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The Cauchy–Born Hypothesis, Nonlinear Elasticity and Mechanical Twinning in Crystals

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Abstract

The bridge between the molecular descriptions of crystalline configurations and the continuum theories of crystal mechanics such as linear and nonlinear elasticity is given by a natural hypothesis that goes back to Cauchy and Born, referred to as the 'Born rule'. This paper reports on an extensive investigation on the validity of the Born rule and the possibility of applying nonlinear elasticity to describe the behavior of crystalline solids. This is done by studying the phenomenon of mechanical twinning and its implications for the invariance group of the energy density of the crystal. The analysis leads to the conclusion that, in the 'generic' case, the Born rule does not hold and that nonlinear elasticity theory cannot provide an adequate model for crystal mechanics because an unphysical energy invariance is derived. However, the Born rule works and elasticity theory can be used for crystals whose twinning shears satisfy certain quite restrictive 'nongeneric' conditions. Relevant experimental data confirm these theoretical negative conclusions. It is remarkable that two very important classes of 'nongeneric' materials to which an elastic model safely applies do emerge experimentally: shape-memory alloys and materials whose crystalline structure is given by a simple Bravais lattice.

1. Introduction. Motivation and results

Linear elastic theories have been successfully used for a long time for modeling various aspects of the behavior of crystalline solids, and the molecular theories of elasticity provide a way to ascertain the properties of the energy density of crystals considered as continua. In order to do so, a way of relating the macroscopic deformation to the changes in atomic arrangements is needed. Cauchy (1828, 1829) put forward the hypothesis that the atomic motion agrees with the gross deformation; Born (1915), who appreciated that this is not always the case, modified Cauchy's hypothesis and made the physically natural assumption that only the skeletal structure of the crystalline lattice is embedded in the macroscopic deformation, while the microstructural 'motif' is free to adjust so as to reach equilibrium (see also Born & Huang, 1954). This has become the standard assumption in the molecular theories of elasticity, not only linear, and is often referred to as the 'Born rule' [see also Love (1944), Ericksen (1984) and Stakgold (1950) for critical presentations and historical remarks].

In more recent years, there has also been a quite successful effort to adopt nonlinear elasticity theory, based on molecular considerations, for modeling the behavior of crystals in the range of finite deformations, such as those encountered in mechanical twinning or in symmetry-breaking diffusionless phase transitions. The latter typically lead to the formation of coherent microstructures in which the phase variants are mixed in a great variety of configurations and these effects are important for the understanding of the macroscopic behavior of materials, which can make them very interesting also from the point of view of applications. For instance, certain alloys exhibit shape-memory properties as a consequence of the ability of the material to form, in response to the imposed boundary conditions such as given loads or deformations, an array of self-accommodating equilibrium phase mixtures involving periodic twinned microstructures.

The nonlinear elastic model for phase transitions and twinning in crystals originated in the work of Ericksen (1977, 1980, 1984, 1987, 1989); he utilized the Cauchy–Born hypothesis in order to obtain from the molecular theories some new invariance properties for the energy function used in the classical framework for phase transitions by Landau (see, for instance, Landau, 1965). The Cauchy–Born–Ericksen route to elasticity leads to a global energy invariance, which is described by a group conjugate to the infinite discrete group of 3×3 invertible matrices with integral entries. This group has several unusual features: for instance, it contains nonorthogonal transformations, the role of which is of importance for describing mechanical twinning in the context of elasticity theory (Ericksen, 1987). This point of view is, of course, quite different from the traditional one adopted in classical linear and nonlinear theories, according to which the energy invariance is given by the crystallographic point group describing the geometrical symmetry of the crystalline lattice (see Truesdell & Noll, 1965). A reconciliation of the two positions is given by Pitteri (1984, 1985*b*).

Ericksen's approach renders elasticity theory flexible enough to encompass the phenomena above, which lay for long outside its range. This has led in recent times to an increasing bulk of literature especially aimed at the understanding and prediction of microstructure formation during phase transitions; see, for instance, the works by Ball & James (1987, 1992), Bhattacharya (1991, 1992), Bhattacharya & Kohn (1996), Chu & James (1995), Ericksen (1980, 1986, 1987, 1989, 1991, 1993, 1996), Gurtin (1983), James (1981, 1992), James & Kinderlehrer (1989), Kinderlehrer (1988), Luskin (1966), Pitteri (1985*a*, 1986, 1990), Pitteri & Zanzotto (1996*a*,*b*), Simha & Truskinovsky (1996) and Zanzotto (1988, 1992, 1996).

