset of twinning in a fatigue test.

It is known that deformation twin growth followed by contraction in ionic solids and in b.c.c. and c.p.h. metals generates lattice defects in the vicinity of the twin interface; this damage will be particularly severe under fatigue conditions. Since both large lenticular twins and twin fragments behave in a similar manner when subjected to cyclic stresses it seems reasonable to assume that twin fragmentation occurs as a consequence of the defects produced during the twin interface motion.
Fig. 4.49 Fatigue crack in cadmium parallel to $\{10\overline{1}2\}$ twin boundary at A, and basal planes at B, after $10^4$ cycles. x 400

Fig. 4.50 Fatigue crack in magnesium parallel to basal plane at B and twin boundary at A. x 75
Fig. 4.51 Pretwinned magnesium fatigued to failure in $10^5$ cycles.

Note very irregular crack path at A


Fig. 4.52a Area from fig. 4.51 after electropolishing.

Crack following twin interfaces at A.

x 50
x 310
Fig. 4.52b Area from fig. 4.51 after electropolishing.
Crack following twin interfaces at A. x 310

Fig. 4.53 Titanium electropolished and fatigued to failure in $6 \times 10^4$ cycles. Fatigue crack 1 - 2 - 3 - 4 - 5. Parts 2 - 3 and 4 - 5 parallel to $\{11\bar{2}1\}$ twin interface. x 750
Fig. 4.54 Crack path in titanium.
Smooth crack at 1 and 2, irregular crack path at 3 and 4, where extensive slip has occurred x 550
The surface filamentary growths associated with twin boundary fatigue damage have not hitherto been reported. The predominance of oxide diffraction patterns from extraction replicas of the filaments from magnesium specimens suggested an oxidation mechanism for the formation of the filaments and hence possibly for crack nucleation. An analogous situation was considered for fatigue slip band cracking by Fujita.333

Some indication of the differences in surface behaviour resulting from twinning was obtained in a magnesium specimen. A twin was grown, and the surface chemically, polished to mark the twin boundary positions and then untwinned slightly. The appearance of the surface after exposure to laboratory air overnight is shown in Fig. 4.55. The parent is uniformly tarnished (at A), the twin only slightly changed (at B) and the untwinned region (at C) most severely tarnished.

The shape changes produced by the twinning shears have been summarised for \{10\overline{1}2\} and \{11\overline{2}1\} twins in Chapter 1. A free surface is tilted by the twinning shear and its orientation is changed. Some examples of the sense of the stresses and the orientation changes involved are given below for these twins in titanium.

<table>
<thead>
<tr>
<th>Twin</th>
<th>Orientation of Surface before Twinning</th>
<th>Orientation of Surface after Twinning</th>
<th>Stress in Surface</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10\overline{1}2)</td>
<td>(0001) \hspace{1cm} (10\overline{1}0)</td>
<td>5° off (\overline{7}010) \hspace{1cm} 5° off (0001)</td>
<td>compressive \hspace{1cm} tensile</td>
</tr>
<tr>
<td>(\overline{1}1\overline{2}1)</td>
<td>(0001) \hspace{1cm} (0\overline{1}10)</td>
<td>3° off (11\overline{2}n) \hspace{1cm} 6 &gt; n &gt; 3 \hspace{1cm} 5° off (0\overline{1}70)</td>
<td>no dimensional change \hspace{1cm} compressive</td>
</tr>
</tbody>
</table>

A conceivable oxidation model for whisker growth may thus be based upon the disruption of the epitaxial oxide layer by repeated twin growth and contraction.

For example, after growth of a (10\overline{1}2) twin in a (10\overline{1}0) surface, the oxide may be cracked by the simultaneous change in substrate orientation and the tensile stresses. Further oxide formation at the exposed surface will be epitaxially related to the (0001) plane in the twin. However during untwinning these areas revert to (10\overline{1}0) and the oxide is subjected to compressive stresses. It is possible that repetition of this process
Effect of orientation on the oxidation of magnesium in air. Specimen twinned and electropolished to mark positions of twin boundaries at A and B. Twin untwinned slightly by bending, new twin boundary positions at A' and B'. Exposed to air for 24 hours.
during fatigue could lead to progressive degradation of the surface and crack nucleation. The effects will be greater in \{11\overline{2}1\} twinning because of the large twinning shear for this system.

The absence of twin boundary whiskers in zinc is not readily explained on this model, nor the magnesium diffraction obtained from some filaments. The similarity between these filaments and the slip band extrusions suggests the possibility that a similar dislocation model is applicable to both phenomena. The dislocation debris associated with untwining has already been invoked to explain the subsequent formation of slip band extrusion in untwinned crystal. It is therefore suggested that the dislocation debris produced during cyclic twinning is responsible for the whisker growth.

In the following Chapters the interactions between dislocations and \{10\overline{7}2\} and \{11\overline{2}1\} twin boundaries are considered. A more detailed discussion of the origin of the twin boundary debris and the mechanism of whisker growth will then be presented in the final discussion based upon the analysis of the above interactions.
Chapter 5
Role of \{10\overline{7}2\} Twinning in the Deformation
of H.C.P. Metals

5.1 Resolved Shear Stress Factors for Slip and \{10\overline{7}2\}<\overline{1}0\overline{1}1> Twinning

It is clear from the present results that interactions between
dislocations and twin boundaries influence the behaviour of twins.
Furthermore, it was noted in Chapter 1, that although the requisite
five independent slip modes may not be available in h.c.p. metals, the
ductility is often considerable. It has therefore been suggested \(^{193,202c}\)
that twinning provides additional deformation modes, although the
mechanism whereby this is achieved is not yet clear.

One possibility, frequently stated in the literature, \(^{5,14,334}\) is
that twinning promotes ductility by reorienting the crystal into
positions more favourable for slip. However no comprehensive study of
the role of twinning in promoting slip has been reported, although some
specific examples have been discussed for basal slip and \{10\overline{7}2\} twinning
in zinc \(^{7,5,14,149}\) and magnesium \(^{335}\) and for \{30\overline{3}4\} twinning in magnesium \(^{153}\).

In the following Chapters an attempt is made to define the role of
twinning in the deformation of h.c.p. metals. Two aspects of the problem
have been considered. Firstly, to what extent does twinning reorientate
the parent so that the ability to slip is increased? Secondly, does
twinning increase the ductility by nucleating slip in \(<c+a>\) directions?

The work done by the applied stress provides the energy for twinning
and the resolved shear stress in the twinning plane and twinning direction
should be positive \(^4\). The resolved shear stress is proportional to the
Schmid factor, given by \(\cos \lambda \cos \varphi\), where \(\lambda\) and \(\varphi\) are the angles between
the direction of the applied stress and the twin plane normal and the
shear direction respectively. The operative twin system should be that
having the maximum Schmid factor. In b.c.c. metals the observed twin
systems are those with the highest Schmid factors \(^{336}\). This criterion
has been used by Williams \(^{337}\) to derive the orientations for which twinning
on one system is most likely to occur in b.c.c. crystals and a stereographic technique for determining the Schmid factors for slip in any
crystal structure has been reported \(^{339}\). Reed-Hill has discussed the
availability of slip and twin modes in zirconium by comparing curves of
Schmid factors \(^{142}\).

It has proved difficult to determine a critical resolved shear

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stress for twinning in h.c.p. metals\(^4,5,97,149\). Although the Schmid factor criterion can account for Gough's observation\(^308\) that twinning in zinc is absent on those \(\{10\bar{7}2\}\) planes containing the slip direction, it is less successful in predicting which of the remaining \(\{10\bar{7}2\}\) twins should operate\(^339,340\). In single crystals extensive \(\{10\bar{7}2\}\) twinning has been reported when the tensile axis is near \([0001]\) (in magnesium\(^224\) and titanium\(^341\) or when the compression axis is nearly normal to \([0001]\) (in magnesium)\(^335\). Then twinning on six \(\{10\bar{7}2\}\) systems occurred, but two twin systems belonging to the same zone predominated\(^335,224\). A different result was obtained by Rosi\(^139\) who found only one operative twin system in similarly oriented titanium crystals.

In a recent detailed study of \(\{10\bar{7}2\}\) twins in zinc, Cooper and Washburn\(^166\) found that the presence of one such twin reduced the stress for nucleation of a second twin which almost always occurred on a conjugate plane. In rhenium\(^158\), \(\{11\bar{2}1\}\) type twins were nucleated with Schmid factors of 0.31 and 0.36 but no \(\{10\bar{7}2\}\) type twins were detected, although the Schmid factor for this system was approximately 0.45.

It is equally difficult to predict the active twin systems in polycrystals. In polycrystalline magnesium, for example, many of the active twin systems appeared to oppose the applied stress\(^342\). In mercury single crystal twins occurred in pairs even when the resolved shear stress for one was unfavourable\(^343\). Clearly the relief of local strains around twins is an important factor controlling subsequent twin nucleation and growth and then the Schmid factor alone may not determine the operative twin system. A similar conclusion has been reached for twinning in metals subjected to shock loading conditions\(^257\).

There is no doubt that in the majority of experiments, slip processes control both twin nucleation and growth, and hence a critical resolved shear stress for twinning would not be expected\(^4\). For this reason a knowledge of the Schmid factor for the active twin and slip systems is likely to be important in any future analysis of the twinning mode of deformation. It is therefore proposed in this Chapter to compare the Schmid factors for twinning and for slip in parent and twinned crystal as a function of the orientation and sense of the stress. Schmid factors for \(\{10\bar{7}2\}\) twinning in titanium have been calculated for stress axes lying in \(\{10\bar{7}0\}\) and \(\{11\bar{2}0\}\) planes. The Schmid factors for all basal and prism slip systems in twin and parent matrices are then compared. Given the stress axis and the sense of the stress, a method has been developed
which allows the Schmid factor to be determined for any twin system and for any slip system in the parent crystal and in any twin. The general conclusions apply equally well to any h.c.p. metal having \( c/a < \sqrt{3} \). Thus magnesium and beryllium, which slip on basal planes, can be compared with titanium and zirconium which slip on prism planes.

5.2 Method Adopted for Describing Schmid Factor Curves

There are two alternatives, either the stress axis is fixed and all twins and their relevant slip systems are considered in turn, or the twin system is fixed and the stress axis varied. The results obtained in the two cases are equivalent, but the second alternative is convenient for computing the Schmid factor curves.

Only stress axes lying in \( \{10\bar{1}0\} \) and \( \{11\bar{2}0\} \) are considered. The stress axis is defined by the plane in which it lies, and \( \theta \), the angle it makes with \([0001]\) in the parent matrix.

A sign convention is adopted for \( \theta \), the significance of which will become apparent in the text. For this purpose a particular twin is considered and the stereogram divided into two halves, each half bisected by the plane of shear of the twin. The angle \( \theta \) is then taken as positive in that half containing the twin pole and negative in that half containing the twinning shear direction (Fig. 5.1). The stress axis planes are lettered (a) to (d), positive and negative signs indicating that portion of the plane for which \( \theta \) is positive or negative respectively.

It must be remembered that letter symbols relate the planes to a particular twin i.e. \((10\bar{1}2)\) in Fig. 5.1. Equivalent symbols for other twin systems are listed in Table 5.1.

It will be shown that stress axes lying in planes having identical letter symbols will give rise to identical Schmid factor curves for twinning and for slip. This applies to all twin systems if account is taken of the relationships in Table 5.1.

5.3 \( \{10\bar{1}2\} <\overline{70}11> \) Twinning

5.3.1 Crystallography of Twinning

The crystallography of twinning in h.c.p. metals is summarised in Chapter 1. In this Chapter the \((10\bar{1}2)\) twin in titanium is considered having twinning elements.

\[
K_1 = (10\bar{1}2) \quad \eta_1 = [\overline{70}11] \\
K_2 = (\overline{70}12) \quad \eta_2 = [10\bar{1}1]
\]
Fig. 5.1 Stereographic projection of poles in parent and in (10\bar{1}2) matrix (subscript $T$). Burger's vector enclosed in $[\cdot]$. Note that positive $\theta$ lies in semi-circle $\bar{1}2\bar{1}O-10\bar{1}O-1\bar{2}\bar{1}O$. 
Table 5.1
INDICES OF STRESS AXIS PLANES FOR \{10\overline{1}2\} TWINS

<table>
<thead>
<tr>
<th>Stress axis plane in standard triangle (parent matrix)</th>
<th>{10\overline{1}2}&lt;\overline{1}011&gt; twin systems</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 01\overline{1}2  2 \overline{1}102  3 \overline{1}102  4 \overline{1}012  5 0\overline{1}12  6 1702</td>
</tr>
<tr>
<td>(1\overline{2}10)</td>
<td>a  c  (-c)  (-a)  (-c)  c</td>
</tr>
<tr>
<td>(1\overline{1}00)</td>
<td>b  b  d  (-b)  (-b)  (-d)</td>
</tr>
</tbody>
</table>

- indicates that negative values of 0 should be taken when referring to the Schmid factor curves.

Table 5.2
EFFECT OF SENSE OF STRESS ON TWINNING

<table>
<thead>
<tr>
<th>Sense of applied stress</th>
<th>Sign of Schmid factor for twinning</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Tensile</td>
<td>Twin grows</td>
</tr>
<tr>
<td>Compressive</td>
<td>Twin contracts</td>
</tr>
</tbody>
</table>
These elements $K_1$ and $\eta_1$ are shown in fig. 1.12, on a standard [0001] stereogram. The positions of $\frac{1}{3} <11\overline{2}0>$ Burgers vectors in the parent matrix and in the twinned crystal are shown in fig. 5.1. The twin poles are numbered according to the convention adopted elsewhere$^{14}$, and the \{10\overline{7}0\} and \{11\overline{2}0\} planes lettered according to the convention described in paragraph 2.

The shape change produced by the twinning shear is shown schematically in fig. 1.11b. It is possible to calculate the change in length along any given direction after complete twinning using the following equation$^{5,14,42}$:

$$1 + \delta = \frac{\ell}{\ell_0} = (1 + 2S \cos \varphi \cos \lambda + S^2 \sin^2 (90 - \varphi))^{\frac{1}{2}}$$

where

- $\ell_0$ = length before twinning
- $\ell$ = length after twinning
- $S$ = twinning shear
- $\varphi$ and $\lambda$ are the angles between $\ell_0$ and the normal to $K_1$, and $\ell_0$ and the direction $\eta_1$ respectively.

Maximum values of $\delta$ occur for axes lying in the plane of shear, i.e. \{1\overline{2}10\} for the \{10\overline{7}2\} twin. For axes lying in $K_1$ and $K_2$, $\delta$ becomes zero, but has negative values in the acute angle between $K_1$ and $K_2$ (i.e., contraction occurs) and positive in the obtuse angle between $K_1$ and $K_2$ (i.e., extension occurs). Equation (1) only applies when a crystal is completely converted to twin orientation. The dimensional changes produced by different \{10\overline{7}2\} twins are summarised in fig. 5.2 where the standard triangle is subdivided by the $K_1$ planes of twins 4, 5 and 3.

For small twin lamellae and for axes lying between $K_2$ and the plane normal to $\eta_1$, the dimensional changes are not those depicted by $\delta$, for the axes contract instead of extend$^{39}$. Fig. 5.3 summarises the dimensional changes produced by small twin lamellae. The diagram is constructed by drawing great circles corresponding to planes normal to $\eta_1$ for each twin. There are nine distinct fields compared with four in fig. 5.2.

5.3.2 Schmid Factors for Twinning ($F_T$)

An indication of the effect of the orientation of an applied stress ($\tau_A$) on the shear mode of either slip or twinning may be obtained by
Fig. 5.2 Change in length as a function of orientation for complete twinning on \{10\overline{1}2\}

A  All twins cause extension
B  1,4 cause contraction
   2,3,5,6 cause extension
C  1,4,2,5 cause contraction
   3,6  extension
D  All twins cause contraction
   Boundary lines 4,5,3 represent \(K_1\) planes for these twins

Fig. 5.3 Change in length as a function of orientation for incomplete twinning on \{10\overline{1}2\}

\begin{align*}
A_1 & \text{ All twins cause extension} \\
A_2 & \text{ 1 causes contraction} \\
       & 2,3,4,5,6 cause extension \\
A_3 & \text{ 1,2 cause contraction} \\
       & 3,4,5,6  \parallel \text{ extension} \\
B_1 & \text{ 1,4  \parallel contraction} \\
       & 2,3,5,6  \parallel \text{ extension} \\
B_2 & \text{ 1,2,4  \parallel contraction} \\
       & 3,5,6  \parallel \text{ extension} \\
B_3 & \text{ 1,2,4,6  \parallel contraction} \\
       & 3,5  \parallel \text{ extension} \\
C_1 & \text{ 1,2,4,5 cause contraction} \\
       & 3,6  \parallel \text{ extension} \\
C_2 & \text{ 1,2,4,5,6  \parallel contraction} \\
       & 3  \parallel \text{ extension} \\
D & \text{ All twins cause contraction} \\
       \text{ Boundary lines 4,5,3 represent } K_1 \text{ planes for these twins} \\
       \text{ Lines 1,2,6 represent plane normal to } \eta_1 \text{ for these twins}
\end{align*}
resolving the stress in the shear plane and in the shear direction. 

\[ \tau_R = \tau_A \cos \phi \cos \lambda \]  

(5.1)

where \( \tau_R \) = resolved shear stress
\( \phi \) = angle between shear plane normal and the stress axis
\( \lambda \) = angle between the shear direction and the stress axis.

