On the Kinematics of Mechanical Twinning in Crystals

M. PITTERI

Dedicated to Jerry Ericksen on his 60th birthday

Contents

§ 1. Introduction

In nature the existence of well-formed single crystals is more the exception than the rule. Often, crystals show various forms of parallel growth and of intergrowth that crystallographers have known for a long time. One of the most common forms of intergrowth is twinning. Good accounts of crystallographers' description of twinning are contained in the book [9] by FRIEDEL and in the article [3] by DONNAY. Roughly, in a twinned crystalline specimen we can distinguish two different orientations of the crystal lattice. Regions of different orientation are separated by planar interfaces, and the orientations on either side of an interface, say $\mathscr{S}$, are related by a reflection across $\mathscr{S}$ or by a rotation of π about an axis orthogonal to $\mathscr{S}$. These conditions characterize Type 1 twins according to [16, p. 294]. We shall consider Type 2 twins elsewhere.

Another view is that each one of the two regions separated by $\mathscr{S}$ is homogeneously deformed, and the two deformations differ by a simple shear. CAHN [2], HALL [11], KLASSEN-NEKLIUDOVA [17] and KELLY & GROVES [16], among others, describe the geometry of twinning for various crystalline species. Although it is clear to FRIEDEL [9] that a perfect crystal and a twinned crystal should be regarded as different possible equilibrium configurations for a periodic crystalline structure, not much more than the geometry of twinning is described in the aforementioned references. There the main interest lies in describing and justifying the twinning elements, for instance the twinning plane $\mathscr{S}$, the direction of shear and the magnitude of shear. As far as I know, FRIEDEL [9] provides the most

successful condition for twinning. According to this condition, twinning occurs if the crystal lattice itself, or some multiple of it, is left almost invariant by the reflection or rotation associated with $\mathscr{S}$ that we described above. These orthogonal transformations should not belong to the point group of the crystal. Using the technique of coincidence-site lattices introduced in [24], SANTORO [25] has generalized FRIEDEL'S condition as follows: if we denote by C the matrix of scalar products of three linearly independent vectors generating the crystalline lattice, then twinning occurs when

$$mCm^T \approx C. \tag{1.1}$$

Here m is a 3×3 matrix of rationals with determinant ± 1, m^T is the transpose of m, and $\approx$ means "almost equal to".

Twinning occurs during the growth of crystals but, in addition, twinning can be induced by mechanical and thermal means in crystals that are initially homogeneous, as is described in [17]. In many cases an increase of temperature causes a twinned crystal to undergo a martensitic phase transition from solid to solid, with a change of symmetry. After the transition the specimen is homogeneously deformed, but it becomes twinned again if we lower the temperature below the temperature of the transition. Also, in a twinned crystal, the region where one of the two orientations is present can grow at the expense of the other one when we apply a load or an electric field. In many cases this action is reversible: upon release of the load or the field, the orientations recover their initial arrangement. Here, as in the description of the phase transition above, *we recover the relative amount* of one orientation with respect to the other, *but not the locations* where that orientation is present in the specimen. These experimental facts, among others, suggest that we should be able to describe mechanical twinning by means of thermoelasticity.

The fact that many twinned crystals show a martensitic phase transition when we increase the temperature has been used by WASILEWSKI [29] to propose the following kinematic description of mechanical twinning: under the action of the applied stress, at constant temperature, the crystal undergoes a martensitic phase transition to a parent phase which is unstable at that temperature. Part of the specimen, in the reverse transformation from the unstable parent phase to the martensitic phase, changes its orientation. Using a suitable parent phase, WASILEWSKI [29] shows that his geometric mechanism is in agreement with the behavior observed in body-centered cubic lattices and in fair agreement with that reported for hexagonal close-packed lattices. He presents a qualitative reasoning based on energy considerations to justify his way of looking at twinning, and that reasoning is interesting. On the other hand, there is no clear relation in [29] between the aforementioned reasoning and the geometric model proposed.

In most of the papers we have mentioned so far there is little more than pure geometry. Exceptions are the results of VLADIMIRSKIY, presented in [17, p. 146], and of THOMAS & WOOSTER [27], in both of which a linear theory is used. More recently PARRY [19], ERICKSEN [7], GURTIN [10] and JAMES [14] have analyzed various aspects of the phenomenon of twinning within non-linear thermoelasticity. In this paper I propose a kinematic definition of twinning which is strictly connected

with a suitable notion of material symmetry for the constitutive equations of a crystalline solid. This point of view is slightly different than that of JAMES [14], who stresses more than I the fact that twinned equilibrium configurations belong to a certain class of piecewise homogeneous configurations that he classifies fully. On the other hand, I show my definition of twinning to be compatible with James's. Hence, it is feasible to use the kinematics proposed here and James's stability analysis [14] to examine simple equilibrium problems like that considered by PARRY [19]. I leave this task for further study, as well as to analyze Type 2 twins according to [16].

Unlike JAMES [14], who considers a general, unspecified group of material symmetry, in this paper I use a specific group G for simple monatomic crystals, following ERICKSEN [6]. I present an explicit algebraic rule by means of which we construct the element m of G corresponding to a given twinning mode and vice-versa, generalizing conditions presented by ERICKSEN [7]. It turns out that $m^2 = 1$, necessarily. The rule above provides a simple framework for a number of twinning modes known to crystallographers. In § 2 and in the Appendix we examine explicitly the cases of body-centered and of face-centered cubic crystals; of primitive and of body-centered tetragonal crystals; of primitive and of one-face-centered orthorhombic crystals, and one twinning mode of hexagonal close-packed crystals, which is not the most common. For all these modes the normal $\boldsymbol{n}$ to the twinning plane and the amplitude $\boldsymbol{a}$ of the shear are those we expect, as reported in Table I in the Appendix. The rule above, when applied to the most common twinning mode of hexagonal close-packed crystals, provides the right orientations for $\boldsymbol{n}$ and $\boldsymbol{a}$, but the magnitude of $\boldsymbol{a}$ is ten times the observed one. Also, the rule above cannot account for the twinning mode of β-tin. This mode, by the way, is scarcely mentioned except by reporting the values of $\boldsymbol{n}$ and $\boldsymbol{a}$, in the sources I have seen. Among these are [11], [16] and [17]. HALL [11] provides the best description I know of that twinning mode.

The analysis of twinning in § 2 refers to simple monatomic crystals, but most crystals are more complex than this. The definition of twinning in § 2 has an easy and immediate extension to complex crystals, and we present it in § 3. This extension rests on the description of $\nu+1$-lattices and their invariance group Γ, generalizing G, that I introduce in [22]. Also, in [23] I show the relation of certain subgroups of Γ to the classical crystallographic space groups. The aforementioned extension, as introduced, is essentially a mathematical one. Furthermore, we must notice, twinning in complex crystals is more difficult to analyze than twinning in monatomic crystals. On the one hand, it seems that the theory of simple materials does not suffice to describe complex crystals from a continuum point of view, and there is no well established theory of material symmetry for non-simple materials. On the other hand, in many cases the description of twinning in terms of simple shear works only for some atoms of the twinned crystal. To describe the atomic displacements that cause twinning, shuffle displacements are usually added to the shear displacement. As far as I know, there is no rationale of shuffle displacements, even for hexagonal close-packed metals, whose structure is relatively simple. The situation is described by KELLY & GROVES [16]. Some account of twinning modes in complex crystals is provided by JASWON & DOVE [15], whose mechanisms seem to apply to 2-lattices and provide informations on the amount

of shear as a function of the twinning plane. Those mechanisms are nevertheless too rough to account for the details of shuffle displacements.

In § 3 I provide arguments in favor of my mathematical extension to complex crystals of the kinematics of twinning introduced in § 2 for simple monatomic crystals. First of all, the theory for complex crystals states precisely what the shuffle displacements are, for any element μ of Γ such that $\mu^2 = 1$. For 2-lattices, the theory incorporates and corrects the mechanisms proposed by JASWON & DOVE [15]. Secondly, the theory accounts for the main twinning mode of hexagonal close-packed metals and the twinning mode of β-tin, using a lattice cell which is twice as large as as the unit cell. Roughly, we regard the crystal as having a translational invariance group which is a subgroup of index 2 of the group of all translations which map the crystal onto itself, and we introduce additional descriptors of the positions of the atoms inside the enlarged cell. Enlarged cells have been considered by ERICKSEN [8] and KOPTSIK & ÉVARESTOV [18]. Thirdly, in the cases of β-tin and of hexagonal metals the theory accounts not only for the directions of $\boldsymbol{n}$ and $\boldsymbol{a}$ and the amount of shear, which all agree with the data reported in [16] and [17], but also for the shuffle displacements, which agree with those reported in [11], [16] and [17]. These data are presented in Table 2 in the Appendix and in Figures 3 and 4. Fourthly, the theory allows us to analyze pseudotwinning in the same way as twinning. The former is a mode of deformation which differs somewhat from twinning. I present an example of pseudotwinning as a non-trivial modification of two deformation modes presented by BOLLING & RICHMAN [1] and by CAHN [2]. To describe pseudotwinning we only have to enlarge the symmetry of crystals to include colored symmetry. This extended class of symmetry transformations is described, for instance, by SHUBNIKOV & KOPTSIK [26].

Finally, in § 4 we show that SANTORO's generalization (1.1) of FRIEDEL's condition for twinning, if supplemented by the condition $m^2 = 1$, implies that m satisfies the condition for twinning proposed here.

The notation in this paper is essentially that of [21] and [22], although most of the terms are described in the text. By $:=$ $[=:]$ we mean that the equality defines the left-hand [the right-hand] side, and by (C_{ab}) we mean the matrix whose typical element is C_{ab}. We denote by V the vector space of translations associated with 3-dimensional Euclidean space, endowed with the Euclidean scalar product, and by Orth (V) the group of orthogonal transformations of V. Also, GL $(n, \mathbb{R})$ denotes the general linear group over the reals $\mathbb{R}$, in n dimensions, det A denotes the determinant of $A \in \mathrm{GL}(n, \mathbb{R})$, and sgn denotes the sign function. In most of the computations we represent vectors in components, for instance $\boldsymbol{v} = (a, b, c)$, which are always components in rectangular cartesian co-ordinates. Since we desire to compare our results with the crystallographic literature, we use also crystallographic indices for congruences of planes and lines, for instance $\boldsymbol{n} \sim (a\ b\ c)$, following standard practice. Indices are described, for instance, in the International Tables [12]. On the other hand, to follow the bulk of the paper it is not necessary to be familiar with crystallographic indices.

§ 2. Twinning in 1-lattices

Let us consider a crystalline body B whose typical configuration is described by means of a 1-lattice. According to [22], the position P_i of any atom of B can be expressed as follows:

$$P_i = 0 + M_i^a e_a, \quad i = 1, \ldots, \quad a = 1, 2, 3. \tag{2.1}$$

Here, 0 is an origin, e_1, e_2 and e_3 are linearly independent 3-dimensional vectors and the coefficients M_i^a are in the ring $\mathbb{Z}$ of integers. Moreover, unless otherwise stated, we apply the summation convention over repeated indices. The vectors e_a, usually called *lattice vectors*, generate the group of translational automorphisms of B. As is known, the triple of vectors

$$\bar{e}_a = m_a^b e_b \tag{2.2}$$

is a triple of lattice vectors if and only if the matrix $m := (m_a^b)$ is in the group G of unimodular 3×3 matrices with integral entries, that is, GL $(3, \mathbb{Z})$.

We can connect the molecular description of B with the continuum description of the deformation of a solid through the Cauchy-Born hypothesis: if we select a triple of lattice vectors E_a as reference vectors, then each triple of vectors e_a uniquely determines a linear map F such that

$$e_a = FE_a, \tag{2.3}$$

and F shall be interpreted as the deformation gradient of B in the continuum description. If, in particular, we choose the vectors e_a to have the same orientation as the vectors E_a, then F has a positive determinant. Using (2.3) we can translate (2.2) in terms of changes of the reference configuration as follows:

$$\bar{F}E_a := \bar{e}_a = m_a^b e_b = m_a^b F E_b = F m_a^b E_b = FHE_a, \tag{2.4}$$

where

$$HE_a := m_a^b E_b. \tag{2.5}$$

As is discussed in [5], the stored energy density W of B, which depends upon the configuration, reduces to a function $W = \hat{W}(e_a)$ of the lattice vectors e_a or, taking (2.3) into account, to a function $W = \tilde{W}(F)$. Since changing the lattice vectors according to (2.2) does not affect the lattice itself, hence leaves the stored energy density invariant, we have that

$$\hat{W}(e_a) = \hat{W}(m_a^b e_b) \quad \text{or equivalently,} \quad \tilde{W}(F) = \tilde{W}(FH) \tag{2.6}$$

for any $m \in G$ or any H provided by (2.5). Either G or its conjugate group $\mathcal{G}$ of unimodular matrices H given by (2.5) are basic invariance groups for the potential W. In addition, ERICKSEN [5] shows that a molecular calculation based on the assumption of central forces implies that W depends on e_a only through the scalars

$$C_{ab} := e_a \cdot e_b = E_a \cdot F^T F E_b, \tag{2.7}$$

and this is also necessary and sufficient for $\hat{W}(e_a)$ to be frame—indifferent. Notice that this condition is equivalent to requiring W to depend on F only through the right Cauchy-Green tensor $C = F^T F$, whose components in the reference basis E_a are given by $(2.7)_2$. In addition, $C := (C_{ab})$ belongs to the set $\mathscr{C}$ of positive-definite and symmetric elements of GL (3, R).