However, Zanzotto (1988) notes that the procedure to obtain an elastic model outlined above often may not be viable because in various cases, especially (but not only) involving twinning deformations in a variety of crystals, the Born rule is *not* in agreement with observations.

Here we briefly report the results of a careful investigation regarding the validity of the rule and the actual extent of applicability of nonlinear elasticity in crystal mechanics (see Zanzotto, 1992). While we refer to the latter work for more details, here we show the essential effects in a general energy setting.

A consequence of the fact that the Born rule does not always hold is that we are left without any *definite* way to connect the molecular and macroscopic continuum pictures. Yet such a definite connection between the two descriptions is clearly necessary for having a useful continuum model capable of theoretical predictions regarding for instance twin or phase boundaries, microstructures *etc*. This suggests that some of the above-mentioned ideas regarding the macroscopic material symmetry of elastic crystals need to be reconsidered. Indeed, without a hypothesis like Born's, it is unclear how to assess from molecular arguments any features of the energy invariance group G and, with the lack of a connection between the atomic positions to the gross deformation of the macroscopic body, it is even difficult to judge *a priori* whether, and how, elasticity theory might be adopted at all for such materials.

The situation is clarified by studying two questions: the first problem is to establish in which cases the Born rule can hold for a crystal, at least in twinning; the second one is to investigate the possibility of a purely macroscopic elastic approach to crystal mechanics in which the theory is developed independently of the Cauchy–Born hypothesis when the rule itself does not hold.

To address these two issues, in this work we tentatively take the point of view of nonlinear elasticity, but on the energy-invariance group G we only make the physically reasonable assumptions that are standard in continuum mechanics, with no hypotheses especially tailored to suit crystalline substances. We then obtain interesting information about G directly from experimental data on twinning. To do so, following the consensus among mineralogists and metallurgists, we regard a mechanical twinning mode as a particular configuration of stable equilibrium for a crystalline body (see, for example, Ericksen, 1987). This is shown to produce a generalized reflection in the group G, which can be calculated on the basis of the standard data available from twin observations. Twinning thus has definite implications regarding the invariance of the energy functions of crystals, and here we indicate some main consequences of this fact.

We notice that this operates a reversal of the perspective adopted in the literature: indeed, we do not obtain the energy-invariance group G from the molecular theories *via* the Cauchy–Born hypothesis and use this to calculate the twinning equilibria, checking thereafter whether the theoretical results match the observed modes. On the contrary, we take direct advantage of the experimental data on twins and gather information about the invariance group G by studying the elements of G that can be computed explicitly from experimentally observed twinning modes. When a number of twins are known for a material, a whole 'twinning (sub)group' of G can be determined and its properties investigated.

The conclusion is that, 'generically', the Born rule does not apply to twinning deformations, in that the twinning subgroups are not consistent with the discrete groups that the rule implies. Indeed, in the generic case, the twinning subgroups exhibit features that are in contrast with most of the common ideas associated with crystalline behavior. For instance, non-isolated energy minimizers, as for transversely isotropic materials, turn out to be rather the rule than the exception. In some cases, the groups turn out to be high-dimensional continuous groups, possibly forcing G to coincide with the whole unimodular group (the group of matrices with determinant ± 1), implying for the material an absurd fluid-like behavior. This makes it quite clear that in these generic cases an elastic approach definitely proves inadequate. An equilibrium theory suitable for crystals in these circumstances has recently been developed by Ericksen (1996).

Although the class of nongeneric twinning groups, generated by the particular twins for which the Born rule does hold (at least in a weaker sense), is theoretically very special, it turns out to have great experimental relevance: a number of remarkable materials in fact exhibit nongeneric behavior. They are essentially of two types: crystals whose structure is described by *one* simple Bravais lattice and shape-memory alloys; for all of them, we were unable to find any evidence of failure of the rule when suitable lattice vectors were chosen and a nonlinear elastic model safely applies.

To conclude, our analysis answers in a rather complete way the questions posed above; it turns out that an elastic model for crystals can be formulated only when the Born rule holds so that its fundamental role in crystal mechanics is clearly made evident. We also give explicit conditions for the validity of the rule, setting in this way some definite boundaries to the range of applicability of elastic theories for crystals.