The orientation dependence of twinning can be considered in terms of the Schmid factor \( F_T = \tau_R / \tau_A \). Values of \( F_T \) were obtained for applied stressing acting along directions lying in \{1010\} and \{1120\} planes (fig.5.4). If a (10\( \overline{1} \)2) twin is considered, the curves (a), (b), etc. represent values of \( F_T \) for (10\( \overline{1} \)2) \{\( \overline{1} \)011\} twins when the stress axes lie in planes (a), (b), etc. in fig.5.1.

Fig.5.4 may also be used to determine values of \( F_T \) for any of the six \{10\( \overline{1} \)2\}<\( \overline{1} \)011> systems for stress axes lying in the planes of the standard triangle, (fig.5.3). Table 5.1 shows that the \( F_T \) curves for all twins are either (a) or (c) type for the (1\( \overline{2} \)10) plane and either (b) or (d) type for the (1\( \overline{0} \)00) plane. Given a stress axis in the standard triangle (defined by \( \theta \) and the stress axis plane), the Schmid factor for twinning, \( F_T \), on any system can be determined by referring to Table 5.1, selecting the particular twin and noting the Schmid factor curve characteristic of that twin. This curve in fig.5.4, together with the value of \( \theta \) defines the appropriate Schmid factor.

The convention adopted is such that tensile stresses and positive values of \( F_T \), or alternatively compressive stresses and negative values of \( F_T \), indicate that the work done favours twin growth. It is well known that stress reversal after twin growth can cause twins to contract (i.e. untwin). The effects of stresses having different senses of twin behaviour are summarised in Table 5.2.

Curves (a) - (c) in fig.5.4. are similar, reaching maximum values close to [0001], and passing through zero when the stress axis lies either in \( K_1 \) (-\( \theta \)) or in the plane normal to \( \eta_1 \) (+\( \theta \)). Curve (d) is unique since it is symmetrical about the c-axis and the \( F_T \) values remain positive for all values of \( \theta \) excepting \( \pm 90^\circ \).

Values of \( \theta \) for which \( \delta = 0 \), are superimposed on the \( F_T \) curves in fig.5.4. For axes lying in \( K_1 \), both \( \delta \) and \( F_T \) are zero for equal values of \( \theta \). However \( F_T \) becomes negative, whilst \( \delta \) remains positive for stress
Fig. 5.4 Schmid factors for twinning for stress axes in planes a, b, c, d. 
\( \theta \) is angle between stress axis and \([0001]_M\). \( \delta = 0 \) at points marked \( \dagger \).
axes lying between the plane normal to \( \eta_1 \) and \( K_2 \). This anomaly is effectively due to the fact that \( \delta \) applies to complete twinning (see para. 5.3.1), whilst the growth of a small twin lamella is controlled by the Schmid factor\(^{39} \). It is proposed in this thesis to discuss twin lamellae. Fig. 5.3 indicates the twins favoured by an applied stress and the relative \( F_T \) values are derived from Table 5.1 and fig. 5.4.

5.4 Slip Systems

The following transformation of Burgers vectors occur when \( \frac{1}{3} \langle 1120 \rangle \) type dislocations enter a (10\( \overline{1} \)2) twin\(^{202(a)} \).

\[
\begin{align*}
\frac{1}{3} [72\overline{7}0]_M & \rightarrow \frac{1}{3} [72\overline{7}0]_T \quad \text{Type (1)} \quad (5.2) \\
\frac{1}{3} [2\overline{7}0]_M & \rightarrow \frac{1}{6} [1\overline{2}13]_T - b_t \quad \text{Type (2)} \quad (5.3) \\
\frac{1}{3} [1\overline{1}20]_M & \rightarrow \frac{1}{6} [72\overline{3}]_T - b_t \quad (5.4)
\end{align*}
\]

where \( b_t \) represents a twinning dislocation. In type (1) interactions the vector is unchanged in magnitude and direction. Only glissile \( \frac{1}{3} \langle 1120 \rangle \) dislocations gliding in (0001) and \{1700\} planes are considered initially.

The Schmid factor curves were determined by measuring values of \( \theta \) and \( \lambda \) in equation (2) for Burgers vectors in the twin, \( (F_{BT} \) and \( F_{PT} \) curves for basal and prism slip respectively) and in the parent matrix \( (F_{BM} \) and \( F_{PM} \) curves for basal and prism slip respectively). The variation in the Schmid factors for stress axis planes (a) - (d) are presented. The slip systems are indexed with respect to the (10\( \overline{1} \)2) twin for convenience. \( F_T \) curves for this twin and the maximum \( F_T \) values, on any twin system, are superimposed on the curves for slip.

5.4.1 Schmid Factors for Basal Slip in Parent and Twin

The Schmid factor curves are shown in fig. 5.5. for axes in the four stress axis planes. In both (a) and (c) planes, the \( F_{BM} \) curves are similar, remaining zero for one slip system, whilst the other two slip systems have equal \( F_{BM} \) values. Moreover \( F_{BM} \) curves in planes (b) and (d) are also identical. \( \frac{1}{4} F_T \) values approach a maximum as \( F_{BM} \) tends to zero and vice versa, excepting values of \( \theta = \pm 90^0 \) in planes (d).

For slip in the twin crystal only near \( \theta = 0 \) are \( F_{BT} \) values minimum,
Fig. 5.5 Schmid factors for twinning (—), basal slip in parent matrix (—O—), and twin matrix (—x—). Curve---indicates maximum Schmid factor on any \{1012\} twin system.

a Stress axis lying in \((1210)_M\) or (a) type plane. Schmid factor for \([1210]_M|T\) is zero.
Fig. 5.5b Stress axis lying in (110) or (b) type plane.
Fig. 5.5c  Stress axis lying in $(2\overline{1}10)_M$ or (c) type plane

Schmid factor for $[2\overline{1}10]_M$ is zero
Fig. 5.5d Stress axis lying in \((10\overline{1}0)_M\) or \((d)\) type plane
when $F_T$ values approach maximum. $F_{BT}$ values are large in plane (b), very small in plane (d), and remain zero for one system in plane (a).

5.4.2 Relative Schmid Factors for Basal Slip in Parent and Twin

From fig. 5.5 the relative Schmid factors can be decided for any twin system and for any position of the stress axis.

5.4.2.1 Ratio of Maximum Schmid Factors

The ratio of the maximum Schmid factors for slip in twin and parent matrix can be determined for any given value of $\theta$. This data is presented in fig. 5.6. Slip is favoured in the twin when the Schmid factor ratio is $\geq 1$ and in the matrix when the ratio is $< 1$. Care must be taken in interpreting these curves for values of $\theta$ near $0^\circ$ and $+90^\circ$, for when the Schmid factor for slip in one matrix tends to zero, even a small Schmid factor for slip in the other matrix gives an infinitely small value for the ratio. Nevertheless the general trend is apparent.

For negative $\theta$ and positive Schmid factors, for twinning, the ratio is $<1.0$ for all planes (a) - (d), except near $[0001]$M. For positive $\theta$, the ratio has values $<<1.0$ over a large orientation range in plane (d). For all planes (a) - (d) extreme values of the Schmid factors ratios occur either in the twin or in the matrix near $\theta = 0$ or $+90^\circ$ (see para. 5.5.1).

5.4.2.2 Ratios of Schmid Factors for Type (1) Dislocations in Parent and Twin

For any twin system only one $\frac{1}{3} <11\bar{2}0>$ type Burgers vector can glide through the twin interface without transforming to a different vector. For the (1012) twin the vector is $+ [1\bar{2}10]$. The ratios of the values of the Schmid factors for this Burgers vector, in the twin and in the matrix, are given in fig. 5.7.

In stress axis planes (a), the Schmid factor for this system remains zero. The ratios suggest slip should continue through the twin boundary for approximate values of $\theta$ of $-65^\circ$ and $+60^\circ$ for (c) and $-50^\circ$ and $+45^\circ$ for (b), i.e. when the ratio of Schmid factors in the twin and parent matrices for the glissile dislocations, approach unity. But at these values of $\theta$, the Schmid factor for twinning is very small.

5.4.3 Schmid Factors for Prism Slip in Parent and Twin

In the parent crystal $F_{PM}$ curves are identical in all planes (a) to (d) in fig. 5.8. since $F_{PM}$ for one slip system remains zero, whilst the
Fig. 5.6 Ratio of maximum Schmid factors for basal slip in the twin to maximum values in parent matrix. $F_T = 0$ for values of $\theta$ marked 1.
Fig. 5.7 Ratio of Schmid factors for type (l) dislocations and basal slip in twin and matrix. Note ratio=0 for (a). F_T=0 for values of $\theta$ marked 1.
other two slip systems have equal \( F_{PM} \) values. In all the planes, \( F_T \) values are nearly maximum, when the \( F_{PM} \) values are near zero, i.e., when \( \theta \) is near \( [0001]_M \); \( F_T \) values are large, but negative, at \( \theta = \pm 90^\circ \), where \( F_{PM} \) values are also large. Note that \( F_T \) for curve (d) is zero at \( \theta = \pm 90^\circ \).

In twin crystal the simplest behaviour is exhibited in plane (a), fig. 5.8 in which the \( F_{PT} \) and \( F_{PM} \) curves are \( 90^\circ \) out of phase, with one system having \( F_{PT} \) equal to zero for all values of \( \theta \). No system has \( F_{PT} \) zero for all values in (b) – (d). In (d) all systems reach approximately maximum \( F_{PT} \) values.

5.4.4 Relative Schmid Factors for Prism Slip in Parent and Twin

5.4.4.1 Ratio of Maximum Schmid Factors

Fig. 5.9 shows the variation in the ratio of the maximum Schmid factors in parent and twin. For positive \( F_T \) values the ratio is always greater than unity, i.e. slip is favoured in the twinned matrix. This is especially so near the \( [0001]_M \) axis. However for negative \( F_T \) values the ratio becomes less than unity, for all planes other than (d).

5.4.4.2 Ratio of Schmid Factors for Type (1) Dislocations

in Parent and Twin

The variation in the ratio, \( F_{PT}/F_{PM} \), for type (1) dislocations is shown in fig. 5.10. For this slip system the ratios for plane (a) and (d) are zero and infinity respectively for all values of \( \theta \).

The optimum ratio for slip to penetrate the twin interface, i.e. unity, occurs only for (b) and (c) planes and for values of \( \theta \) equal to that found for basal slip, i.e. when \( F_T = 0 \). For positive \( F_T \) values, the ratio tends to be much greater than 1.0 (especially near \( [0001]_M \)). For negative \( F_T \) values the ratio indicates greater slip in the parent matrix.

5.5 Discussion

It has often been stated that twinning can increase ductility in h.c.p. structures by reorienting the parent crystal into positions more favourable for slip. However this generalisation can be misleading, since often when twinning is favoured subsequent slip in the twinned crystal is not favoured in comparison to slip in the original untwinned crystal. In the following discussion \([10\bar{1}2]\) twinning is considered and a comparison made between slip on basal and prism systems in \(<11\bar{2}0>\) directions.
Fig. 5.8 Schmid factors for twinning (−), prism slip in parent matrix (−O−) and twin matrix (−x−). Curve-- indicates maximum Schmid factor on any {1012} twin system.

a Stress axis lying in (1210)_M or (a) type plane.
Schmid factor for [1210]_M/T is zero.
Fig. 5.8b Stress axis lying in (1100)_M or (b) type plane

Schmid factor for [1120]_M is zero
Fig. 5.8c  | Stress axis lying in (10\bar{1}0) or (c) type plane
Schmid factor for [2\bar{1}10]_M is zero
Fig. 5.8d Stress axis lying in (1010) or (d) type plane
Schmid factor for $[1210]_M$ is zero
Fig. 5.9 Ratio of maximum Schmid factors for prism slip in twin and parent. Notation as in Fig. 7

Fig. 5.10 Ratio of Schmid factors for type (1) dislocations and prism slip systems. Note ratio is zero for (a), infinitely large for (d)
The ratio \[ \frac{\text{maximum Schmid factor for slip in twin}}{\text{maximum Schmid factor for slip in matrix}} \] has been calculated for all twins and for the appropriate axes in the standard triangle. Results obtained with magnesium single crystals suggest the ratio must exceed \( \sim 1.3 \) before slip predominates in twinned crystal\textsuperscript{335}. This corresponds to a difference in Schmid factor of not less than 0.1. In Table 5.3 differences less than and greater than approximately 0.1 are distinguished by small (m, t) and capital (M, T) letters respectively.

Two practical situations will be discussed separately. The first involves the effect of applied stresses on pre-existing twins introduced into a polycrystalline aggregate during processing. The second case considers the effect of applied stresses on initially twin-free crystal.

5.5.1 Relative Slip in Pre-existing Twins

When all twins are present, each twin matrix will respond according to the Schmid factor curves indicated in Table 5.1. The relative slip in twinned and parent crystal is summarised in Table 5.3.

For pre-existing twins, the relative slip in twin and parent matrix is independent of the sense of the stress, but the sign of \( F_T \) is important. E.g. In the \( F_T \) positive regions all pre-existing twin systems favour prism slip under both tensile and compressive stresses. In \( F_T \) negative regions all twin systems favour prism slip in the matrix.

From the Schmid factor curves it is possible to determine the effect of the presence of twins on the ability to slip. A measure of the ability to slip was estimated from the difference in maximum Schmid factors in twin and parent. Slip in one matrix was assumed to predominate when its Schmid factor exceeded that in the other by more than 0.1.

This data is summarised in Table 5.4 for the case of pre-existing twins, assuming all twins are equally represented. The table shows clearly that in the basal slip case, for the majority of orientations considered, the presence of twins has little effect on the ability to slip, but when they do have an effect, it is more likely to decrease the ability to slip.

In the prism slip case however, (Table 5.4), twins greatly enhance the ability to slip in the majority of orientations considered.
Table 5.3

RELATIVE SLIP IN $\{10\overline{7}2\}$ TWINS AND IN PARENT

<table>
<thead>
<tr>
<th>Predominant slip system</th>
<th>Sense of stress required for twin growth</th>
<th>Twin systems</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stress axis plane in standard triangle</td>
<td>1  2  3  4  5  6</td>
</tr>
<tr>
<td>Basal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tensile $(F^*_T$ positive)</td>
<td>$1\bar{2}10$ t* m/t M m M m/t</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$1\bar{7}00$ t t M M M M</td>
<td></td>
</tr>
<tr>
<td>Compression $(F^*_T$ negative)</td>
<td>$1\bar{2}10$ m T t T t T T</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$1\bar{1}00$ t/T t/T does not occur (M pre-existing)</td>
<td></td>
</tr>
<tr>
<td>Prism</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tensile $(F^*_T$ positive)</td>
<td>$1\bar{2}10$ T T T T T T</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$1\bar{7}00$ T T T T T T</td>
<td></td>
</tr>
<tr>
<td>Compression $(F^*_T$ negative)</td>
<td>$1\bar{2}10$ M m m M m m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$1\bar{7}00$ M M does not occur M (pre-existing)</td>
<td></td>
</tr>
</tbody>
</table>

$m(t)$ indicates $F^*_{BM}$ $(F^*_{BT})$ curve is greater than $F^*_{BT}$ $(F^*_{BM})$ by less than $\sim 0.1$ in the Schmid factor.

$M(T)$ indicates $F^*_{BM}$ $(F^*_{BT})$ curve is greater than $F^*_{BT}$ $(F^*_{BM})$ by more than $\sim 0.1$ in the Schmid factor.
TABLE 5.4
THE EFFECT OF PRE-EXISTING TWINS ON THE ABILITY TO SLIP, ASSUMING
ALL TWIN SYSTEMS OF A PARTICULAR FORM ARE EQUALLY REPRESENTED

<table>
<thead>
<tr>
<th>Twin System</th>
<th>Slip System</th>
<th>% Stress Axes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ability to slip increased by twinning</td>
</tr>
<tr>
<td>[1121]</td>
<td>Basal</td>
<td>40%</td>
</tr>
<tr>
<td></td>
<td>Prism</td>
<td>38%</td>
</tr>
<tr>
<td>[1012]</td>
<td>Basal</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>Prism</td>
<td>57</td>
</tr>
</tbody>
</table>
5.5.2 Relative Slip in Growing Twins

The effect of orientation on twin systems favoured under tensile and compressive stresses is shown in fig. 5.3.

For the tensile case, there is a large region in which only two twins are favoured (0,) but their Schmid factors are < 0.25 for stress axes in the [1700] zone. Twins 3 and 6 are most favoured when $\theta$ is greater than boundary 1. Table 5.3 indicates that prism slip is greatly enhanced by all twin systems. When no twins are favoured, prism slip in the parent matrix is expected to be easy. Under tensile stresses twinning is now expected to enhance basal slip and for axes near [0001] the strain must be produced largely by the twinning shear. Neither twinning nor matrix slip can contribute significantly to the strain normal to [0001] for materials slipping on basal planes.

The separation of the Schmid factor curves for twinning is greater when $F_T$ is negative (fig. 5.4). Thus in order of increasing negative $F_T$ values $c < b < a$. In compression twins 1 and 4 will predominate for stress axes in [1210] zones, whilst twins 1, 2, 4 and 5 will predominate for axes in the [1700] zone.