Each $m \in G$ generates through (2.2) the bijection

$$g_m : \mathscr{C} \to \mathscr{C}, \quad g_m C := m^T C m. \tag{2.8}$$

For any choice of lattice vectors e_a, we shall consider the elements m of G such that

$$m_a^b e_b = Q e_a, \quad \text{hence} \quad g_m C = C, \quad \text{for some} \quad Q \in \text{Orth}\,(V). \tag{2.9}$$

As ERICKSEN [6] shows, any finite subgroup of G is conjugate to one of the crystallographic point groups. In addition, for any $C \in \mathscr{C}$ we uniquely determine a finite subgroup of G each element of which satisfies $(2.9)_2$. As a consequence of well known properties of point groups, the finite cyclic subgroups of G have order 1, 2, 3, 4 or 6.

Let the lattice vectors e_a generate a configuration of the crystal B, and let C be given by (2.7). We are interested in the elements m of G such that

$$m^2 = 1 \quad \text{and} \quad g_m C \neq C, \tag{2.10}$$

and upon these we shall construct below our definition of twinning.

According to standard descriptions of twinning, at least locally and away from boundaries a twinned crystal consists in two regions, say $\mathscr{R}_1$ and $\mathscr{R}_2$, in each of which the deformation is homogeneous. The two regions have in common a part $\mathscr{S}$ of their boundary which is assumed to be plane and is called *the twinning plane*. From the molecular point of view, $\mathscr{R}_1$ and $\mathscr{R}_2$ are related by means of an *orthogonal map Q which does not belong to the point group of either $\mathscr{R}_1$ or $\mathscr{R}_2$*. For Type 1 twins, Q is either the reflection across $\mathscr{S}$ or a rotation of π about an axis orthogonal to $\mathscr{S}$. In either case $Q^2 = \mathbf{1}$. From the continuum point of view, in most cases there is no appreciable slip along the twinning plane when the twins form, and so we can assume that the displacement vector remains continuous across $\mathscr{S}$, whereas the deformation gradient F has a jump. As JAMES [14] remarks, under these hypotheses the surface $\mathscr{S}$ is necessarily plane if it is smooth.

Let E_a be a triple of reference vectors, let $e_a = F_1 E_a$ generate the crystal in $\mathscr{R}_1$, and let F_2 denote the deformation gradient in $\mathscr{R}_2$. Then, from the molecular point of view, there are lattice vectors $\tilde{e}_a$ which generate the crystal in $\mathscr{R}_2$, such that

$$\tilde{e}_a = Q e_a, \quad \text{where } \tilde{e}_a \neq m_a^b e_b \quad \text{for all } m \in G, \tag{2.11}$$

$$Q = D(2\boldsymbol{n} \otimes \boldsymbol{n} - \mathbf{1}), \quad D := \det Q = \pm 1, \tag{2.12}$$

and $\boldsymbol{n}$ is, for definiteness, the unit normal vector to $\mathscr{S}$ pointing into $\mathscr{R}_2$.

From the continuum point of view, the deformation gradient F has a jump discontinuity $[F] := F_2 - F_1$ across $\mathscr{S}$ and, at least for mechanical twinning[1],

[1] For instance, JAMES [14] assumes $\det F$ to be positive throughout his paper.

it is reasonable to assume that

$$\operatorname{sgn}\det \boldsymbol{F}_1 = \operatorname{sgn}\det \boldsymbol{F}_2 . \tag{2.13}$$

If we consider the molecular description of $\mathscr{R}_2$, we see that there are lattice vectors $\bar{\boldsymbol{e}}_a$, which generate the crystal in $\mathscr{R}_2$, such that

$$\bar{\boldsymbol{e}}_a = \boldsymbol{F}_2 \boldsymbol{E}_a , \tag{2.14}$$

and the condition (2.13) asserts that the vectors $\boldsymbol{e}_a$ and $\bar{\boldsymbol{e}}_a$ have the same orientation. Since the displacement is continuous across $\mathscr{S}$, Hadamard's theorem, presented for instance by TRUESDELL [28], implies that

$$\boldsymbol{F}_2 = \boldsymbol{F}_1 + \boldsymbol{a} \otimes \hat{\boldsymbol{N}}, \quad \text{where } \hat{\boldsymbol{N}} := \boldsymbol{F}_1^T \boldsymbol{n} \quad \text{and } \hat{\boldsymbol{N}} \cdot \boldsymbol{E}_a = \boldsymbol{n} \cdot \boldsymbol{e}_a . \tag{2.15}$$

Notice that the direction of $\hat{\boldsymbol{N}}$ is unaffected if we replace $\boldsymbol{F}_1$ in $(2.15)_2$ by $\boldsymbol{F}_2$, and that $\boldsymbol{a}$ is unrestricted so far. Hence the conclusions below, resting on $(2.15)_2$, do not depend on our using $\boldsymbol{F}_1$ instead of $\boldsymbol{F}_2$ in $(2.15)_2$.

Since $\bar{\boldsymbol{e}}_a$ and $\tilde{\boldsymbol{e}}_a$ are both triples of lattice vectors generating the crystal in $\mathscr{R}_2$, there is an $m \in G$ such that

$$\bar{\boldsymbol{e}}_a = m_a^b \tilde{\boldsymbol{e}}_b, \quad \text{where } \det m = D, \tag{2.16}$$

as a consequence of (2.11) to (2.14). From (2.11) and (2.14) to (2.16) we deduce that

$$(\boldsymbol{F}_1 + \boldsymbol{a} \otimes \hat{\boldsymbol{N}})\, \boldsymbol{E}_a = \boldsymbol{S}\boldsymbol{e}_a = m_a^b \boldsymbol{Q}\boldsymbol{e}_b, \quad \text{where } \boldsymbol{S} := \boldsymbol{1} + \boldsymbol{a} \otimes \boldsymbol{n} . \tag{2.17}$$

This relation and $(2.16)_2$ imply that

$$1 = \det \boldsymbol{S} = 1 + \boldsymbol{a} \cdot \boldsymbol{n}, \quad \text{hence } \boldsymbol{a} \cdot \boldsymbol{n} = 0, \tag{2.18}$$

that is, $\boldsymbol{S}$ is a simple shear, $\det \boldsymbol{F}_1 = \det \boldsymbol{F}_2$ and $\boldsymbol{F}_1^T \boldsymbol{n} = \boldsymbol{F}_2^T \boldsymbol{n}$.

A simple shear is introduced in the standard geometric description of twinning modes, as can be seen in [11] or [17], and the shear affects all the atoms in the crystal or, more often, some of them only. In the latter case, we divide the deformation into the shear deformation of a sublattice, this being defined in [8], and the deformation of the remaining atoms, which is not a shear and is usually called a "shuffle deformation". We obtain here a simple shear in any case because we consider the simplest class of crystals, namely 1-lattices, and the simplest class of twinning modes for these crystals. We shall introduce sublattices and shuffle displacements, also for 1-lattices, in § 3 below.

Another consequence of (2.17), besides (2.18), is that

$$(\boldsymbol{QS})^2 = \boldsymbol{1}, \quad \text{hence} \quad m^2 = 1 , \tag{2.19}$$

the implication being easy to prove. To verify that $(2.19)_1$ holds, notice that

$$\boldsymbol{Qa} = -\boldsymbol{Da} \quad \text{and} \quad \boldsymbol{Qn} = \boldsymbol{Dn}; \tag{2.20}$$

hence

$$\boldsymbol{QSQ} = \boldsymbol{1} - \boldsymbol{a} \otimes \boldsymbol{n} = \boldsymbol{S}^{-1}, \tag{2.21}$$

from which $(2.19)_1$ follows immediately. Moreover, if $(2.10)_2$ fails to hold, then S must be orthogonal and hence reduce to the identity. This fact and (2.17) contradict $(2.11)_2$.

We have just shown that if $\mathscr{R}_1$ and $\mathscr{R}_2$ are regions of pairwise homogeneous deformation constituting twins, then (2.17) holds for a suitable m satisfying (2.10). We can express m in terms of Q, S, the vectors e_a and their duals e^a as follows:

$$m_a^b = e^b \cdot QSe_a. \tag{2.22}$$

Moreover, we are going to prove that the converse holds, that is, for any choice of lattice vectors e_a and any $m \in G$ such that (2.10) hold, there are a non-zero vector a and a unit vector n such that (2.17) holds. If Q satisfies $(2.11)_2$, we can work backwards from (2.17) to show the kinematic possibility of a pairwise homogeneous deformation as described above. Our proof that (2.10) implies (2.17) generalizes conditions presented by ERICKSEN [7] in his discussion of twinning. In addition, the proof below is purely algebraic and does not require any assumption on the existence of pairwise or piecewise homogeneous deformations. Although such deformations are kinematically compatible with the definition of twinning we give below, they need not constitute the only possibility, and I prefer to let the equilibrium theory decide if and under what conditions on the loads they can be stable equilibria.

Any $m \in G$ such that $m^2 = 1$ has a 1-dimensional proper space corresponding to the proper number $D = \det m$, and a 2-dimensional proper space corresponding to the proper number $-D$. One way to check this assertion is to recall that, as ERICKSEN [6] shows, there is a choice of $C \in \mathscr{C}$ such that $(2.9)_2$ holds for the given m; hence there is a choice of vectors e_a, satisfying (2.7), such that $(2.9)_1$ holds for some orthogonal Q. Since $Q^2 = \mathbf{1}$, as is easy to see, Q is given by (2.12), and hence its proper numbers and proper spaces can be characterized easily. Moreover, m and Q have the same proper numbers, and proper spaces which are simply related. Indeed

$$Qv = \lambda v \iff m_a^b v^a = \lambda v^b \quad \text{when } v = v^a e_a; \tag{2.23}$$

hence the assertion above about proper numbers and proper spaces of m easily follows.

For any $m \in G$ such that $m^2 = 1$, let $v_1 := (v_1^1, v_1^2, v_1^3)$ be a proper vector of m corresponding to the proper number D and $v_i := (v_i^1, v_i^2, v_i^3)$, $i = 2, 3$, be two linearly independent proper vectors of m corresponding to the proper number $-D$. In addition, for any choice of linearly independent vectors e_a, let e^a denote their dual vectors; let C be given by (2.7), and let

$$v_i := v_i^a e_a \quad \text{for } i = 1, 2 \text{ and } 3. \tag{2.24}$$

Since the elements of m are integers, we can certainly choose v_i^a to be integers. Moreover, we see that the vectors v_i are linearly independent and, denoting by v^i their duals, we define

$$n := v^1 / \| v^1 \|. \tag{2.25}$$

Notice that the equality

$$w^a m_a^b e_b = Lw \tag{2.26}$$

holds for any vector $w = w^a e_a$ when

$$L = D(2v_1 \otimes v^1 - 1). \tag{2.27}$$

Indeed, it is easy to verify that (2.26) holds when w equals any of the v_i's. From (2.26) we deduce that

$$m_a^b e_b = Le_a. \tag{2.28}$$

In addition, letting

$$a = 2(v^1/\|v^1\| - \|v^1\| v_1), \tag{2.29}$$

we can verify that on the one hand $a \cdot n = 0$, on the other hand that

$$L = D(2n \otimes n - a \otimes n - 1) = QS, \tag{2.30}$$

where Q and S are given by (2.12) and $(2.17)_3$, respectively. It is easy to see that Q is orthogonal and that L is so if and only if $a = 0$, which is equivalent to making v_1 orthogonal to v_2 and v_3. If this happens, then m is conjugate to an element of the point group for the crystal generated by e_a and violates $(2.10)_2$. Therefore, for e_a and m satisfying the conditions (2.10) there are a non-zero vector a and a unit vector n such that (2.17) holds.

Notice that all the considerations above, which we decided to phrase in terms of e_a and m, can be rephrased in terms of F and H effortlessly by using the definitions (2.3) and (2.5). For instance, (2.17) and $(2.11)_2$ can be written as follows:

$$SF = QFH \quad \text{and} \quad QF + F\hat{H} \quad \text{for all} \quad \hat{H} \in \mathcal{G}. \tag{2.31}$$

The condition $(2.31)_1$ has been used by JAMES [14] in his definition of twinning, and the condition $(2.31)_2$ will allow us to separate "true twins" from "false twins" according to JAMES [14, p. 150].