2. Crystal elasticity

2.1. *Lattice configurations*

A description of the configurations of a crystalline lattice can be given, in general, by means of a 'multilattice', that is, by means of a number of interpenetrating simple Bravais lattices whose points are given by

$$x = \sum_a M^a \mathbf{e}_a + \mathbf{p}_k, \tag{1}$$

with M^a integers, $a = 1, 2, 3$. In (1), $\mathbf{e}_a$ are suitable linearly independent 'lattice vectors' and $\mathbf{p}_k$ are 'shift' vectors, with k ranging from 0 to some integer N (see, for instance, Engel, 1986; Pitteri, 1985*b*). The vectors $\mathbf{p}_k$ can be interpreted as describing the microstructural 'motif' in the crystalline lattice.

2.2. *Lattice energy*

Granted (1), the free-energy density of the lattice per unit volume, φ say, is obtained in molecular theories as a function of the lattice vectors $\mathbf{e}_a$, of the shifts $\mathbf{p}_k$ and of the temperature θ,

$$\varphi = \varphi(\mathbf{e}_a, \mathbf{p}_k, \theta), \tag{2}$$

where all the arguments vary within some appropriate domain. We assume, as usual, that the function in (1) is smooth enough.

2.3. *Born rule*

A macroscopic, phenomenological, theory, such as thermoelasticity theory, is brought into the picture by connecting the molecular description to the continuum one. As discussed in §1, this is done by means of the Born rule, which is utilized, explicitly or implicitly, in all the literature we know.

In order to state the rule, let any reference configuration R be chosen for the crystalline body viewed as a continuum, the position of whose points are described by the variable position vector $\mathbf{x}$. We assume R is a bounded region of the Euclidean 3-space. The macroscopic deformation of R is given by an invertible function $\mathbf{y} = \mathbf{y}(\mathbf{x})$, which, in a system of rectangular Cartesian coordinates, is given by $y_i = y_i(x_r)$ $(i, r = 1, 2, 3)$. This maps the point $\mathbf{x}$ to its new position $\mathbf{y}$ and thus maps R onto another region in space giving the deformed shape of the body. For physical reasons, the deformations are considered to be continuous, piecewise differentiable and orientation preserving. The deformation gradient $\mathbf{F} = D\mathbf{y}$, which is a matrix whose entries are $F_{ir} = \partial y_i / \partial x_r$, is thus assumed to have positive determinant: $\det(F_{ir}) > 0$ (see, for instance, Truesdell & Noll, 1965). Furthermore, we assume that the crystalline lattice in the reference configuration R is generated by 'reference' lattice vectors $\mathbf{E}_a$.

Suppose now that the macroscopic body in the configuration R experiences a homogeneous deformation with gradient $\mathbf{F}$. The Born rule states that the lattice vectors behave as *material vectors*, *i.e.* that they are 'embedded' in the macroscopic deformation. Precisely, according to the Born rule, the vectors $\mathbf{e}_a$, defined by

$$\mathbf{e}_a = \mathbf{F}\mathbf{E}_a, \quad a = 1, 2, 3, \tag{3}$$

are assumed to constitute a set of possible lattice vectors for the crystal in the deformed configuration (Born & Huang, 1954; Ericksen, 1984; Stakgold, 1950). No analogous assumptions are made regarding the evolution of the internal variables $\mathbf{p}_k$. For instance, Born assumed that the microstructural motif would not evolve according to a kinematical rule such as (3) but by solving equations that depend on the material, so as to reach an equilibrium configuration in the deformed crystal. This means that the vectors $\mathbf{p}_k$ may be 'minimized out' of the energy function to obtain the free energy φ of the lattice as a (possibly multivalued) function of the sole lattice vectors $\mathbf{e}_a$ (see, for instance, Ericksen, 1980, 1982). We will not need to do so here and indeed can avoid making any specific hypothesis on the behavior of $\mathbf{p}_k$.

2.4. *Continuum energy*

By using the Born rule, one obtains from the molecular constitutive function in (2) a constitutive function $\tilde{\varphi}$ for the free-energy density of the crystal viewed as a macroscopic continuum; this is done by means of the definition

$$\tilde{\varphi}(\mathbf{F}, \mathbf{p}_k, \theta) = \varphi(\mathbf{F}\mathbf{E}_a, \mathbf{p}_k, \theta) = \varphi(\mathbf{e}_a, \mathbf{p}_k, \theta), \tag{4}$$

where the reference lattice vectors $\mathbf{E}_a$ are held fixed. Except for the presence of the 'internal variables' $\mathbf{p}_k$, the constitutive function in (4) gives an energy that depends on the macroscopic deformation gradient, suitable for a nonlinear elastic model. As usual, it is then possible to introduce the free-energy functional of the unloaded body:

$$\Phi[\mathbf{y}] = \int_R \tilde{\varphi}\big(D\mathbf{y}(\mathbf{x})\big)\,d\mathbf{x}, \tag{5}$$

where the internal variables and the temperature are omitted for brevity. The minimizers of (5) at a given temperature are the stable stress-free equilibria of the crystal.