Under compressive stresses twins facilitate basal slip only for about half the stress axes considered, whilst no twins facilitate prism slip, (Table 5.3). For axes nearly normal to [0001] when all twins are favoured (D, fig. 5.3) prism slip in the parent matrix is also highly favoured. But basal slip is not favoured and if the 1 and 4 twin systems predominate twinning is not likely to enhance basal slip; however the opposite is true if twins 2 and 5 occur, (fig. 5.3). For axes near [0001] under compressive stresses neither twinning nor slip can contribute significantly to the strain in materials slipping on either prism or basal systems, remembering that initially twin free material is considered.

It is clear from figs. 5.6 and 5.9 that extremes of slip in twinned crystal may occur for certain values of $\theta$. When a twin nucleates under these conditions a slip avalanche could be initiated within the twin. The conditions necessary for this to occur are listed in Table 5.5. Under tensile stresses, prism slip produces ideal conditions, since large values of Schmid factor exist both for twinning and for prism slip in twinned crystal. Suitable conditions arise only for basal slip in compression. The favoured twin systems (1, 4) only have small Schmid factors for basal
<table>
<thead>
<tr>
<th>Twin System</th>
<th>Sense of Stress</th>
<th>Slip System</th>
<th>Orientation of Stress Axis</th>
<th>Operative Twin System</th>
<th>Schmid factors for twinning</th>
<th>Schmid factors in twin and parent</th>
</tr>
</thead>
<tbody>
<tr>
<td>{10\overline{7}2}</td>
<td>Tension Basal Prism</td>
<td>parallel to c-axis</td>
<td>All twins</td>
<td>0.5</td>
<td>0.06/0</td>
<td>0.4/0</td>
</tr>
<tr>
<td></td>
<td>Compression Basal</td>
<td>normal to c-axis</td>
<td>All twins</td>
<td>$0.5(1,4)$, $0.1(2,3,5,6)$, $0.38(1,2,4,5)$</td>
<td>0.06/0</td>
<td>0.43/0</td>
</tr>
<tr>
<td>{11\overline{2}1}</td>
<td>Tension Basal Prism</td>
<td>parallel to c-axis</td>
<td>All twins</td>
<td>0.28</td>
<td>.47/0</td>
<td>.15/0</td>
</tr>
<tr>
<td></td>
<td>Compression Basal</td>
<td>normal to c-axis</td>
<td>All twins</td>
<td>$0.28(1,4)$, $0.21(1,3,4,6)$</td>
<td>.23-0.47/0</td>
<td>0.35/0</td>
</tr>
</tbody>
</table>
slip in the twin matrix, but twins 1, 2, 4 and 5 are nearly ideally suited when stress axes lie in \([1\bar{1}00]\) zone.

5.5.3 Twin Boundaries as Obstacles to Slip

Only type (1) dislocations can glide through twin interfaces and leave no defect in the interface. The appearance of slip traces produced by such dislocations is shown schematically in fig. 5.11. Figs 5.7 and 5.10 give the orientations of stress axes for which these dislocations should pass through the twin interface. This will occur most readily for values of \(\theta\) corresponding to ratios near unity. Here the Schmid factor for twinning is very small and only pre-existing twins are then relevant.

For both basal and prism slip a suitable combination of Schmid factors in twin and matrix only occurs for axes lying in \((h)\) and \((c)\) planes and for values of \(\theta\) near \(\pm 50^\circ\) and \(\pm 60^\circ\) respectively. Clearly for other orientations the Schmid factors in one matrix will be much less than that in the other and the twin boundary will become effectively a barrier to slip even for type (1) dislocations. A good example of this occurs for prism slip and plane \((a)\) when the glissile slip system in the matrix has zero Schmid factor whereas that in the twin approaches 0.5 at \(\theta \approx \pm 45^\circ\).

Individual type (2) dislocations cannot glide readily through \([10\overline{1}2]\) twin interfaces since they become sessile dislocations after transformation. This was confirmed experimentally by Price \(^{162}\) using zinc platelets; moving \([10\overline{1}2]\) twin interfaces sweep type (2) dislocations ahead of the interface. The progressively increasing stress required for continuous twin boundary displacement in zinc \(^{166}\) has also been attributed to the accumulation of dislocations swept up by the boundary. Twins also prevent geometrical softening in magnesium by acting as barriers to slip \(^{206}\).

It is therefore concluded that when twins are nucleated, the twin interface is effectively a barrier to slip of \(\frac{1}{3}[1\overline{1}20]\) type dislocations on all basal and prism slip systems and twin interfaces will then behave like grain boundaries. Whilst extensive twinning may allow increased slip, the grain size is effectively reduced by twinning, which may thereby increase the work hardening rate and ductility. There is some evidence for this in zinc \(^{344}\), titanium \(^{85,186}\), magnesium \(^{224}\) and zirconium \(^{345}\). The large twinned volume fraction possible in h.c.p. metals \(^{142,186}\) is likely to enhance this effect of twinning.
Fig. 5.11 Schematic diagram of slip traces produced by type (l) dislocations gliding in basal or prism planes through a $\{10\bar{1}2\}$ twin. Section parallel to plane of shear of twin.
5.6 Summary

1. Pre-existing twins greatly enhance the ability to slip on prism planes (57% at the stress axes) and slip is unaffected or decreased for 24% and 19% of the stress axes respectively.

   Basal slip is not affected by pre-existing twins for the majority of stress axes (59%) but when twins do have an effect it is more likely to decrease (25% of the stress axes) than to increase (16% of the stress axes) the ability to slip.

2. All twins nucleated under tensile stresses increase the ability to slip on prism planes, but these twins have little effect on the ease of basal slip. When twins are nucleated under compressive stresses, no twins help prism slip, but some twins enhance basal slip.

3. Except for small ranges of orientation, twin boundaries are expected to act as barriers to slip in <1120> directions. Twins can then be considered to behave as individual grains and by effectively reducing the grain size, twinning can increase the work hardening rate and the ductility.

4. For some orientations of stress axis, slip avalanches can occur within the matrix of a growing twin.

5.7 Slip Planes for Transformed Dislocations

   It has been shown that when {1012} type twins are nucleated, the applied stress is unlikely to cause glide of \( \frac{1}{3} <11\bar{2}0> \) type dislocations through twin interfaces. Under these conditions dislocation pile-ups will occur at twin interfaces causing high local stresses. Twins will also be required to grow through the dislocation forest. Consequently the dislocation/twin interface reactions are expected to play an important role in the deformation of h.c.p. metals.

   The incorporation of slip dislocations into mechanical twins has been discussed for twinning in tin and b.c.c. metals and for twinning in zinc. Interactions between {1012} twins and \( \frac{1}{3} <11\bar{2}0> \) dislocations gliding in prism and basal planes are now considered and the possible effects of these interactions in titanium and other hexagonal metals are examined.

   The transformation of Burgers vectors is described by equations 5.2 - 5.4. In equation (5.2) the vector is unchanged in magnitude and direction but in equations (5.3) and (5.4) both vector magnitudes and directions are changed. In the subsequent discussion dislocations will
be described as type (1) or type (2) according to their Burgers vectors after transformation.

Although type (1) dislocations may glide through twin interfaces, for the stress axes considered in para.5.2 suitable shear stresses only exist in a very small range of orientation and twin interfaces will normally act as barriers to the glide of these dislocations.

The transformation product in equations 5.3 and 5.4 is not a glissile dislocation and will be associated with stacking faults in the twin. However two parent matrix dislocations together can produce a glissile pyramidal dislocation according to the reaction.

\[
\frac{2}{3} [2\overline{7}0]_M \rightarrow \frac{1}{3} [\overline{2}1\overline{3}]_T + 2b_t
\]  

(5.5)

The zonal twinning dislocation in (5.5) is expected to result in a lower twin interface energy than the twinning dislocations produced in (5.3) and (5.4). The relative positions of the vectors (5.3) and (5.4) before and after twinning, are shown in fig.5.12.

The effects of the twin interface on type (2) dislocations is dependent on the slip planes in the parent matrix. The basal plane in the parent matrix and the (1010) plane in the twin (fig.5.12) intersect the (10\overline{7}2) twin boundary along [1\overline{2}10]. Thus type (2) dislocations in the parent basal planes, after transformation to \(\frac{1}{3} <1\overline{1}23>\) type Burgers vectors, can slip in \{10\overline{7}0\} in the twin. The sequence is shown schematically in fig.5.13. Note the dislocation segments parallel to the twin boundary are of mixed orientation.

Type (2) dislocations gliding in prism planes in the parent will intersect the twin boundary along \(<\overline{4}223>\) directions (fig.5.12). These are also the directions of intersection of \{1\overline{1}22\} type planes in the twin matrix with the twin boundary. Thus type (2) dislocations can cross-slip from prism planes in the parent to \{1\overline{1}22\} planes in the twin, as shown schematically in fig.5.14.

In both examples described above, twinning dislocations are produced where the glissile dislocations pass through the twin interface (figs.5.13 and 5.14).

5.8 Schmid Factors for Slip in \(<1\overline{1}23>\) Directions in Twinned Crystal

5.8.1 \[10\overline{1}0\] \(<1\overline{1}23>\) Slip Systems

When basal slip utilising type (2) dislocations predominates in the
Fig. 5:12 Stereographic projection of poles and $\frac{1}{3} <11\overline{2}0>$ Burgers vectors in parent matrix and in $(10\overline{2}2)$ twin (subscript T). Stress axis zones lettered a–d, dash indicating negative $\theta$. Burgers vectors enclosed in [ ]. Pyramidal Burgers vectors produced by transformation are also indicated.
FIG. 5.13

FIG. 5.14
metal, prism slip in \( <11ar{2}3 > \) directions is most likely to operate after transformation according to equation (4) above. In order to consider the subsequent behaviour of these glissile pyramidal dislocations, Schmid factors for these systems are presented in fig. 5.15.

The Schmid factor curves for basal slip in the parent matrix have been compared with the appropriate curves in fig. 5.15. For all stress axis planes, type (2) dislocations have similar Schmid factors before and after transformation for all values of \( \theta \).

Since type (2) Burgers vectors are equally favoured in parent and twin matrices for stress axes in (a) type planes, the \( \frac{1}{3} <11\bar{2}0 > \) type dislocations are likely to operate in both parent and twin matrices.

Similarly for (b) type planes, a type (2) Burgers vector has the maximum Schmid factor in the parent. It is greater than the Schmid factors for any \( \frac{1}{3} <11\bar{2}0 > \) Burgers vector in the twin when \( F_T \) is positive. Since Schmid factors for type (2) are large in the twin for both \( \pm F_T \), they could produce \( \frac{1}{3} <11\bar{2}3 > \) dislocations in the parent matrix.

In (c) type planes, a type (1) Burgers vector has a maximum Schmid factor in a parent, but when \( F_T \) is positive, its Schmid factor in the twin is much less. However the other operative parent Burgers vector is of type (2); its Schmid factor in the twin is greater than any \( \frac{1}{3} <11\bar{2}0 > \) type Burgers vector when \( F_T \) is positive. When \( F_T \) is negative, \( \frac{1}{3} <11\bar{2}3 > \) Burgers vectors may arise in parent matrix.

In (d) type planes, a type (1) Burgers vector has a large Schmid factor in the parent, but all \( <11\bar{2}0 > \) Burgers vectors in the twin have values \( <0.1 \). Values for type (2) dislocations lie between 0.1 and 0.2 in parent, but after transformation lie between 0.1 and 0.3, much greater than any \( <11\bar{2}0 > \) in the twin.

5.8.2 \{1212\} \{12\bar{1}3\} Slip Systems

When prism slip predominates in the metal type (2) dislocations can give rise to \( \frac{1}{3} <11\bar{2}3 > \) dislocations gliding in \{11\bar{2}2\} twin planes. Curves for the system having the maximum Schmid factor are shown in fig. 5.16. The Schmid factor for prism slip (para. 5.4.3) has been compared with the appropriate curve in fig. 5.16.

For all stress axis planes the Schmid factor for type (2) dislocations before and after transformation is approximately equal in both parent and twin for all values of \( \theta \).

In the (a) type plane, type (1) dislocations have zero Schmid factors.
Fig 5.15 Schmid factors for \{\bar{1}010\} <\bar{1}2\bar{1}3> slip systems produced in twin matrix after transformation
in the parent matrix and only type (2) dislocations operate. In the
twin, when $F_T$ is positive $\frac{1}{3} <1\bar{1}20>$ slip predominates but for negative
$F_T <1\bar{1}20>$ is much less favoured, while $<1\bar{1}23>$ slip resulting from
transformation is highly favoured. Similarly for the type (b) plane.

In the (c) plane, Schmid factors for type (2) $<1\bar{1}20>$ dislocations
in the twin are similar to those for $<1\bar{1}23>$ when $F_T$ is negative. Thus
$<1\bar{1}23>$ slip may also operate in the parent by transformation of type (2)
dislocations active in the twin. Only type (2) dislocations are active
in the (d) plane. Although the $\frac{1}{3} <1\bar{1}20>$ dislocations in the twin have
greater Schmid factors than the $\frac{1}{3} <1\bar{1}23>$, values for the latter are quite
significant. Again where $F_T$ is negative, $\frac{1}{3} <1\bar{1}23>$ are likely to be
produced in the parent matrix.

5.8.3. Prism to Pyramidal Slip in $<1\bar{1}23>$ Directions

For slip in $<1\bar{1}23>$ directions the Schmid factor curves repeat about
every $90^\circ$ and $180^\circ$ for slip in $\{1\bar{1}00\}$ and $\{\bar{1}1\bar{2}2\}$ planes respectively
(figs. 5.15 and 5.16). If a Schmid factor greater than 0.2 is considered
necessary for slip, then $\{1\bar{1}00\}$ and $\{\bar{1}1\bar{2}2\}$ slip may occur together for
values of $\theta$ between about $40^\circ$ and $70^\circ$. Thus cross-slip from $\{1\bar{1}00\}$ to
$\{\bar{1}1\bar{2}2\}$ is possible within this orientation range. However if a higher
Schmid factor is required for slip on these systems, the favourable
orientation range for cross-slip is reduced.

5.9. Slip Traces in Parent and Twin Matrices

Experimental evidence for the operation of slip systems in bulk
material is normally obtained from slip trace analysis. Fig. 5.11 shows
the traces produced by type (1) dislocations after penetrating a $(10\bar{1}2)$
twin. Parallel traces are produced by type (2) dislocations nucleated in
each matrix.

Traces produced when type (2) dislocations penetrate the twin inter-
face are shown in fig. 5.17. When basal slip predominates, prism slip in
$<1\bar{1}23>$ directions would be apparent, but $\{1\bar{1}22\}$ traces cannot be
distinguished from basal slip in the twin. When prism slip predominates
$\{1\bar{1}22\} <\bar{1}1\bar{2}3>$ traces in the twin may be identified if basal slip can be
assumed to be absent. However it is apparent that the unambiguous
identification of the $\{1\bar{1}22\} <\bar{1}1\bar{2}3>$ slip system from slip traces in the
plane of shear is not easy.

Type (1) dislocations produce no visible slip traces when the parent
Fig. 5.17 Schematic diagram of slip traces in twin and parent matrices. Section parallel to the plane of shear.

(a) Produced by type (2) dislocations gliding in basal planes.
(b) Produced by type (2) dislocations gliding in prism planes.
crystal surface is parallel to (0001) (fig. 5.18a). The (7010)[1213] is not distinguishable from (7010)[1210] (fig. 5.18b). However there is no easy slip system parallel to (7212)[1213] in the twin, which may now be identified unambiguously (fig. 5.18b, c).

5.10 Summary

Dislocations in h.c.p. metals e.g. magnesium, titanium, zirconium and beryllium, tend to be confined to a single prism or basal slip plane and pile-ups against twin boundaries will cause large stress concentrations. These stresses may eventually be relieved by cross-slip in the parent matrix or by the pile-up dislocations penetrating the twin boundary.

Individual type (2) dislocations are unlikely to relieve the stress by penetrating the twin boundary since they become immobile dislocations associated with stacking faults in the twin matrix. However two pile-up dislocations may penetrate the twin boundary together and nucleate $\frac{1}{3}<11\bar{2}3>$ type dislocations; subsequent glide of these dislocations would relieve the stresses at the head of the pile-up.

Pairing of dislocations prior to glide in the twin matrix seems most likely when glissile dislocations impinge on a stationary twin interface, whereas the immobile dislocations are more likely when a moving twin interface sweeps through the dislocation forest.

The ratio of the Schmid factor before and after transformation is about unity for all values of $\theta$, a result unattainable with type (1) dislocations. Thus the Schmid factor curves show clearly that the shear stresses favour the subsequent glide of $<c+a>$ dislocations. Furthermore the magnitude of the Schmid factor for the $<c+a>$ dislocations is often greater than for any $\frac{1}{3}<11\bar{2}0>$ T dislocation.

It is concluded that {1072} type twins may nucleate $<c+a>$ dislocations, in either the parent or twin matrix, which may then glide away under high shear stresses. This implies that the twin interfaces may cease to be barriers to slip of type (2) dislocations at high stresses.
Fig. 5.18 Schematic diagram of slip traces in twin and parent matrix.
Section parallel to basal plane
(a) Produced by type (1) dislocations gliding on basal or prism planes
(b) Produced by type (2) dislocations gliding on basal planes
(c) Produced by type (2) dislocations gliding on prism planes
CHAPTER 6
The Role of \{11\bar{2}1\} Twinning in the Deformation of H.C.P. Metals

6.1 Resolved Shear Stress Factors for Slip and Twinning

The most frequently observed twin systems in titanium are \{10\bar{1}2\} and \{11\bar{2}1\}. The role of \{10\bar{1}2\} twinning in titanium was considered in Chapter 5. It was concluded that at low stresses \{10\bar{1}2\} twins increase the ability to slip on prism planes but have much less effect when basal slip predominates. Twin interfaces are expected to act as barriers to slip at low stresses. At higher stresses, dislocation interactions at twin boundaries can lead to \(<c+a>\) type slip and could thereby enhance the ductility. This effect is expected to be greater when prism slip predominates.