For any $m \in G$ such that $m^2 = 1$, and any e_a, let a, n, S and Q be the vectors and tensors associated with m and e_a according to (2.24) to (2.30). Moreover, let C be given by (2.7).

Definition 1. The matrix $m \in G$ is kinematically compatible with a twinning mode of the crystal B in the configuration generated by the lattice vectors e_a if and only if it satisfies (2.10) and the orthogonal matrix Q associated with m and e_a satisfies $(2.11)_2$.

In (2.11) to (2.22) we proved the following result: if B occupies two regions $\mathscr{R}_1$ and $\mathscr{R}_2$ such that $F_1 = F$ and $F_2 = SF$, where S is given by $(2.17)_3$, and such that the relations (2.31) hold, then the matrix m generating H through (2.5) is kinematically compatible with a twinning mode of B in the configuration generated by e_a. To prove the converse, remember that we can write (2.17) for any $m \in G$ satisfying (2.10) and for any e_a, when Q and S are given by (2.24) to (2.30). Therefore, we can consider regions $\mathscr{R}_1$ and $\mathscr{R}_2$ separated by a plane $\mathscr{I}$ whose normal is n, and assign e_a as lattice vectors in $\mathscr{R}_1$ and Se_a as lattice vectors

in $\mathscr{R}_2$. The corresponding deformation gradients have a jump across $\mathscr{S}$ whereas the displacement remains continuous. Equality (2.17) then implies that the vectors $\boldsymbol{Q}\boldsymbol{e}_a$ are also lattice vectors in $\mathscr{R}_2$, but it can well be that

$$\boldsymbol{Q}\boldsymbol{e}_a = \mu_a^b \boldsymbol{e}_b, \quad \text{hence} \quad \boldsymbol{S}\boldsymbol{e}_a = \nu_a^b \boldsymbol{e}_b \tag{2.32}$$

for a suitable choice of μ and for $\nu = \mu m$. In this case we have a "false twin" and, in fact, the pairwise homogeneous configuration in $\mathscr{R}_1$ and $\mathscr{R}_2$ can be better described as a slip along a symmetry plane of B or orthogonal to a twofold symmetry axis of B. The converse also holds: if $\boldsymbol{Q}$ is any element of order 2 in the point group of B when $\boldsymbol{e}_a$ are the lattice vectors, and if $\boldsymbol{S}$ is *any one* of the infinitely many shears of the form $(2.17)_3$ mapping B to itself, then $\boldsymbol{QS}$ satisfies (2.17) and (2.19). In terms of $\boldsymbol{F}$ and $\boldsymbol{H}$, "false twins" are present if and only if $(2.31)_1$ holds but $(2.31)_2$ is violated, that is, if $\boldsymbol{Q}$ *is already an element of the point group of the actual configuration characterized by* $\boldsymbol{F}$ (or $\boldsymbol{e}_a$).

Remark 1. As is clear from Definition 1, we intend to describe twinning in terms of certain elements of the invariance group of the potential W rather than in terms of pairwise homogeneous configurations. On the one hand, we have shown Definition 1 to be consistent with the standard description of pairwise homogeneous configurations which are twin-related. On the other hand, intuitively, if Definition 1 applies to some m and $\boldsymbol{e}_a$, then it will apply to m and any vectors $\boldsymbol{e}_a$ which differ little from $\boldsymbol{e}_a$. Although this can be made precise and proved using [21, Theorem 2], we will not pursue it here. We argue that twinning modes are not affected by small perturbations of lattice vectors. On the contrary, the point group may change considerably in a neighborhood of $\boldsymbol{e}_a$, no matter how small we choose it, unless the $\boldsymbol{e}_a$'s correspond to triclinic symmetry. Again on intuitive grounds, the kinematically possible twinning modes are to a large extent unaffected by the specific choice of $\boldsymbol{e}_a$, the only restricting conditions being $(2.10)_2$ and $(2.11)_2$, which are violated by a finite number of m's. Therefore, energy considerations become more important than pure kinematics to decide which twinning modes will be present when a crystal deforms. This line of thought seems to be consistent with crystallographer's opinion that a twinning mode is difficult to observe if the amplitude $\|\boldsymbol{a}\|$ of the shear $\boldsymbol{S}$ is large, and in § 4 we show that SANTORO's condition (1.1) includes this requirement. The remarks above also shed some light on a statement[2] of FRIEDEL [9, p. 454] which remains otherwise obscure.

The vectors $\boldsymbol{n}$ and $\boldsymbol{a}$ introduced in (2.25) and (2.29) can be expressed in terms of the reference vectors

$$\boldsymbol{N} = \boldsymbol{F}^T\boldsymbol{n}\,\|\boldsymbol{v}^1\| \quad \text{and} \quad \boldsymbol{A} = \boldsymbol{F}^{-1}\boldsymbol{a}(\|\boldsymbol{v}^1\|)^{-1}, \quad \text{when} \quad \boldsymbol{e}_a = \boldsymbol{F}\boldsymbol{E}_a. \tag{2.33}$$

[2] "Il faut en conclure que *les macles ne nous enseignent absolument rien sur la symétrie ou la pseudo-symétrie du réseau, et* a fortiori *sur celles du crystal.* Elles ne sont que le résultat de la rencontre fortuite de mailles multiples suffisamment petites qui présentent une pseudo-symétrie; ou encore, elles ne sont que le résultat de la rencontre accidentelle, dans le réseau, d'un plan réticulaire et d'une rangée suffisamment denses qui se trouvent etre à peu près rectangulaires ...".

Since the vectors $\boldsymbol{v}_i$ in (2.24) are integral combinations of $\boldsymbol{e}_a$, their duals $\boldsymbol{v}^i$ are rational combinations of $\boldsymbol{e}^a$. Indeed, letting $\boldsymbol{v} = (v_i^a)$, we can easily see that

$$\boldsymbol{v}^i = V_a^i \boldsymbol{e}^a, \quad \text{where} \quad V = \boldsymbol{v}^{-T} \quad \text{and} \quad V := (V_a^i). \tag{2.34}$$

In particular, denoting by $\boldsymbol{E}^a$ the duals of $\boldsymbol{E}_a$ and by $C^{-1} = (C^{ab})$ the inverse of C, we have

$$\boldsymbol{N} = V_a^1 \boldsymbol{E}^a; \tag{2.35}$$

hence $\boldsymbol{N}$ does not depend on the choice of $\boldsymbol{e}_a$, or of $\boldsymbol{F}$, and the plane orthogonal to $\boldsymbol{n}$ is a rational plane whose indices are determined by m alone. On the other hand

$$A^b := \boldsymbol{A} \cdot \boldsymbol{E}^b = 2 \frac{V_a^1 C^{ab}}{V_r^1 V_s^1 C^{rs}} - 2v_1^b, \tag{2.36}$$

hence both $\boldsymbol{A}$ and $\boldsymbol{a}$ in general depend upon the choice of $\boldsymbol{e}_a$, or of $\boldsymbol{F}$, besides that of m, and need not have rational indices, although they do so in some important cases. Table 1 in the Appendix lists the elements m, $\boldsymbol{a}$, $\boldsymbol{n}$ and $s := \|\boldsymbol{a}\|$, calculated according to the aforementioned rules, for a number of commonly observed twinning modes. Notice that all the data, including the amount of shear s, agree with those presented by KLASSEN-NEKLIUDOVA [17, Table 1a] and KELLY & GROVES [16, p. 303] with the exception of the most common hexagonal twinning mode, for which our s is much larger than that reported in [16] or [17]. Also, the twinning mode of β-tin is not contained in Table 1 and cannot be easily accounted for on the basis of the theory presented so far. As we shall see in § 3, both the aforementioned twinning modes can be described if we replace the lattice vectors corresponding to the unit cell by lattice vectors corresponding to a larger cell, and apply the theory above, or its extension in § 3, to the larger vectors. Crystals have been described in terms of a cell larger than the fundamental cell by ERICKSEN [8], KOPTSIK & ÉVARESTOV [18] and PARRY [20]. Table 2 in the Appendix lists the elements for the two aforementioned twinning modes, and these elements agree with those listed in [16] and [17].

BOLLING & RICHMAN [1] discuss, among other things, twinning in Fe–Be alloys. The alloys are in general disordered and, if we do not distinguish the atoms of Fe from those of Be, have the structure of a body-centered cubic 1-lattice. Alloys containing 15–30% of Be atoms twin easily. It seems reasonable to presume that, in such disordered Fe–Be alloys, the potential energy density function does not differ much from the one we had if only Fe atoms were present. Hence, the translational invariance of that function is in practice that of a body-centered cubic 1-lattice. If such is the case, then the theory of twinning presented above applies to the alloy, which has the twinning mode reported in Table 1 for body-centered cubic 1-lattices. This mode is precisely the one observed. On the other hand, the shear $\boldsymbol{S}$ will produce a crystal in $\mathscr{R}_2$ which is the mirror image of the crystal in $\mathscr{R}_1$ as far as the positions of atoms are concerned irrespective of the atomic species which occupy them, whereas a number of Fe atoms in $\mathscr{R}_1$ have a mirror image in $\mathscr{R}_2$ which is an atom of Be, and conversely. In § 3 we shall analyze ordered alloys and discuss twinning modes for them in wich the mirror image of an atom can be an atom of a different atomic species.

Let us consider a 1-lattice generated by lattice vectors whose components with respect to a rectangular cartesian co-ordinate system are

$$e_1 = (b, 0, 0), \quad e_2 = (0, c, 0) \quad \text{and} \quad e_3 = (0, u, d), \tag{2.37}$$

where b, c and d are positive constants, and u is a parameter. In particular, we have a tetragonal primitive lattice if $cu = u^2 + d^2$. Using the defining relations (2.25) and (2.29), we see that the lattice has the twinning mode

$$m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & -1 \end{pmatrix}, \quad n = (0, 0, 1), \quad \text{and} \quad a = (0, -2u/c, 0), \tag{2.38}$$

whose shear component leaves e_1 and e_2 unaffected and changes the y-component of e_3 into its negative. If we only consider u as variable, we have that the stored energy density W of the lattice depends on u and is such that $W(u) = W(-u)$. Therefore, if we assume W to have a locally unique proper minimum at $u = u_0$, then we have another minimum at $u = -u_0$ by symmetry. If we assume these minima to be the only ones in the interval of values of u we are interested in, we conclude that the graphs of $W(u)$ and $W'(u)$ have the qualitative features shown in Figure 1. Moreover, remembering (2.3), we see that, in the present one-dimensional

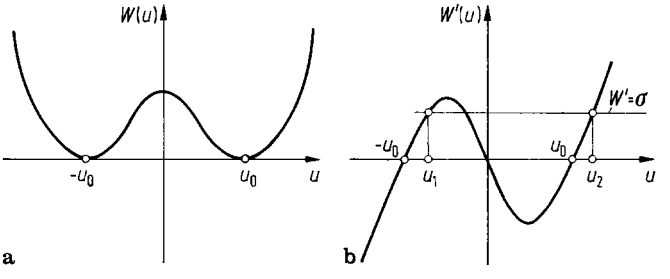

Fig. 1

model, u is the only relevant component of F. Then we can consider a one-dimensional homogeneous bar having $W(u)$ as stored energy per unit reference mass and subjected, for instance, to a dead load. If X and x denote reference and actual co-ordinates along the bar, then $x = \hat{x}(X)$ describes the actual placement and $u(X) = \hat{x}'(X)$. According to the theory of JAMES [13] and his definition of metastability, the metastable equilibrium configuration of the bar under the load σ is homogeneous if the line $W' = \sigma$ intersects the graph of $W'(u)$ in only one point. Otherwise, using the notation of Fig. 1b and letting L be the reference length of the bar, we can describe the metastable configurations by means of

$$\hat{x}'(X) = u_1 \text{ on } S_1 \quad \text{and} \quad \hat{x}'(X) = u_2 \text{ on } S_2, \tag{2.39}$$

for any choice of the measurable sets S_1 and S_2 such that $S_1 \cup S_2 = [0, L]$. Moreover, the absolutely stable configuration is homogeneous and corresponds to u_2 for $\sigma > 0$ and to u_1 for $\sigma < 0$. For $\sigma = 0$ any choice of S_1 and S_2 will produce a neutrally stable equilibrium configuration.

The one-dimensional model just discussed produces one-dimensional equilibrium solutions having some qualitative features one expects to find in single crystals that twin under uniaxial load. On the other hand, we expect the simplifications introduced in the model to be too drastic. In the one-dimensional model, the twinning plane $\mathscr{S}$ reduces to a point and no compatibility conditions across the boundary are necessary, whereas these conditions are required in the 3-dimensional theory, as JAMES [14] shows. Moreover, as ERICKSEN remarked[3], only two different orientations, or phases, come out of the one-dimensional model whereas, for instance, also three different orientations should be possible when we apply a ternary symmetry element of the cubic point group to a tetragonal lattice.