2.5. *Energy invariance; discussion*

The invariance properties of the free-energy function $\tilde{\varphi}$ are the central ingredient by means of which the notion that the material is 'crystalline' is introduced in the theory. Ericksen (1977, 1980, 1989) proposed to obtain the invariance of $\tilde{\varphi}$ suitable for describing crystalline behavior by deriving it from the invariance of the lattice-energy function φ [the invariance properties of φ in (2) for a multilattice (1) are given by Pitteri (1985*b*); see also Pitteri & Zanzotto (1996*a*)]. This proposal by Ericksen is based on the validity of the rule (3) and it leads to an invariance for $\tilde{\varphi}$ described by a group conjugate to the infinite discrete group of 3×3 matrices with integral entries and unimodular determinant. As mentioned above, this point of view, used in the elastostatic variational calculations based on the functional (5), makes it possible to model phenomena such as transformation twinning and the formation of fine twinned microstructures in crystals undergoing solid-to-solid phase transitions (see the literature quoted in §1).

However, here we do not follow this train of thought regarding the invariance properties of $\tilde{\varphi}$. The reason is that the Born rule is observed not to hold on a number of occasions, especially in mechanical twinning deformations (see §3.4). Our aim here is to *test* the validity of the rule and check whether and to what extent elasticity theory can be applied to model crystal mechanics.

Consequently, here we only accept the hypothesis that a macroscopic free-energy function such as (4) can be written for the crystalline body but do not make any *a priori* assumptions regarding its invariance properties. We only assume for $\tilde{\varphi}$ the physically reasonable standard invariance requirements (i) and (ii) – see §2.6 below – made for any strain-dependent constitutive function in a continuum theory (see Truesdell & Noll, 1965). In the next sections, we investigate the consequences of twinning on the invariance group of $\tilde{\varphi}$. Also, we do not assume the validity of the Born rule (3) and actually seek to determine when it holds for twinning deformations.

Remark. It will become clear that, for the purposes of investigating the main implications of twinning about the invariance of $\tilde{\varphi}$, it is enough to consider the dependence and invariance of $\tilde{\varphi}$ with respect to its argument $\mathbf{F}$ only, disregarding the shifts $\mathbf{p}_k$ and the temperature θ. Thus from now on we will drop the latter variables from all formulas.

2.6. *Energy invariance; assumptions*

(i) The constitutive function $\tilde{\varphi}$ is assumed to be Galilean invariant, that is, it must be invariant under rigid-body motions; this means that it must satisfy

$$\tilde{\varphi}(\mathbf{F}) = \tilde{\varphi}(\mathbf{RF}) \tag{6}$$

for any orthogonal transformation $\mathbf{R}$ and any deformation gradient $\mathbf{F}$.

(ii) We also assume, as usual in continuum mechanics, that there is a 'material symmetry group' G of *unimodular* matrices $\mathbf{H}$ describing the invariance of the response function $\tilde{\varphi}$ under changes of the reference configuration for the body. Explicitly, we assume that

$$\tilde{\varphi}(\mathbf{F}) = \tilde{\varphi}(\mathbf{FH}) \tag{7}$$

for any tensor $\mathbf{F}$ and any $\mathbf{H}\in G$. The specific choice of G contributes to the characterization, in the mathematical model, of the physical properties of the material. Here we assume that the point group of the crystal is contained in G. The full invariance of $\tilde{\varphi}$ in its argument $\mathbf{F}$ is hence summarized by the condition

$$\tilde{\varphi}(\mathbf{F}) = \tilde{\varphi}(\mathbf{RFH}), \tag{8}$$

which must hold for any $\mathbf{H}$ in G, any orthogonal transformation $\mathbf{R}$, and any deformation gradient $\mathbf{F}$ within an appropriate domain. Deformation gradients $\mathbf{F}_1$ and $\mathbf{F}_2$ such that

$$\mathbf{F}_2 = \mathbf{RF}_1\mathbf{H} \tag{9}$$

for some orthogonal $\mathbf{R}$ and some $\mathbf{H}$ in G are called 'symmetry related'.

3. Mechanical twinning

To proceed, we must study in some detail the mechanical-twinning deformations of crystals, whose physical characteristics, as described for instance by Cahn (1954), Kelly & Groves (1970) and Klassen-Nekliudova (1964), are modeled here following Ericksen (1981, 1987), Pitteri (1985*a*), James (1981), Gurtin (1983) and Pitteri & Zanzotto (1996).

