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A Single Surface Analysis of Deformation Twins in Crystalline Mercury

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Abstract

Deformation twins are reported to occur in crystalline mercury on the {110} planes of the face-centred rhombohedral cell, but a recent study of slip in this material suggests that this result may be incorrect. In the present paper we first give an analysis of the geometry of the possible twinning modes in mercury, including modes of a new type with four irrational elements, and show that the mode which is most likely to arise in practice does indeed have a {110} habit. A detailed single surface analysis, not involving the use of x-ray techniques, of one grain of a mercury specimen exhibiting four sets of twins is then described. None of the twins belong to the {110} mode. However, the traces and surface features of all four twins are consistent with the Type II mode with K_1 K_2 η_1 η_2 elements given by:

$$'\{\bar{1}\bar{3}5\}'\{\bar{1}11\}\langle\bar{1}21\rangle'\langle 0\bar{1}1\rangle'.$$

This mode has been confirmed using the same technique on further grains and also conventional single crystal methods.

Neither the {110} nor the '{$\bar{1}\bar{3}5$}' mode involves atomic shuffling but the '{$\bar{1}\bar{3}5$}' mode has a much larger twinning shear. The occurrence of this mode thus violates the basic hypothesis of recent theories of deformation twinning. The significance of this result and of the power of the single surface analysis technique are discussed.

§ 1. Introduction

The deformation modes of crystalline mercury were first investigated by Andrade and Hutchings (1935). By measuring angles between pairs of surface traces on cylindrical single crystal specimens, they deduced that slip and twinning occur on {100} and {011} planes respectively. These indices are given relative to the face-centred rhombohedral cell of axial angle 98° 22′ (Barrett 1957), to which the structure is most conveniently referred. It was later shown by Fisher (1943) that the Andrade and Hutchings results on slip could equally well be interpreted as slip on {11$\bar{1}$}, which seemed more likely as this is the closest-packed plane of the mercury structure. A single surface analysis by Crocker *et al.* (1963), which involved the study of the shapes of triangles formed by triplets of slip traces, showed that the traces were consistent with {11$\bar{1}$} slip but

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not {100} slip, and very surprisingly suggested that the predominant slip direction is not ⟨101⟩, the closest-packed direction, but ⟨1$\bar{1}$0⟩. A more recent conventional single crystal investigation by Rider and Heckscher (1966) has proved conclusively that the slip plane is {11$\bar{1}$}. It also showed that at liquid nitrogen temperature the slip direction is always ⟨1$\bar{1}$0⟩, but both ⟨1$\bar{1}$0⟩ and ⟨101⟩ are operative at −70°c. An interpretation of these results in terms of dislocation geometry has been given recently by Heckscher and Crocker (1966).

These observations on the slip of crystalline mercury suggest that the twinning behaviour may also be of considerable interest. Indeed, the fact that the designation of indices to the slip plane by Andrade and Hutchings (1935) was incorrect, indicates that the operative twinning plane is unlikely to be {011} as reported by these authors. However, as demonstrated by Jaswon and Dove (1956), the twinning mode which, on geometrical grounds, is most likely to be operative in the mercury structure, does have an {011} habit. The prediction of twinning modes is in fact comparatively straightforward in this case as mercury crystallizes on a single lattice and not on two interpenetrating lattices as do the other rhombohedral metals antimony, arsenic and bismuth. Thus, as in the b.c.c. and f.c.c. metals and indium, all of which are based on a single lattice, no shuffling of atoms need accompany the twinning shear in mercury. However, whereas in these other metals each of the most likely twinning modes involves two crystallographically equivalent twinning planes, in mercury the two twinning planes are {011}, as reported by Andrade and Hutchings, and {100}. The question thus arises why twins on {100} have not been observed, as the magnitudes of the twinning shears on the two planes are identical. Jaswon and Dove (1956) suggested that {100} did not operate as a twinning plane because it is the slip plane, but as explained above this is now known to be incorrect. In any case slip and twinning both occur on {111} planes in f.c.c. metals. The shear associated with the mercury twinning mode with {011} and {100} twinning planes has magnitude 0·46. This value is unusual, most twinning modes having shears either much smaller or larger than this value. Finally it is interesting to compare the twinning behaviour of mercury with that of f.c.c. metals, to which its structure approximates.

Deformation twinning of crystalline mercury would thus appear to be a fruitful field of research and in this paper we describe the results we have obtained from a single surface analysis of a single grain of a flat mercury specimen. As in the case of slip we have been able to arrive at very definite and surprising conclusions about the operative twinning mode without making use of conventional x-ray techniques. In §2 we describe the geometry of twinning in mercury, including the prediction of possible twinning modes, and in §3 the experimental procedure adopted is described and our observations summarized. These observations are analysed in §4 and the significance of our conclusions is discussed in §5.

§ 2. Geometry of Twinning in Mercury

2.1. *General Relations*

The crystallography of deformation twinning is described in general terms in the books by Hall (1954) and Christian (1965), the review articles by Cahn (1954, 1964) and, more recently, in a paper by Bilby and Crocker (1965). Only a brief summary, relevant to the case of single lattice structures, will therefore be given here. It is found convenient to describe a deformation twinning process by means of four twinning elements $K_1 K_2 \eta_1 \eta_2$ which form a twinning mode, although a twinning shear is in fact uniquely defined by either K_1 and η_2 or K_2 and η_1. The elements K_1 and η_1 are the shear or twinning plane and direction respectively; K_2 and η_2 are the reciprocal twinning plane and direction. The plane containing η_1 and η_2 is known as the plane of shear. By interchanging the planes K_1 and K_2 and the directions η_1 and η_2 one obtains the reciprocal twinning mode, which involves the same shear strain g as the original mode. Classical twinning modes are normally divided into those with four rational elements, which are termed compound, and those with two rational elements, either K_1 and η_2 or K_2 and η_1, which are labelled Types I and II respectively. The reciprocal of a Type I mode is clearly of Type II and vice versa. Degenerate cases of Type I and Type II modes with three rational elements also arise (Crocker 1965). The orientation relationship associated with a Type I twin is reflection in K_1 and with a Type II twin is rotation of π about η_1; the two relationships are identical for compound twins. It has been shown recently (Crocker 1962, Bevis and Crocker, to be published) that shears which restore a lattice in a new orientation may be described by unconventional twinning modes, which in general have four irrational elements, although some or all of these may become rational in degenerate cases. These twins do not obey the conventional orientation relationships.

General expressions for the shear magnitude and general relationships between the twinning elements have been given by Bilby and Crocker (1965). In a rhombohedral lattice, for the case of a compound or Type I mode with rational elements $K_1 = (hkl)$ and $\eta_2 = [uvw]$ these become:

$$g^2 = 4\{UH[(1-c)(1+2c)p^2]^{-1} - 1\}, \quad \ldots\ldots \quad (1)$$

$$K_2 = \begin{bmatrix} Uh - p[u + c(v+w)] \\ Uk - p[v + c(w+u)] \\ Ul - p[w + c(u+v)] \end{bmatrix}, \quad \ldots\ldots \quad (2)$$

$$\eta_1 = \begin{bmatrix} p[(1+c)h - c(k+l)] - Hu \\ p[(1+c)k - c(l+h)] - Hv \\ p[(1+c)l - c(h+k)] - Hw \end{bmatrix}, \quad \ldots\ldots \quad (3)$$

where

$$U = [(u^2+v^2+w^2) + 2c(uv+vw+wu)],$$
$$H = [(1+c)(h^2+k^2+l^2) - 2c(hk+kl+lh)],$$
$$p = (uh+vk+wl),$$

and c is the cosine of the axial angle of the rhombohedral cell. Similar relations hold for Type II twins on interchanging K_1, η_2 and K_2, η_1. For a given twinning mode only a fraction of the parent lattice points are in general sheared to lattice points of the twin. This fraction may be determined from the quantity $q = I^{-1}p$. For face-centred cells the factor I is unity when h, k, l are all odd and otherwise is one-half and, in determining p, $[uvw]$ must be a primitive lattice vector. When q is odd a fraction q^{-1} of the lattice points are sheared correctly and when q is even the fraction is $2q^{-1}$. In particular when q equals either 1 or 2 no shuffles are necessary.

2.2. *Possible Twinning Modes*

As explained by Bilby and Crocker (1965), eqn. (1) may be used to determine twinning modes with small shears for a given value of the parameter q defined in §2.1. We are here primarily interested in modes involving no shuffles and thus set $q = 1$ or 2. This gives rise to five modes with shears less than unity together with the corresponding five reciprocal modes. These modes are listed in order of increasing shear magnitude as modes 1 to 5 of table 1. It will be seen that three of the modes are compound and two are of Type I, the corresponding reciprocal modes being compound and of Type II respectively. Mode 1 is the one predicted by Jaswon and Dove (1956), the K_2 plane being the twinning plane reported by Andrade and Hutchings (1935). Dove (1956) also showed that modes 3, 4 and 5 are crystallographically possible but did not obtain mode 2. In another theoretical investigation Kiho (1954) reported mode 1 and also three modes with shears between 1 and 3/2 but did not give modes 2 to 5. One interesting feature of the modes is that, of the eight rational twinning planes, three are $\{11\bar{1}\}$, the observed slip planes, and a further two are $\{100\}$, which were formerly thought to operate as slip planes.

Mode 6 of table 1 is the mercury twinning mode with the smallest shear in which only one-half of the atoms are sheared to correct twin sites. It will be seen that it has an exceptionally small shear, much smaller than that for mode 1, but is not expected to operate in practice due to the large shuffles involved. No non-conventional twinning modes with four irrational elements, involving no shuffles and shears less than unity, arise for the mercury structure. However, mode 7 of table 1, in which half the atoms must shuffle does have four irrational elements and has a comparatively small shear. A feature of this kind of mode is the fact that the indices of the twinning plane and the other twinning elements are different relative to the parent and twin bases. Each of these modes can thus be defined in two distinct ways, the mode corresponding to mode 7 being given as mode 8 in table 1. Again due to the large shuffles involved, modes 7 and 8 are unlikely to be operative in practice.

The f.c.c. twinning modes corresponding to the f.c. rhombohedral modes of Table 1 may be obtained by letting $c = 0$. Mode 1 then degenerates to a mode with zero shear and both modes 2 and 5 become the operative

Table 1. Possible twinnidg modes of crystalline mercury

	K_1	K_2	η_1	η_2	g
1	011	100	100	011	0·457
2	$\bar{1}11$	'$\bar{1}35$'(a)	'$0\bar{1}1$'(b)	$\bar{1}21$	0·633
3	100	$1\bar{1}\bar{1}$	$0\bar{1}\bar{1}$	211	0·880
4	$3\bar{1}1$	'$3\bar{1}\bar{3}$'(c)	'$1\bar{1}\bar{4}$'(d)	101	0·888
5	111	$11\bar{1}$	$\bar{1}\bar{1}2$	$\bar{1}\bar{1}\bar{2}$	0·901
6	$11\bar{1}$	113	112	$33\bar{2}$	0·007
7	$22\alpha^+$	$22\alpha^-$	$33\alpha^-$	$33\alpha^+$	0·453
8	β^+22	β^-22	β^-33	β^+33	0·453

No shuffles are necessary in modes 1–5 but half of the atoms must shuffle in modes 6–8. The rational approximations to the irrational elements have been obtained by letting $c=-1/7$. The algebraic expressions for these elements are:

(a) $(-1-5c,\ -1-c,\ 1-3c)$; (b) $[-1-7c,\ -2-6c,\ 1-c]$

(c) $(1+c,\ -1-5c,\ -1-c)$; (d) $[1-c,\ -4-20c,\ -7-17c]$.

In addition $\alpha^{\pm}=2[(-1+9c)\pm 2(57c^2+6c+1)^{1/2}](1+7c)^{-1}$,

$\beta^{\pm}=2[(1+15c)\pm 2(57c^2+6c+1)^{1/2}](1-c)^{-1}$.

f.c.c. twinning mode with elements identical to those of mode 5 and shear equalling $2^{-1/2}$. The f.c.c. mode arising from mode 3 is a compound mode with the same twinning elements and shear equalling $2^{1/2}$. The K_2 and η_1 elements of mode 4 become $\{1\bar{1}\bar{1}\}$ and $\langle 1\bar{4}\bar{7}\rangle$ and the twinning shear $(3/2)^{1/2}$. This f.c.c. mode is particularly interesting as, although the four twinning elements are rational, it is not a conventional compound mode, but a degenerate case of a mode with four irrational elements. The shears restore the structure directly for twinning on both K_1 and K_2, no shuffling being necessary, if the operative orientation relationships are taken to be Type I and Type II respectively. However, for the alternative orientation relationships to be obeyed, two-thirds of the atoms must shuffle in each case. Finally, modes 6, 7 and 8 all become variants of the f.c.c. mode with elements identical to those of mode 6 and twinning shear equalling $8^{-1/2}$. This mode was suggested by Jaswon and Dove (1957) as a possible mode for twinning of materials with the diamond structure.

2.3. *Surface Features*

In §4 we shall be using all the available experimental information which can be obtained from a single surface of a flat specimen. This includes the magnitude of the surface tilt associated with a twin and the displacement of slip lines and other traces when they are sheared by the twin. Analytic expressions for these quantities are obtained below.

Figure 1 (*a*) is a schematic representation of a twin meeting the surface of a crystal at an angle α to the vertical. The surface tilt is given by θ and the twinning direction makes an angle $\pi/2-\gamma$ with the trace of the twin in the surface. From this diagram it is readily shown that θ and the apparent surface shear s are given by:

$$\tan\theta = g\cos\gamma[\sec^2\alpha + g\cos\gamma\tan\alpha]^{-1}, \quad \ldots\ldots (4)$$

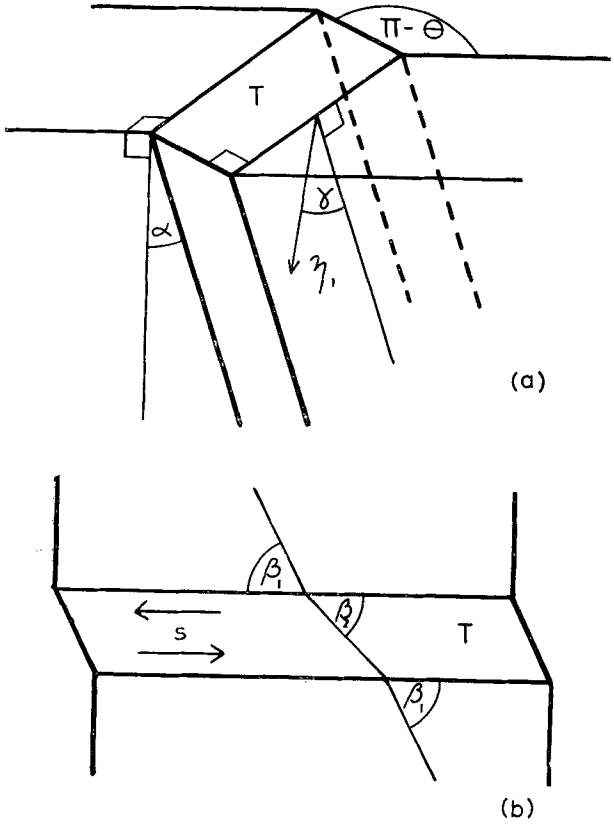
$$s = g\sin\gamma[\sec\alpha + g\cos\gamma\sin\alpha]^{-1}, \quad \ldots\ldots (5)$$

where the signs of the angles are as indicated in the diagram. A plan view of the crystal surface showing a slip line sheared by the twin is given in fig. 1 (*b*). The angles β_1 and β_2 which the slip line makes with the twin trace can be measured and enable s to be determined, using the relation:

$$s = \cot\beta_1 - \cot\beta_2, \quad \ldots\ldots (6)$$

and compared with the value predicted by eqn. (5). The angle θ may be

Fig. 1



Surface features associated with a twin T meeting the surface of a crystal. Diagram (*a*) shows the surface tilt θ and (*b*), which is a plan view of the surface, indicates the apparent shears.

measured directly as described in § 3 and compared with that given by eqn. (4).

A feature of single surface analyses based on the angles between traces is that it is not possible to distinguish between the true crystal orientation and the mirror image of this orientation in the specimen surface (Bevis *et al.* 1964). Reference to fig. 1 (*a*) indicates that the effect of reflecting the crystal in this way is to reverse the sign of α and to change γ to its supplement. Hence, using eqns. (4) and (5), the sign of θ is reversed but s remains unchanged. Thus when some of the traces are produced by twins, and the sense of the surface tilts can be determined, it is possible to ascribe a unique orientation to the crystal.

§ 3. Experimental Procedure and Observations

Flat polycrystalline specimens containing elongated grains about 1 cm across were prepared by carefully freezing pools of mercury, using the procedure described previously (Crocker *et al.* 1963). After the specimens had solidified they were covered with ethyl alcohol which removed frost from the surfaces and made them suitable for observation. They were then deformed, at various temperatures between that of liquid nitrogen and -50°C, by tapping a thin pre-cooled rod placed in contact with their surfaces. Deformation twins on several different planes were observed to form in individual grains throughout this temperature range. One particular grain was chosen for detailed analysis as it clearly showed three sets of slip traces and four sets of twins. It is shown in fig. 2, the slip lines being labelled S_1, S_2, S_3 and the twins T_1, T_2, T_3, T_4. In addition, a uniform set of growth ripples R is present over the whole surface together with various accommodation features including some wavy slip (Greenland 1937).

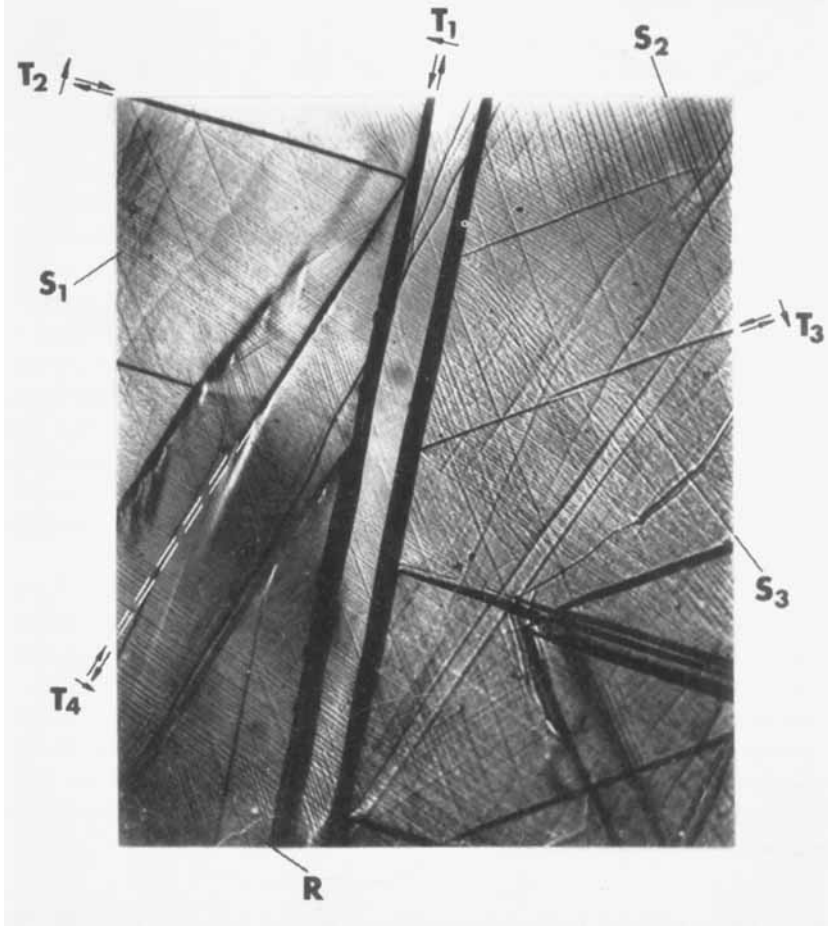
The angles between trace S_1 and traces S_2, S_3, T_1, T_2, T_3, T_4 were measured to $\pm\frac{1}{2}$° using the rotating stage of the microscope and found to be $78\frac{1}{2}$°, 100°, 49°, 134°, 170°, 27° respectively. The senses of the surface tilts associated with the twins could be distinguished very readily and are indicated in fig. 2. An estimate of their magnitudes was also obtained by determining the position of a lamp which gave maximum intensity of reflected light when viewing the twins through a microscope set normal to the specimen surface. The tilt θ could then be calculated from the angle of incidence ϕ using the relation:

$$\mu \sin 2\theta = \cos\phi, \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad (7)$$

where μ, the refractive index of ethyl alcohol, was taken to be 1·36. The results for the four twins are given in table 2. Compared with the measurements of the angles between the traces these results are very inaccurate but, as described in § 4, they prove an invaluable check in the analysis of the observations. Finally the apparent surface shear s was determined by examining the shear of slip lines and ripples which pass through the twins. Again the sense of the shear is very clear in all four cases, being

as indicated in fig. 2. The magnitudes of the shears were determined by measuring the angles β_1 and β_2, defined in fig. 1 (*b*), for the four twins, and substituting in eqn. (6). The accuracy of the results depends critically on the magnitudes of β_1 and β_2, when either departs appreciably from $\pi/2$. In addition the angle β_2 is difficult to measure, particularly for the narrow twins. The results, together with an estimate of the errors Δs involved in each case, are given in table 2.

Fig. 2



Three sets of straight slip traces S_1, S_2, S_3, four sets of twins T_1, T_2, T_3, T_4 and a set of ripples R, on the surface of a mercury crystal. The sense of the surface shear associated with each twin is indicated by a pair of arrows along the twin trace and the sense of the surface tilt by a transverse arrow pointing downhill. (Mag. × 70.)

Table 2. Comparison of observed and predicted tilts and shears

		T_1	T_2	T_3	T_4
Observed	θ	20°	17°	<3°	17°
	s	0·30	0·37	0·38	0·39
	Δs	±0·02	±0·05	±0·15	±0·05
Predicted	θ_1	2°	22°	23°	1°
	θ_2	28°	14°	4°	25°
	s_2	0·30	0·38	0·48	0·41

§ 4. Analysis of Observations

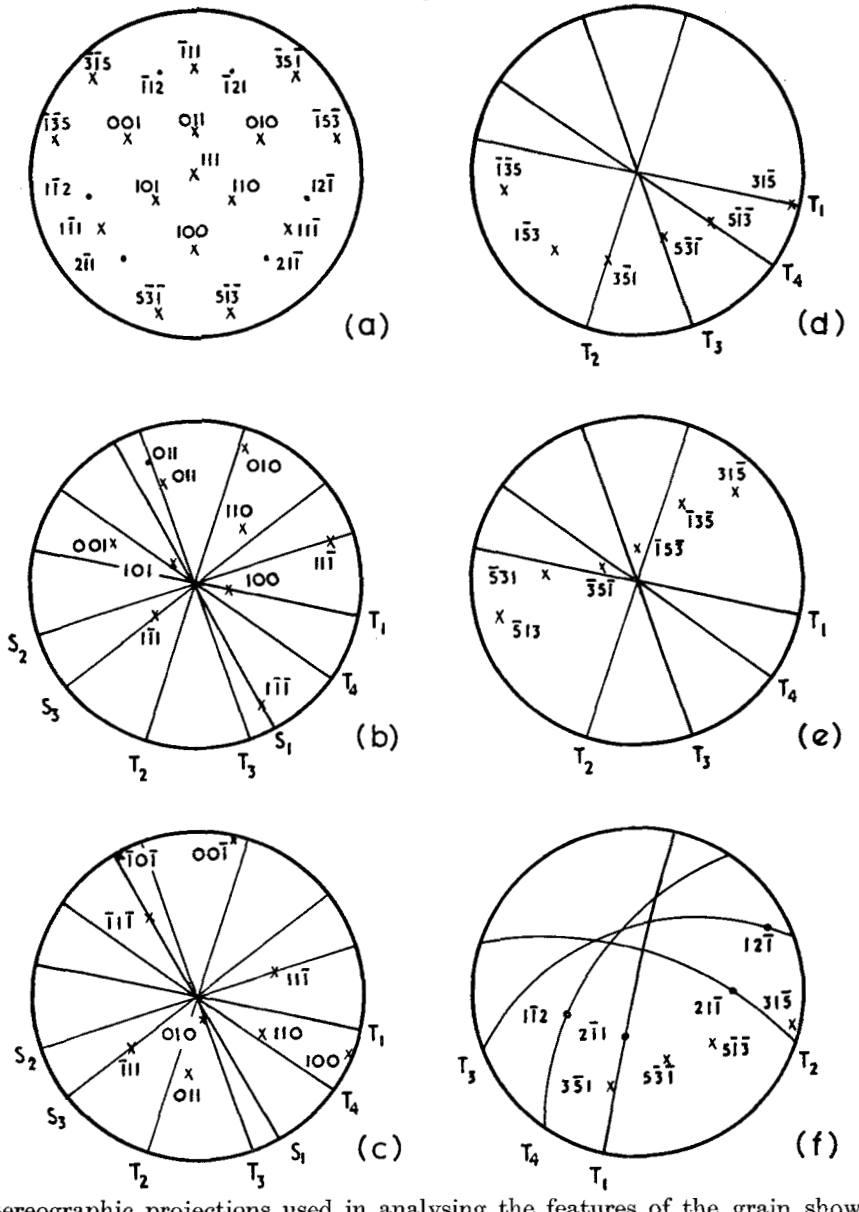
4.1. *Orientation Determination*

In a previous paper (Bevis *et al.* 1964) we described methods of determining the orientation of rhombohedral crystals, and in particular mercury, from the angles between three sets of crystallographically equivalent slip traces on a single surface. Essentially three different procedures are available, one based on stereographic manipulations, another on the use of simple physical models and a third, an exact analytic method involving the solution of a quartic equation. These produce four, two or no possible orientations, depending on the angles between the traces. In the present application, in which the traces are produced by slip on the three $\{11\bar{1}\}$ mercury planes, the first method was found to be most inadequate. The analytic method was therefore employed and for the grain shown in fig. 2 gave two possible orientations which will be labelled I and II. The Miller indices of the surface corresponding to these orientations were calculated to be $\{1, 0{\cdot}422, \overline{0{\cdot}1}\,\overline{2}\,\overline{1}\}$ and $\{1, \overline{0{\cdot}1}\,\overline{7}\,\overline{3}, \overline{0{\cdot}1}\,\overline{3}\,\overline{1}\}$ respectively. The method using models was also used to orient this grain and the results were found to agree with the analytic solutions to within $1\frac{1}{2}°$. In order to decide which of the two possible orientations is correct it is necessary to make use of the additional information provided by the twins. This is done in §§ 4.2 and 4.3.

4.2. *Interpretation in Terms of* {100} *and* {011} *Twins*

The most obvious deduction to make from the appearance of four twins on different planes in a single grain of mercury is that both {100} and {011}, the K_1 and K_2 planes of mode 1 of table 1, are acting as composition planes, as there are only three variants of each set of planes. In order to test this hypothesis the standard mercury stereogram shown in fig. 3 (*a*) (Bacon *et al.* 1964) was rotated to the two orientations deduced in § 4.1. The resulting projections, with the poles of the {100} and {011} planes indicated, are given in figs. 3 (*b*) and (*c*), together with the traces of the normals to the slip and twin traces. The $\{11\bar{1}\}$ poles do of course lie exactly on the normals to the slip traces for both orientations, providing

Fig. 3



Stereographic projections used in analysing the features of the grain shown in fig. 2. The standard mercury projection is shown in (*a*), crosses and closed circles indicating the poles of planes and directions respectively. Orientation I is shown in (*b*) and (*d*) and orientation II in (*c*) and (*e*). The poles of the {100} and {011} planes are plotted in (*b*) and (*c*) and the poles of the '{$\bar{1}35$}' planes in (*d*) and (*e*) and in all four cases the normals to the twinning traces are shown. In addition, in diagrams (*b*) and (*c*) the poles of the {11$\bar{1}$} planes and the normals to the slip traces are indicated. The traces of the four twins and the poles of the operative twinning planes and directions are plotted in (*f*).

a useful check on the orientation determinations described in § 4.1. However, in neither case is there very satisfactory agreement for the twins. Using a 40 cm diameter stereographic projection, the angles between the normals to T_1, T_2, T_3, T_4 and the nearest {100} or {011} twin pole were 0°, 3½°, 2°, 3° and 10°, 4½°, ½°, 2° respectively for the two orientations.

Orientation II can thus be discarded immediately, if all the twins are to belong to mode 1 or its reciprocal. There is however a possibility that the discrepancies for orientation I are due to errors in measurement, but on examining the surface tilts and displacements, which would be associated with the suggested twins, it is readily seen that the approximate agreement is fortuitous. This is clearly illustrated by twin T_1 which in fig. 3(*b*) appears to have a (100) composition plane. The twinning direction corresponding to this plane is [011] which, as indicated on the stereogram, is approximately parallel to the specimen surface. The surface tilt associated with this twin would thus be very small and quite inconsistent with the measured value of 20°. The actual tilts θ_1 for the four twins have in fact been calculated using eqn. (4), the angles γ and α being measured from the stereogram. They are given in table 2. Comparing them with the observed values it is clear that the hypothesis that the four twins belong to mode 1 or its reciprocal must be abandoned.

4.3. *Interpretation in Terms of '{$\bar{1}\bar{3}5$}' Twins*

Following the failure of the attempt described in § 4.2 to index the twins shown in fig. 2 in terms of the {100} and {011} composition planes of mode 1, it was decided to see whether they were consistent with any of the other modes given in table 1. We do not consider modes 6, 7 and 8 which involve shuffles and can also eliminate the {100} and {11$\bar{1}$} habits of modes 2, 3 and 5 which were considered in figs. 3(*b*) and (*c*). This leaves the '{$\bar{1}\bar{3}5$}' habit of mode 2, both twinning planes of mode 4 and the (111) habit of mode 5. As the shear of mode 2 is much smaller than that of modes 4 and 5, we shall first examine whether the twins may lie on four of the six variants of '{$\bar{1}\bar{3}5$}'.

The stereograms of figs. 3(*d*) and (*e*) give the two possible orientations of the specimen with the '{$\bar{1}\bar{3}5$}' poles indicated. It is seen immediately that there is very good agreement between the normals to the twin traces and four of the '{$\bar{1}\bar{3}5$}' poles in fig. 3(*d*) for orientation I, the discrepancies being ½°, ½°, 2½°, 0° for twins T_1, T_2, T_3, T_4 respectively. There is no such agreement for orientation II. The magnitudes of the surface tilts θ_2 for orientation I, calculated using eqn. (4), are given in table 2 and are in satisfactory agreement with the measured values. They are however all in the wrong sense indicating, as discussed in § 2.3, that the correct orientation of the grain is the mirror image in the specimen surface of the orientation shown in fig. 3(*d*). The senses of these tilts can be readily deduced by referring to fig. 3(*f*), which shows orientation I with the poles and traces of the relevant twin planes and the poles of the corresponding

twin directions indicated. It must be borne in mind when using this stereogram that the positive side of the '{$\bar{1}\bar{3}5$}' twinning plane shears in the positive $\langle \bar{1}21 \rangle$ direction.

The magnitudes of the surface shears were calculated using eqn. (5) and the results are again given in table 2. They are in very good agreement with the measured shears for these twins, and as shown by fig. 3(*f*) the senses are correct in all four cases. There is thus overwhelming evidence that all four traces are produced by the reciprocal of mode 2 of table 1 and incidentally that orientation I is the mirror image in the specimen surface of the true orientation of the grain. It is therefore unnecessary to consider the possibility of modes 4 and 5 being operative.

§ 5. Discussion

This paper has clearly illustrated the wealth of information which can be obtained from a detailed single surface analysis of a single grain of a specimen. This technique has proved particularly valuable in the case of crystalline mercury, where, due to the dangers of losing specimens through melting, x-ray work and other lengthy experimental procedures are inconvenient. In these circumstances it is also necessary to obtain clear micrographs, providing as much detailed information as possible, so that flat specimens are ideal. It has certainly been satisfying to supplement our earlier single surface analysis, which enabled the slip plane and direction of mercury to be deduced, by the present work on the operative twinning mode. It should be stressed however that the technique is potentially of very wide application, particularly in the case of small grained polycrystalline specimens where x-ray orientation determinations may be difficult.

The full single surface analysis of twinning in one grain of crystalline mercury, which has been described in this paper, has been repeated on one other grain containing two twins and three sets of slip traces. The agreement between the observed traces, tilts and shears and the features expected to arise from the '{$\bar{1}\bar{3}5$}' twinning mode was again excellent. In addition, preliminary results by Heckscher and Guyoncourt (unpublished work), involving x-ray orientation determinations and conventional single crystal specimens, have also indicated that the operative twinning plane is '{$\bar{1}\bar{3}5$}'. There is thus overwhelming evidence in favour of this mode.

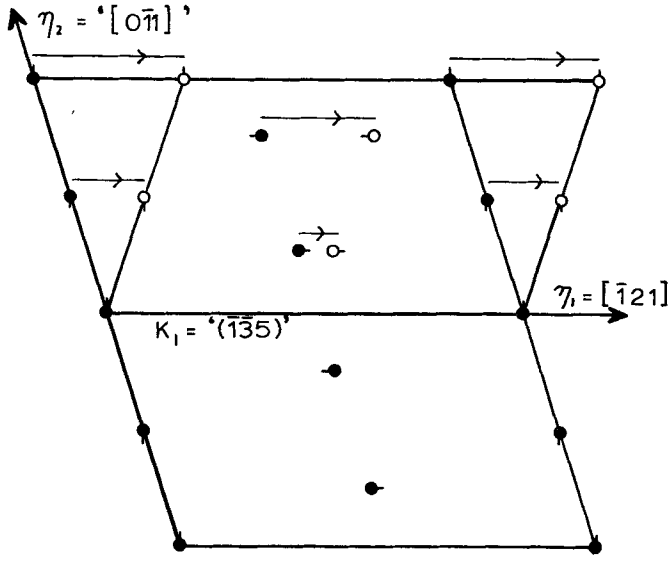
This result is very surprising. In only one other metal, α-uranium, have Type I or Type II twinning modes been observed (Cahn 1953) and even then the predominant mode is compound. Also, in mercury, not only is the operative mode of Type II, but it is preferred to a compound mode with a smaller shear. Indeed, for a metal which twins so profusely, the twinning shear of mercury is exceptionally high. This behaviour cannot be attributed to unfavourable shuffle mechanisms as the structure of mercury is based on a single lattice and not a double lattice, as is α-uranium. Thus, whereas atomic shuffles are unavoidable for twinning

in α-uranium, this is not the case for mercury, so that the twinning mechanisms should be particularly simple. In addition, no twins have been oberved on $\{11\bar{1}\}$ the twinning plane reciprocal to '$\{\bar{1}\bar{3}5\}$', although this might be explained by the fact that this is the operative slip plane and the corresponding twinning direction, which is irrational, is approximately parallel to the predominant slip direction.

Unfortunately, owing to the irrational nature of both the K_1 plane and the plane of shear, it is not possible to present an accurate simple plot of the atomic movements associated with the '$\{\bar{1}\bar{3}5\}$' twinning mode. However an indication of the movements involved may be obtained by making the approximation $c = -1/7$ for $c = -0{\cdot}1454$, the cosine of the axial angle of the rhombohedral cell. The elements K_1 and η_2 then become $(\bar{1}\bar{3}5)$ and $[0\bar{1}1]$ respectively, as indicated in Table 1, and the plane of shear becomes (311), which has a four-fold stacking sequence. The resulting plot is shown as fig. 4. It clearly illustrates the simple nature of the twinning shear in this case. It should be noted however that, although the mode is now apparently compound, the orientation relationship must remain that of a Type II twin, rotation of π about η_1, if shuffles are to be avoided.

As mentioned in § 1, the previously reported twinning mode of crystalline mercury was unusual in that other operative modes have either much smaller or larger shears. Now that it is known that this mode is not

Fig. 4



Approximate plane of shear plot illustrating the atomic movements associated with the '$\{\bar{1}\bar{3}5\}$' mercury twinning mode. Parent and twin atom sites are indicated by closed and open symbols respectively. The stacking sequence of the plane of shear is fourfold, sites in successive planes being distinguished by bars at 90° intervals.

the predominant twinning mode, the division of operative modes into two groups becomes very marked. This may well indicate that low and high shear twins are nucleated homogeneously and inhomogeneously respectively. Well known dislocation models do, of course, exist for the nucleation of twins with shear equalling $2^{-1/2}$ in b.c.c. and f.c.c. metals (Cottrell and Bilby 1951, Venables 1964) and the correspondence, noted in § 2.2, between the f.c.c. mode and the '$\{\bar{1}\bar{3}5\}$' mode may thus be significant. However, whereas twinning dislocations may be produced by elementary dissociations of slip dislocations in cubic crystals this is not possible in mercury, where no simple relation exists between the Burgers vectors of partial slip dislocations and twinning dislocations. The same problem arises for the well-established $\{11\bar{2}1\}$ twins in h.c.p. metals (Reed-Hill 1964), for which the magnitude of the twinning shear is γ^{-1}, where γ is the axial ratio.

In order to clarify the problems which have arisen from this investigation, further experimental work is clearly necessary. Some additional information can still be obtained using single surface analyses, particularly now that the twinning plane is known. Thus, for example, accommodation effects at twin intersections can be studied. An interesting example of this does in fact arise at the lower right-hand side of the grain shown in fig. 2, where, at the intersection of twins T_2 and T_3, a considerable amount of slip has occurred on system S_2. These traces are produced by '$(3\bar{5}1)$', '$(5\bar{3}1)$' and $(11\bar{1})$ planes respectively, which have an approximately common line of intersection along [112]. Other well-known features associated with twinning, such as cross-twinning (Cahn 1964) and indented twin boundaries (Hull 1964) have been noted on flat specimens of mercury and require further investigation. However, in order to obtain an adequate understanding of the operation of the '$\{\bar{1}\bar{3}5\}$' mode, a conventional single crystal study of the effects of orientation and temperature on the operative deformation modes in single crystals is also being carried out. In particular detailed information on the inter-relation of twinning and slip is necessary, particularly at low temperatures where the operative slip directions all lie in the unique (111) plane. This investigation should also enable effects of elastic anisotropy to be evaluated. Another topic of interest is the martensitic transformation which has been reported to occur, on the basis of x-ray evidence only, at very low temperatures (Schirber and Swenson 1962). For all these phenomena it is of course desirable to obtain direct information on the dislocations and faults present in the mercury structure and it is hoped that this will be possible using either electron microscopy or x-ray techniques.

The importance of the results of the present paper to the general theories of deformation twinning cannot be over-emphazised. These theories are based on the hypothesis that the operative twinning mode in a given structure is the one with the smallest shear, consistent with a simple shuffle mechanism. In mercury this hypothesis has been shown to be violated in a very striking way as, of the modes involving no shuffles,

the operative mode does not have the smallest shear. The apparent understanding of the crystallography of deformation twinning which has developed in recent years would thus seem to be open to serious questioning. Another important feature of the results is that modes in which half of the atoms must shuffle are not operative, despite the fact that one of these involves an exceptionally small shear. It thus appears that shuffles can not be tolerated in single lattice structures even when associated with modes having very favourable shears. Deformation twinning of crystalline mercury has certainly proved to be just as fascinating a topic of study as the slip behaviour. In both cases the previously reported modes were incorrect and it is remarkable that in neither case does the operative mode conform to the well-established theories of these deformation mechanisms.

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