The twinning shear for \{11\bar{2}1\} twins is large\(^{150,157,158}\). It is difficult to predict the active twin system in both single crystal and polycrystalline materials, a situation which also prevails in \{10\bar{1}2\} twinning. Only \{11\bar{2}1\} twins were found in rhenium single crystals\(^{158}\), although the resolved shear stresses were greater on \{10\bar{1}2\} twin systems. This differs from the results obtained with titanium\(^{349}\), in which only \{10\bar{1}2\} twins were detected when \{11\bar{2}1\} twin systems experienced similar resolved shear stresses. It is probable that the difference arises because basal slip predominates in rhenium whilst prism slip predominates in titanium and the nucleation of twins is dependent on suitable dislocation interactions. This explanation is supported by the work of Reed-Hill et al.\(^{149,192}\), who found \{11\bar{2}1\} twins were not nucleated in zirconium at low strain rates at room temperature. However \{11\bar{2}1\} twins nucleated at low temperatures grew significantly during subsequent room temperature deformation.

Another anomaly frequently encountered is the occurrence of \{11\bar{2}1\} twins which appear to oppose the applied stress\(^{158}\). This is undoubtedly associated with the complex accommodation stresses around twins.

It has been shown by Reed-Hill et al.\(^{142,192}\) that \{11\bar{2}1\} twinning is a significant deformation mode in zirconium at low temperatures and is responsible for increased ductility. The ductility of titanium at cryogenic temperatures has similarly been attributed to twinning\(^{85,186,193a,202c}\).

It is therefore proposed in this Chapter to consider the effect of \{11\bar{2}1\} twinning on the ability to slip on prism and basal planes. The technique developed for the analysis of \{10\bar{1}2\} twinning will be used.
Each stress axis plane is lettered A to D, a negative sign (-A etc.) indicating regions in which $\theta$ is negative.

The stereogram in fig.6.1 shows all six \{1121\} twin poles and the twin boundary for the (1121) twin. Stress axis planes are lettered with respect to (1121) twin. By consulting Table 6.1 the equivalent Schmid factor curve for any twin and stress axis plane can be determined. The Burgers vectors on the curves relate to stress axes lying in the quadrant 0001-1120-1100 of the stereogram in fig.6.1.

It should be noted that the plane denoted by (a) in the analysis for \{10\overline{7}2\} twinning, (Chapter 5) is equivalent to a (B) type plane in the present analysis of \{11\overline{2}1\} twinning (Table 6.2).

As in the analysis for \{10\overline{7}2\} twinning, stress axes lying in planes having identical letter symbols give rise to identical Schmid factor curves for either twinning or slip.

6.2 \{11\overline{2}1\} <\overline{1}7\overline{2}6> Twinning

6.2.1 Crystallography of Twinning

The \{11\overline{2}1\} type twin in titanium has the following twinning elements (Table IV, Chapter 1):

\begin{align*}
  K_1 &= (11\overline{2}1) \; \eta_1 = [\overline{7}726] \\
  K_2 &= (0001) \; \eta_2 = [11\overline{2}0]
\end{align*}

These elements are shown in fig.6.1 on the standard stereogram. The positions of $\frac{1}{3} <1\overline{2}0>$ Burgers vectors before and after transformation by twinning are also shown.

The shape change caused by twinning is described schematically in fig.1.11d, and the change in length in complete twinning along any given direction is summarised in fig.6.2. However for small twin lamellae the diagram is modified, as shown in fig.6.3.

6.2.2 Schmid Factors for Twinning

Fig.6.4 shows that only stress axes lying in D type planes give rise to a Schmid factor curve symmetrical about the c-axis of the parent. All twins will grow under a tensile stress parallel to the c-axis or a compressive stress normal to the c-axis.
Fig. 6.1 Stereographic (0001) projection showing (1121) twinning elements, stress axis planes and twin poles. Position of \( \frac{1}{3} \langle 11 \bar{2} 0 \rangle \) Burgers vectors in parent and (1121), twin are also shown.
**TABLE 6.1**

**INDICES OF STRESS AXIS PLANES FOR \{1\bar{1}21\} TWINS**

<table>
<thead>
<tr>
<th>Stress axis plane in standard triangle (parent matrix)</th>
<th>{1\bar{1}21} \times \bar{1}726 \text{ twin systems}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>({1\bar{1}21})</td>
<td>B</td>
</tr>
<tr>
<td>({\bar{1}100})</td>
<td>A</td>
</tr>
</tbody>
</table>

**TABLE 6.2**

<table>
<thead>
<tr>
<th>Stress axis plane in standard triangle (parent matrix)</th>
<th>{1\bar{1}21} twin notation in Chapter 5</th>
<th>{1\bar{1}21} twin notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>({1\bar{1}21})</td>
<td>a</td>
<td>B</td>
</tr>
<tr>
<td>({\bar{1}100})</td>
<td>b</td>
<td>A</td>
</tr>
</tbody>
</table>
Dimensional changes as a function of orientation. Great circles 3, 4, 5 represent $K_1$ planes for these twin systems, and 1, 6, 2 represent planes normal to $\eta_1$ for these twin systems.

**Fig. 6.2** For complete twinning on $\{1121\}$ systems

A All twins produce extension
B Twins 4 produce contraction.
   Twins 1, 2, 3, 5, 6 produce extension
C 1, 3, 4, 6 produce contraction.
   2, 5 produce extension
D All twins produce contraction

**Fig. 6.3** For incomplete twinning on $\{11\overline{2}1\}$ systems

A All twins produce extension
B Twin 4 produce contraction
   1, 2, 3, 5, 6 produce extension
C$_1$ 4, 3 produce contraction.
   1, 2, 5, 6 produce extension
C$_2$ 1, 3, 4 produce contraction.
   2, 5, 6 produce extension
C$_3$ 1, 3, 4, 6 produce contraction.
   2, 5 produce extension
D$_1$ 3, 4, 5 produce contraction.
   1, 2, 6 produce extension
D$_2$ 1, 3, 4, 5 produce contraction.
   2, 6 produce extension
D$_3$ 1, 3, 4, 5, 6 produce contraction.
   2 produce extension
D All twins produce contraction
Fig 6.4  Schmid factors for twinning for stress axes in planes (A), (B), (C) and (D). $\theta$ is angle between stress axis and $[000]_M$.
6.3 Slip Systems

Since all $\frac{1}{3} <11\overline{2}0>$ Burgers vectors lie in $K_2$, the indices and magnitudes of the Burgers vectors are similar after transformation, although their positions are changed to $K_1$ (Fig. 6.1). For the $(11\overline{2}1)$ twin, the following transformations occur.

Type 1: $\frac{1}{3} [11\overline{2}0]_M \rightarrow \frac{1}{3} [\overline{1}7\overline{2}0]_T + 2t$

$$b_1 \rightarrow b_1^*$$

$$\left\{ \begin{array}{l}
\frac{1}{3} [\overline{1}7\overline{2}0]_M \rightarrow \frac{1}{3} [\overline{2}110]_T + t \\
-b_3 \rightarrow -b_3^*
\end{array} \right.$$  (6.2)

Type 2

$$\left\{ \begin{array}{l}
\frac{1}{3} [2\overline{1}10]_M \rightarrow \frac{1}{3} [1\overline{2}10]_T + t \\
-b_2 \rightarrow -b_2^*
\end{array} \right.$$  (6.3)

No dislocations having these Burgers vectors can glide through a twin interface without raising the energy of the interface by generating twinning dislocations. For the present the dislocations are assumed to nucleate either in the twin or in the parent.

6.3.1 Schmid Factors for Basal Slip in Parent and Twin

In Fig. 6.5, for stress axis planes type (A) and (C) the Schmid factors for basal slip in the parent ($F_{BM}$) are identical, attaining maxima at $\theta = \pm 45^0$ and a value of zero at $\theta = 0$ or $\pm 90^0$.

Similarly $F_{BM}$ curves in planes (B) and (D) are identical, remaining zero for one slip system, whilst the other two slip systems have equal $F_{BM}$ values.

Unlike $\{10\overline{1}2\}$ type twinning, the Schmid factor for $\{11\overline{2}1\}$ type twinning, $F_T$, is a maximum, when $F_{BM}$ values are high, excepting plane (D).

Schmid factors for basal slip in the twinned matrix, $F_{BT}$, are also shown in Fig. 6.5. $F_{BT}$ values remain large in regions of the stress axis planes where $F_{BM}$ is tending to become small.

In general $F_{BT}$ values are high, no consistently low values are obtained, as they were for the (d) type planes in $\{10\overline{1}2\}$ twinning.

6.3.2 Ratio of Maximum Schmid Factors for Basal Slip in Parent and Twin

From Fig. 6.5, the relative Schmid factors can be determined for any
Fig. 6.5a Schmid factors for twinning (---), basal slip in parent matrix (--O--), and twin matrix (--x--).
(a) Stress axis lying in (100)_M or (A) type plane.
Fig. 6.5b. Stress axis lying in $(\overline{2}1\overline{1}0)_M$ or (B) type plane
Fig. 6.5c Stress axis lying in (1010)_M or (C) type plane
Fig. 6.5d  Stress axis lying in $(1 \bar{2} 0)_M$ or (D) type plane
twin system and for any stress axis lying in the lettered planes. The relative Schmid factors are expressed as a ratio of the maximum Schmid factor for basal slip in the twin to the maximum Schmid factor for basal slip in the parent. This ratio, $F_{BT}:F_{BM}$, is shown in fig. 6.6 for the slip systems possessing maximum Schmid factors in the twin or parent matrices, at any given value of $\theta$. Slip is favoured in the twin matrix when the Schmid factor ratio exceeds unity, and is favoured in the parent matrix, when the ratio is less than unity. As proposed in Chapter 5, a difference in Schmid factor greater than 0.1 is considered to result in greater slip in that matrix having the higher Schmid factor. Fig. 6.6 shows that when the ratio is unity the Schmid factor for twinning, $F_T$, may be large or zero, while $F_{BT}\gg F_{BM}$ for $\theta = 0^\circ$, or $\pm 90^\circ$ and $F_{BM}\gg F_{BT}$ for $\theta = 60^\circ$ and $-40^\circ$.

The amount of slip in particular twins relative to that in the parent is summarised in Table 6.3.

6.3.3 Schmid Factors for Prism Slip in Parent and Twin

Schmid factor curves for prism slip in the parent ($F_{PM}$) are identical in all planes A to D in fig. 6.7, since two slip systems have equal $F_{PM}$ values while the third has a value of zero.

In the twin (fig. 6.7) the curve of $F_{PT}$ values for the stress axis in the A-type plane is identical in shape to the $F_{PM}$ curve, but is displaced by $\sim 40^\circ$. In A and D type planes one system has zero $F_{PT}$ values while in A the other two systems are equal. In B and C-type planes no system has zero $F_{PT}$ values for all values of $\theta$.

6.3.4 Ratio of Maximum Schmid Factors for Prism Slip in Parent and Twin

In planes A, B and C when $F_T$ is negative, $F_{PM} > F_{PT}$; the opposite is true for positive $F_T$. For D-type planes, $F_T$ is positive and $F_{PT} > F_{PM}$ for all values of $\theta$. This is illustrated in fig. 6.8. When ratios are near unity, $F_T$ values approach zero in all planes except D. The data for individual twins is presented in Table 6.3.

6.4 Discussion

The Schmid factor curves have proved useful when considering data obtained by other authors. For example the Schmid factors for twinning quoted in Ref. 158 were rapidly confirmed by referring to fig. 6.4 and Table 6.1. Similarly an error in the table included in Ref. 171 was
Fig. 6.6 Ratio of maximum Schmid factors for basal slip in the twin to maximum values in parent. $F_T = 0$ for values $\theta$ marked 1.
<table>
<thead>
<tr>
<th>Predominant slip system</th>
<th>Sense of stress required for twin growth</th>
<th>Stress axis plane</th>
<th>Twin systems</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BASAL</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tensile</td>
<td>1210</td>
<td>t/M</td>
<td>1 2 3 4 5 6</td>
</tr>
<tr>
<td>(F&lt;sub&gt;T&lt;/sub&gt; positive)</td>
<td>1700</td>
<td>t/M</td>
<td></td>
</tr>
<tr>
<td>Compressive</td>
<td>1210</td>
<td>M/t</td>
<td></td>
</tr>
<tr>
<td>(F&lt;sub&gt;T&lt;/sub&gt; negative)</td>
<td>1700</td>
<td>t/T</td>
<td></td>
</tr>
<tr>
<td><strong>PRISM</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tensile</td>
<td>1210</td>
<td>T/t</td>
<td></td>
</tr>
<tr>
<td>(F&lt;sub&gt;T&lt;/sub&gt; positive)</td>
<td>1700</td>
<td>T/t</td>
<td></td>
</tr>
<tr>
<td>Compressive</td>
<td>1210</td>
<td>m/M</td>
<td></td>
</tr>
<tr>
<td>(F&lt;sub&gt;T&lt;/sub&gt; negative)</td>
<td>1700</td>
<td>m</td>
<td></td>
</tr>
</tbody>
</table>

- m(t) indicates that $F_{BM}(F_{BT}) > F_{BT}(F_{BM})$ by 0.1
- M(t) indicates that $F_{BM}(F_{BT}) > F_{BT}(F_{BM})$ by 0.1

* Twin does not form in compression but the results are valid for pre-existing twins.
Fig. 6.7a. Schmid factors for prism slip systems in twin and parent.
Notation as for Fig. 6.5
Fig. 6.7b
Fig. 6.7d
Fig. 6.8 Ratio of maximum Schmid factors for prism slip in twin and parent. Notation as in Fig. 6.6
revealed; the Schmid factor for twin b should be negative. It is also clear that the stereographic projection in Rosi's paper is incorrect; either the twin poles or the stress axis must be changed to correspond with the text.

As in the previous analysis, a difference in Schmid factor of greater than 0.1 is used as a criterion for deciding whether slip in one matrix predominates over that in the other. Table 6.3 summarises the data for individual twins, the notation being similar to that used previously. The role of pre-existing twins and of twins nucleated under an applied stress will be considered separately since the effects are different in these two cases.

6.4.1 Relative Slip in Pre-existing Twins

If it is assumed that all twins are equally represented the effect of the presence of a twin on the ability to slip can be determined from Table 6.3. A quantitative estimate of the effects of twinning is given in Table 5.4. The percentages were obtained by measuring the total angle over which the Schmid factors for slip were greatest in twin (column 1) and in parent (column 2). Angles for which there was little change were also measured (column 3).

It is apparent from Table 5.4. that twinning reorients the crystal to favour prism and basal slip to about equal extent. However basal slip is made more difficult by twinning more often than is prism slip. Thus pre-existing twins might be expected to favour prism slip more than basal slip, although the effect is not so marked as when \{10\overline{1}2\} twins occur.

It must be emphasised that the percentage figures in Table 5.4. refer to arrays of axes lying in the planes already defined. It is not possible from the present data to obtain values for regions within the standard triangle, and thus the case of a random array of axes cannot be dealt with. However the method does indicate a possible approach to the problem of the role of twinning in the deformation of a polycrystalline aggregate.

6.4.2 Relative Slip in Growing Twins

It is worth noting here that twin nucleation often occurs in a co-operative manner on \{11\overline{2}1\} planes having a particular relationship to each other. The result is a zig-zag pattern of twins in a free surface. This was observed in titanium by Rosi et al and Rosi. Reed-Hill and
Buchanan have analysed zig-zag twinning in zirconium. The twins occurred in pairs such that their twinning shears were within 17° i.e. twins 1 and 2 or 1 and 6 in fig. 6.1 in agreement with Rosi's observations. In zirconium the active twins had Schmid factors >0.38, whereas non-operative twin systems had values <0.16. Jeffery and Smith found the predominant twin systems had Schmid factors >0.3, but there was also some small twins with values as low as 0.06 and with negative signs. Anderson et al also found {1121} twins occurred after considerable plastic strain by slip.

Clearly these facts should be borne in mind when considering which twin system is likely to operate under an applied stress.

An indication of the orientation dependence of twinning can be deduced from fig. 6.3. The relative slip in the twin and the parent matrices can be determined from Table 6.3 which has been derived from Table 6.1 and figs. 6.5 and 6.7.

For tensile stresses parallel to the c-axis no slip system operates, but all twin systems are favoured with a Schmid factor of 0.28. Slip will be pronounced in all twins relative to the parent, particularly when basal slip predominates. Neither basal slip nor twins are favoured when tensile stresses act normal to the c-axis, but prism slip then has a maximum Schmid factor. (It is noteworthy that pre-existing twins would facilitate basal slip under these conditions, fig. 6.6.)

No slip or twin system is favoured by compressive stresses parallel to the c-axis, although pre-existing twins would again greatly enhance basal, and to a lesser extent, prism slip. All twin systems operate for orientations normal to the c-axis, together with prism slip in the parent. These twins will not enhance prism slip but will greatly enhance basal slip.