3.1. *Mechanical twins as stable equilibria for a crystal*

In elasticity theory, mechanical twins are considered as pairwise homogeneous stress-free stable equilibrium states of an unloaded crystal. Twinning is thus regarded as a continuous deformation $\mathbf{y}$ of the reference configuration R such that: (*a*) $\mathbf{y}$ minimizes the functional (5) for fixed temperature; (*b*) $\mathbf{y}$ is continuous and 'pairwise homogeneous', *i.e.* it is specified by *constant* deformation gradients $\mathbf{F}_1$ and $\mathbf{F}_2$ defined on two complementary subregions R_1 and R_2 of R, meeting along a plane in R with normal $\mathbf{N}$, say. The plane in the deformed configuration whose normal is $\mathbf{n} = \mathbf{F}_1^t\mathbf{N}$ is called the 'composition plane' or 'twin interface'.

In order for (*a*) and (*b*) to be verified (away from phase transitions), $\mathbf{F}_1$ and $\mathbf{F}_2$ must both be *symmetry-related minimizers* of the energy function $\tilde{\varphi}$ of the crystal [see (9)] and, as a consequence of the well known Hadamard compatibility conditions for the

continuity of $\mathbf{y}$ (see, for instance, Truesdell & Noll, 1965), they must also satisfy the following 'twinning equation':

$$\mathbf{F}_2 = \mathbf{Q}\mathbf{F}_1\mathbf{H} = (\mathbf{1} + \mathbf{a} \otimes \mathbf{n})\mathbf{F}_1, \tag{10}$$

where $\mathbf{a}$ and $\mathbf{n}$ are suitable vectors, $\mathbf{Q}$ is a suitable orthogonal transformation *not* in the point group of the crystal and $\mathbf{H}$ is a suitable element of the invariance group G of the energy $\tilde{\varphi}$:

$$\mathbf{H} \in G. \tag{11}$$

In (10), the symbol $\otimes$ denotes the dyadic or tensor product of vectors, which is a matrix whose components, in rectangular Cartesian coordinates, are $(\mathbf{a} \otimes \mathbf{n})_{ir} = a_i n_r$. Since $\det \mathbf{F}_1$ and $\det \mathbf{F}_2$ in (10) have the same sign, so must $\det \mathbf{H}$ and $\det \mathbf{Q}$, and this implies $\det(\mathbf{1} + \mathbf{a} \otimes \mathbf{n}) = 1$; therefore, in (10) we have

$$\mathbf{n} \cdot \mathbf{a} = 0, \quad \text{so that} \quad \mathbf{S} = \mathbf{1} + \mathbf{a} \otimes \mathbf{n} \tag{12}$$

is necessarily a simple shear, called the 'twinning shear'. The orthogonal transformation $\mathbf{Q}$ appearing in (10) is called the 'twinning operation'.

3.2. *Implications of twinning regarding the energy invariance*

Away from phase transitions, it is assumed that the minimizers for the constitutive function $\tilde{\varphi}$ are only those dictated by the energy invariance (9). Thus, the condition that in (10) the tensor $\mathbf{H}$ be an element of the group G is necessary to guarantee that the twinning deformation $\mathbf{y}$ defined by the two gradients $\mathbf{F}_1$ and $\mathbf{F}_2$ in (10) be a minimizer of the functional (5), *i.e.* that it gives a *stable* equilibrium state for the body under zero loads. Indeed, $\mathbf{y}$ minimizes (5) only if both $\mathbf{F}_1$ and $\mathbf{F}_2$ are minimizers of the free-energy density $\tilde{\varphi}$ and, under our hypothesis for $\tilde{\varphi}$, by (8) if the tensor $\mathbf{F}_1$ is a minimizer of $\tilde{\varphi}$, the tensor $\mathbf{F}_2 = \mathbf{Q}\mathbf{F}_1\mathbf{H}$ in (10) is also a minimizer of $\tilde{\varphi}$ *only* if $\mathbf{H} \in G$. Thus, in order to have a mechanical twin, the twinning equation (10) must be satisfied with (11).

From our point of view, this is the central observation because it means that to any twinning mode of a crystal can be associated an element $\mathbf{H}$ of its energy-invariance group G: such $\mathbf{H}$ can be calculated explicitly when the usual data on twinning modes are known [see (14) and (15) below].