§ 3. Twinning in $\nu + 1$-lattices and additional twinning modes in 1-lattices

As the Appendix shows, the theory presented in § 2 can account only for the directions of $\boldsymbol{n}$ and $\boldsymbol{a}$ in the most common twinning mode of hexagonal close-packed crystals. Those directions have indices $(0\ 1\ -1\ 2)$ and $[0, -1\ 1\ 1]$ respectively, but the amount of shear s is largely different from the amount observed. Also, the twinning mode of β-tin seems not to fit into the theory in § 2. To account for these twinning modes, one must suitably extend the analysis in § 2 to complex lattices. On the one hand, there is no clear indication in the literature on what governs the kinematics of shuffle twins, except that the shear mechanism applies to some of the atoms only. On the other hand it is tempting to adopt a definition of twinning for $\nu + 1$-lattices which mimics Definition 1, and we shall do so. Since Definition 1 is phrased in terms of elements of a certain invariance group, we shall use the group Γ, introduced in [22] as the extension of G to the case of $\nu + 1$-lattices, and regard it as the invariance group of the potential W, which will be a function

$$W = \hat{W}(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_\nu) = \hat{W}(\boldsymbol{\varepsilon}_i) \tag{3.1}$$

of the lattice vectors $\boldsymbol{e}_a$ and of the shifts $\boldsymbol{p}_i$. As is discussed in [22], we can replace the lattice vectors and shifts $\boldsymbol{\varepsilon}_i$ by a new set, say $\bar{\boldsymbol{\varepsilon}}_i$, of lattice vectors and shifts:

$$\bar{\boldsymbol{\varepsilon}}_i = \mu_i^j \boldsymbol{\varepsilon}_j, \tag{3.2}$$

where, for $a, b = 1, 2, 3$ and $i, j = 1, \ldots, \nu$,

$$\mu_a^b = m_a^b, \quad \mu_a^{j+3} = 0, \tag{3.3}$$

$$\mu_{j+3}^a = l_j^a \quad \text{and} \quad \mu_{j+3}^{i+3} = A_j^i. \tag{3.4}$$

Here l_j^a are integers, m is in G and the matrix $\mathfrak{A} := (A_j^i)$ is the product of a permutation matrix and a matrix which either is the identity or has the form

$$A_j^i = \delta_j^i \quad \text{for } j \neq r \quad \text{and} \quad A_r^i = -1 \quad \text{for any } i, j \text{ and for some } r. \tag{3.5}$$

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[3] In a lecture given at the 1982 meeting of the Society for Engineering Science in Rolla, Missouri, U.S.A.

We can rewrite (3.2) explicitly as

$$\bar{e}_a = m_a^b e_b, \quad \bar{p}_i = A_i^j p_j + l_i^a e_a, \tag{3.6}$$

and introduce the symmetric matrix

$$K = (K_{ij}), \quad K_{ij} = \varepsilon_i \cdot \varepsilon_j, \quad i,j = 1, \ldots, \nu + 3, \tag{3.7}$$

which generalizes C in (2.7). If we consider W to depend on K, as it must if W is invariant under the full orthogonal group, then

$$W(K) = W(g_\mu K), \tag{3.8}$$

where

$$(g_\mu K)_{ij} := (\mu^T K \mu)_{ij} = \mu_i^r K_{rs} \mu_j^s \tag{3.9}$$

is the transformation induced on K by (3.2). We shall denote by Γ the subgroup of $\mathrm{GL}(\nu + 3, \mathbb{Z})$ defined by (3.3) to (3.5) and by $\mathcal{K}$ the set of symmetric matrices in $\mathbb{R}^{\nu+3}$ defined by (3.7) when e_a and p_i satisfy the conditions

$$e_1 \cdot e_2 \times e_3 \neq 0, \quad p_i \neq l_i^a e_a \quad \text{and} \quad p_i \neq p_j + l_{ij}^a e_a, \tag{3.10}$$

for $i,j = 1, \ldots, \nu$, $i \neq j$, and for l_i^a and l_{ij}^a in $\mathbb{Z}$. For any choice of ε_i, hence of $K \in \mathcal{K}$,

$$g_\mu K = K \Leftrightarrow \mu_i^j e_j = Q e_i \tag{3.11}$$

for some orthogonal Q, and the relation between crystallographic space groups and lattice groups, which are suitable finite subgroups of Γ, has been considered in [23]. We propose to extend Definition 1 to $\nu + 1$-lattices as follows.

Definition 2. The matrix $\hat{\mu} \in \Gamma$ is kinematically compatible with a twinning mode of the crystal B in the configuration generated by the lattice vectors e_a and the shifts p_i if and only if

$$\hat{\mu}^2 = 1 \quad \text{and} \quad g_{\hat{\mu}} K \neq K \tag{3.12}$$

when K is given by (3.7), and the orthogonal Q associated with the m component of μ does not satisfy $(3.11)_2$ for any $\mu \in \Gamma$.

To promote confidence in this definition, let us consider a twinned $\nu + 1$-lattice locally and away from boundaries. According to experience, the twinned crystal occupies two regions $\mathcal{R}_1$ and $\mathcal{R}_2$ as described in § 2. Moreover, it is still true that the configuration of B in $\mathcal{R}_2$ can be obtained from the configuration in $\mathcal{R}_1$ by means of the orthogonal Q introduced in (2.12); hence the crystal in $\mathcal{R}_2$ is generated by the vectors

$$\tilde{\varepsilon}_i = Q \varepsilon_i. \tag{3.13}$$

If we assume that the configuration in $\mathcal{R}_2$ can be obtained from the one in $\mathcal{R}_1$ by the simple shear S introduced in (2.17), then the configuration in $\mathcal{R}_2$ is generated by the vectors

$$\bar{\varepsilon}_i = S \varepsilon_i. \tag{3.14}$$

We know that this assumption is not reasonable in general because the shuffle deformation cannot be reduced to S, but let us assume (3.14) for the sake of argument. Then, from (3.13) and (3.14) we deduce that

$$S\varepsilon_i = \mu_i^j Q\varepsilon_j \quad \text{for some } \mu \in \Gamma, \tag{3.15}$$

because both the vectors $\bar{\varepsilon}_i$ and $\tilde{\varepsilon}_i$ generate B in $\mathscr{R}_2$. Moreover, $(3.12)_1$ follows from $(2.19)_1$, and $(3.12)_2$ and the negation of $(3.11)_2$ follow if we assume that Q does not transform B into itself.

Let us assume now that $\mu \in \Gamma$ satisfies Definition 2. Since the lattice vectors e_a transform under the m component of μ as in § 2, we can still construct vectors a and n such that (2.17) hold. Let us define

$$\Delta_i := QSp_i - A_i^j p_j - l_i^a e_a \tag{3.16}$$

and notice that the condition $(3.12)_1$ implies that

$$m_a^b l_i^a + l_j^b A_i^j = 0 \quad \text{and} \quad \mathfrak{A}^2 = 1. \tag{3.17}$$

Therefore, using (3.16) twice and (3.17), we conclude that

$$\begin{aligned} QS\Delta_i &= p_i - A_i^j QSp_j - l_i^a QSe_a \\ &= p_i - A_i^j(\Delta_j + A_j^k p_k + l_j^a e_a) - l_i^a m_a^b e_b \\ &= -A_i^j \Delta_j. \end{aligned} \tag{3.18}$$

Using (3.18), we can write (3.16) in the form

$$Sp_i - Q\Delta_i = S(p_i + A_i^j \Delta_j) = A_i^j Qp_j + l_i^a Qe_a, \tag{3.19}$$

which states that a new set of shifts on $\mathscr{R}_2$ differs from Sp_i by the vectors $Q\Delta_i$ or, equivalently, by $A_i^j S\Delta_j$. In this context "shuffling" has a precise meaning, namely, that provided by (3.19). Before we comment on (3.19), let us observe that if $(3.11)_2$ holds for some $\tilde{\mu}$, then (3.19) still holds but the combined effect of S and of the reshufflings $Q\Delta_i$ leaves B invariant across $\mathscr{S}$. In this case we have a transformation which could be better described as a slip along a symmetry plane of B. To avoid this possible deformation we added in Definition 2 the condition that Q should not satisfy $(3.11)_2$ for any $\mu \in \Gamma$. Notice that here, abandoning a requirement in Definition 1, we allow Q to map the lattice generated by e_a onto itself. In this case, however, Q must act on the shifts in a way which is not equivalent to mapping B onto itself. Then the combination of shear and shuffling produces in $\mathscr{R}_2$ a crystal whose lattice is identical with the lattice in $\mathscr{R}_1$ but whose shifts differ essentially from those in $\mathscr{R}_1$. A twinning mode having these properties is usually classified as "twinning without change of form" or also "shuffle twinning". Such is, for instance, the Dauphiné twinning mode in β-quartz, which is described, for instance, in [14] and [27].

The discussion of twinning in β-tin and in hexagonal crystals below provides evidence in favor of our Definition 2. In addition, when only one shift is involved, that is, $\nu = 1$, we see that $\mathfrak{A}$ reduces to a number which is either 1 or -1. Then

(3.18) reduces to

$$QS\boldsymbol{\Delta} = \mp\boldsymbol{\Delta} \quad \text{if } \mathfrak{A} = \pm 1, \text{ respectively.} \tag{3.20}$$

If $\mathfrak{A} = -1$, then $\boldsymbol{\Delta} \cdot \boldsymbol{n} = 0$; if $\mathfrak{A} = 1$, then $\boldsymbol{\Delta} = k(2\boldsymbol{n} - \boldsymbol{a})$ for some constant k, and this is the way we rationalize the X and Y mechanisms proposed by JASWON & DOVE [15]. As is shown in Figure 2, the X mechanism corresponds to $\mathfrak{A} = -1$ and $\boldsymbol{\Delta}$ parallel to the twinning plane, whereas the Y mechanism corresponds to $\mathfrak{A} = 1$ and $\boldsymbol{\Delta}$ having a component orthogonal to the twinning plane. Although the Y mechanism in [15] requires $\boldsymbol{\Delta}$ to be parallel to $\boldsymbol{n}$, I consider my condition acceptable because in most cases $\|\boldsymbol{a}\|$ is much smaller than 1, and so $\boldsymbol{\Delta}$ is practically parallel to $\boldsymbol{n}$. I regard JASWON & DOVE'S as one of the few attempts to give a rationale to shuffle twinning, although the mechanisms they proposed are not powerful enough to justify the details of the suffle displacements in this type of twinning.

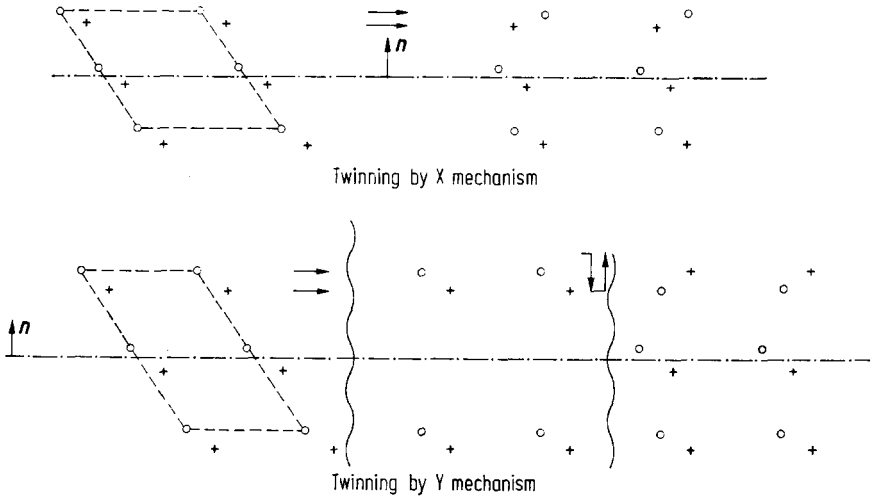

Fig. 2

The description of twinning modes in $\nu + 1$-lattices can be used to deal with certain twinning modes in less complex lattices. These modes should be classified as "twinning by reticular merohedry" according to FRIEDEL [9]. First of all, we can replace the translational invariance group T of a crystal B by a subgroup $\hat{T}$ of T. That is equivalent to considering as lattice vectors for B the vectors

$$\boldsymbol{\eta}_a = \hat{m}_a^b \boldsymbol{e}_b, \quad |\det \hat{m}| = |T : \hat{T}| > 1, \tag{3.21}$$

where $\hat{m}$ is a matrix with integral entries and $|T : \hat{T}|$ denotes the order of the quotient group $T/\hat{T}$. ERICKSEN [8] considers the relation between the original lattice vectors and the vectors $\boldsymbol{\eta}_a$ generating $\hat{T}$, and KOPTSIK & ÉVARESTOV [18] study the relation between the groups of isometries which leave invariant T and $\hat{T}$,

respectively. As I have observed in [23], when we multiply the edges of the elementary cell of a $\nu + 1$-lattice by factors r, s and t, respectively, we must add $(rst - 1)(\nu + 1)$ shifts to the original ones. Also, there are transformations which map the crystal onto itself and are permutable with $\hat{T}$, which are not in the class of those permutable with T. Roughly speaking, such transformations act as affine maps on the lattices $\hat{T}$ or T, respectively, whereas they need not do so on the shifts. Therefore, when we enlarge the primitive cell, we introduce new possible twinning modes in which the relative number of atoms which need not shear increases. As KOPTSIK & ÉVARESTOV [18, p. 5] put it, this increase produces "... expansion of the content of the physical theory on account of the appearance of internal degrees of freedom ...".

Instead of constructing a general theory of twinning which puts together the theory of twinning in $\nu + 1$-lattices presented above and the use of enlarged cells, we shall show in two important cases, namely β-tin and hexagonal close-packed crystals, how the theory presented above works. For the hexagonal crystals, already one twinning mode is described in the Appendix using the simpler theory in § 2. We analyze below the most common mode, providing a complete rationale for the shuffle displacements, and we do so for β-tin also. The procedure below is applicable in general although, of course, it becomes less manageable when the number of shifts grows. Anyway, this is, to my knowledge, the first kinematic, and not only geometric, description of twinning in complex lattices which can account for shuffle displacements. In their description of twinning in hexagonal crystals, KELLY & GROVES [16, p. 300] conclude that "... the twinning shear is not capable of describing the atom movements. In this case there is no obvious, simple way in which the atom movements can be described.", and also "... It will be evident that, physically, twinning in hexagonal metals is not well understood.".

Using Figure 3 as a reference throughout the argument, we see that hexagonal close-packed crystals are 2-lattices generated by the lattice vectors $\boldsymbol{e}_a$ in (A.13) in the Appendix and by the shift

$$\boldsymbol{p}_1 = \left(\frac{d}{2}, \frac{\sqrt{3}d}{6}, \frac{b}{2}\right). \tag{3.22}$$

We introduce the new lattice vectors

$$\boldsymbol{\eta}_1 = \boldsymbol{e}_1, \quad \boldsymbol{\eta}_2 = (0, \sqrt{3}d, 0) = \boldsymbol{e}_1 + 2\boldsymbol{e}_2 \quad \text{and} \quad \boldsymbol{\eta}_3 = \boldsymbol{e}_3, \tag{3.23}$$

and notice that the matrix $\hat{m}$ introduced in (3.21) has determinant 2 in this case. Therefore we introduce the additional shifts

$$\boldsymbol{p}_2 = \tfrac{2}{3}\boldsymbol{\eta}_2 + \tfrac{1}{2}\boldsymbol{\eta}_3 \quad \text{and} \quad \boldsymbol{p}_3 = \tfrac{1}{2}(\boldsymbol{\eta}_1 + \boldsymbol{\eta}_2) \quad (\boldsymbol{p}_1 = \tfrac{1}{2}(\boldsymbol{\eta}_1 + \tfrac{1}{3}\boldsymbol{\eta}_2 + \boldsymbol{\eta}_3)). \tag{3.24}$$

We show in the Appendix that, when m is given by $(A.29)_3$, then

$$\begin{gathered} \boldsymbol{n} = \lambda(\boldsymbol{\eta}^2 + \boldsymbol{\eta}^3), \quad \boldsymbol{a} = 2k\lambda(\boldsymbol{\eta}_3 - \boldsymbol{\eta}_2), \\ \lambda = \frac{\sqrt{3}db}{\sqrt{3d^2 + b^2}} \quad \text{and} \quad k = \frac{3d^2 - b^2}{6d^2b^2}. \end{gathered} \tag{3.25}$$

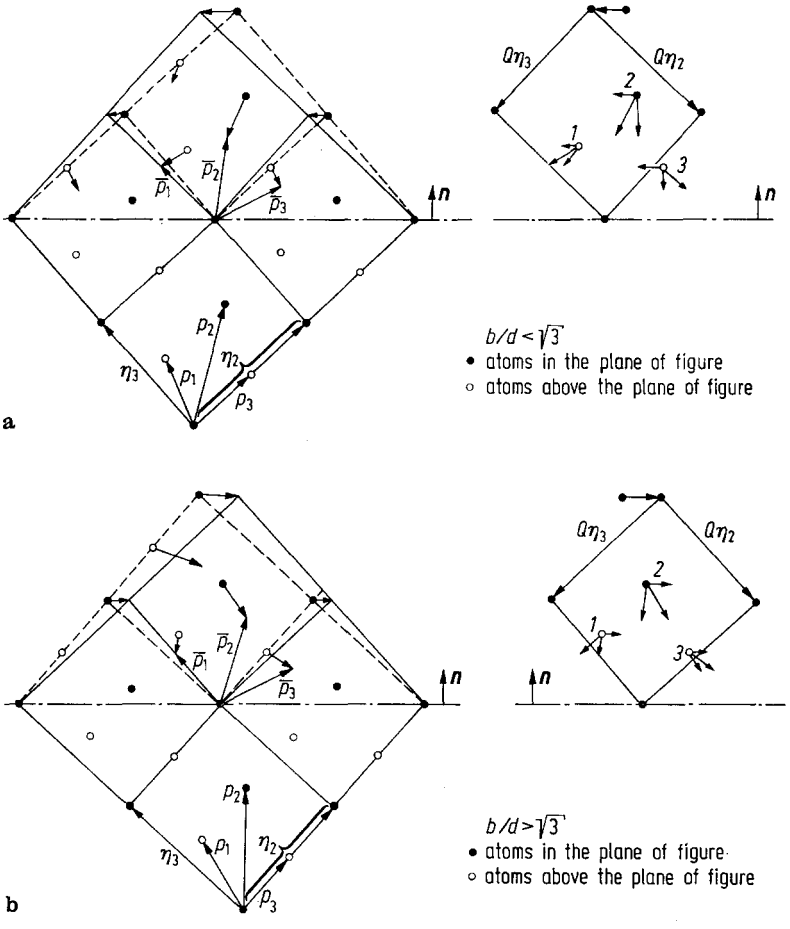

Fig. 3a and b

We comment there on the indices of $\boldsymbol{n}$ and $\boldsymbol{a}$ as well as on the sign of the shear and its magnitude for various hexagonal metals. The numbers obtained there are those we should get.

As we can see in Figure 3, a set of shifts $\bar{\boldsymbol{p}}_i$ in $\mathscr{R}_2$, to be regarded as the left-hand sides of $(3.19)_1$, are given by

(3.26)

$$\bar{\boldsymbol{p}}_1 = Q(\boldsymbol{p}_3 - \boldsymbol{\eta}_2), \quad \bar{\boldsymbol{p}}_2 = Q(\boldsymbol{p}_2 - \boldsymbol{\eta}_2 - \boldsymbol{\eta}_3) \quad \text{and} \quad \bar{\boldsymbol{p}}_3 = Q(\boldsymbol{p}_1 - \boldsymbol{\eta}_3).$$

Therefore, by (3.19)

$$(3.27)\quad \mathfrak{l}_1 = (0,-1,0),\ \mathfrak{l}_2 = (0,-1,-1),\ \mathfrak{l}_3 = (0,0,-1) \text{ and } \mathfrak{A} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

Furthermore, by (3.16)

(3.28) $\Delta_1 = -\frac{1}{6}\eta_3, \quad \Delta_2 = -\frac{1}{6}(\eta_2 + \eta_3)$ and $\Delta_3 = -\frac{1}{6}\eta_2$;

hence

(3.29) $\bar{p}_1 = Sp_1 + \frac{1}{6}Q\eta_3, \quad \bar{p}_2 = Sp_2 + \frac{1}{6}Q(\eta_2 + \eta_3)$ and $\bar{p}_3 = Sp_3 + \frac{1}{6}Q\eta_2$.

This result is in good agreement with the mechanism for atomic displacements presented, for instance, by KELLY & GROVES [16], as can be seen in Figure 3. There we decompose $\bar{p}_i - p_i$ according to (3.29), that is, along the common direction of $(S - 1)\,p_i$, which is that of a, and along the direction of the second summand in $(3.29)_i$. There is good agreement between the shuffle displacements drawn in Figure 3, which look quite different in the two cases $b/d < \sqrt{3}$ and $b/d > \sqrt{3}$, and the theoretic prediction provided by (3.29). Notice that the vectors Δ_i in (3.28) satisfy (3.18), as they ought to.

Using Figure 4 as a reference throughout the argument, we see that β-tin has the structure of a body-centered tetragonal 2-lattice, generated by the lattice vectors e_a in (A.1) in the Appendix, and by the shift

(3.30) $p_1 = (0, \frac{1}{2}d, (x - 1)\,b)$ for a suitable x, $0 < x < 1$.

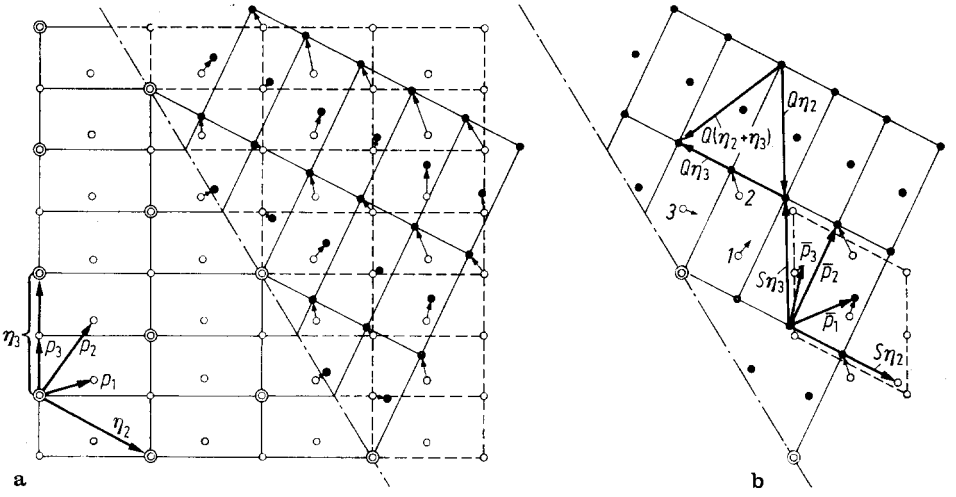

Fig. 4a and b

We introduce the new lattice vectors

(3.31) $$\eta_1 = e_1, \ \eta_2 = (0, d, -b) = e_1 + 2e_2 - 2e_3 \text{ and}$$
$$\eta_3 = (0, 0, 2b) = -2(e_1 + e_2) + 4e_3$$

and notice that the matrix $\hat{m}$ in (3.21) has determinant 2. We introduce the two additional shifts

(3.32) $p_2 = \frac{1}{2}\eta_2 + \frac{1}{2}(x + 1)\,\eta_3$ and $p_3 = \frac{1}{2}\eta_3$ $(p_1 = \frac{1}{2}\eta_2 + \frac{1}{2}x\eta_3)$,

and claim that the twinning mode of β-tin is associated with $\mu \in \Gamma$ such that

$$\mathfrak{l}_1 = \mathfrak{l}_2 = \mathfrak{l}_3 = (0, -1, -1)$$

$$m = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix} \quad \text{and} \quad \mathfrak{M} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{3.33}$$

In the Appendix we assume $(3.34)_{1,2}$ below, and prove $(3.33)_4$ and $(3.34)_{3,4}$ to hold:

$$\boldsymbol{n} = \lambda(\eta^1 + \eta^2 + \eta^3), \quad \boldsymbol{a} = 2k\lambda(\eta_3 - \eta_2),$$
$$\lambda = \frac{2db}{\sqrt{d^2 + 9b^2}}, \quad k = \frac{d^2 - 3b^2}{8d^2b^2} > 0. \tag{3.34}$$

It is not difficult to see that the twinning plane and the twinning direction, which have indices (1, 1, 1) and [0, −1, 1] with respect to the enlarged cell, have indices (0, 1, 3) and [0, −1,3] with respect to the primitive tetragonal cell, as required. Moreover, the shear has the right sign and its magnitude s is 0.113, which differs by 0.6% from the value of 0.119 reported in [17]. This difference seems acceptable. Moreover, from (2.17), (3.16) and (3.33) we deduce that

$$\boldsymbol{\Delta}_1 = \tfrac{1}{2}(1 - x)(\eta_2 + \eta_3), \quad \boldsymbol{\Delta}_2 = \tfrac{1}{2}(1 - x)\,\eta_2 \quad \text{and} \quad \boldsymbol{\Delta}_3 = \tfrac{1}{2}(1 - x)\,\eta_3. \tag{3.35}$$

Hence, a set of shifts $\bar{\boldsymbol{p}}_i$ in the region $\mathscr{R}_2$ is given, according to $(3.19)_1$, by

$$\bar{\boldsymbol{p}}_1 = S\boldsymbol{p}_1 + \tfrac{1}{2}(x - 1)\,Q(\eta_2 + \eta_3), \quad \bar{\boldsymbol{p}}_2 = S\boldsymbol{p}_2 + \tfrac{1}{2}(x - 1)\,Q\eta_2 \quad \text{and}$$
$$\bar{\boldsymbol{p}}_3 = S\boldsymbol{p}_3 + \tfrac{1}{2}(x - 1)\,Q\eta_3. \tag{3.36}$$

This result is in good agreement with the mechanism for atomic displacements proposed by HALL [11], as can be seen in Figure 4. There, we have decomposed $\bar{\boldsymbol{p}}_i - \boldsymbol{p}_i$ according to (3.36), that is, along the directions of $\boldsymbol{a}$ and of the second summand in $(3.36)_i$. Since the magnitude of $\boldsymbol{a}$ is much smaller than that of the second summand in $(3.36)_i$, in practice $\bar{\boldsymbol{p}}_i - \boldsymbol{p}_i$ coincides with the second summmand in $(3.36)_i$, and this is consistent with the description of the shuffle displacements in Figure 4, as can be seen directly on the points marked 1, 2 and 3 in Figure 4(b). Notice that the vectors $\boldsymbol{\Delta}_i$ in (3.35) satisfy (3.18), as they ought to.

In [1] BOLLING & RICHMAN consider an ordered alloy of Fe–Be which is denoted by Fe_3Be. If we do not distinguish atoms of Fe and of Be, the alloy has the structure of a body-centered cubic 1-lattice. The true periodicity of the alloy actually involves a primitive cell which is a multiple of the aforementioned cubic cell. For this alloy BOLLING & RICHMAN report a mode of deformation which is similar to twinning: it would be twinning if we could not distinguish Fe and Be. Since Fe_3Be has the structure of a complex lattice, its twinning modes should be discussed using the theory we presented in this section. On the other hand, the number of shifts involved in the description of this alloy is large, and we prefer to analyze one of the aspects of the aforementioned deformation mode on a hypothetical compound $\mathscr{L}$ having $\nu = 1$ and the following generating elements, referred to a

cartesian co-ordinate system:

$$(3.37)\qquad \boldsymbol{e}_1 = (d, 0, 0), \quad \boldsymbol{e}_2 = \tfrac{1}{2}(d, b, 0), \quad \boldsymbol{e}_3 = (0, 0, c), \quad 2\boldsymbol{p}_1 = \boldsymbol{e}_1.$$

Let us assume the atoms in the base lattice L_0 to be different from those in the lattice L_1 which is displaced by $\boldsymbol{p}_1$ with respect to L_0. Altogether, the 2-lattice we consider is orthorhombic, with one face centered. Consider the element μ of Γ such that

$$(3.38)\qquad m = \begin{pmatrix} -1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathfrak{A} = -1 \quad \text{and} \quad \mathfrak{l}_1 = (0, -1, 0),$$

whose twinning elements $\boldsymbol{a}$ and $\boldsymbol{n}$ are reported in Table 1. We see that

$$(3.39)\qquad \boldsymbol{S}\boldsymbol{e}_1 = Q(2\boldsymbol{e}_2 - \boldsymbol{e}_1), \text{ hence } \boldsymbol{S}\boldsymbol{p}_1 = Q(\boldsymbol{e}_2 - \boldsymbol{p}_1).$$

We conclude that $\boldsymbol{\Delta}_1 = \boldsymbol{0}$ and that the crystal structure in the region $\mathscr{R}_2$ can be obtained from the structure in $\mathscr{R}_1$ by means of $\boldsymbol{S}$ alone, as is shown in Figure 5(a).

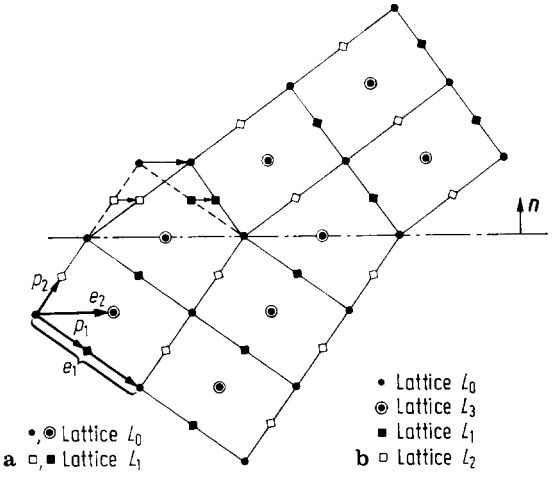

Fig. 5a and b

As an example of how the technique of enlarged cells works, let us regard $\mathscr{L}$ to be generated by the vectors

$$(3.40)\qquad \boldsymbol{\eta}_1 = \boldsymbol{e}_1, \quad \boldsymbol{\eta}_2 = (0, b, 0), \quad \boldsymbol{\eta}_3 = \boldsymbol{e}_3, \quad \boldsymbol{\pi}_1 = \boldsymbol{p}_1, \quad 2\boldsymbol{\pi}_2 = \boldsymbol{\eta}_2, \quad \text{and} \quad \boldsymbol{\pi}_3 = \boldsymbol{e}_2.$$

In this case, as is sketched in Figure 5(b), $\mathscr{L}$ has a primitive orthorhombic lattice whose cell is twice as large as the actual unit cell, and is regarded as a 4-lattice such that L_0 and L_3 [L_1 and L_2] are occupied by identical atoms. The twinning mode of

$\mathscr{L}$ described in (3.37) to (3.39) is now generated by

$$(3.41)\qquad m = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathfrak{A} \quad \text{and} \quad l_i^a = 0, \quad \text{for} \quad a, i = 1, 2 \text{ and } 3.$$

Indeed, using the technique in § 2 as we do in the Appendix, we find that

$$(3.42)\qquad \boldsymbol{n} = \frac{db}{\sqrt{d^2 + b^2}}(\boldsymbol{\eta}^1 - \boldsymbol{\eta}^2), \quad \text{where} \quad \boldsymbol{\eta}^1 - \boldsymbol{\eta}^2 = \left(\frac{1}{d}, \frac{1}{b}, 0\right),$$

and that

$$(3.43)\qquad \boldsymbol{a} = \frac{b^2 - d^2}{db\sqrt{d^2 + b^2}}(\boldsymbol{\eta}_1 + \boldsymbol{\eta}_2) \quad \text{and} \quad s = \frac{|b^2 - d^2|}{db}, \quad \text{where}$$

$$\boldsymbol{\eta}_1 + \boldsymbol{\eta}_2 = (d, b, 0).$$

These vectors $\boldsymbol{n}$ and $\boldsymbol{a}$ coincide with those reported in Table 1 for the twinning mode associated with $(3.37)_{1-3}$ and $(3.38)_1$. In addition, it is easy to deduce from (3.16), (3.40) and (3.41) that

$$(3.44)\qquad \boldsymbol{\Delta}_1 = \boldsymbol{QS\pi}_1 - \boldsymbol{\pi}_2 = \boldsymbol{0}, \quad \boldsymbol{\Delta}_2 = \boldsymbol{QS\pi}_2 - \boldsymbol{\pi}_1 = \boldsymbol{0}, \quad \text{and} \quad \boldsymbol{\Delta}_3 = \boldsymbol{QS\pi}_3 - \boldsymbol{\pi}_3 = \boldsymbol{0}.$$

Therefore, we recover the result that, as above, S and Q are sufficient to describe the twinning mode in Figure 5.

Let us denote by A_i the atomic species occupying the lattice L_i, which is displaced by $\boldsymbol{p}_i$ with respect to L_0 for $i > 0$. We now replace $\mathscr{L}$ by a primitive orthorhombic 4-lattice $\tilde{\mathscr{L}}$, which is generated by the vectors in (3.40) and is such that

$$(3.45)\qquad A_1 \dotplus A_0 = A_3 \dotplus A_2 \quad \text{and} \quad A_1 \dotplus A_2.$$

Notice that $\mathscr{L}$ satisfies $(3.45)_{1-3}$ but not $(3.45)_4$; hence $\boldsymbol{\pi}_3$ in (3.40) is for it a translational automorphism. This is not true for $\tilde{\mathscr{L}}$, and the enlarged cell considered above for $\mathscr{L}$ is a unit cell for $\tilde{\mathscr{L}}$. In the case of $\tilde{\mathscr{L}}$, the product $\boldsymbol{QS}$ transforms $\boldsymbol{\eta}_a$ according to (2.17) and $(3.41)_1$, and the shifts according to (3.19), $(3.41)_{2,3}$ and (3.44), generating a lattice which differs from $\tilde{\mathscr{L}}$ by the interchange of A_1 and A_2. In contrast with what happens in "ordinary twins", in the "pseudotwin" drawn in Figure 5(b) for $\tilde{\mathscr{L}}$ the mirror image of an atom A_1 is an atom A_2, and conversely. Notice that by interchanging A_1 and A_2 in the 4-lattice above, we obtain a 4-lattice which is simply a translate of the original one, a possible translation being, for instance, $\boldsymbol{\pi}_3$. Such combinations of orthogonal maps of a repetitive pattern to itself and of change in some local property of points or of regions in the pattern fall into the category of colored symmetry transformations. These transformations are described, for instance, by SHUBNIKOV & KOPTSIK [26]. Since interchanging

A_1 and A_2 is equivalent to translating the lattice, quantities like the energy density W will remain unaffected by this interchange, which will be an additional invariance transformation for W. It seems then that "pseudotwins" like that of the hypothetical alloy $\tilde{\mathscr{L}}$ in Figure 5(b) are not very different from "ordinary twins", and that a mechanical theory of equilibrium based on the energy criterion for stability should be able to treat both types of twinning similarly. For the first category of twins, the symmetry of W must be extended to include also "colored symmetry". We shall not pursue this task here.

In spite of the apparent similarity, the deformation mode of Fe_3Be, considered by BOLLING & RICHMAN [1], and that of the iron-brass alloy considered by CAHN [2, p. 386], are not "pseudotwins" like that of $\tilde{\mathscr{L}}$ in Figure 5(b), because the shear S produces in $\mathscr{R}_2$ a crystal whose structure is different from the one in $\mathscr{R}_1$. To give an example of this situation, we consider again the 4-lattice in Figure 5, assume the crystal to be generated by the vectors in (3.40) with the additional requirement that $\eta_1 = 2\eta_2$, and replace (3.45) by the following:

$$A_1 = A_0 \quad \text{and} \quad A_2 = A_3 + A_0. \tag{3.46}$$

Then, the crystal is a primitive tetragonal 2-lattice, generated by

$$\tilde{e}_1 := \pi_1, \quad \tilde{e}_2 := \eta_2, \quad \tilde{e}_3 := \tilde{\eta}_3, \quad \text{and} \quad \tilde{p}_1 := \pi_2, \tag{3.47}$$

and the cell associated with (3.40) is twice as large as the unit cell. By inspection of Figure 5(b) we see that the shear S produces in $\mathscr{R}_2$ a crystal which is primitive orthorhombic, hence essentially different from the crystal in $\mathscr{R}_1$. Alternatively, by the argument presented above for $\tilde{\mathscr{L}}$, the action of QS on the vectors in (3.40) is equivalent to interchanging A_1 and A_2, and this produces a crystal which is essentially different from the original one. For this reason CAHN [2] puts the aforementioned deformation mode of the iron-brass alloy in the category of martensitic transformations.

§ 4. Conclusions

We have described the kinematics of twinning in terms of certain elements of the invariance group of the stored energy density W of a crystalline solid. When the solid can be regarded as a 1-lattice from the molecular point of view, we have shown the aforementioned elements to be kinematically compatible with the existence of piecewise homogeneous configurations having the properties commonly imputed to twinned configurations. This description applies to $\nu + 1$-lattices also, for $\nu > 0$, if we restrict our attention to lattice vectors alone. In addition, any $\nu + 1$-lattice can be regarded as a lattice of larger complexity if we replace its unit cell by a cell whose volume is k times larger, for any integer k greater than 1. This is equivalent to choosing a new set of lattice vectors according to (3.21). SANTORO'S [25] generalization of FRIEDEL'S condition for twinning asserts that twinning is possible for a lattice referred to lattice vectors e_a whenever

$$\hat{m}^T C \hat{m} \approx C \tag{4.1}$$

where $\hat{m}_a^b$ are rationals and $\approx$ means approximately equal. I wish to show that, if $\hat{m}^2 = 1$, then all the twinning modes given by (4.1) are included in Definition 1. Indeed, by the reasoning that leads to (2.24), $\hat{m}$ has linearly independent proper vectors v_1, v_2 and v_3, corresponding to the proper numbers D, $-D$ and $-D$, respectively, and the components (v_i^a) of v_i form a matrix V with rational entries. Letting (v_a^i) denote the inverse of V and λ_i the proper number corresponding to v_i^a, we observe that v_a^i are the components of the vectors v^i dual of v_i, and that

$$\hat{m}_a^b = \sum_i v_i^b \lambda_i v_a^i = (V^T \tilde{m} V^{-T})_a^b \quad \text{for} \quad \tilde{m}_i^j = \lambda_i \delta_i^j, \quad \tilde{m} \in G. \tag{4.2}$$

Moreover, we can always choose V to be a matrix of integers, and we find that

$$\hat{m}^T C \hat{m} = V^{-1} \tilde{m}^T \tilde{C} \tilde{m} V^{-T}, \quad \text{where} \quad \tilde{C} = VCV^T \quad \text{and} \quad \tilde{m}^2 = 1. \tag{4.3}$$

Then the vectors

$$\tilde{e}_i = v_i^a e_a, \quad \tilde{C}_{ij} = \tilde{e}_i \cdot \tilde{e}_j, \tag{4.4}$$

are sublattice vectors of the lattice generated by e_a, and so are $\tilde{m}_i^j \tilde{e}_j$. Conversely, for any choice of sublattice vectors (4.4) and of $\tilde{m} \in G$ satisfying $(4.3)_3$, we can construct a unimodular rational matrix $\hat{m}$ such that (4.3) holds. The analysis in § 2, applied to $\tilde{e}_a$ and $\tilde{m}$, implies that

$$(\tilde{m}^T \tilde{C} \tilde{m})_{ab} = \tilde{e}_a \cdot S^T S \tilde{e}_b; \tag{4.5}$$

hence, by (4.3), (4.1) is equivalent to

$$\tilde{m}^T \tilde{C} \tilde{m} \approx \tilde{C}; \quad \text{hence } S^T S \approx 1 \quad \text{or} \quad a \approx 0. \tag{4.6}$$

Therefore we can interpret (4.1) as selecting, among all the twinning modes associated with e_a and all the sublattice vectors given by $(4.4)_1$, those for which the amount of shear is small. This condition, which is not included in Definition 1, seems to be not purely kinematic. I think that the smallness of the shear should characterize, among the kinematically possible twinning modes, those which are energetically favored within an equilibrium theory based on the energy criterion for stability. Such a theory wants. The kinematics we introduced in §§ 2 and 3 is phrased in such a way to be useful in an equilibrium theory, and includes the geometric conditions proposed by FRIEDEL, as we have just seen. Besides, the reasonable extension of Definition 1 that we proposed for complex lattices, namely Definition 2, allows us to rationalize, perhaps for the first time, some of the kinematic features of shuffle displacements in shuffle twins. An additional success of the kinematics proposed above is the description of the twinning elements and of the shuffle displacements in the most common twinning mode of hexagonal close-packed metals and in the twinning of β-tin. The former mode has been described geometrically, for instance in [16], but has not been understood, whereas the latter has received little more than mention, the best account of it being that of HALL [11].

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Appendix

In this appendix I show how some of the data in Tables 1 and 2 are obtained. Let us consider the *body-centered tetragonal* lattice generated by the lattice vectors

$$\text{(A.1)} \qquad e_1 = (d, 0, 0), \quad e_2 = (0, d, 0) \quad \text{and} \quad e_3 = \tfrac{1}{2}(d, d, b),$$

where, as throughout the appendix, the components of vectors are taken with respect to a rectangular cartesian co-ordinate system. Notice that the aforementioned 1-lattice *is face-centered cubic* when $b = \sqrt{2}\, d$.

Let us consider the matrix

$$\text{(A.2)} \qquad m \in G, \quad m = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & -2 & -1 \end{pmatrix}, \quad m^2 = 1,$$

which has proper vectors

$$\text{(A.3)} \qquad v_1 = (1, 0, -2), \quad v_2 = (0, -1, 1) \quad \text{and} \quad v_3 = (1, 0, 0)$$

corresponding to the proper numbers -1, 1 and 1 respectively. The vectors $\boldsymbol{v}_i$ in (2.24) are given by

$$\text{(A.4)} \qquad \boldsymbol{v}_1 = (0, -d, -b), \quad \boldsymbol{v}_2 = \tfrac{1}{2}(d, -d, b) \quad \text{and} \quad \boldsymbol{v}_3 = (d, 0, 0);$$

hence

$$\text{(A.5)} \qquad \boldsymbol{v}^1 = -\tfrac{1}{2}\left(0, \frac{1}{d}, \frac{1}{b}\right), \quad \|\boldsymbol{v}^1\| = \tfrac{1}{2}\frac{\sqrt{d^2 + b^2}}{db} \quad \text{and}$$

$$\boldsymbol{n} = -\frac{db}{\sqrt{d^2 + b^2}}\left(0, \frac{1}{d}, \frac{1}{b}\right).$$

Therefore the congruence of planes orthogonal to $\boldsymbol{n}$ is rational and has crystallographic indices (0 1 1) with respect to the tetragonal primitive cell generated by

$$\text{(A.6)} \qquad \tilde{\boldsymbol{e}}_1 = \boldsymbol{e}_1, \quad \tilde{\boldsymbol{e}}_2 = \boldsymbol{e}_2 \quad \text{and} \quad \tilde{\boldsymbol{e}}_3 = (0, 0, b).$$

Equivalently, $\boldsymbol{n}$ is proportional to $\tilde{\boldsymbol{e}}^2 + \tilde{\boldsymbol{e}}^3$, if we denote by $\tilde{\boldsymbol{e}}^a$ the duals of $\tilde{\boldsymbol{e}}_a$, and this can be also checked directly from (A.1), (A.3) and (A.6), without using

Table 1

Crystal structure	Basis	m	n ($\sim$ indices)	a ($\sim$ indices)	s
B.C.T.	$(d, 0, 0)$ $(0, d, 0)$ $\frac{1}{2}(d, d, b)$	$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & -2 & -1 \end{pmatrix}$	$\frac{db}{\sqrt{d^2 + b^2}}\left(0, \frac{1}{d}, \frac{1}{b}\right)$ $\sim (0\ 1\ 1)$	$\frac{b^2 - d^2}{db\sqrt{d^2 + b^2}}(0, d, -b)$ $\sim [0\ 1\ -1]$	$\frac{\lvert b^2 - d^2 \rvert}{db}$
F.C.C.	Same as B.C.T. for $b = \sqrt{2}\, d$		$\sim (1\ 1\ 1)$	$\sim [1\ 1\ -2]$	$\frac{\sqrt{2}}{2}$
B.C.C.	$(d, 0, 0)$ $(0, d, 0)$ $\frac{1}{2}(d, d, d)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & -1 & -1 \end{pmatrix}$	$\frac{\sqrt{6}}{6}(1, 1, 2)$ $\sim (1\ 1\ 2)$	$-\frac{\sqrt{6}}{6}(1, 1, -1)$ $\sim [-1\ -1\ 1]$	$\frac{\sqrt{2}}{2}$
Orthorhombic (Tetragonal $b = d$) primitive	$(d, 0, 0)$ $(0, b, 0)$ $(0, 0, c)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$	$\frac{bc}{\sqrt{b^2 + c^2}}\left(0, \frac{1}{b}, \frac{1}{c}\right)$ $\sim (0, 1, 1)$	$\frac{c^2 - b^2}{bc\sqrt{b^2 + c^2}}(0, b, -c)$ $\sim [0\ 1\ -1]$	$\frac{\lvert c^2 - b^2 \rvert}{bc}$
Orthorhombic one-face-centered	$(d, 0, 0)$ $\frac{1}{2}(d, b, 0)$ $(0, 0, c)$	$\begin{pmatrix} -1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\frac{db}{\sqrt{d^2 + b^2}}\left(\frac{1}{d}, -\frac{1}{b}, 0\right)$ $\sim (1, -1, 0)$	$\frac{b^2 - d^2}{db\sqrt{d^2 + b^2}}(d, b, 0)$ $\sim [1\ 1\ 0]$	$\frac{\lvert b^2 - d^2 \rvert}{db}$
			(orthorhombic primitive axes)		
H.C.P.	$(d, 0, 0)$ $\frac{1}{2}(-d, \sqrt{3}\, d, 0)$ $(0, 0, b)$	$\begin{pmatrix} 1 & -1 & -1 \\ 0 & -1 & -2 \\ 0 & 0 & 1 \end{pmatrix}$	$\frac{\sqrt{3}\, db}{\sqrt{3\, d^2 + 4b^2}}\left(0, \frac{2}{\sqrt{3}\, d}, \frac{1}{b}\right)$ $\sim (0\ 1\ -1\ 1)$	$-\frac{\sqrt{3}\, d}{b\sqrt{3\, d^2 + 4b^2}}(0, 3d, -2b)$ $\sim [0\ -1\ 1\ 2]$	$\frac{\sqrt{3}\, d}{b}$

Table 2

Crystal structure	Basis	m	n ($\sim$ indices)	a ($\sim$ indices)	s
H.C.P.	$(d, 0, 0)$ $(0, \sqrt{3}\,d, 0)$ $(0, 0, b)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$	$\dfrac{\sqrt{3}\,db}{\sqrt{3\,d^2 + b^2}}\left(0, \dfrac{\sqrt{3}}{3d}, \dfrac{1}{b}\right)$ $\sim (0\ 1\ -1\ 2)$	$\dfrac{3d^2 - b^2}{\sqrt{3}\,db\sqrt{3\,d^2 + b^2}}(0, -\sqrt{3}\,d, b)$ $\sim [0\ -1\ 1\ 1]$	$\dfrac{\lvert 3d^2 - b^2\rvert}{\sqrt{3}\,db}$
β-tin	$\frac{1}{2}(d, d, b)$ $(0, d, -b)$ $(0, 0, 2b)$	$\begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix}$	$\dfrac{2db}{\sqrt{d^2 + 9b^2}}\left(0, \dfrac{3}{2d}, \dfrac{1}{2b}\right)$ $\sim (0, 3, 1)$	$\dfrac{d^2 - 3b^2}{2db\sqrt{d^2 + 9b^2}}(0, -d, 3b)$ $\sim [0, -1, 3]$	$\dfrac{\lvert d^2 - 3b^2\rvert}{2db}$
			(tetragonal primitive axes)		

(A.5)$_3$. From (2.29)

$$\boldsymbol{a} = -2\left(\frac{db}{\sqrt{d^2+b^2}}\left(0, \frac{1}{d}, \frac{1}{b}\right) + \frac{\sqrt{d^2+b^2}}{2db}(0, -d, -b)\right)$$

$$= \frac{b^2-d^2}{db\sqrt{d^2+b^2}}(0, -d, b) = \frac{b^2-d^2}{db\sqrt{d^2+b^2}}(2\boldsymbol{e}_3 - 2\boldsymbol{e}_2 - \boldsymbol{e}_1) \tag{A.7}$$

$$= \frac{b^2-d^2}{db\sqrt{d^2+b^2}}(\tilde{\boldsymbol{e}}_3 - \tilde{\boldsymbol{e}}_2), \quad \text{and} \quad s := \|\boldsymbol{a}\| = \frac{|b^2-d^2|}{db}.$$

If the same calculation is performed on the *primitive tetragonal* 1-lattice generated by the lattice vectors $\tilde{\boldsymbol{e}}_a$ in (A.6) when

$$m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad \text{and hence} \quad \begin{cases} v_1 = (0, 1, 1) \\ v_2 = (0, 1, -1), \\ v_3 = (1, 0, 0) \end{cases} \tag{A.8}$$

then

$$\boldsymbol{v}^1 = \tfrac{1}{2}(\tilde{\boldsymbol{e}}^2 + \tilde{\boldsymbol{e}}^3), \quad \|\boldsymbol{v}^1\| = \frac{\sqrt{d^2+b^2}}{2db}, \quad \boldsymbol{a} = \frac{b^2-d^2}{db\sqrt{d^2+b^2}}(\tilde{\boldsymbol{e}}_2 - \tilde{\boldsymbol{e}}_3). \tag{A.9}$$

Hence $\boldsymbol{a}$ is the negative of the vector in (A.7) and has indices (0 1 −1), and s has the same value as in (A.7)$_5$. If in (A.7)$_5$ we put 1.078 for the ratio b/d for Indium, reported in [17, Table 1a], we obtain for s the value 0.1503, in agreement with [17]. Therefore we obtain the most common twinning mode for both primitive and body-centered tetragonal lattices, and the right amount of shear for Indium. The case of β-tin is discussed below. If in (A.7) we put $b = \sqrt{2}\,d$, which corresponds to a *cubic face-centered* 1-lattice, we obtain $s = \sqrt{2}/2$, which is the amount of shear reported in [17, Table 1a]. It is also easy to see that, in this case, the indices of $\boldsymbol{n}$ and $\boldsymbol{a}$ with respect to the cubic unit cell are

(1 1 1) and [1 1 −2] respectively, (A.10)

as we expect.

A calculation similar to the one above shows that if we choose for a *body-centered cubic* 1-lattice

$$\begin{cases} \boldsymbol{e}_1 = (d, 0, 0) \\ \boldsymbol{e}_2 = (0, d, 0) \\ \boldsymbol{e}_3 = \tfrac{1}{2}(d, d, d) \end{cases} \text{and} \quad m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & -1 & -1 \end{pmatrix}, \quad \text{hence} \quad \begin{cases} v_1 = (0, 0, 1) \\ v_2 = (0, 2, -1), \\ v_3 = (2, 0, -1) \end{cases} \tag{A.11}$$

then

$$\boldsymbol{n} = \frac{d}{\sqrt{6}}(\boldsymbol{e}^1 + \boldsymbol{e}^2 + 2\boldsymbol{e}^3) = \frac{1}{\sqrt{6}}(1, 1, 2),$$

$$\boldsymbol{a} = \frac{2}{\sqrt{6}d}(-\boldsymbol{e}_1 - \boldsymbol{e}_2 + \boldsymbol{e}_3) = -\frac{1}{\sqrt{6}}(1, 1, -1) \quad \text{and} \quad s := \|\boldsymbol{a}\| = \frac{\sqrt{2}}{2}. \tag{A.12}$$

Therefore s and the indices of $\boldsymbol{n}$ and $\boldsymbol{a}$ have the values reported in [17, Table 1a].

The calculation presented above for tetragonal primitive lattices can be used to construct the elements of a common twinning mode in *orthorhombic primitive* crystals. We omit the details and only report in Table 1 the elements involved in the calculations, for both primitive and *one-face-centered orthorhombic* crystals.

Let us consider a hexagonal 1-lattice, generated by the lattice vectors

$$\text{(A.13)} \quad \boldsymbol{e}_1 = (d, 0, 0), \quad \boldsymbol{e}_2 = \left(-\frac{d}{2}, \frac{\sqrt{3}}{2} d, 0\right) \quad \text{and} \quad \boldsymbol{e}_3 = (0, 0, b)$$

whose duals are

$$\text{(A.14)} \quad \boldsymbol{e}^1 = \left(\frac{1}{d}, \frac{1}{\sqrt{3}d}, 0\right), \quad \boldsymbol{e}^2 = \left(0, \frac{2}{\sqrt{3}d}, 0\right) \quad \text{and} \quad \boldsymbol{e}^3 = \left(0, 0, \frac{1}{b}\right).$$

We look for the matrix m to be associated with the most common twinning mode in *hexagonal crystals*, in which, when the four-indices convention is used, $\boldsymbol{n}$ has indices (0 1 −1 2) and $\boldsymbol{a}$ has indices [0 −1 1 1]. Equivalently,

$$\text{(A.15)} \quad \boldsymbol{n} = \lambda(\boldsymbol{e}^2 + 2\boldsymbol{e}^3) \quad \text{and} \quad \boldsymbol{a} = 2k\lambda(\boldsymbol{e}_3 - 2\boldsymbol{e}_2 - \boldsymbol{e}_1),$$

where

$$\text{(A.16)} \quad \lambda = \|\boldsymbol{e}^2 + 2\boldsymbol{e}^3\|^{-1} = \frac{\sqrt{3}\, db}{2\sqrt{3d^2 + b^2}}$$

and k is a parameter to be determined. We look for $m \in G$ such that (2.17) holds, and we deduce from (2.17) and (A.15) that

(A.17)

$$\boldsymbol{Q}\boldsymbol{S}\boldsymbol{e}_1 = \boldsymbol{e}_1, \quad \boldsymbol{Q}\boldsymbol{S}\boldsymbol{e}_2 = \boldsymbol{e}_2 + \lambda(\boldsymbol{a} - 2\boldsymbol{n}) \quad \text{and} \quad \boldsymbol{Q}\boldsymbol{S}\boldsymbol{e}_3 = \boldsymbol{e}_3 + 2\lambda(\boldsymbol{a} - 2\boldsymbol{n}).$$

Since the right-hand sides of the equalities in (A.17) must be integral combinations of $\boldsymbol{e}_a$, we must choose k such that $\lambda(\boldsymbol{a} - 2\boldsymbol{n})$ is such a combination. By (A.13) to (A.16) and the expressions for $\boldsymbol{e}^a$ as linear combinations of $\boldsymbol{e}_a$, which are easy to compute, we conclude that

$$\text{(A.18)} \quad \lambda(\boldsymbol{a} - 2\boldsymbol{n}) = 2\lambda^2\left[-\left(k + \frac{2}{3d^2}\right)\boldsymbol{e}_1 - \left(2k + \frac{4}{3d^2}\right)\boldsymbol{e}_2 + \left(k - \frac{2}{b^2}\right)\boldsymbol{e}_3\right].$$

Therefore, necessarily,

$$\text{(A.19)} \quad k + \frac{2}{3d^2} = \frac{l}{2\lambda^2} \quad \text{for some integer } l,$$

hence

$$2\lambda^2\left(k - \frac{2}{b^2}\right) = l - 1, \quad \lambda(\boldsymbol{a} - 2\boldsymbol{n}) = (l-1)\,\boldsymbol{e}_3 - l(\boldsymbol{e}_1 + 2\boldsymbol{e}_2),$$

$$\text{(A.20)} \quad \text{and} \quad m^T = \begin{pmatrix} 1 & 0 & 0 \\ -l & 1-2l & l-1 \\ -2l & -4l & 2l-1 \end{pmatrix}.$$

On the other hand

$$(A.21)\quad s := \|\boldsymbol{a}\| = 2\,|k|\,\lambda\,\|\boldsymbol{e}_3 - 2\boldsymbol{e}_2 - \boldsymbol{e}_1\| = \frac{2}{\sqrt{3}\,db}\,|l(3d^2 + b^2) - b^2|,$$

and the smallest value of s corresponds to either $l = 0$ or $l = 1$, in which case

$$(A.22)\qquad s = \frac{2\sqrt{3}\,b}{3d} \approx 2 \quad \text{and} \quad s = 2\sqrt{3}\,\frac{d}{b} \approx 2, \quad \text{respectively.}$$

The values in $(A.22)_2$ and $(A.22)_4$ are based on $b/d \approx \sqrt{3}$, according to [17, Table 1 a] for hexagonal close-packed crystals; they differ by an order of magnitude from the amount of shear actually observed for the twinning mode we just examined.

The technique we just used gives satisfactory results for the twinning mode shown, for instance, by Mg and having indices (0 1 −1 1) for $\boldsymbol{n}$ and [0 −1 1 2] for $\boldsymbol{a}$. Equivalently,

$$(A.23)\quad \boldsymbol{n} = \lambda(\boldsymbol{e}^2 + \boldsymbol{e}^3), \quad \boldsymbol{a} = 2k\lambda(2\boldsymbol{e}_3 - 2\boldsymbol{e}_2 - \boldsymbol{e}_1), \quad \lambda = \frac{\sqrt{3}\,db}{\sqrt{3d^2 + 4b^2}}.$$

Skipping the intermediate steps, we have the minimum s for

$$(A.24)\qquad m = \begin{pmatrix} 1 & -1 & -1 \\ 0 & -1 & -2 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad s = \sqrt{3}\,\frac{d}{b},$$

and the value of s for the ratio $\dfrac{b}{d} = 1.624$ of Mg is $s = 1.066$, as reported in [17, Table 1 a].

We wish to apply the technique we used above to find the twinning elements for the hexagonal close-packed metals and β-tin according to the description in § 3. We shall construct m from the required $\boldsymbol{n}$ and $\boldsymbol{a}$ since this procedure can be handled more quickly than the inverse one, that is, to obtain $\boldsymbol{n}$ and $\boldsymbol{a}$ from m.

For hexagonal crystals, the lattice vectors are given by (3.23) and $\boldsymbol{n}$ and $\boldsymbol{a}$ by $(3.25)_{1-3}$, where the dual lattice vectors $\boldsymbol{\eta}^\alpha$ are

$$(A.25)\quad \boldsymbol{\eta}^1 = \left(\frac{1}{d}, 0, 0\right), \quad \boldsymbol{\eta}^2 = \left(0, \frac{1}{\sqrt{3}\,d}, 0\right) \quad \text{and} \quad \boldsymbol{\eta}^3 = \left(0, 1, \frac{1}{b}\right).$$

We have

$$(A.26)\quad \boldsymbol{QS}\eta_1 = \eta_1, \quad \boldsymbol{QS}\eta_2 = \eta_2 + \lambda(\boldsymbol{a} - 2\boldsymbol{n}) \quad \text{and} \quad \boldsymbol{QS}\eta_3 = \eta_3 + \lambda(\boldsymbol{a} - 2\boldsymbol{n}),$$

where

$$(A.27)\qquad \begin{aligned} \boldsymbol{a} - 2\boldsymbol{n} &= 2\lambda[k(\eta_3 - \eta_2) - (\eta^2 + \eta^3)] \\ &= 2\lambda\left[-\eta_2\left(k + \frac{1}{3d^2}\right) + \left(k - \frac{1}{b^2}\right)\eta_3\right]. \end{aligned}$$

For the right-hand sides on (A.26) to be linear combinations of η_a, it is necessary that

$$k = \frac{1}{b^2} + \frac{l}{2\lambda^2}, \quad \text{hence} \quad 2\lambda^2\left(k + \frac{1}{3d^2}\right) = l + 2 \quad \text{and}$$

(A.28)

$$s := \|\boldsymbol{a}\| = \left|2\sqrt{3}\,\frac{d}{b} + l\frac{3d^2 + b^2}{\sqrt{3}\,db}\right|.$$

The minimum of s is attained for $l = -1$. For this choice of l

$$s = \frac{|3d^2 - b^2|}{\sqrt{3}\,db}, \qquad \lambda(\boldsymbol{a} - 2\boldsymbol{n}) = -\eta_2 - \eta_3 \quad \text{and}$$

(A.29)

$$m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix},$$

as asserted before (3.35). We wish to compare the values of s obtained from (A.29) with those reported in [16] and [17], using the values of b/d reported there. We obtain 0.199 for Be, 0.175 for Ti, 0.168 for Zr, 0.129 for Mg, −0.138 for Zn, and −0.170 for Cd. The signs are the opposites of those in [16] because we used the opposite orientation for $\boldsymbol{n}$, but otherwise the data differ at most by two units in the last figure from their counterparts in [16]. The same can be said of the data in [17] with the exception of Ti, the reported value of which is 0.189.

For β-tin, the lattice vectors are given by (3.31), and $\boldsymbol{a}$ and $\boldsymbol{n}$ are given by $(3.34)_{1-3}$, where the dual lattice vectors $\boldsymbol{\eta}^a$ are

$$\text{(A.30)} \quad \boldsymbol{\eta}^1 = \left(\frac{2}{d}, 0, 0\right), \quad \boldsymbol{\eta}^2 = \left(-\frac{1}{d}, \frac{1}{d}, 0\right) \quad \text{and} \quad \boldsymbol{\eta}^3 = \left(-\frac{1}{d}, \frac{1}{2d}, \frac{1}{2b}\right).$$

We conclude that

$$\text{(A.31)} \qquad \boldsymbol{QS}\eta_i = \eta_i + \lambda(\boldsymbol{a} - 2\boldsymbol{n}), \quad i = 1 \text{ to } 3,$$

where

$$\text{(A.32)} \qquad \begin{aligned} \boldsymbol{a} - 2\boldsymbol{n} &= 2\lambda[k(\eta_3 - \eta_2) - (\boldsymbol{\eta}^1 + \boldsymbol{\eta}^2 + \boldsymbol{\eta}^3)] \\ &= 2\lambda\left[-\left(k + \frac{3}{2d^2}\right)\eta_2 + \left(k - \frac{d^2 + 3b^2}{4d^2b^2}\right)\eta_3\right]. \end{aligned}$$

The right-hand sides of the equalities in (A.31) are integral combinations of η_i if and only if

$$k = -\frac{3}{2d^2} + \frac{l}{2\lambda^2}; \quad \text{hence} \quad 2\lambda^2\left(k - \frac{d^2 + 3b^2}{4d^2b^2}\right) = l - 2, \text{ and}$$

(A.33)

$$s := \|\boldsymbol{a}\| = 4db\left|-\frac{3}{2d^2} + \frac{l}{2\lambda^2}\right|.$$

The minimum of s is attained for $l = 1$, for which choice

$$\text{(A.34)}\quad s = \frac{d^2 - 3b^2}{2db},\quad \lambda(\boldsymbol{a} - 2\boldsymbol{n}) = -\boldsymbol{\eta}_2 - \boldsymbol{\eta}_3;\quad \text{hence}\quad m = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix}$$

as asserted in $(3.33)_1$.

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Seminario Matematico
Università di Padova

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