Other important orientations lie in regions C and D in fig. 6.3, since these orientations are obtained in textured sheets. For axes in (1700), D, in fig. 6.3, tensile and compressive stresses favour twins 1, 2, 6 and 3, 4, 5 respectively. For axes in (1210), C, the corresponding twin systems are 1, 2, 5, 6 and 4, 3. However only prism slip is enhanced by any of these twins, and then only under tensile stresses.

Extremes of slip occur in twins nucleated in certain orientations. The conditions are summarised in Table 5.5. The greatest effect will arise when basal slip predominates and twins nucleate under tensile or compressive
stresses acting parallel and normal to the c-axis respectively. In the former case the results differ from those for \{1012\} twinning, when prism slip produced the greatest effect.

6.4.3 Twin Boundaries as Obstacles to Slip

None of the dislocations with \( \frac{1}{3} <11\bar{2}0> \) Burgers vectors can glide through \{11\bar{2}1\} twin interfaces without producing a defect in the interface and thus raising the interfacial energy. At low stresses therefore the interface will probably act as a barrier to slip. There is evidence that twinning does increase the strain hardening exponent of titanium at low temperatures. When twins nucleate, the dislocation density on either side of the boundary will normally be unequal, because the resolved shear stresses are greater in one matrix than in the other. Exceptions occur when basal slip predominates and for certain stress axes having 0 values of approximately 30\(^\circ\) and -60\(^\circ\). Then the ratio of the maximum Schmid factors is unity (fig.6.6) and high Schmid factors occur for both twinning and slip in parent and twin matrices. This result is not found in \{10\bar{7}2\} twinning, when a ratio of unity only coincided with a zero Schmid factor for twinning.

6.5 Summary

The curves presented allow rapid determination of Schmid factors for \{11\bar{2}1\} twinning and for basal and prism slip systems in parent and twin. If a specimen contains twins and all twin systems are equally represented, then the number of stress axes for which the ability to slip is increased by the presence of a twin is about the same for basal and prism slip systems. However the ability to slip is decreased for many more stress axes when basal slip predominates than when prism slip predominates. Twinning on \{11\bar{2}1\} systems thus favours slip on prism planes, but the difference is not nearly so great as is found for \{10\bar{7}2\} twinning.

Slip avalanches within twin matrices are expected when twins nucleate under tensile stresses parallel or compressive stresses normal to the c-axis respectively. The effect is expected to be greater when basal slip predominates, whereas in the case of \{10\bar{7}2\} twinning the effect was greatest when prism slip predominated. In general, when twins nucleate under an applied stress, either basal slip or prism slip may be enhanced, depending on the orientation.

At low stresses the \{11\bar{2}1\} twin boundaries will act as barriers to all \( \frac{1}{3} <11\bar{2}0> \) type dislocations. When twins can nucleate there are
orientations in which basal slip is equally favoured in twin and parent, a result not obtained for the prism slip case and not found for either slip system in \{10\overline{7}2\} twinning.

6.6 Slip Planes for Transformed Dislocations

The effect of \{11\overline{2}1\} twinning on the subsequent ability to slip has been discussed. It was assumed that only the normal \frac{1}{3}<11\overline{2}0> type dislocations were nucleated within the twin and parent matrices. However the observed ductilities in polycrystalline titanium are not easily accounted for in terms of this Burgers vector (Chapter 1.VIII).

Dislocation interactions at \{11\overline{2}1\} twin interfaces have not previously been discussed in the literature, although such interactions may be particularly important in the deformation of polycrystalline titanium. It is therefore proposed in this report to consider the interactions between \{11\overline{2}1\} twins and \frac{1}{3}<11\overline{2}0> type dislocations gliding in basal and prism planes.

Since all \frac{1}{3}<11\overline{2}0> Burgers vectors lie in \textit{K}_2, their positions are changed to \textit{K}_2 by the twinning shear (fig.6.1). For the \{1121\} twin, the transformations occur according to equations 6.1-6.3.

6.6.1 Basal Slip in Parent

The basal planes in both twin and parent matrices intersect the twin boundary along [\overline{1}100]_{\text{TT}} (fig.6.9). Any \frac{1}{3}<11\overline{2}0> type dislocation gliding in the parent basal planes may penetrate the twin boundary and slip on basal planes in the twin after transformation. The segments of dislocation parallel to the coherent twin boundary have either mixed (type (1) dislocations) or edge character (type (2) dislocations). Thus where these dislocations pass through the twin interface they will produce twinning dislocations associated with steps in the twin interface. This is shown schematically in figs.6.10 and 6.15a.

6.6.2 Prism Slip in Parent

Prism slip predominates in titanium (Chapter 1.VII). Type (1) dislocations will glide on a plane which is parallel in twin and parent i.e. (1\overline{7}00) in fig.6.9. Thus for each \{11\overline{2}1\} twin, one third of all the possible \frac{1}{3}<11\overline{2}0> type dislocations may glide on prism planes undeviated through the twin interface, as shown in fig.6.11.

Type (2) dislocations gliding in prism planes intersect a coherent \{11\overline{2}1\} twin boundary parallel to \textit{<11\overline{2}3> directions}. The Burgers vector of the dislocation after transformation does not lie in the prism plane.
Fig. 6.9 Stereographic projection of slip planes for transformed dislocations in type 1 ($b_1$ Burgers vector) and type 2 ($-b_3$ Burgers vector) interactions (see text)
Fig. 6.10 Schematic diagram of a type I dislocation gliding in a basal plane and interacting with a $(1121)$ twin boundary.

Fig. 6.11 Schematic diagram of a type I dislocation gliding in a prism plane and interacting with a $(1121)$ twin boundary.
containing the dislocation line e.g. in fig. 6.9, \( \frac{1}{3} [\overline{2}1110]_T \) transforms
\( \frac{1}{3} [\overline{2}110]_T \), which does not lie in \((\overline{1}010)_T\) passing through \([\overline{1}2\overline{1}3]_T\).
This dislocation will lie in \((01\overline{1}1)_T\) and may glide away from the twin
boundary in this plane. However in titanium single crystals and poly-
crystals slip in \(<c+a>\) directions has been observed. In zinc and
cadmium the preferred slip plane for dislocations with this Burgers
vector is \{11\overline{2}2\}. It is therefore proposed in this Chapter to consider
only prism slip in \(<1\overline{1}20>\) directions and \{11\overline{2}2\} slip in \(<c+a>\) directions.
The following possible dissociations are now relevant.

\[
\frac{1}{3} [\overline{2}110]_T \rightarrow \frac{1}{3} [\overline{7}2\overline{7}0]_T + \frac{1}{3} [\overline{7}1\overline{2}0]_T \quad (6.4)
\]

\( -b_3^* \quad b_2^* \quad b_1^* \)

produced in glissile in immobile

equation (6.2) above \((\overline{1}010)_T\)

One of the product dislocations, lying parallel to the appropriate \(<1\overline{2}13>\)
direction, can now glide in \([\overline{7}010]_T\) in the twin (fig. 6.9), a sessile
dislocation remaining in the twin interface.

An alternative to the reactions 6.2 and 6.4 above involves pyramidal
Burgers vectors e.g.

\[
\frac{1}{3} [72\overline{7}0]_M \rightarrow \frac{1}{3} [\overline{7}2\overline{7}3]_M/T + [001]_M \quad (6.5)
\]

The \( \frac{1}{3} [\overline{7}2\overline{7}3] \) dislocation so nucleated, at the twin interface, can glide
away in the \((\overline{7}2\overline{7}2)_T\) plane. (Further reaction of the type

\[
\frac{1}{3} [\overline{7}2\overline{7}3]_{M/T} \rightarrow \frac{1}{3} [\overline{7}2\overline{7}0]_T + [000\overline{1}]_T \quad (6.6)
\]

produces the \( \frac{1}{3} [\overline{7}2\overline{7}0]_T \) dislocation, glissile in \((\overline{7}010)_T\) i.e. equations
(6.2) and (6.4) are equivalent to (6.5) and (6.6). For a given \{11\overline{2}1\}
twin, two thirds of the \( \frac{1}{3} <1\overline{1}20> \) dislocations can interact at the twin
interface in this manner. Fig. 6.12 illustrates these interactions. Note
that one third of all the \( <c+a> \) dislocations gliding in \{11\overline{2}2\} planes can
cross slip through a given \{11\overline{2}1\} twin interface without producing defects
in the interface.
Fig. 6.12 Schematic diagram of a type 2 dislocation \((b_2)\) gliding in a parent prism plane. Dislocation \(-b_2^\ast\) is produced by reaction (4) and dislocation \(b_p^\ast\) \((<c+a>)\) is produced by reaction (5) in text.
6.7 Relative Schmid Factors in Twin and Parent After Transformation of Burgers Vectors

The mobility of the dislocations produced by the above transformations will be dependent on the resolved shear stress acting on the product dislocation in a particular slip plane. Thus a parent dislocation gliding under a high resolved shear stress may impinge on the twin interface and give rise to a dislocation for which the resolved shear stress in its slip plane is much smaller. The greater the difference between the Schmid factors before and after transformation the more effective will be the barrier effect of the twin boundary. If the difference in Schmid factors is small, the product dislocations may glide away and relieve the stress due to the pile-up at the twin interface. The active slip system nucleated in the twin may of course have a higher Schmid factor than the product dislocation from the interactions.

The relative Schmid factors may be determined by comparing the appropriate curves for each slip system before and after transformation. For basal and prism slip systems and \( \frac{1}{3} <1\bar{1}20> \) Burgers vectors, the relative Schmid factor values before transformation can be obtained from the curves described in para 6.3. Curves for \{1\bar{2}12\} and \{1\bar{2}13\} slip systems are given in figs. 6.13 and 6.14 for the (11\bar{2}1) twin.

6.7.1 Basal Slip in \(<1\bar{1}20>\) Directions

Type (1) dislocations are unlikely to glide easily through the interface, since large differences in Schmid factor exist for the majority of values, although a ratio of unity is obtained for particular values of \( \pm \theta \). This is analogous to the situation found for type (1) dislocations and \{10\overline{7}2\} twinning.

For type (2) dislocations the most favourable conditions for slip after transformation exist in \( D \) type planes. Then the Schmid factors are nearly equal over an extensive range of \( \theta \) values near \( +90^\circ \).

It is concluded that for the majority of orientations considered basal slip dislocations are not likely to penetrate \{1\bar{1}21\} twin interfaces and nucleate \( \frac{1}{3} <1\bar{1}20> \) type dislocations in the twin.

6.7.2 Prism Slip in \(<1\bar{1}20>\) Directions

Type (1) dislocations are favoured before and after twinning for stress axes in \( C \) and \( B \) type planes and for positive \( \theta \) values. The Schmid factor ratio is unity at high Schmid factor values when \( \theta \) approaches \( 90^\circ \).
For type (2) dislocations very favourable Schmid factors exist in the D type plane when the Schmid factor for twinning is small. The product dislocations are also those having the maximum Schmid factor in the twin crystal.

Thus $\frac{1}{3} <11\bar{2}0>$ type dislocations may readily penetrate $\{1\bar{2}1\}$ twin interfaces over a range of orientations.

6.7.3 $\{1\bar{2}1\}2<2\bar{1}3>$ Slip

There are two possible pyramidal systems that may be nucleated at a $(1\bar{2}1)$ twin interface by $\frac{1}{3} <11\bar{2}0>$ dislocations gliding in prism planes. These are $(\bar{7}2\bar{7}2)$ $[\bar{1}\bar{2}13]_T$ nucleated by $(10\bar{1}0)$ $[\bar{1}\bar{2}10]_M$ and $(\bar{2}\bar{1}\bar{7}2)[\bar{2}113]_T$ nucleated by $(01\bar{7}0)[\bar{2}110]_M$. These may be referred to as $b_3'$ and $b_2'$ reactions respectively according to the dislocations giving rise to these $<c+a>$ dislocations (fig. 6.9).

The Schmid factor curves for the $<c+a>$ dislocations produced in the $b_3'$ reactions are plotted in fig. 6.13 with the single Schmid factor curve for the matrix superimposed. The relevant slip planes are shown in fig. 6.9.

It should be noted that when comparing Schmid factor curves to determine whether $<c+a>$ slip will be nucleated by $\frac{1}{3} <11\bar{2}0>$ type dislocations, care must be taken to ensure that the curves used relate to Burgers vectors having the correct sense:

- e.g. $b_3'$ reaction $\frac{1}{3}[\bar{7}2\bar{7}0]_M$ and $\frac{1}{3}[\bar{7}2\bar{7}3]_T$
  or $\frac{1}{3}[\bar{1}\bar{2}10]_M$ and $\frac{1}{3}[\bar{1}\bar{2}13]_T$

- $b_2'$ reaction $\frac{1}{3}[\bar{2}1\bar{1}0]_M$ and $\frac{1}{3}[\bar{2}1\bar{1}3]_T$
  or $\frac{1}{3}[\bar{2}\bar{1}\bar{7}0]_M$ and $\frac{1}{3}[\bar{2}\bar{1}\bar{7}3]_T$

For the A type plane $<c+a>$ slip is only likely when $\theta$ is negative. The Schmid factors are then large and $F_{c+a} >> F$ parent for the majority of $\theta$ values, and become equal at $\theta = -68^\circ$ when the Schmid factor is 0.37. The Schmid factors for $\frac{1}{3} <11\bar{2}0>$ slip nucleated in the twin is then 0.14 and for twinning in compression is 0.49. Thus for this stress axis twins nucleated in compression favour $<c+a>$ slip.

In B type planes again for negative $\theta$ the Schmid factor for slip is favourable though low, becoming equal at $\theta = -46^\circ$ when the Schmid factors
Fig. 6.13 Schmid factor curves for stress axes in quadrant, 0001-1120-1000 and 0001-1120-1100 and for b\text{1} interaction (see text)
for slip and compression twinning are 0.25 and 0.35 respectively. Then the maximum Schmid factor for \( \frac{1}{3} <11 \bar{2}0 > \) slip in the twin is \( \sim 0.1 \).

In D type planes and positive \( \theta \), when the Schmid factors favour \( <c+a> \) slip, the Schmid factor for twinning is very low e.g. at \( \theta = +90^\circ \), \( F_{<c+a>} = 0.34 \) \( F_{\text{parent}} = 0.44 \). For \( -\theta \) the situation is much more favourable. Tensile twinning may nucleate \( <c+a> \) slip, but pre-existing twins are especially beneficial since for \( \theta = -78^\circ \) the Schmid factors for slip are equal in twin and parent (0.42). The maximum Schmid factor for \( \frac{1}{3} <11 \bar{2}0 > \) slip in the twin is also large (0.47); note that the reaction (6.2) and (6.4) would only give \( \frac{1}{3} <11 \bar{2}0 > \) slip with a Schmid factor of 0.32.

Fig. 6.14 shows the Schmid factor curves for the \( <c+a> \) system produced by the \( h_2^* \) reaction. The curve for the A type plane is similar to that for the \( h_3^* \) reaction and \( <c+a> \) slip is favoured when \( \theta \) is negative and for twins nucleated in compression. For the C type plane positive \( \theta \) provides the most favourable orientations, since for \( \theta = 0-90^\circ \) high slip and tensile twin Schmid factors prevail. The slip factors become equal at \( \theta = +76^\circ \) (0.4) when the Schmid factor for twinning is 0.07; then pre-existing twins will be most effective in nucleating \( <c+a> \) slip.

For the D plane and \( +\theta \) tensile twinning is likely to nucleate \( <c+a> \) slip as in the C plane above. At \( \theta = +78^\circ \), Schmid factors for slip become equal at 0.41. For \( -\theta \) and over a restricted range i.e. -70 to \( -90^\circ \) conditions favour the nucleation of \( <c+a> \) slip by pre-existing twins or twins produced under tensile stresses e.g. \( \theta = -90^\circ \), \( F_{<c+a>} = 0.33 \) \( F_{\text{parent}} = 0.44 \). However the Schmid factor for \( \frac{1}{3} <11 \bar{2}0 > \) slip in the twin is also large (0.44). (Note that the Schmid factor is zero for \( h_3^* \) and \( h_2^* \) in planes C and B respectively).

In general the Schmid factors for \( <c+a> \) slip in the twin and for \( \frac{1}{3} <11 \bar{2}0 > \) in the parent differ by more than 0.1: However the Schmid factors are often equal at high values for slip but low values for twinning. It is therefore concluded that pre-existing twins would be particularly beneficial in nucleating \( <c+a> \) slip (It also follows that slip nucleated within twins can nucleate \( <c+a> \) slip in the parent). Particular examples can also be found where \( <c+a> \) will be nucleated for twinning either in tension or compression. A detailed example can now be presented.

Consider an annealed material subjected to a stress, the axis of which lies in the plane (\( \bar{T}1\bar{0}0 \)) and region D_1 of the standard stereographic
Fig. 6.14 As for fig. 6.13 but for $b_2^1$ interaction (see text)
triangle (fig. 6.3). The resolved shear stresses on each of the twin systems is such that twins 1, 2 and 6 cause extension and 3, 4 and 5 cause contraction in the direction of the stress axis. For the above stress axis and from curves constructed in figs. 6.13 and 6.14, it is possible to determine the resolved shear stress factors for these twin systems and any slip mode studied as follows. Let the material slip on prism planes.