3.3. *Type 1 and type 2 twins*

Let us confine our attention to the geometrically simplest twins, *i.e.* type 1 and type 2 twins,* which appear to be the only ones to have been experimentally observed without doubt (Zanzotto, 1988, 1992). These twins constitute the class of solutions to (10) that are best understood: for them, it is always possible to choose the twinning operation $\mathbf{Q}$ in (10) to be the mirror symmetry about the planes with normals $\mathbf{n}$ or $\mathbf{a}$, that is,

$$\begin{aligned} \mathbf{Q}_\mathbf{n} &= \mathbf{1} - 2(\mathbf{n} \cdot \mathbf{n})^{-1}\mathbf{n} \otimes \mathbf{n}, \\ \mathbf{Q}_\mathbf{a} &= \mathbf{1} - 2(\mathbf{a} \cdot \mathbf{a})^{-1}\mathbf{a} \otimes \mathbf{a}, \end{aligned} \tag{13}$$

respectively, for type 1 and type 2 twins. It is well known that, if the motif of the crystalline structure is not taken into account, a type 1 twin can be equivalently described by means of a twinning operation that is a 180° rotation about the axis n normal to the composition plane (see Fig. 1); this is often used in the literature as a

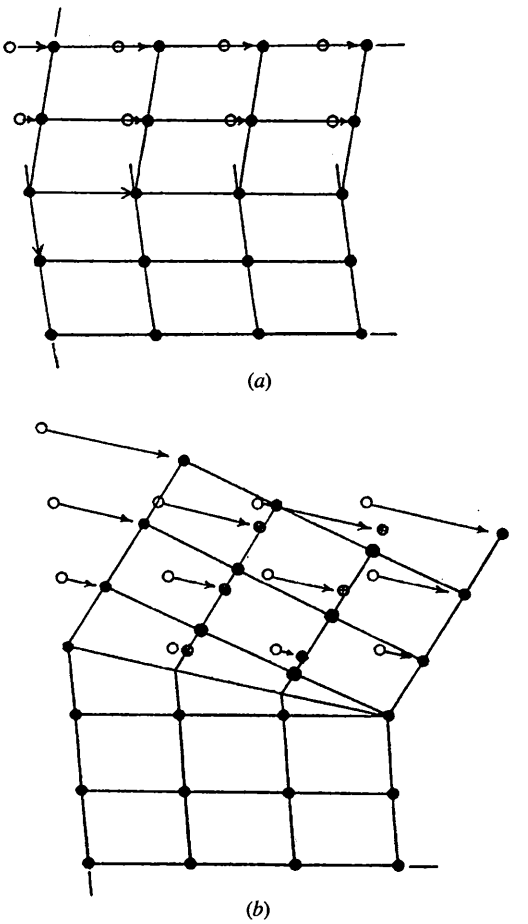

Fig. 1. ● Actual positions of the lattice points in the twinned individuals. ○ Lattice points before shearing. ⊕ Lattice points after shearing according to the macroscopic twinning shear. Two schematized twinning modes of type 1 are shown. Notice that in (*b*) the Born rule [equation (3)] does not hold *stricto sensu* because the sheared lattice vectors are not lattice vectors for the twinned lattice (the twinning shear only restores a *sublattice* in mirror symmetry; additional shuffle movements of the atoms are needed to reconstruct the whole lattice in a twinned configuration; see also §3.4). Condition (18) holds for these two twinning shears.

* Zanzotto (1988) notices that there are in the literature two different definitions of type 1 and type 2 twins, which are not equivalent. One definition refers to certain properties of rationality of some elements of the twinning shear, the other is the one given in the text, which we follow.

definition of type 1 twins. In what follows, we mostly consider type 1 twins, which are predominant in the observations.

3.4. *Failures of the Born rule*

The shear **S** [in (10)] is always experimentally observed in connection with mechanical twinning (Cahn, 1954) and often it is explicitly measured. Suppose, as is usually done in the experimental literature, that the reference lattice vectors $\mathbf{E}_a$ are those giving one of the individuals of the twin. Fig. 1 shows schematically the effect of two type 1 twinning deformations on a crystalline lattice. The Born rule holds for the shear **S** of the twin in Fig. 1(*a*): the portion of the lattice on one side of the contact plane is left undeformed, while on the other side the twinning shear produces lattice vectors $\mathbf{SE}_a$ that generate the twinned lattice as dictated by (3), related to the original lattice by the orthogonal twinning operation $\mathbf{Q}_\mathbf{n}$.

Now, while in Fig. 1(*a*) the twinning shear restores the *whole* lattice in mirror symmetry, it is known (Cahn, 1954) that in several materials the restoration of a *sublattice* suffices, so that in a mechanical twin a fraction of the lattice points must undergo inhomogeneous shuffling in order to reach the correct positions in the twinned lattice. Fig. 1(*b*) illustrates one such twinning mode. Zanzotto (1988) observed that in this case the Born rule (3) does *not* hold *stricto sensu* because the sheared lattice vectors $\mathbf{SE}_a$ do *not* generate the twinned lattice. Thus, in spite of its widespread and very common use, the validity of the Born rule for crystalline substances should not be taken for granted. We will return later to the consequences of this phenomenon regarding the invariance of the energy function of the crystal.

3.5. *Explicit computation of some elements of the invariance group G*

In the case of type 1 twins, there is a rapid way of computing explicitly the matrix $\mathbf{H} \in G$ connected to a twinning mode experimentally observed in a given crystal. To this end, we consider, as is usual in the mineralogical and metallurgical literature, the 'elements' K_1, K_2, η_1 and η_2 of the twinning shear **S**; the twin interface, normal to **n**, is the 'invariant plane' of the shear, denoted by K_1; K_2 is the 'second undistorted plane', *i.e.* the unique plane that is only rotated by **S**; S is the 'plane of shear' containing **a** and **n**; η_1 is the 'shear direction', parallel to **a**; η_2 is the oriented intersection of S and K_2 (see Fig. 2).

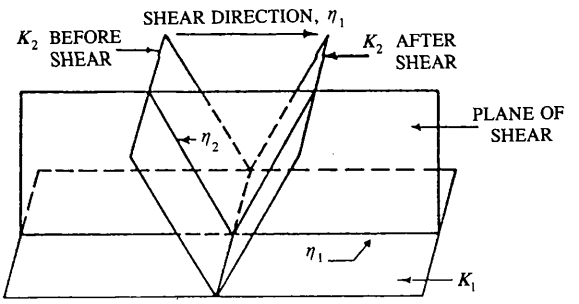

Fig. 2. The elements K_1, K_2, η_1, η_2, introduced in §3.5 for a shear $\mathbf{S} = \mathbf{1} + \mathbf{a} \otimes \mathbf{n}$.

A shear is determined by either couple, (K_1, η_2) or (K_2, η_1), of its elements, and in the literature the macroscopic shear **S** is always given by means of the crystallographic indices of such elements; for instance, the indices (K_{1i}) and $[\eta_2^i]$ of K_1 and η_2 are given for type 1 twins. Tables reporting experimental data for K_1 and η_2 for many twins in different materials can be found in various metallurgy and mineralogy textbooks [see, for instance, Kelly & Groves (1970) and Klassen-Nekliudova (1964); see also §5].

Now, it is possible to utilize such data to calculate the element **H** connected to an observed twin by means of the following formulas:

$$\mathbf{H} = \mathbf{1} - 2(\boldsymbol{\eta}_2 \cdot \mathbf{K}_1)^{-1} \boldsymbol{\eta}_2 \otimes \mathbf{K}_1, \quad \boldsymbol{\eta}_2 \cdot \mathbf{K}_1 \neq 0, \qquad (14)$$

where

$$\boldsymbol{\eta}_2 = \eta_2^i \mathbf{E}_i \quad \text{and} \quad \mathbf{K}_1 = K_{1i} \mathbf{E}^i; \qquad (15)$$

here, (K_{1i}) and $[\eta_2^i]$ are the indices of the shear elements K_1 and η_2 and the lattice vectors $\mathbf{E}_i$ of the unsheared individual of the twin are chosen as reference lattice vectors ($\mathbf{E}^i$ denotes the dual or reciprocal-lattice vectors). The expressions (14) and (15) for **H** are obtained by making the definition of K_1 and η_2 explicit in terms of the shear vectors **a** and **n**, and by considering the twinning equation (10) for a type 1 twin with the reference configuration chosen above, that is, when in (10) we set $\mathbf{F}_1 = \mathbf{1}$ and $\mathbf{Q} = \mathbf{Q}_\mathbf{n}$ [see (13)].

An analysis of the twinning equation actually shows that even for type 2 twins the element **H** can be calculated in a similar way by exchanging K_2 and η_1 for K_1 and η_2 in (14) and (15) (Zanzotto, 1992). We recall that the shears of type 2 twins are always given in the experimental literature in terms of their elements K_2 and η_1.

3.6. *Twin-connected generalized reflections in the group G*

It can be easily verified that the elements **H** connected to type 1 and type 2 twins, given by (14) and (15), are (nonorthogonal) 'generalized reflections' in the sense of Bourbaki (1981, p. 67), that is, they are matrices **H** such that $\mathbf{H}^2 = \mathbf{1}$ and $\mathbf{H} - \mathbf{1}$ has rank 1. This means that, given a crystalline material of which some twinning modes are known, it is possible to calculate explicitly a number of generalized reflections belonging to the invariance group G of its energy $\tilde{\varphi}$. Such generalized reflections generate groups whose properties are investigated in the literature on group theory.

4. Properties of the invariance group of the energy when twinning is observed. Validity of the Born rule and conditions to apply elasticity theory

4.1. *Twinning subgroups of G*

According to the discussion in §§3.4 and 3.5, let us assume that, for a given crystal whose energy $\tilde{\varphi}$ has an invariance group G, a number of twinning modes of type 1 or type 2 are known and that, consequently, also a finite number of 'twin-connected' generalized reflections $\mathbf{H}_\alpha \in G, \alpha = 1, \ldots, n$, have been determined. The twin-connected $\mathbf{H}_\alpha$ generate a 'twinning subgroup', H say, of G.

4.2. *Twinning subgroups and validity of the Born rule*

By using (3), (10), (14) and (15), it is not hard to check the following properties of the twinning subgroup H of G:

(i) The group H is, in general, constituted by invertible 3×3 matrices with *rational* entries. This follows from the fact, mentioned in §3.4, that, in any twinning deformation observed experimentally, at least a sublattice is restored in mirror symmetry by the twinning shear.

(ii) The Born rule (3) holds *stricto sensu*, that is, *all* the twinning shears restore the whole lattice in mirror symmetry if and only if the group H is constituted by invertible 3×3 matrices with *integral* entries. When the Born rule holds, it is possible to apply the Cauchy–Born–Ericksen procedure discussed in §1 and consider an elastic model for the crystal. The invariance group G of the energy proposed by Ericksen as mentioned in §2.5 is a discrete group that physically describes well the properties of the crystal and contains the twinning group H in a natural way.

(iii) If the Born rule (3) does not hold, there is still the possibility that the group H is *conjugate* to a group of invertible integral matrices. This is true if and only if a weaker version of the Born rule holds, in which the lattice vectors in (3) are replaced by a suitable set of 'sublattice vectors'. In this case, the twinning shears, each of which, as we know, separately restores a sublattice, do so for a suitable *common* sublattice, the same for all shears. To such a sublattice, (3) applies if a suitable set of sublattice vectors is used in place of the lattice vectors $\mathbf{E}_a$. This constitutes a weak version of the Born rule that can be utilized to obtain an elastic model for the behavior of the crystal by means of the same procedure. Also, in this case, it is possible to bridge the continuum and the molecular descriptions and the energy-invariance group obtained from the molecular considerations describes well the crystalline properties of the material.

(iv) If the group of rational matrices H is *not* conjugate to a group of integral matrices, the Born rule does not hold even in the weak sense. Although each twinning shear does restore a sublattice in mirror symmetry, they cannot do so for any common sublattice and it is not possible to follow the route to elasticity theory mentioned above. In this case, it is necessary to check whether elasticity can be applied at all to model the behavior of the material.

4.3. *Explicit conditions selecting the alternatives above*

In the case of *two* generic twin-connected reflections, there is a simple way to check which of the alternatives above holds for H. Since this case is enough to illustrate all the important conclusions, we give some details about it. It will turn out that the more interesting cases (ii) and (iii) above are very special ones and that (iv) is the generic one. If the twin-connected elements are $\mathbf{H}_1$ and $\mathbf{H}_2 \neq \mathbf{H}_1$, given explicitly by

$$\mathbf{H}_1 = \mathbf{1} - \mathbf{a} \otimes \mathbf{b},\ \mathbf{H}_2 = \mathbf{1} - \mathbf{c} \otimes \mathbf{d} \text{ with } \mathbf{a} \cdot \mathbf{b} = 2 = \mathbf{c} \cdot \mathbf{d}, \tag{16}$$

the twinning subgroup H is, abstractly, a dihedral group that is finite or infinite depending on the period p of the element $\mathbf{H}_1\mathbf{H}_2$ (when p is finite, the number of elements of H is $2p$). It turns out that p and the other interesting properties of H are determined by the value of the 'cross product' $(\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \cdot \mathbf{d}) = \operatorname{tr} \mathbf{H}_1\mathbf{H}_2 + 1 \in \mathbb{Q}$ ($\mathbb{Q}$ denotes the field of rational numbers). