TWINNED MARTENSITE*

A. G. CROCKER†

In view of the recent thin film work which has shown that at least some plates of martensite are twinned on a fine scale, the possible twinning modes of the martensite structure are examined in detail. These reduce to fourteen different shear modes, which are used as initial data for a current theory of martensite crystallography. It is shown that only six of these modes can in fact result in twinned martensite plates and a comparison of the corresponding predictions and the observed crystallographic features indicates that only one type of twinned martensite is likely to occur in practice. This type has been observed in several steels. Further developments of the theory which appear to be necessary in order to explain all the observed features are also discussed.

MARTENSITE MACLEE

Sur la base de récents travaux sur des lames minces qui ont montré qu'au moins quelques plaquettes de martensite sont maclées à petite échelle, l'auteur étudie en détails les mécanismes possibles du maclage de la structure martensitique. Ils sont réduits au nombre de 14 modes de cisaillement différents, qui sont utilisés comme dossiers initials pour une théorie courante de la cristallographie martensitique. L'auteur montre que six seulement de ces modes peuvent en fait conduire à des plaquettes de martensite maclées, et indique par comparaison des prédictions correspondantes et des caractéristiques cristallographiques observées, qu'en pratique seulement un type de martensite maclée peut se présenter. Ce type a été observé dans plusieurs aciers. Il discute aussi les développements théoriques subséquents qui semblent être nécessaires en vue d'expliquer toutes les caractéristiques observées.

ZWILLINGSBILDUNG IN MARTENSIT

Im Hinblick auf die neureen Arbeiten an dünnen Schichten, nach denen wenigstens manche Martensitplättchen eine feinstrukturierte Zwillingsbildung aufweisen, werden die möglichen Arten der Zwillingsbildung in der Martensitstruktur in einzelnen untersucht. Diese lassen sich auf vierzehn verschiedene Scherungsarten reduzieren, die als notwendige Angaben für eine geläufige Theorie der Martensitkristallographie dienen. Es wird gezeigt, daß nur sechs dieser Arten wirklich zur Zwillingsbildung in Martensitplättchen führen, und ein Vergleich der diesbezüglichen Prognosen mit den beobachteten kristallographischen Eigenschaften ergibt, daß wahrscheinlich nur ein Typ von Zwillingsbildung in Martensit wirklich auftritt. Dieser Typ wurde in mehreren Stählen beobachtet. Weitere Entwicklungen der Theorie, die zur Deutung aller beobachteten Einzelheiten notwendig erscheinen, werden ebenfalls diskutiert.

1. INTRODUCTION

The recent examination of thin foils by transmission electron microscopy has indicated that at least some plates of martensite in steels of various compositions are twinned on a fine scale. Thus Kelly and Nutting[1,2] have shown that martensite in high carbon steels and also in an Fe–Ni–C steel is twinned on one of the $\{112\}_\alpha$ planes. Assuming that lattice planes are related by the Bain correspondence[3] it is found that these planes can derive from either $\{110\}_\gamma$ or $\{113\}_\gamma$ austenite planes and it appears that in these steels the martensite is always twinned on a plane which was a $\{110\}_\gamma$ plane in the parent phase. Venables,[4] examining martensite produced by low temperature deformation in an austenitic stainless steel (18 per cent Cr, 8 per cent Ni), has also obtained evidence of twinning on $\{112\}_\alpha$ but on planes which derive from $\{113\}_\gamma$.‡ He reports that the nucleation of the martensite plates appears to be associated with the presence of h.c.p. ε-martensite and thus considers the transformation to take place in two stages. He suggests that the f.c.c. austenite is first transformed into ε-martensite by means of an inhomogeneous shear on a $\{111\}_\gamma$ plane. This structure is then transformed into b.c.c. martensite by means of a shear on a $\{112\}_\alpha$ plane accompanied by small shuffles and dimensional changes. This second shear occurs in different directions in different regions of the crystal resulting in a product twinned on $\{112\}_\alpha$. An examination of the relations between parent planes and directions indicates that this mechanism is in fact equivalent to the Bain strain followed by twinning on a $\{112\}_\alpha$ plane which derives from $\{113\}_\gamma$. If the first shear of the mechanism is taken to be homogeneous, no shuffling is necessary in the second shear, and the resulting process reduces to the well-known Kurdjumov–Sachs double shear mechanism.[5]

The current theories of martensite crystallography, which have been reviewed recently by Bilby and Christian[6,7] are based on the hypothesis that the interface between the two phases (the habit plane)

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† Department of Physics, Battersea College of Advanced Technology, London.

‡ The present paper shows that martensite plates of this type are not expected to occur regularly in practice, and Venables, in a recent private communication (28/9/61), states that the original interpretation of his results was in fact incorrect and that he now has no experimental evidence for this type of substructure. The experimental facts about the nucleation of martensite still stand however.

must be, at least approximately, invariant (i.e. unrotated and undistorted). This implies that in addition to the lattice deformation, which converts the parent structure into the product martensitic structure, a further lattice invariant deformation is also necessary. The various theories make different assumptions about this additional deformation. Wechsler *et al.*, in their earliest treatment of the transformations in steels[8] considered it to be slip or twinning on a $\{112\}_\alpha$ plane which, using the Bain correspondence, derives from a $\{110\}_\gamma$ austenite plane. In more recent work this theory has been generalized[9,10] and some other shear systems considered.[11,12] Bowles and Mackenzie[13–15] who introduce an additional degree of flexibility by allowing a uniform dilatation of the interface, consider the product to be twinned, the two twin components being formed from the parent by equivalent correspondences. This restricts the additional deformation mode considerably and, in the case of steels, limits it to the same twinning mode as that considered by Wechsler *et al.*[8]. The theory of Bullough and Bilby[16] imposes no restrictions on the lattice invariant deformation mode and a trivial addition to the algebra enables the effect of a uniform dilatation of the interface to be examined.[17] This theory has been programmed for an electronic digital computer and numerical results obtained on transformations in steels,[18] uranium, titanium and zirconium.[17,19] In studying the transformations in steels the shear plane and shear direction of the lattice invariant deformation mode were varied extensively and the results have been tabulated and deposited at the library of Sheffield University, England.[20] In the original discussion of these predictions Crocker and Bilby[18] attempt to explain both the large scatter of experimental results for a given steel and also the widely differing results obtained for different steels. The additional deformation was considered to occur either by means of the usual deformation modes of the parent or product structures, or by suitable combinations of such modes. In this way mechanisms by which the observed habit planes and other crystallographic features can be explained were described, but some of these appear unlikely to occur in practice.

As discussed earlier[16] the predictions can be interpreted in terms of twinning of the product phase, each twinning mode corresponding to a certain slip mode of the martensite structure. However, whereas the direction and magnitude of the shear associated with the additional deformation (the dislocation shear) are unrestricted for slip, in the case of twinning they must clearly not exceed the twinning shear (equality of the shears corresponding to the whole plate being twinned) and also the two shears must have the same sign.[21] These conditions have not been rigorously imposed in a previous consideration of twinned martensite resulting in some misleading conclusions.[12]

Following a brief review of the relevant features of the crystallography of mechanical twinning, this paper discusses in detail the possible twinning modes of the martensite structure. The results obtained when these twinning modes are used as initial data for the current theories of martensite crystallography are then presented and assessed, and finally possible generalizations of the theories which appear necessary are discussed.

2. CRYSTALLOGRAPHY OF MECHANICAL TWINNING

Since the publication of the review articles on mechanical twinning by Hall[22] and Cahn[23] several theories have been presented which attempt to predict the operative twinning modes of crystalline materials.[19,24–28] The most recent of these theories[19] is as yet unpublished so the results which are relevant to the subject of this paper will be discussed briefly below.

Mechanical twinning is best described by the four interdependent twinning elements K_1, K_2, η_1, η_2, which together define a twinning mode. These elements are shown in Fig. 1, K_1 being the twinning or composition plane, η_1 the twinning or shear direction which is contained in K_1, K_2 the conjugate or reciprocal twinning plane and η_2 the conjugate twinning direction which is contained in K_2. The plane of shear is defined as the plane containing η_1 and η_2. Two types of twin can arise depending on the rationality of the four twinning elements. In type I twinning K_1 and η_2 are rational* and at least one of the other elements is

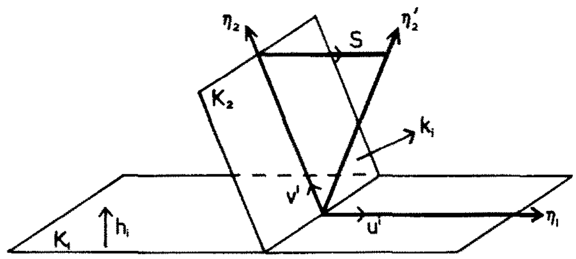

FIG. 1. The twinning elements: K_1—twinning plane, K_2—conjugate twinning plane, η_1—twinning direction, η_2—conjugate twinning direction. The Miller indices of these four elements are represented by h_i, k_i, u^i and v^i, respectively (i = 1, 2, 3). On twinning, the material above K_1 is sheared to the right by an amount determined by the twinning shear s, the η_2 direction becoming the η_2' direction in the twinned crystal.

* A rational direction is defined as one which passes through an infinite number of lattice points and a rational plane contains an infinite number of rational directions. Irrational directions and planes are those which do not satisfy these conditions.

irrational and in type II twinning K_2 and η_1 are rational and at least one of K_1 and η_2 is irrational. Earlier definitions have stated that two of the elements in each type of twin are irrational. However, recent[19,26] work has indicated that modes are possible in some crystal systems which have three rational elements and one irrational element so that the above definitions seem preferable. Degenerate compound twinning modes also arise in which all four elements are rational.

A twinning mode is uniquely defined by its two rational elements. Thus in type I twinning when K_1 and η_2 are known, K_2 and η_1 can always be determined. Letting the Miller indices of the four elements K_1, K_2, η_1, η_2 be h_i, k_i, u^i, v^i, respectively, $(i = 1, 2, 3)$ we have the following equations giving K_2 and η_1 in terms of K_1 and η_2:

$$Ak_i = (c_{lm}v^l v^m)h_i - (h_j v^j)c_{ik}v^k$$
$$Bu^i = (h_j v^j)c^{ik}h_k - (c^{pq}h_p h_q)v^i.$$

Here $c_{ij} = c_{ji} = \mathbf{a}_i \cdot \mathbf{a}_j$ where the triad of vectors $\mathbf{a}_i$ defines the direct lattice basis, $c^{ij} = (c_{ij})^{-1}$ and A and B are arbitrary constants. Indices occurring twice in any expression are to be summed over the values 1, 2, 3 and thus $h_j v^j = h_1 v^1 + h_2 v^2 + h_3 v^3$ and $c_{lm}v^l v^m = c_{11}v^1 v^1 + c_{22}v^2 v^2 + c_{33}v^3 v^3 + 2(c_{12}v^1 v^2 + c_{23}v^2 v^3 + c_{31}v^3 v^1)$ etc. A positive twinning shear in the twinning direction given by the above equation for u^i occurs if the vectors representing K_1 and η_2 both point to the region of crystal which is sheared. Thus in Fig. 1 the material above the twinning plane moves to the right. The magnitude of the twinning shear s can also be determined from K_1 and η_2 and is given by:

$$s^2 = 4\left[\frac{(c_{lm}v^l v^m)(c^{pq}h_p h_q) - (h_j v^j)^2}{(h_j v^j)^2}\right].$$

Equivalent expressions for type II twinning can be obtained by interchanging h_i and k_i, and u^i and v^i in the above equations.

The quantity $q = h_j v^j$, which occurs above, plays an important part in the theory. When h_i and v^i are unit lattice vectors, it gives the number of lattice planes parallel to K_1 which cut the vector η_2. As in general these planes will not all shear to their correct twin sites large values of q are associated with complicated shuffle mechanisms. However modes with very small twinning shears arise if large values of q are allowed and the prediction of twinning modes is thus concerned with the balancing of these two opposing criteria, operative modes being usually associated with small twinning shears and simple shuffle mechanisms[23] (see Fig. 2).

In the observed twinning modes of single lattice metal structures (i.e. metals with atoms situated at the lattice points of a single lattice) the atoms all shear directly to their correct twin sites so that no shuffling is necessary.[22] This occurs only when $q = 1$ or 2 and the modes are readily predicted on substituting these values in the above expression for s and using a minimum shear hypothesis. These modes are all compound and, except in the case of mercury, a further degeneracy arises in that K_1 and η_2 are crystallographically equivalent to K_2 and η_1, and the two possible composition planes are thus indistinguishable. In double lattice structures shuffles are in general necessary and the above degeneracies do not usually occur.

3. TWINNING OF MARTENSITE

Body centred cubic martensite

For cubic materials we have

$$c_{ij} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{pmatrix} \quad \text{and} \quad c^{ij} = \begin{pmatrix} a^{-2} & 0 & 0 \\ 0 & a^{-2} & 0 \\ 0 & 0 & a^{-2} \end{pmatrix}$$

and the expressions of Section 2 therefore become independent of the lattice parameter a. All possible modes are thus compound, the predicted mode in b.c.c. metals being

$$\{112\},\ \{\bar{1}\bar{1}2\},\ \tfrac{1}{2}\langle\bar{1}\bar{1}1\rangle,\ \tfrac{1}{2}\langle 111\rangle;\quad s = 2^{-1/2};\quad q = 2.$$

The twinning elements here and subsequently in this section are given in the order K_1, K_2, η_1, η_2, followed by the twinning shear s, and the value of q as defined in the last section. The signs of the elements are such that η_2 and η_1 make acute angles with the normals to K_1 and K_2, respectively, and on twinning the positive side of the composition plane shears in the positive sense in the twinning direction. The mode gives rise to two crystallographically equivalent composition planes. There are twelve variants of this $\{112\}_\alpha$ twinning plane and, using the Bain correspondence,[3] four of these derive from the $\{110\}_\gamma$ planes and eight from the $\{113\}_\gamma$ planes of the parent f.c.c. austenite. Two types of martensite may thus occur in practice, both twinned on $\{112\}_\alpha$, but exhibiting entirely different macroscopic crystallographic features. The atom movements which occur when twinning is achieved by means of this mode are indicated in Fig. 2(a).

In the above mode $q = 2$ and thus no atomic shuffling is necessary. This is the case for all observed mechanical twinning modes of single lattice structures, but in the formation of martensite it appears that shuffles may occur, particularly if the transformation

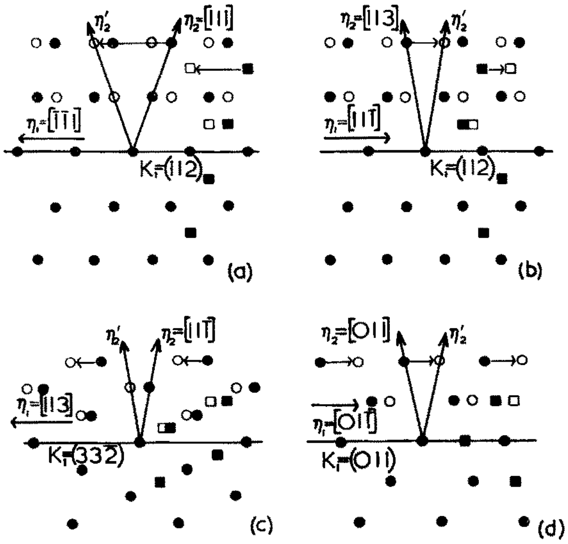

FIG. 2. The possible martensite twinning modes. The twinning elements and planes of shear for the four types of twinning shown are (a) (112) $(\bar{1}\bar{1}2)$ $[\bar{1}\bar{1}1]$ [111]; $(1\bar{1}0)$. (b) (112) $(33\bar{2})$ $[11\bar{1}]$ [113]; $(1\bar{1}0)$. (c) $(33\bar{2})$ (112) [113] $[11\bar{1}]$; $(1\bar{1}0)$. (d) (011) $(01\bar{1})$ $[01\bar{1}]$ [011]; (100). In each case the planes of shear are stacked - - -$ABABAB$- - - and the following notation is used.
Untwinned atom positions ●—plane A, ■—plane B. Twinned atom positions ○—plane A, □—plane B. To avoid overcrowding plane B sites are indicated only at the right of each plot. The plane A atoms are sheared directly to their correct twin sites in all four types of twinning, but in (b) and (c) additional shuffles are seen to be necessary for the plane B atoms. This arises because unit lattice vectors along η_2 in these two cases intersect four lattice planes parallel to $K_1 (q = 4)$, whereas in (a) and (d) $q = 2$. Plots (a), (b) and (c) show cubic martensite but an axial ratio of 5/4 has been used in (d) in order to emphasise the twinning shear of this mode.

occurs in two stages. Thus the mechanism suggested by Venables[4] indicates that the following twinning mode may be responsible for the fine structure of the martensite plates in an 18/8 stainless steel:

$$\{112\},\ \{33\bar{2}\},\ \tfrac{1}{2}\langle 11\bar{1}\rangle,\ \tfrac{1}{2}\langle 113\rangle;\quad s = 8^{-1/2};\quad q = 4.$$

This mode requires that one half of the atoms must shuffle to their correct twin sites, but if the transformation occurs via an intermediate h.c.p. phase, the magnitude of these shuffles may be reduced. The mode again gives a $\{112\}_\alpha$ composition plane, as does the usual b.c.c. mode discussed above, but the direction of the twinning shear is reversed and its magnitude halved. Also the two planes K_1 and K_2 are not crystallographically equivalent, and this mode thus gives rise to several other possible shear modes which may be utilized in the transformation. These are discussed in Section 4. The atom movements which occur during twinning on the $\{112\}_\alpha$ and $\{332\}_\alpha$ composition planes are indicated in Fig. 2 (b) and (c).

Body centred tetragonal martensite

Modes equivalent to those discussed above also occur in the b.c.t. structure. For this structure we have

$$c_{ij} = \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix} \text{ and } c^{ij} = \begin{pmatrix} a^{-2} & 0 & 0 \\ 0 & a^{-2} & 0 \\ 0 & 0 & c^{-2} \end{pmatrix}$$

and the twinning elements are thus not necessarily rational but depend on the lattice parameters a and c. For the cases in which the $\{112\}_\alpha$ composition planes arise from $\{110\}_\gamma$ planes however, the two modes remain compound, the twinning elements being equivalent to those of the corresponding b.c.c. modes. Typical modes are

$$(112),\ (\bar{1}\bar{1}2),\ \tfrac{1}{2}[\bar{1}\bar{1}1],\ \tfrac{1}{2}[111];$$
$$s = \frac{2 - \gamma^2}{\gamma\sqrt{2}};\quad q = 2.$$
$$(112),\ (33\bar{2}),\ \tfrac{1}{2}[11\bar{1}],\ \tfrac{1}{2}[113];$$
$$s = \frac{3\gamma^2 - 2}{2\gamma\sqrt{2}};\quad q = 4.$$

the twinning shear depending on the axial ratio $\gamma = c/a$. The corresponding modes for the other $\{112\}_\alpha$ planes are typified by:

$$(121),\ (\gamma^2 - 2,\ 2\gamma^2,\ 2 - 3\gamma^2),$$
$$\tfrac{1}{4}[-1 - \gamma^2,\ 3\gamma^2 - 1,\ 3 - 5\gamma^2],\ \tfrac{1}{2}[111];$$
$$s = \frac{1}{2\gamma}(2 - 5\gamma^2 + 5\gamma^4)^{1/2};\quad q = 2.$$
$$(121),\ (2 + \gamma^2,\ 2\gamma^2 - 4,\ 10 - 7\gamma^2),$$
$$\tfrac{1}{4}[3\gamma^2 - 1,\ \gamma^2 - 3,\ 7 - 5\gamma^2],\ \tfrac{1}{2}[131];$$
$$s = \frac{1}{4\gamma}(10 - 13\gamma^2 + 5\gamma^4)^{1/2};\quad q = 4,$$

which reduce to the compound b.c.c. modes when $\gamma = 1$. Both the twinning shear and the irrational elements of these modes vary considerably with axial ratio.

The $\{110\}_\alpha$ planes are mirror planes of the b.c.c. structure and can thus not operate as composition planes of mechanical twins. However in tetragonal structures only two of these planes, $(110)_\alpha$ and $(1\bar{1}0)_\alpha$, are mirror planes and twinning is possible on the other four variants, the predicted mode being

$$(011),\ (01\bar{1}),\ [01\bar{1}],\ [011];\quad s = \frac{\gamma^2 - 1}{\gamma};\quad q = 2.$$

This mode is compound, involves no shuffles ($q = 2$), and again contains two crystallographically equivalent composition planes. As expected, the twinning shear s reduces to zero when $\gamma = 1$ corresponding to the cubic case, and for axial ratios not differing greatly

TABLE 1. The b.c.c. shear modes

	Twinning shear	Shear mode in product	Shear mode in parent
1	$\frac{1}{\sqrt{2}}$	$(112)\,[\bar{1}\bar{1}1]$	$(101)\,[\bar{1}01]$
2		$(121)\,[\bar{1}1\bar{1}]$	$(311)\,[01\bar{1}]$
3	$\frac{1}{2\sqrt{2}}$	$(112)\,[11\bar{1}]$	$(101)\,[10\bar{1}]$
4		$(33\bar{2})\,[113]$	$(30\bar{1})\,[103]$
5		$(121)\,[1\bar{1}1]$	$(311)\,[0\bar{1}1]$
6		$(3\bar{2}3)\,[131]$	$(1\bar{5}3)\,[211]$

from unity the shear is small. As twinning modes with small shears are favoured in practice, this mode seems likely to occur in martensite, which has an axial ratio satisfying $1.0 \leqslant \gamma \leqslant 1.1$. The atom movements involved in this type of twinning are shown in Fig. 2(d).

4. RESULTS

Introduction

The b.c.c. twinning modes discussed in Section 3 result in six non-equivalent shear modes and these are listed in Table 1, together with the parent shear modes with which they correspond. Similarly the eight shear modes which may result in the twinning of b.c.t. martensite are given in Table 2. Putting $\gamma = 1$ in Table 2 the modes reduce to variants of those quoted in Table 1; the b.c.c. mode corresponding to mode 14 is not however given as it involves a zero twinning shear. The predictions which resulted when these fourteen shear modes were used as initial data for the Bullough and Bilby theory of martensite crystallography[16–18] are presented in this section. In obtaining these results the parent and product structures were assumed to be related by the Bain correspondence.[3] The lattice parameters used for the b.c.c. modes were such that a volume increase of 2.6 per cent occurs on transformation, and the parameters of the Fe–0.8% C–22% Ni alloy examined by Greninger and Troiano[29] were used in the calculations involving tetragonal modes.

The choice of shear mode is not unrestricted, being limited by the **m**-restriction and the **l**-restriction, which are imposed on the shear plane and shear direction respectively by the principal strains of the lattice deformation associated with the correspondence.[30] Thus in the present investigation no results arise for modes 4 and 11 as they involve a shear direction which violates the **l**-restriction. However, the remaining modes do result in real solutions and these are discussed below.

The dislocation shears

The algebra of the theories is simplified if it is assumed that the additional lattice invariant deformation takes place formally prior to the lattice deformation[16] and the dislocation shears are thus most conveniently given relative to the parent phase. However, in the present application of the theory the additional deformation clearly takes place in the product phase and a direct comparison of the dislocation shear and twinning shear cannot thus be made. The parent shear s' to which the twinning shear s corresponds, if the dislocation shear precedes the lattice deformation, may however be calculated using a relation given elsewhere.[30] The restriction imposed by the twinning shear on the dislocation shear g may then be written $0 \leqslant g \leqslant s'$.

In general two dislocation shears arise for each shear mode[18] and the magnitudes of these shears for modes 7 to 14 are given in Table 2. Only four of the values of g quoted satisfy the restriction discussed above. Thus both shears for mode 7 are positive and smaller than the limiting value, and modes 12 and 13 may also occur, one of the shears being suitable in each case. The values of g are not critically dependent on the

TABLE 2. The b.c.t. shear modes and the resulting dislocation and shape shears

	Twinning shear (s)	Shear mode in product	Shear mode in parent	Dislocation shears (g)		Shape shears (θ)
7	$(2-\gamma^2)/\gamma\sqrt{2}$	$(112)[\bar{1}\bar{1}1]$	$(101)\,[\bar{1}01]$	$+0.234$	$+0.353$	10.3°
8	$\frac{(2-5\gamma^2+5\gamma^4)^{1/2}}{2\gamma}$	$(121)[-1-\gamma^2, 3\gamma^2-1, 3-5\gamma^2]$	$(311)\,[\gamma^2-1, 2\gamma^2, 3-5\gamma^2]$	-0.294	$> +1$	18.6°
9		$(\gamma^2-2, 2\gamma^2, 2-3\gamma^2)\,[111]$	$(3\gamma^2-2, \gamma^2+2, 2-3\gamma^2)\,[101]$	-0.261	$> +1$	17.4°
10	$\frac{(3\gamma^2-2)}{2\gamma\sqrt{2}}$	$(112)\,[11\bar{1}]$	$(101)\,[10\bar{1}]$	-0.234	-0.353	10.3°
11		$(33\bar{2})\,[113]$	$(30\bar{1})\,[103]$	L	L	L
12	$\frac{(10-13\gamma^2+5\gamma^4)^{1/2}}{4\gamma}$	$(121)\,[3\gamma^2-1, \gamma^2-3, 7-5\gamma^2]$	$(311)\,[2\gamma^2-2, -\gamma^2-1, 7-5\gamma^2]$	$+0.243$	-0.63	19.1°
13		$(2+\gamma^2, 2\gamma^2-4, 10-7\gamma^2)\,[131]$	$(3\gamma^2-2, \gamma^2-6, 10-7\gamma^2)\,[211]$	$+0.228$	-0.517	19.2°
14	$(\gamma^2-1)/\gamma$	$(011)\,[01\bar{1}]$	$(111)\,[11\bar{2}]$	-0.257	-0.357	10.3°

L indicates that no solutions arise due to the operation of the **l**-restriction.

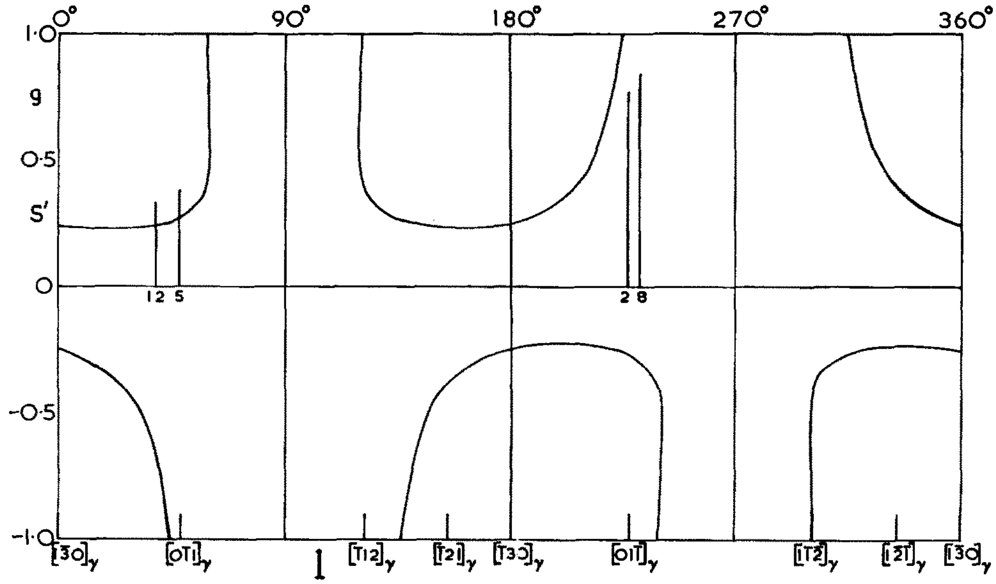

FIG. 3. The two values of the dislocation shear g for shear directions $\mathbf{l}$ lying in the $(311)_\gamma$ shear plane. The angular displacement of $\mathbf{l}$ from $[1\bar{3}0]_\gamma$ is indicated at the top of the figure and specific shear directions are shown at the bottom. The twinning directions of modes 2, 5, 8 and 12 are also indicated, the magnitude of the twinning shear for these modes relative to the parent structure s' (see text) being represented by vertical bars.

axial ratio of the product phase and thus, of the b.c.c. modes of Table 1, only modes 1, 5 and 6—corresponding to modes 7, 12 and 13 of the b.c.t. structure—may result in satisfactory solutions. The striking feature of these results is that modes 2, 8 and 14 are precluded. These modes have been discussed by Otte[12] who claims that they may give rise to twinned martensite products. This author however did not examine the signs of the dislocation shears and quotes incorrect indices for mode 8.

The exclusion of modes 2 and 8 and the acceptable shears for modes 5 and 12 are indicated in Fig. 3. Here the variation of the two possible values of g is shown as the shear direction $\mathbf{l}$ rotates through its full 360° range in the $(311)_\gamma$ shear plane. The values given are for the b.c.t. lattice parameters, the corresponding cubic results differing only slightly from these. A change in sign of $\mathbf{l}$ in the initial data causes a change in sign of g in the results and thus the part of the plot lying between 180° and 360° may be obtained by inverting the first 180° range of values. The two halves of the plot are also themselves symmetrical about the 90° and 270° positions, respectively. No solutions arise for certain ranges of the shear directions used due to the effect of the $\mathbf{l}$-restriction. Also for certain values of $\mathbf{l}$ one of the two shears becomes infinite; this occurs when the predicted habit plane and the shear plane coincide.[18] The parent shears s' for modes 2, 5, 8 and 12, all of which have a $(311)_\gamma$ twinning plane, are indicated by vertical bars at positions corresponding to the twinning directions of these four modes. One of the dislocation shear curves intersects the bars for modes 5 and 12 indicating their suitability but no such intersection occurs for modes 2 and 8.

Mechanisms giving rise to low dislocation shears are thought to be favoured in practice[16] and as shown previously[18] the minimum value of $|g|$ for the tetragonal lattice parameters and correspondence being used in this study is 0.22732. Table 2 indicates that the shears for the tetragonal modes which may give rise to twinned products are only slightly greater than this value, and the corresponding shears for modes 1, 5 and 6 are also very low. As shown in Fig. 3 the minimum value of $|g|$ is attained for certain shear directions lying in $(311)_\gamma$ and the shears for modes 5 and 12 do not greatly exceed this value.

The shape shears

A convenient measure of the total shape deformation which occurs on the formation of a plate of martensite is the angle θ between the normal to the habit plane, as measured in the parent phase, and the direction this becomes after the transformation. The values of this angle which arise for habits associated with the smaller of the two dislocation shears for modes 7 to 14, are given in Table 2, the related values for the modes of Table 1 not differing greatly from these. Modes with small shape shears are again favoured and the minimum possible value for the tetragonal modes of 10.3° is attained by modes 7, 10 and 14. However of these modes only mode 7 can result in twinned martensite, and the shears for the other possible modes (12 and 13) are rather high. However as indicated by Fig. 4, which shows the variation of θ as the shear direction rotates in the $(311)_\gamma$ shear plane, the value for mode 12 lies near the minimum for this system of modes. This figure again shows the restricted range of solutions due to the operation of the l-restriction.

The habit planes

The habit planes of the twinned martensite plates which can arise from the shear modes of Tables 1 and 2 are plotted on the standard austenite stereographic triangle of Fig. 5. As described elsewhere the solutions for mode 7 are degenerate and all four habits are crystallographically equivalent; only one pole 7 thus appears in the figure. This mode, which predicts the $\{3, 10, 15\}_\gamma$ habit observed by Greninger and Troiano[29], has been discussed exhaustively in several theoretical treatments of martensite crystallography, and plates of martensite containing fine twins of this type have been observed recently by Kelly and Nutting[1,2]. Similarly only one pole arises for mode 1, the b.c.c. mode corresponding to mode 7. Two habit planes are possible for each of the other four modes which may result in twinned plates and these are indicated in Fig. 5 by primed and unprimed poles. The poles fall into two groups, one of which is near the observed $\{225\}_\gamma$ pole.

The shear elements of modes 1 and 7 are identical and thus any differences in the predictions of these two modes are due primarily to adjustments of the lattice deformation associated with the different lattice parameters. Fig. 5 indicates that the effect is in fact small, poles 1 and 7 lying very close together.

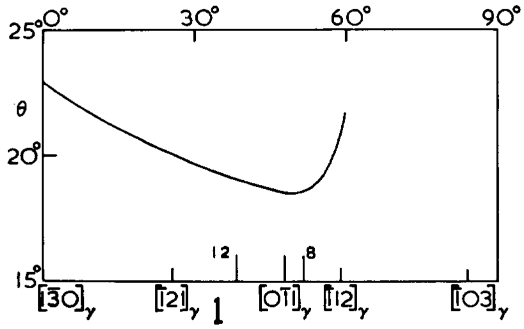

FIG. 4. The variation of the shape shear θ, corresponding to the smaller of the values of g shown in Fig. 3, as the shear direction l varies in the $(311)_\gamma$ shear plane. The angular displacement of l from $[1\bar{3}0]_\gamma$ is indicated at the top of the figure and specific shear directions, including those of modes 8 and 12, are shown at the bottom.

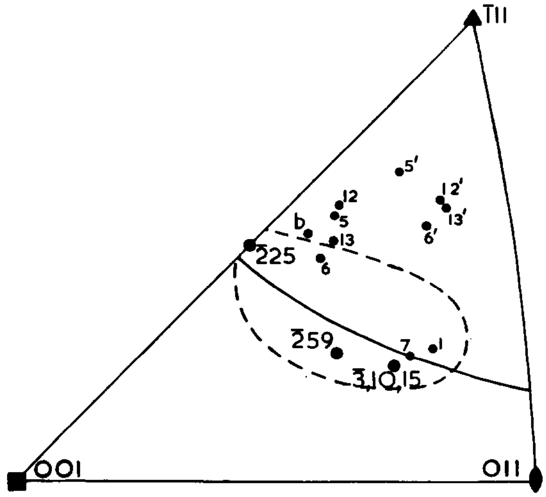

FIG. 5. Standard austenite stereographic triangle showing the possible twinned martensite habit planes. The way in which the pole predicted by mode 7 varies on the introduction of a uniform dilatation into the interface is represented by a full curve, and the region in which the observed habits fall (other than those with an orientation near $\{111\}_\gamma$) by a broken curve.

The shear elements of modes 12 and 13 are not however the same as those of modes 5 and 6, to which they reduce in the cubic structure, as they depend on the axial ratio of the martensite. Differences in the predictions of these modes will thus be due partly to a change in the lattice invariant deformation and partly to a change in the lattice deformation, as above. The combined effect of these changes is not however large as shown by the habit plane poles of Fig. 5

All the observed habit plane poles, other than those lying near $\{111\}_\gamma$, lie within the broken curve of Fig. 5. It is thus clear that the primed poles do not arise from operative mechanisms but the unprimed poles lie near the boundary of the observed scatter region and are worthy of further consideration.

The orientation relationship

The orientation relationship associated with habit 7 has been discussed fully elsewhere[8,15,18,31] and is consistent with that of the observed $\{3, 10, 15\}_\gamma$ habit. The results for pole 1 are again almost identical with those for pole 7. The primed habit plane poles are not consistent with experimental results and the orientation relationships of these planes will not thus be discussed. The other poles lie near $(\bar{2}25)_\gamma$ and it will thus be convenient to compare the orientation relationship predictions for these poles with the Kurdjumov–Sachs relationship[5] which is associated with $\{225\}_\gamma$ habits. This relationship is most conveniently defined by quoting parallelism between lattice planes of the two structures and between directions contained in these planes. Thus for the $(522)_\gamma$ variant of the habit we have $(111)_\gamma \parallel (011)_\alpha$; $[01\bar{1}]_\gamma \parallel [\bar{1}1\bar{1}]_\alpha$ or $(\bar{1}11)_\gamma \parallel (\bar{1}01)_\alpha$; $[01\bar{1}]_\gamma \parallel [\bar{1}1\bar{1}]_\alpha$, the parent lattice direction quoted being contained in the habit plane. This relationship is not predicted for poles 6 and 13, the angle between the relevant $\langle 011 \rangle_\alpha$ and $\langle 111 \rangle_\alpha$ directions being large. However for pole 12 this angle is about $\frac{1}{2}°$ and the angle between the associated planes is about 2°. An orientation relationship consistent with that of Kurdjumov and Sachs also arises for pole 5, the predictions not being critically dependent on either lattice parameters or shear direction.

Discussion

The results presented in this section have shown that only six of the fourteen shear modes examined may give rise to twinned plates of martensite. Of the modes excluded special mention should be made of mode 2, one of the variants of the usual mechanical twinning mode of b.c.c. materials and of modes 8 and 9 to which it corresponds in the b.c.t. structure. These modes have to be rejected because they involve dislocation shears which do not fall within the limits set by the magnitude and sign of the twinning shear. This restriction was not rigorously applied by Otte[12] who discussed modes 2 and 8, and also mode 14, consequently arriving at misleading conclusions. Three of the satisfactory modes are for b.c.t. martensite and these reduce to the three possible b.c.c. modes when the axial ratio is taken to be unity. As shown by several investigators[8,15,18,31] mode 7 predicts satisfactorily all the crystallographic features of a martensite plate observed in an Fe-0.8% C–22% Ni alloy by Greninger and Troiano.[29] Earlier work has shown that permissible changes in lattice parameters do not greatly influence the predictions[8,18] and thus the results for the b.c.c. mode 1 are very similar to those for mode 7, the shear elements of the two modes being identical. The shear direction of mode 12 and the shear plane of mode 13 are not the same as the corresponding elements of modes 5 and 6 as they depend on the axial ratio of the structure. However no great differences again occur between the predictions for these two pairs of modes.

Modes 5, 6, 12 and 13 arise from twinning modes which involve atomic shuffling. Modes of this type have not been observed in single lattice structures but may arise in mechanisms such as that suggested by Venables[4] in which some shuffling is of necessity associated with the additional deformation. One of the two possible habit planes predicted by mode 13 is unsatisfactory (pole 13′) and the orientation relationship of the other habit (pole 13) is not consistent with the observed Kurdjumov–Sachs relationship. The predictions of mode 6, the corresponding b.c.c. mode, are also untenable. Similarly pole 12′, one of the two possible habits predicted by mode 12 is unsatisfactory but the other habit (pole 12), although lying outside the accepted region in which experimental habit plane poles fall, is not far from $\{225\}_\gamma$ and has an orientation relationship not inconsistent with that of Kurdjumov and Sachs. The corresponding habit from mode 5 lies very near pole 12, due to the fact that in this case the effects due to the change of lattice deformation and the change of shear direction associated with the adjustment of the lattice parameters compensate each other. This is indicated by the relative positions of poles 5, 12 and b in Fig. 5, pole b corresponding to a shear on the $(311)_\gamma$ plane in the $[0\bar{1}1]_\gamma$ direction of the tetragonal structure, thus involving the lattice strains of mode 12 and the shear direction of mode 5. It does in fact appear that the results predicted by the (311) $[0\bar{1}1]_\gamma$ shear mode, which is equivalent to (121) $[1\bar{1}1]$ slip of martensite, are in closer agreement with the experimental results than the predictions of either mode 5 or mode 12. Following a detailed examination of a single plate of martensite Otte[32] has recently suggested that this mode is operative in an Fe–2.8% Cr–1.5% C alloy, but as shown previously[18] the habit plane predictions of this mode are not in general agreement with earlier results on this steel.[33]

Venables[34] claims that the habits he observes in thin films of 18/8 stainless steel are within 2° of the predicted pole 5, and have an orientation relationship near that of Kurdjumov and Sachs. However this mode involves shuffles and results in a shape shear of nearly twice that predicted for the $\{3, 10, 15\}_\gamma$ habit and it is thus unlikely to form part of a general mechanism. It should also be noted that Kelly and Nutting[2] have reported that the martensite they observe in this steel consists of untwinned needles and not twinned plates.

The present results have thus shown that the only type of twinned martensite product which is expected to arise regularly in practice is twinned by means of the usual twinning mode of the b.c.c. structure on a $\{112\}_\alpha$ plane which corresponds to a $\{110\}_\gamma$ parent austenite plane. Plates twinned on those $\{112\}_\alpha$ planes which arise from $\{113\}_\gamma$ planes must use a twinning mode involving atomic shuffling and are not thought to be of general occurrence.

5. GENERAL DISCUSSION

The feature of the experimental results on martensite crystallography which is most difficult to explain is the large scatter of the observed habit planes which is indicated by the broken curve of Fig. 5. Two approaches have been made to this problem. Bowles and Mackenzie[15] assume that the additional deformation always takes place by means of shear mode 7 (or mode 1) of the present study but allow a uniform dilatation of the interface. On varying the parameter which fixes the magnitude of this dilatation the pole of the predicted habit plane traces out a curve on the stereogram. This curve, for the case of the Greninger and Troiano alloy[29] discussed above, is shown in Fig. 5. Pole 7 of course lies on the curve, corresponding to an undistorted interface, but in order to predict a habit in the region of $\{225\}_\gamma$ a large uniform dilatation of about 1.5 per cent is necessary. Recent experimental work[1] has shown that some habits near $\{225\}_\gamma$ are twinned by means of mode 7, but this treatment cannot explain the full scatter of results as the lateral displacement of the curve associated with permissible changes in the lattice parameters is small.

The second approach is to assume that the mode of additional deformation varies for different habits. The most extensive study of this kind is by Crocker and Bilby[18] who obtained results[20] for over three hundred different deformation modes of the parent and product structures. They found that some of the observed crystallographic features could be predicted in this way only if it is assumed that the additional mode of deformation is composed of slip on two or more planes in two or more directions. Such modes of deformation result in complications in the motion of the interface and seem unlikely to be the true explanation of the experimental results. The present paper discusses the predictions for the cases in which the additional deformation is twinning of the product martensite. The results show that the large scatter of experimental results cannot be explained in this way and, excepting shear modes 1 and 7, none of the shear modes examined is expected to occur regularly in practice.

Neither of the above approaches thus seems satisfactory in predicting the observed results and as suggested by Bilby and Christian[7] it appears that both the additional shear mode and the uniform dilatation of the interface may have to be varied in order to explain all the observations. Another possibility is that the Bain correspondence is not obeyed in the formation of some of the plates. This correspondence has been used, in some cases indirectly, in all recent work on the martensite transformation in steels on account of the small strains which it involves. If the principal strains associated with a correspondence are represented by $\eta_i - 1$ $(i = 1, 2, 3)$ the correspondence may be classified by means of the quantity $Q = \Sigma \eta_i^2$; the smaller the value of Q, the more likely is the correspondence to occur in practice.[35] For the martensite transformation between β and α uranium many correspondences exist with the values of Q between 3.0 and 3.1[35] and several of these are thought to be operative giving rise to different crystallographic features.[19] In this transformation the correspondences are of necessity associated with atomic shuffling due to the complexity of the two structures. In steels however no such shuffles need occur and if it is assumed that all austenite atoms move directly to their correct martensite sites only the Bain correspondence has $Q \leqslant 3.2$, the second best correspondence having $Q > 4$.[35] This correspondence is of much lower symmetry than the Bain correspondence and thus gives rise to a host of possible shear mode variants, and consequently a large scatter of predicted results However considering the large strains involved and the present state of the experimental work on martensite it seems unwise to embark on a detailed examination of these modes. Smaller values of Q do arise for correspondences in which atomic shuffling occurs, and it is conceivable that these correspondences might be operative if the additional deformation of the transformation involves shuffling, as in some of the modes discussed above.

An explanation of the results may also be obtained by the introduction of a non-uniform strain into the interface. At present none of the general theories enables this hypothesis to be examined, but some earlier treatments of the transformation in steels do embody uniaxial interfacial strains.[36,37] Some progress is at present being made[35,38] towards generalising the theory of Bullough and Bilby to enable these cases to be studied in detail.

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