From Table 6.1 the equivalent stress axis plane for each twin can be determined. The Schmid factor curve for each twin system and for \( \frac{1}{3} <11\overline{2}0> \) slip in the parent and in each twin can be derived from figs. 6.4 and 6.7 respectively. The Schmid factor curves for \( \frac{1}{3} <11\overline{2}0> \) slip can then be compared with the curves for \( <c+a> \) slip in the twin shown in fig. 6.13 and 6.14. The data is summarised in Table 6.4.

It can be seen that a tensile stress will cause twin 1 to nucleate. In this twin system the Schmid factor for \( \frac{1}{3} <11\overline{2}0> \) slip is much greater than either \( \frac{1}{3} <11\overline{2}0> \) slip in the parent or \( <c+a> \) slip in the twin. However twins 2 and 6 have fairly large Schmid factors. In these twins the Schmid factor for \( <c+a> \) slip is equal to that for \( \frac{1}{3} <11\overline{2}0> \) slip in the twin and greater than that for \( \frac{1}{3} <11\overline{2}0> \) slip in the parent.

Thus under a tensile stress the two twin systems 2 and 6 may nucleate \( <c+a> \) slip.

Under a compressive stress twin 4 is likely to predominate since it has a large Schmid factor whilst twins 3 and 5 have much smaller Schmid factors. Twin 4 is ideally oriented for nucleating \( <c+a> \) slip, since the Schmid factor for \( \frac{1}{3} <11\overline{2}0> \) slip in the twin is less than that in the parent, which is much less than that for \( <c+a> \) slip in the twin.

The possibility that all these twins may exist together in fabricated material can also be considered. This may be of considerable practical importance. The above data indicates that pre-existing twins would have a greater effect than twins nucleated in this orientation. For example, twin 4 would nucleate \( <c+a> \) slip in tension also, together with twins 3 and 5. Consequently for the stress axis defined above and assuming twins 2, 3, 4, 5 and 6 are already present in the metal, they will all nucleate \( <c+a> \) slip in the twinned crystal under both tensile and compressive stresses.
### TABLE 6.4

RELATIVE SCHMID FACTORS FOR PRISM SLIP AND \{11\bar{2}1\} TWINNING

FOR A STRESS AXIS IN (11\bar{1}0) AND REGION D₁ OF

THE STANDARD STEREOGRAPHIC TRIANGLE (FIG. 6.3)

<table>
<thead>
<tr>
<th>Twin System</th>
<th>Equivalent Stress Axis Plane</th>
<th>Schmid Factor for Twinning</th>
<th>Relative Schmid Factors *</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( +A )</td>
<td>(+ 0.5)</td>
<td>( F_T &gt; F_p &gt; F_{c+a} )</td>
<td>( b_3', b_2' )</td>
</tr>
<tr>
<td>2</td>
<td>( +C )</td>
<td>(+ 0.35)</td>
<td>( F_{c+a} = F_T &gt; F_p )</td>
<td>( b_2' )</td>
</tr>
<tr>
<td>3</td>
<td>(-C)</td>
<td>(-0.1)</td>
<td>( F_{c+a} &gt;&gt; F_p = F_T )</td>
<td>( b_3' )</td>
</tr>
<tr>
<td>4</td>
<td>(-A)</td>
<td>(-0.4)</td>
<td>( F_{c+a} &gt;&gt; F_p &gt; F_T )</td>
<td>( b_3', b_2' )</td>
</tr>
</tbody>
</table>

* \( F_p \) Schmid factor for \(10\bar{1}0\) \(\frac{1}{3}\) \(<1\bar{2}10\) in parent

\( F_T \) * * * * * * * in twin

\( F_{<c+a>} \) * * * * \(\{1\bar{2}12\}\) \(\frac{1}{3}\) \(<1\bar{2}13\) slip in
twin produced by twin boundary interactions
6.8 Slip Traces in Parent and Twin

The traces expected in surfaces parallel to (0001)_M and parallel to the plane of shear of the twin have been derived from fig. 6.9.

When basal slip occurs, penetration of the twin boundary by type (2) dislocations will be evident in sections parallel to the plane of shear by the formation of steps in the twin interface (6.15a). Note that similar slip traces will be produced by dislocations nucleated within the twin.

The traces expected when prism slip occurs are shown in fig. 6.16. For clarity twin boundary steps are omitted in this figure. Only type 2 dislocations produce traces in the plane of shear, twin boundary steps again being indicative of dislocation/twin interactions. The traces produced will depend on whether reaction (6.4) above occurs, leading to \( \frac{1}{3} <1120> \) dislocations and \{1070\} slip traces, or reaction (6.5) occurs, leading to \(<c+a>\) dislocations and \{1122\} slip traces. The traces due to these different reactions are easily distinguished both in the plane of shear (fig. 6.16a) and in the basal plane section (fig. 6.16b). In the latter section type (1) dislocations will also become visible in the twin and may produce twin boundary steps if reaction (1) occurs.

6.9 Summary

When \( \frac{1}{3} <1120> \) type dislocations impinge on a \{1121\} twin interface, they may transform to produce similar type dislocations in the twin. However when the dislocations glide on prism planes, two-thirds of the \( \frac{1}{3} <1120> \) type dislocations can also interact with a given \{1122\} twin and nucleate \( \frac{1}{3} <1213> \) type dislocations in \{1212\} type planes. Pre-existing twins are expected to be particularly useful in this respect.

In certain orientations the Schmid factor for the pyramidal slip system may be greater than \( <1120> \) slip in either the parent or the twin.
Fig. 6.15 Basal slip in parent

*a* Section parallel to the plane of shear of the twin. Surface slip steps are produced by type 2 dislocations but not by type 1.

*b* Section parallel to $(0001)_M$

Slip steps are produced by type 1 and 2 dislocations in the twin, but not in parent. Dislocation type indicated by figures in brackets.
Fig. 6.16 Prism slip in parent

a) Section parallel to plane of shear. Slip steps produced by type 2 dislocations and \(<c+a]\) dislocations

\[ \frac{1}{3} \{\{1\bar{2}\bar{0}\} \] type dislocations

\[ \langle c+a\rangle \] dislocations

b) Section parallel to \((\text{OOO})_M\). Type 1 and 2 dislocations will produce steps in twin
7.1 Fatigue Damage in H.C.P. Metals

7.1.1 Slip Band Extrusion

Extrusion formation in fatigued hexagonal metals has not hitherto been reported. The complex dislocation models proposed for slip band extrusion and intrusion in f.c.c. metals have required extensive cross-slip of screws, sometimes in a co-operative manner. This is unlikely, especially in low stacking fault energy metals and in hexagonal metals. The small amount of cross-slip to produce dipole loops appears sufficient to produce extrusions in cadmium, magnesium and titanium for example, whereas the smaller amount of cross-slip in zinc is inadequate.

The preferential sites for extrusions in untwinned crystal must also be accounted for. In view of the similarity between the debris produced by untwining and the dipole loop structures produced in magnesium\(^{320}\), titanium and beryllium\(^{351}\) by cyclic strains, it seems reasonable to relate extrusion formation to the dipole loop structure.

It was concluded in Chapter 4.4 that the occurrence of extrusions on cadmium and magnesium and their absence on zinc, could be explained in terms of the glide of dislocation loops or dipoles to the free surface. Then vacancy type loops would give rise to intrusions and interstitial type loops would form extrusions.

The loops and dipole jogs are assumed to form by cross-slip. The absence of extrusions on zinc is attributed to the difficulty in cross-sliping in this metal. This allows only small jogs and narrow dipole loops to form, which may degenerate into point defects. There is some evidence for this in fatigued zinc\(^{48,110}\). Even assuming a stable dipole loop, it is unlikely to be mobile in zinc, since its short segments will be in the cross-slip plane.

In cadmium, magnesium and titanium the whole loop may glide on its slip cylinder. It is suggested that under suitable stresses\(^{352}\) the dense array of dipole loops will move together to the free surface to leave a column of crystal beneath the extrusion (or intrusion) which will be relatively free of dislocations. Subsequent deformation in this region may differ from that produced by the earlier stress cycles. Thus the
polygon structures found in fatigue striations in copper may be produced by the cyclic plastic strain following extrusion formation.

The preferred sites for extrusions in untwinned crystal is also accounted for, since such regions contain a high density of loops and dipoles. Subsequent slip is inhibited in such regions (as shown in fig. 4.16) although extrusions still occur. This suggests that plastic instability within the defect structure gives rise to the extrusion. This is also indicated by the rapid initial rate of extrusion growth and subsequent cessation of growth observed in fig. 4.9.

However extrusions are not necessarily observed in metals that readily cross-slip, in annealed aluminium for example. The mobility of the dipoles will then be reduced by cross-slip of screw segments of the dipole. The absence of extrusions in cadmium fatigued at room temperature is attributed to climb of the dipole loop segments before sufficient numbers of dipoles accumulate or reach the surface.

In low stacking fault energy metals and alloys the glide of the loops could also be affected by dissociation of the loop segments on the glide cylinder; however extrusions appear to form readily in such metals.

A mechanism based on glissile prismatic dislocation loops can account for extrusion and intrusion in many crystal systems and for the following observations.

(a) The low temperatures and early stages in the life at which extrusions occur, i.e. coincident with a rapid rate of work hardening due to dipole or debris formation.

(b) The rapid rate of formation of extrusions.

(c) The distribution of extrusions in close packed hexagonal metals.

(d) The absence of internal voids beneath extrusions.

There is good evidence for easy cross-slip facilitating fatigue crack nucleation both in metals and ionic crystals and a similar relationship appears to exist for slip band extrusion (intrusion) formation. Foulon reported interstitial loops in unidirectionally deformed copper and subsequent work by Feltner showed both vacancy and interstitial loops to be present in fatigued aluminium. Thus the proposed slip band extrusion model is consistent with the observed defect structures and the experimental data as discussed further by Watt.
It is noteworthy that those metals\textsuperscript{306} and ionic solids\textsuperscript{360} that do not readily cross-slip, exhibit high cyclic strain hardening capacity and good fatigue strength. Statistically roughening the surface by steps to produce a notch or crack nucleus, as proposed by Wood\textsuperscript{326} and May\textsuperscript{327} and discussed by Kuhlmann-Wilsdorf and Nine\textsuperscript{363} might be expected to operate ideally in such materials. The enhanced fatigue strength observed suggests this mechanism is not important in practice.

7.1.2 Cyclic Twinning

Particular attention has been paid to the twinning mode, since this mode occurs in several technologically important metals, e.g. titanium, zirconium, beryllium. Russian\textsuperscript{311,312} workers reported cracks in fatigued titanium at [1121] type twin interfaces. This has been confirmed by Beevers\textsuperscript{314}, who found that when twinning was inhibited by hydride precipitates, the fatigue life was increased. Hempel\textsuperscript{313} also observed twinning in fatigued titanium, but this mode was not detected by Turner and Roberts\textsuperscript{364}. In tensile tests the twinning mode is less common as the grain size is reduced\textsuperscript{193a-195}, although the higher strain rates in fatigue may favour twinning. The role of pre-existing twins in fatigue specimens has not been considered.

The fragmentation of twins and filamentary growths associated with twin boundary fatigue damage have not previously been reported. Again it seems reasonable to relate the occurrence of filamentary growths to the twin boundary debris generated by a moving boundary.

There is extensive evidence that cyclic twinning may produce defects either in the parent or in the twin. These defects may inhibit further twin boundary displacement. Point defects may be produced by twinning\textsuperscript{105b} but are unlikely to impede the boundary\textsuperscript{365}. However the faults observed in the basal plane of magnesium after untwining may arise by condensation of point defects and these would reduce the boundary mobility.

Dislocations are the most likely obstacles to twin boundary movement. It will be shown that dislocation interactions at \{10\{2\}2\} and \{1121\} twin interfaces can give rise to severely jogged dislocations. These dislocations will compose the debris adjacent to twin boundaries during cyclic twinning and can produce the filamentary growths observed by a mechanism similar to that proposed for slip band extrusion.
Consider the transformation of Burgers vectors when $\frac{1}{3} <11\bar{2}0>$ type dislocations enter a (10\bar{7}2) twin, as shown in equations 5.2 - 5.4.

In type (1) interaction the vector is unchanged in magnitude and direction, but in type (2) interactions the product vectors are not the normal lattice translation vectors and the dislocations with these vectors will be sessile and associated with a stacking fault.

For (1\bar{1}21) twinning, the dislocations transform according to equations 6.1-6.3. All the Burgers vectors lie in the $K_2$ plane and are similar after transformation.

The effect of moving a twin boundary through forest dislocations may now be examined. Consider (10\bar{7}2) twinning and a type (1) dislocation gliding on parent basal planes. Let the dislocation have predominantly screw character, with some parts in edge orientation, as shown in fig. 7.1. After twinning the screw portion can continue gliding in the basal plane in the twin (fig. 7.2); however the edge portion will lie in (1\bar{2}10) and becomes a jog on the gliding dislocation. Conversely any parent screw dislocations with jog segments parallel to the c-axis will become unjogged after twinning. The screw segments of a parent dipole (the dipole is dashed in fig. 7.1) will glide in the twin to form a closed loop (fig. 7.2). Thus jogged type (1) dislocations in one matrix will give rise to dipole loops in the other after twinning. Type (1) dislocation segments of mixed orientation also become sessile jogs in the twin. In comparison in {11\bar{2}1} twinning, all edge and screw dislocations gliding in prism planes have the same type Burgers vector after twinning.

Thus a {10\bar{1}2} twin growing through forest dislocations in which all $\frac{1}{3} <11\bar{2}0>$ Burgers vectors are equally represented, will produce dislocation debris containing $\frac{2}{3}$ sessile dislocations and $\frac{1}{3}$ severely jogged glissile dislocations and dipole loops; a {11\bar{2}1} twin will produce entirely jogged glissile dislocations and loops.

The dipoles associated with the twin boundary in fig. 3.12 may now be accounted for. These dipoles associated with a {10\bar{7}2} twin are shown schematically in fig. 7.3. Assuming the dipoles are generated in both twin and parent and glide to the free surface, the resulting extrusion would appear as in fig. 7.4. The {11\bar{2}1} twin boundary debris will produce a similar result, the extrusion emerging parallel to {10\bar{7}0} planes. Clearly if the debris is confined to a narrow band and contains a high
Fig. 7.1 Dislocation in parent gliding in basal planes (see text).

Fig. 7.2 After twinning on (1012). Dislocation gliding in basal planes (see text).
Fig. 7.3 Formation of dislocation dipoles at (10\bar{1}2) twin boundary by dislocation twin interaction.

Fig. 7.4 Formation of "whisker" extrusions near twin boundary during fatigue (see text).
density of dipole loops, the result will be a continuous narrow metal filament. The well developed platelets in \{1\overline{2}1\} twinning in titanium compared with the fragmented ones in \{10\overline{7}2\} twinning can be attributed to the fact that only \(\frac{1}{3}\) of the normal \(\frac{1}{3}\) \langle1\overline{1}20\rangle type Burgers vectors can contribute to filaments in \{10\overline{7}2\} twinning, whereas they all contribute to filament formation in \{11\overline{2}1\} twinning.

Although the filaments will be metallic when formed, they may become converted to oxide on exposure to air and hence give predominantly oxide patterns. The absence of filaments in zinc at room temperature, as in the case of slip band extrusions, is due to the difficulty in retaining and moving the dipole loops.

Crack nucleation at twin boundaries will be analogous to the slip band cracking. When vacancy type dipoles predominate, intrusions will be produced which subsequently give rise to cracks.

The fragmentation of \{10\overline{7}2\} twins is attributed to the pinning of twin interfaces by dislocation debris, particularly sessile dislocations and stacking faults.

Although Price\(^{162}\) found type (2) dislocations were pushed ahead of a moving \{10\overline{7}2\} twin interface in zinc, there is direct evidence that stacking faults are produced by dislocation interactions at \{10\overline{7}2\} twin interfaces in zinc\(^{366}\), magnesium\(^{367}\), titanium and beryllium\(^{105b, 368}\). Stacking faults and sessile dislocations could arise by reactions (2) and (3) above and they may well account for the higher critical resolved shear stress for basal slip measured within \{10\overline{7}2\}.twins in zinc\(^{14,97}\).

Consider a \{10\overline{7}2\} twin interface oscillating to and fro in response to a cyclic stress i.e. fixed stress axis, stress changing sign. If the twin interface sweeps through a volume of crystal previously slipped i.e. containing dislocations, then certain \(\frac{1}{3}\) \langle1\overline{1}20\rangle Burgers vectors will transform to \(\frac{1}{6}\) \langle1\overline{1}23\rangle type. Because of the sessile nature of these \(\frac{1}{6}\) \langle1\overline{1}23\rangle dislocations, it may be more difficult to move the twin interface through regions containing such dislocations, especially if they are associated with stacking faults\(^{348,365}\). The relative amounts of slip in any twin matrix and in the parent matrix has been deduced in chapters 5 and 6. During twin growth faults are expected to be produced in the twin matrix when slip in the parent matrix predominates, but in the parent matrix when twins untwin after slip in the twin matrix.
When slip is equally favoured in twin and parent matrices, the dislocation density and hence the fault density, on either side of the twin boundary, will be similar. Thus the twin boundary may become immobile.

When the dislocation density is greater on one side of the twin interface the twin boundary will move more readily either towards the axis of the twin (for conditions corresponding to twin matrix slip) or away from the twin axis (for conditions corresponding to parent matrix slip). This ratchet mechanism is illustrated schematically in fig. 7.5.

The positions are shown of a twin interface corresponding to the first $\frac{2\pi}{3}$ cycles of stress. A twin boundary AB is assumed to be pinned by obstacles in the parent matrix at $X_M$ and in the twin matrix at $X_T$, fig. 7.5a. The first $\frac{1}{3}$ cycle of stress, favouring twin growth, causes the unpinned segments of the twin boundary to bow outwards, fig. 7.5b; the local displacements of the twin interface are accommodated by kink boundaries. The reverse $\frac{1}{3}$ cycle, favouring untwining, causes the remaining unpinned segments to bow in the opposite direction, fig. 7.5c; and accommodation kinks of opposite sign to be nucleated. It is assumed that the high density of defects produced behind moving twin interfaces (shaded areas in fig. 7.5) will prevent the reversal of these boundary displacements. Thus successive stress cycles will accentuate the boundary displacements. (fig. 7.5d) until the maximum degree of incoherency is reached, when the incoherent interfaces will nucleate twins in either undamaged twin matrix ($T_1$) or undamaged parent matrix ($T_2$) as in fig. 7.5e. Repetition of the above sequence will lead to fragmentation proceeding from the original twin interface either towards the centre of the twin (if $T_1$ type twins predominate) or away from the centre of the twin (if $T_2$ type twins predominate).

The above model is applicable to cyclic twinning in any crystal lattice provided the matrix is sufficiently plastic.

Although at low cyclic stresses fragmentation can proceed in either direction from the twin interface, normally fragmentation is confined to pre-existing twinned crystal. This could be due to the greater tendency for slip to occur within the twin matrix and hence more damage to be produced (in the parent matrix) during untwining than is produced (in the twin matrix) during twin growth. This accounts for the greater stress
Fig. 7.5

Schematic illustration of the effect of cyclic stresses on a twin interface in magnesium.

(a) initial twin boundary position AB, in basal plane surface
(b) after 1/4 stress cycle favouring twin growth
(c) after 3/4 stress cycle favouring untwinning
A +ve and -ve sign denotes accommodation of surface elevation and surface depression respectively
(d) after 23/4 stress cycles
(e) twin nucleation at incoherent twin interfaces
(f) partial untwinning and progressive fragmentation towards the centre of the twin
required for untwining than for twin growth in the simple case of growth followed by contraction, e.g. in magnesium\(^{342}\), titanium\(^{270}\) and iron\(^{271}\). However, it follows that the stress to grow a twin after untwining is likely to be greater than the untwisting stress and progressive untwining is favoured. Thus in fig.7.5d the growth segments, X, can reverse while the untwining segments Y will tend to penetrate more deeply into the twin (fig.7.5f).

The possible effect of orientation on cyclic twinning may now be examined in some detail for \{1072\} and \{1121\} twinning and using the data in chapters 5 and 6.

Consider \{1072\} twinning and a crystal oriented with the stress axis in \{1\1\0\0\} and within region C\(_t\) in fig.5.3. Prism slip is assumed to be the active slip mode. If a compressive stress is applied (fig.7.6a), twins 1, 2, 4 and 5 are nucleated, but slip predominates in the parent matrix (fig.7.6b). When the stress is reversed, twins 3 and 6 nucleate and slip occurs in these twins; twins 1, 2, 4 and 5 contract (fig.7.6c). In fig.7.6d the stress again becomes compressive. Now twins 1, 2, 4 and 5 grow and their twin interfaces sweep through parent crystal containing dislocations, which are transformed to sessile dislocation debris in the twin matrices. Similarly, twins 3 and 6 contract and dislocation debris is produced in the parent matrix. Further tensile stressing (fig.7.6e) has little effect on the position of the twin interfaces, which are pinned by the dislocation debris. However compressive stresses will cause twin interface movement, twins 1, 2, 4 and 5 becoming progressively wider and twins 3 and 6 becoming progressively narrower (fig.7.6f). In these last two twins, crack nucleation during fatigue stressing may be accentuated by preferential slip in these twins.

A similar sequence can occur for \{1121\} twinning. For example, consider a stress axis in region D\(_t\) and \{1\7\0\0\} of the standard triangle on fig.6.3. Twins 3, 4 and 5 grow under compression and twins 1, 2, 6 under tension. The diagram in fig.7.6 therefore describes the behaviour of these twins since the relative slip is greater in the parent for the 3, 4, 5 twin systems and in the twin for 1, 2, 6 twin systems.

7.1.3 Stacking Faults Associated with Deformation Twins

It has been shown that stacking faults are observed only associated with twins in deformed unalloyed polycrystalline magnesium and titanium.
FIG. 7.6 Schematic diagram illustrating the effect of orientation on the behaviour of [1012] twins under cyclic stress conditions. The stress axis lies in (1100) and region $C_1$ of fig. 5.3. Prism slip predominates.

--- slipped regions  
\[\sim\] region containing dislocation debris.
Furthermore, only faults on basal planes were found in magnesium, whereas faults on non-basal planes were frequently observed in titanium. Such faults are likely to act as barriers to the movement of twin interfaces when cyclic twinning occurs and it is appropriate here to briefly discuss the origins of these faults.

Several dislocation dissociation sequences are possible, which could explain the experimental observations. For example, consider equation (5.8), representing two $\frac{1}{3}\{2\overline{7}0\}$ type 2 dislocations impinging on a coherent $(10\overline{7}2)$ twin interface. This is shown schematically for the basal slip in fig. 5.13. The $<c+a>$ dislocation lying along $[1\overline{2}10]$ in the twin boundary can dissociate according to equations 11 and 14, Chapter 1. A Schockley partial may then glide in the basal plane in the twin to produce a stacking fault.

The prism slip is more complex (fig. 5.14). The $<c+a>$ dislocation may glide in $(\overline{7}2\overline{7}2)$ until it intersects the basal plane along $[\overline{7}0\overline{1}0]$. Dissociation may then occur according to equations 11, 14 and 18, Chapter 1, to produce stacking faults in the basal and $(1\overline{2}10)$ planes. Another possibility is that the $<c+a>$ dislocation in the twin boundary dissociates at the twin boundary according to equation 17, to produce a fault in $(\overline{7}2\overline{7}2)$ fig. 5.14 e.g.

\[
\frac{1}{3}\{\overline{7}2\overline{1}3\} \rightarrow \frac{1}{6}\{0\overline{2}2\overline{3}\} + \frac{1}{6}\{2\overline{2}0\overline{3}\}
\]

One of these partials may then dissociate further:

\[
\frac{1}{6}\{2\overline{2}0\overline{3}\} \rightarrow \frac{1}{3}\{10\overline{7}0\} + \frac{1}{6}\{0\overline{2}2\overline{3}\}
\]  \hspace{1cm} (7.1)

The $\frac{1}{3}\{10\overline{7}0\}$ partial can glide and produce a fault in the basal plane. The evidence suggests that the faults arise at the twin interfaces, and so this latter reaction seems most likely for the prism slip case.

It is interesting to note that the above dissociation of the $<c+a>$ dislocation can also occur in $[\overline{14}21]$ twins. However since the $\frac{1}{3}<11\overline{2}0>$ product dislocations lie in $\{1\overline{7}00\}$ planes for this twin system, faults in $\{1\overline{7}00\}$ are also possible by reactions 15 or 16 in Chapter 1. The dislocation energies involved favour the above interactions, excepting that in equation 7.1. However the fault energy is expected to be lower in the basal than in the non-basal plane.
7.2 **Ductility of H.C.P. Metals**

The present results indicate that \{11\overline{2}1\} twins can be responsible for the nucleation of \(<c+a>\) slip when prism slip occurs. The pyramidal slip system may have a Schmid factor when nucleated which is greater than that for any \(\frac{1}{3}<11\overline{2}0>\) prism slip system in either twin or parent. For a given \{11\overline{2}1\} twin, two-thirds of all the \(\frac{1}{3}<11\overline{2}0>\) dislocations can nucleate \(<c+a>\) slip. Pre-existing twins will be particularly beneficial in this respect.

These results may be compared with those obtained for \{10\overline{7}2\} twinning (Chapter 5). Both basal and prism slip can nucleate \(<c+a>\) slip at \{10\overline{7}2\} twin interfaces but only prism slip was able to nucleate slip on the \{11\overline{2}2\} planes, which is the preferred slip plane. Again two-thirds of the \(\frac{1}{3}<11\overline{2}0>\) dislocations can nucleate \(<c+a>\) slip, but the dislocations are required to impinge on the twin boundary in pairs.

It is clear therefore that \(<c+a>\) slip is best nucleated when prism slip occurs and when \{11\overline{2}1\} twinning occurs. This is significant in view of the excellent ductility of titanium particularly at cryogenic temperatures when high twin densities occur (Chapter 1.VIII). The good ductility of this metal in the hexagonal form has not been adequately accounted for in terms of the normally observed slip modes, which are basal and prism slip in \(<11\overline{2}0>\) directions, together with twinning on \{10\overline{7}2\} and \{11\overline{2}1\} planes, and to a lesser extent on \{11\overline{2}2\}. The \(\frac{1}{3}<11\overline{2}0>\) Burgers vector cannot alone produce five independent slip modes. Kocks and Westlake concluded that this paradox existed in other h.c.p. metals. They were therefore forced to conclude that twinning modes must be counted as independent deformation modes. However the limited shear strain attributable to twinning, due to the low twin volume fraction, and the polarity of the shear, argues against this explanation of the ductility. Re-orientation of the parent crystal by twinning may allow slip to occur more readily, but slip within the twinned volume must also satisfy the above 5 independent slip modes criterion to maintain compatibility at crystal interfaces, as pointed out by Kocks and Westlake.

The conflicting data can clearly be reconciled if the reactions at twin boundaries can give rise to \(<c+a>\) slip. This aspect has not hitherto been considered. Direct experimental evidence for \(<c+a>\) slip nucleated at \{10\overline{7}2\} twin boundaries has been obtained by Bevis and Tomsett. Furthermore it is found experimentally that \{11\overline{2}1\} twins enhance the,
ductility of titanium and zirconium. Dislocations with \(<c+a>\) Burgers vectors have been identified in polycrystalline titanium by Blackburn while more recently some careful experiments by Cass have shown \(<c+a>\) dislocations associated with \([11\bar{2}1]\) twins in titanium single crystals. The dislocations appeared to lie in \([10\bar{1}1]\) planes. This is the most direct evidence for type (2) dislocations gliding in prism planes reacting with \([11\bar{2}1]\) twins to produce \(<c+a>\) slip, as described in para. 6.6.2.

Twinning plays an important role in the development of textures in both titanium and zirconium. An important conclusion drawn from the study of textures in these materials is that the normally observed slip and twin systems cannot account for the observed textures. However the textures can be accounted for in terms of \(<c+a>\) slip, which again is consistent with the nucleation of \(<c+a>\) slip by twins.

Since pre-existing twins are likely to be effective in nucleating \(<c+a>\) slip, it is possible that the selection of a suitable texture to cause extensive twinning during fabrication would produce a material with improved ductility. Some evidence for this effect in zirconium has been reported.

Other experimental observations, not hitherto adequately explained, may be accounted for in terms of dislocation/twin interactions. The fact that \([1\bar{1}22]\) slip traces in zirconium and magnesium were associated with twins for example and the increased ductility of magnesium alloyed with lithium. Alloying does not affect the twin density but causes extensive prism slip. This is more likely to nucleate \([1\bar{1}\bar{2}2]\) \(<11\bar{2}3>\) slip at twin interfaces than basal slip which predominates in unalloyed magnesium.

A similar argument could be applied to beryllium. At room temperature basal slip and \([10\bar{1}2]\) twinning are the predominant deformation modes and the metal is brittle. At elevated temperatures prism slip systems also operate and \(\frac{1}{3}<11\bar{2}3>\) type dislocations are detected and the material becomes ductile. However in this metal the poor low temperature ductility is accentuated by the low basal plane cleavage stress. Anisotropic elasticity theory does not appear to account for the active slip systems in beryllium. Again the observed textures in beryllium can only be satisfactorily explained if \(<c+a>\) slip is active.
Further indirect evidence for the nucleation of $\frac{1}{3} <1\bar{1}23>$ type dislocations at $\{10\bar{1}2\}$ twin interfaces is provided by Hartt and Reed-Hill. In a study of the $\{30\bar{3}4\}$ twinning mode in magnesium they concluded that $\frac{1}{3} <1\bar{1}23>$ type dislocations are necessary for the plastic accommodation in the vicinity of the twin boundary. This twinning mode involves second order twinning on $\{10\bar{1}2\}$. Wonsiewicz and Backofen confirmed that enhanced ductility is associated with slip within the matrix of $\{30\bar{3}4\}$ twins in magnesium single crystals.

Slip on the pyramidal system may also be difficult to nucleate and twins may facilitate this process. Furthermore twins frequently occur in local regions of high stress concentration. It is under these conditions that $<c+a>$ slip might be expected to have a particularly beneficial effect on ductility. Although $\frac{1}{3} <1\bar{1}23>$ type dislocations may be nucleated at twin interfaces, the shear stress required to move them in their glide planes is expected to be much greater than that required to move $\frac{1}{3} <1\bar{1}20>$ type dislocations.

In spite of this fact, $<c+a>$ slip is found in cadmium and zinc. According to anisotropic elasticity theory, $<c+a>$ slip should be no more difficult in magnesium, titanium and zirconium. The lack of optical evidence for $<c+a>$ slip is probably due to the difficulty in unambiguously identifying this slip system in a polycrystal by trace analysis, since both prism and basal slip traces may be present in a heavily twinned structure. In zirconium and magnesium $<1\bar{1}22>$ slip traces have been reported; they cannot arise by slip in $<1\bar{1}20>$ directions and so it may be tentatively concluded that slip in $<1\bar{1}23>$ directions did occur in these experiments.

It is concluded that the ductility of titanium and other h.c.p. metals may be attributed to $<c+a>$ type dislocations nucleated at twin interfaces. It is then possible to explain the greater ductility of metals which slip in prism planes and twin on $\{11\bar{2}1\}$ planes. The experimental evidence available is consistent with this explanation of the ductility.

7.3 Future Work

In the conclusions in Chapter 1 several topics in the field of deformation of h.c.p. metals were proposed as suitable for further study. More specific proposals can now be made based upon the present research.
The observations made on twins in unidirectionally and cyclicly deformed metals have shown that dislocations and stacking faults are produced by interactions at twin boundaries. The nature of these faults and the dislocations composing the debris should now be determined. A comparison may then be made with the model proposed for the formation of twin boundary filamentary growth and fatigue crack nucleation in twin boundaries. It would also be interesting to know whether similar effects occur at twin interfaces in other materials e.g. antimony, bismuth and b.c.c. metals.

Elevated temperature fatigue tests on zinc and sodium chloride would also provide information on the effect of cross-slip on the defect structures in these materials as compared with zinc, magnesium and silver chloride at room temperature.

It has been shown that twin fragmentation and twin boundary cracking may occur during a fatigue test. Since twins may enhance tensile ductility, it is important to know whether pre-existing twins in a cold worked structure or in a fine grained material are detrimental under fatigue conditions.

Clearly more definitive experiments can be devised to determine whether the role of twins in the ductility of h.c.p. metals is that suggested in this thesis. Deliberate production of a twinned microstructure prior to tensile testing should be informative, particularly if the material is also cold worked or has a fine grain size. Explosive forming might be expected to be especially effective in introducing twins.

The effects of twinning are likely to be greatest in metals exhibiting prism slip and \{11\overline{2}1\} twinning e.g. titanium and zirconium. However significant effects may be obtained in beryllium twinned on \{10\overline{7}2\} planes and deformed in the temperature range where prism slip is operative and in magnesium alloyed with sufficient lithium to promote prism slip.

The first attempt at defining the relative importance of different twin and slip systems in the deformation of an h.c.p. metal was made by Professor Reed-Hill working with zirconium. In the present research an attempt has been made to measure the effect of twinning on both the ease of primary slip and on the ease of \(<c+a>\) slip. It is suggested that a computer programme might now be developed for calculating, for any stress axis, the Schmid factor values for primary and secondary slip and twin systems. This might give a better indication of the role of twinning in
the deformation of h.c.p. metals and possibly indicate the best
texture for a specific component made from a particular h.c.p. metal.
In polycrystalline magnesium and titanium dislocations are confined predominantly to their slip planes at low stresses and small dipoles and loops are produced by jogs on screw dislocations. Polygonisation begins in titanium after 15% strain and is well developed after 25% strain. Basal plane stacking faults are found associated with {1012} twins in magnesium and titanium and in the latter faults are found in non-basal planes. Faults in {1121} twins were also detected. A high dislocation density is also found in twins adjacent to twin interfaces. This debris is believed to arise from interactions between glissile dislocations and moving twin interfaces.

Examples of non-uniform twin boundary displacements have been found in magnesium and titanium during both twin growth and contraction. Dislocation debris is produced in the parent during untwinnning. Moving twin interfaces containing local incoherent twin boundary regions may generate imperfections in the form of microtwins and tilt boundaries in either the twin or parent matrix. Surface oxide particles on magnesium markedly affect the behaviour of twin boundaries at a free surface.

The first evidence for slip band extrusion in fatigued h.c.p. metals has been obtained. The extrusions are produced in cadmium, magnesium and titanium, but were not found in zinc. Cyclic stresses caused extrusions to form preferentially in regions of crystal previously twinned and untwinned. A qualitative model based upon the glide of dislocation dipoles and loops is proposed to explain the formation and distribution of the extrusions.

In fatigued specimens plastic deformation is accentuated at pre-existing twin interfaces, which subsequently become serrated. Suitably oriented twins break up into smaller irregularly shaped twin fragments. Fatigue cracks are nucleated in twin fragment interfaces before 25% of the fatigue limit has elapsed. A filamentary whisker growth phenomenon has been observed at {1012} twin interfaces in cadmium and magnesium and {1121} twin interfaces in titanium during fatigue. The formation of these whiskers and crack nucleation in twin boundaries is accounted for in terms of the dislocation debris generated by cyclic twinning. This debris can also cause the observed fragmentation of twins.
An attempt has been made to determine the role of twinning in h.c.p. metals using a resolved shear stress criterion to measure the relative ease of slip and twinning. For the stress axes considered and for pre-existing twins, it is concluded that prism slip is favoured by \{10\bar{1}2\} twins, while \{11\bar{2}1\} twins favour both basal and prism slip. When twins nucleate under stress, prism slip is favoured by \{10\bar{1}2\} twinning whereas either basal or prism slip may be enhanced by \{11\bar{2}1\} twinning. Dislocation interactions at twin boundaries may be responsible for nucleating \langle c+a \rangle slip. Prism slip is likely to be most effective in nucleating \langle c+a \rangle slip at \{10\bar{1}2\} and \{11\bar{2}1\} twin interfaces, and the preferred twin system is \{11\bar{2}1\}. This suggests that the ductility of polycrystalline h.c.p. metals may be improved by the presence of twins.
APPENDIX 1
Preparation of Thin Foils of Titanium
for Transmission Electron Microscopy

A.1.1 Introduction

There is a dearth of information on the preparation of thin foils of titanium from the bulk metal. The techniques reported in the literature are summarised in Table A.1.

In pure titanium chemical polishing preferentially attacks grain and twin boundaries and can lead to hydrogen pick-up with titanium alloys severe etching may occur due to differing rates of attack of different phases present.

None of the electropolishing techniques which have been described are completely satisfactory, because a tenacious oxide film can develop which is difficult to remove.

A technique was developed which avoided both hydrogen contamination and surface oxidation and permits large areas to be polished uniformly and without deformation. It has been successfully applied to the preparation of thin foils of complex-titanium alloys as well as those of pure titanium and single phase α alloys.

A.1.2 Experimental Technique

The specimens were initially sheet, 1/16" thick (chemically thinned or mechanically ground to the starting thickness) and protected with lacquer except for the area to be thinned.

In order to avoid the formation of surface oxide films it was found to be essential to severely agitate the electrolyte in contact with the specimen surface. This was done by directing submerged jets of electrolyte at each face of the specimen as shown in Fig.A.1.1. The jets were disposed symmetrically on either side of the specimen but at an angle of ~30° to the surface. This allowed the use of double cathodes each consisting of a small secondary stainless steel cathode close to the specimen backed with a larger plate cathode to which it was connected in parallel. This arrangement lessened preferential polishing at the edge of the protective lacquer, provided the small cathode area/polished area ratio was approximately 2:3. To produce thin foils from sheets 0.5 mm and 0.2 mm thick required the polished areas to be 12.5 mm and 5.0 mm diameter discs respectively. Polishing was continued until perforation of the sheet occurred.
<table>
<thead>
<tr>
<th>Solution</th>
<th>Conditions</th>
<th>Remarks</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 70% HNO₃ 30% HF</td>
<td>Chemical Polish</td>
<td>Pure titanium. Not applicable to alloys due to preferential attack at grain boundaries etc. and hydrogen pick-up</td>
<td>135</td>
</tr>
<tr>
<td>2 5% perchloric acid 95% acetic anhydride</td>
<td>'Window' technique 30-40V at -10 to -20°C Electrolyte stirred vigorously</td>
<td>Pure titanium Solution potentially dangerous</td>
<td>68</td>
</tr>
<tr>
<td>3 Disa-Electropol Solution A-3</td>
<td>Dissapol technique 45V</td>
<td>Ti, Ti-Al-Mn, Ti-Al-V Foil likely to be damaged</td>
<td>66</td>
</tr>
<tr>
<td>4 5% perchloric acid 95% acetic acid</td>
<td>P.T.F.E. holder 50V Electrolyte stirred vigorously and cooled with liquid nitrogen just before perforation</td>
<td>Ti-Al-Mn and other alloys Polishing may occur under an oxide layer. Epitaxial oxide difficult to remove</td>
<td>68</td>
</tr>
<tr>
<td>5 5% perchloric acid 95% acetic anhydride</td>
<td>'Window' technique 40V 0.1A/cm² -20 to 0°C</td>
<td>Quenched pure titanium</td>
<td>109</td>
</tr>
<tr>
<td>6 30 cc perchloric acid 295 cc methanol 175 cc n-butanol</td>
<td>Solution cooled 15V</td>
<td>Ti-8Al-2Mo-1V Electropolishing technique not described</td>
<td>105a</td>
</tr>
<tr>
<td>7 60 cc Perchloric acid (70%) 590 cc Methanol 350 cc 2-Butoxyethanol (Butyl Cellosolve)</td>
<td>30V 0.8A/cm² 0°C to -30°C</td>
<td>Present work</td>
<td></td>
</tr>
</tbody>
</table>
FIG.A.II. SCHEMATIC DIAGRAM OF ELECTROPOLISHING CELL
Satisfactory foils were produced using solutions 6 and 7, Table A.1. For solution 6 a slow rate of 1200 ml/min through jets of 4 mm diameter was adopted and polishing occurred under potentials varying from 15V to 50V, which at -20°C gave current densities from 0.2 to 0.75 A/cm² respectively. As reported for other solutions, the current density was sensitive to the temperature of the electrolyte, typical values being 0.25 A/cm² at -30°C and 0.7 A/cm² at 0°C for the normal operating voltage of 30V. The rate of metal removal at 30V and below 0°C was from 0.025 to 0.050 mm/min.

Polishing conditions could not be re-established if the current was switched off after perforation of the sheet, since etching and oxide formation occurred. However, if the foil edge was lacquered polishing could be continued to produce further thin areas.

A.1.3 Results

Areas greater than 50μm x 50μm may be obtained uniformly thin and free from hydride or oxide contamination. Further thinning in a chemical polishing solution (No.1 Table A.1) kept at less than 0°C produced equiaxed titanium hydride precipitates (fig.A.1.2) varying in size from ~400 Å to 5000 Å. Similar hydride precipitates were detected after chemical polishing in other solutions. These equiaxed particles precipitated at the free surfaces on twin boundaries and dislocations. When thin foils were heated in the electron beam, the residual pressure of hydrogen was sufficient to cause hydrogen absorption. During subsequent cooling, acicular titanium hydride was precipitated within the foil thickness (A in Fig.A.1.3a). A similar effect has been reported in zirconium foils. These precipitates are identical to those found in the α phase in titanium alloys after chemical polishing above room temperature, where the hydrogen content was found to have increased from ~50 to 400 ppm. The acicular hydride precipitates could be confused with martensite plates in complex titanium alloys and it is, therefore, important to avoid hydrogen contamination in thin foils of these materials. Further beam heating may remove the hydride, but the dislocations nucleated by the hydride remained (fig.A.1.3b).
Fig. A.1.2 Hydride precipitates in titanium after chemical polishing. Fine precipitates in the parent and coarse precipitates on the surface of a \{11\overline{2}1\} twin boundary.

x 40,000

Fig. A.1.3(a) Large hydride needle in titanium produced during cooling after electron beam heating. Long basal plane dislocations accommodating needle at A. Dislocations at B arise from climb of slip dislocations during beam heating.

x 25,000

Fig. A.1.3(b) As (a) after reheating to remove hydride. Note residual basal dislocations at A.

x 25,000
Appendix 2

Identification of Twin Spots in Electron Diffraction Patterns From H.C.P. Metals

Extra spots are produced in electron diffraction patterns when twins are present. These reflections may be close to matrix reflections and care must be taken to distinguish between them. Electron diffraction patterns for twinned crystals can be derived analytically. This method has been described for the case of twins in cubic and h.c.p. structures. However in practice it is often extremely tedious to analyse diffraction patterns from twinned h.c.p. metals when several twinning modes are present. A simple stereographic projection technique is described for predicting the position of twin spots in h.c.p. metals.

The three important twinning modes in h.c.p. metals are considered, namely {1012}, {1121} and {1122}. Diffraction patterns are constructed for the case of twins lying in a surface parallel to the basal plane and normal to the electron beam. Special orientations are defined in which twin and parent reflections are related by simple rotation about a single axis. The method allows the identification of twin spots from any twin lying in a foil of any orientation.

A.2.1 Crystallography of Twinning

A (0001) stereographic projection is shown in fig.A.2.1 for titanium. The poles and traces of K planes for the three types of twin are shown.

The twinning elements are listed in Table IV, Chapter 1, and shown on standard projections in figs.12, Chapter 1, A.2.2, A.2.3. The shape changes associated with twinning on these planes are illustrated by sections parallel to the plane of shear, in Chapter 1, IV.

The great circles corresponding to the \( \pi \) zones are in the same position in the projections for both twin and parent whereas the \( \pi \) zones in the parent move to \( \pi \) in the twin. Note the large displacement of \( \pi \) in fig.A.2.2 due to the large twinning shear associated with twinning on \( \{11\overline{2}1\} \). The determination of indices of planes and directions after twinning is also discussed in Chapter 1, IV.

A.2.2 General Case

The construction and indexing of a reciprocal lattice for h.c.p. metals and its use in indexing electron diffraction patterns is well documented in Chapter 1, VI and references 13,15,20,265. The reflecting planes lie in a
Fig. A.2.1. Relative orientations of \((10\bar{1}2)(\bar{1}1\bar{2}1)\) &\((\bar{1}1\bar{2}2)\) twinning modes in titanium
Fig. A.2.2

Position of some poles after (1121) twinning.

Fig. A.2.3

Position of some poles after (1122) twinning.

Also shown are $K_1$, $K_2$, $K'_2$ (after twinning) $\eta_1$, $\eta_2$, $\eta'_2$ (after twinning) and the zones for the last three axes. + parent poles • twin poles + coincident parent and twin poles.
zone, the axis at which is parallel to the electron beam. The stereographic technique for determining twin reflections requires the construction of a standard (0001) projection and also projections showing the poles after twinning on one twin plane in each of the three twin modes, as described in Chapter 1, IV.2.

It will be assumed for the moment that a thin foil is normal to the electron beam and contains an unknown twin. The orientation of the parent foil surface must be determined, and is drawn as a great circle through the poles of the reflecting planes in a (0001) projection. A coherent twin boundary plane, $K_1$, will intersect the foil surface along a certain direction, the twin boundary trace. The pole of $K_1$ will be somewhere on the great circle passing through both the foil normal and the normal to the twin boundary trace in the foil surface. This great circle is drawn on the same (0001) projection.

Possible reflections from any twin can be determined by superimposing the appropriate twin pole projection upon the (0001) projection, so that the trace of the pole of $K_1$ passes through the twin pole in a twin projection. Due to the spikes or relrods in reciprocal space, diffraction is possible when planes deviate appreciably from the exact Bragg reflecting position $^{11,73,260,261,266,267}$. Thus twin reflections are indicated by the low index twin poles nearest to that great circle corresponding to the parent orientation.

A.2.3 Parent Surface Oriented Parallel to Basal Plane

When the electron beam is parallel to $[0001]_M$, the matrix diffraction pattern consists of reflections from planes whose poles lie in the great circle corresponding to the (0001) plane of projection. To determine the possible reflections from a $\{10\bar{7}2\}$ twin, the $(10\bar{7}2)$ twin pole projection is superimposed onto the (0001) standard projection, so that the respective twin poles are coincident figs.12 (Chapter 1) A.2.2, A.2.3. The twin poles which lie nearest the parent basal plane great circle are possible reflecting planes in the twin. The nearest rational plane in the $\{10\bar{7}2\}$ twin is $[7010]$; twinned crystal will therefore give rise to the diffraction pattern shown in fig.1.18a. The relative position of the twin spots can be determined from the stereogram.

By superimposing each twin pole projection in turn upon the same standard projection, e.g. as in figs.A.2.2 and A.2.3, possible reflections can be predicted for any twin. It is clear that although $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$ twins
may give rise to parallel twin boundary traces in a basal plane surface (fig.A.2.1), they can be readily distinguished by comparing their diffraction patterns (figs.1.18 b-c).

Confirmation of the twin plane can be obtained by measuring the projected widths of the twin boundary in the foil plane.

The structure factor becomes zero and there is no diffracted beam when (h + 2k) = 3N and ℓ = 2N + 1, where h, k and ℓ are Miller Bravais indices and N and M are integers. However this condition is frequently relaxed in h.c.p. structures because double diffraction occurs in Chapter 1.

A.2.4 Special Cases

These arise when the twin boundary (K1 plane) is either parallel or normal to the foil surface.

For all twins, when η1 is parallel to the electron beam (K1 parallel to the beam) all twin spots are coincident with matrix spots and only one pattern is obtained (figs. 12, Chapter 1, A.2.2, A.2.3). Coincident spots for the three twin systems are given in Table V, Chapter 1.

When the electron beam is parallel to other directions in K1, the twin spots can be obtained by rotation of the parent pattern 180° about an axis normal to the twin boundary to produce a mirror image of the parent pattern across the twin boundary. This is shown in fig.A.2.4 for a beam parallel to [100] and for reflections from two different twin modes belonging to the [100] zone. The twins give rise to identical patterns and can only be distinguished by the difference in angle between the twin and parent patterns in each case. A similar situation exists when the beam is normal to the plane of shear of two reciprocal {1012} twins.

When K1 is normal to the electron beam and for small twinning shears i.e. {1012}, {1122} twins, the twin and parent diffraction patterns are similar, since they are composed of reflections from η21 and η2 zones. However the twin spots will be displaced slightly from the parent spots.

A.2.5 Identification of Unknown Twin in Titanium

A diffraction pattern from a titanium foil containing an unknown twin is shown in fig.A2.5a. The parent pattern (fig.A2.5b) was indexed and projected as a great circle in fig.A2.6. The great circle corresponding to the trace of the pole of K1 is also shown. This great circle indicates
Diffraction patterns produced when $K_1$ is parallel and the plane of shear normal to the electron beam. Notation as in fig. 1.18 0 indicates forbidden reflection.
(a) Diffraction pattern from twinned titanium.

(b) Parent diffraction pattern.

(c) Indices of twin spots.

Fig.A.2.5
two reciprocal twins, \((10\overline{1}2)\) and \((\overline{7}012)\), would give rise to the observed twin boundary trace. By superimposing the \((10\overline{1}2)\) twin pole projection with its twin pole on either \(10\overline{1}2\) or \(\overline{7}012\) in fig. 2.5 it was found that the \((10\overline{1}2)\) twin poles agreed with the diffraction pattern obtained in fig.A.2.5a. The analysis of the diffraction pattern was completed in terms of a \((10\overline{1}2)\) twin, as shown in fig.A.2.5c. Note the extra reflections produced by double diffraction.

Another example is shown in fig.A.2.7. The parent great circle is shown in fig.A.2.8 together with the trace of the twin boundary normal. Again two twins could produce the twin boundary trace, but only the \((01\overline{7}2)\) twin produces reflections consistent with the pattern in fig.A.2.7a and the indexed pattern is given in fig.A.2.7b. It can be seen in fig.A.2.8 that the poles do not all lie on the same great circle although their planes give rise to diffracted beams. Reciprocal lattice spikes are responsible for this effect. Consequently twin and parent reflections frequently occur together, although rational zone axes are seldom coincident in twin and parent and the planes are not at the exact Bragg reflecting position. Note the \([1\overline{1}2\overline{1}]\) forbidden reflections in fig.A.2.7 produced by two allowed reflections i.e. \(0\overline{7}10 + 1\overline{7}0\overline{7} = 1\overline{2}\overline{1}\overline{7}\).

\subsection*{A.2.6 Summary}

The stereographic technique for determining twin spots in diffraction patterns is applicable to any twin mode in a foil of any orientation. A projection of the poles after twinning in each mode is required, together with a standard basal plane projection.

The technique is particularly useful in h.c.p. metals where the majority of low index planes become irrational after twinning and several twin modes may occur together. The technique is also rapid and can allow for deviations from the exact Bragg reflecting position.
Fig. A.2.6

Stereographic projection of parent diffraction pattern and trace of twin boundary normal (from Fig. A.2) on standard (0001) stereogram. Twinned poles transferred from (1012) twin pole projection.
(a) Diffraction pattern from twinned titanium.

(b) Indices of twin spots in (a).

Notation as Fig. 1.18 Forbidden reflections produced by double diffraction

Fig. A.2.7

Projection of parent diffraction pattern and trace of twin boundary normal (from Fig. A.2.7a on standard (0001) stereogram. Twinned poles transferred from 0TT2 twin pole projection
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I enclose 3 copies of my thesis for the University.

Dr A. G. Gocker is the University supervisor and Mr P. J. E. Forsyth is the R.A.E. Supervisor.

The date for the ORAL is 28th March 1969. The external examiner will therefore require his copy as soon as possible.

Yours faithfully

P. G. Partridge.
     M. J. Blackburn
     W. D. Robertson
     W. A. Backofen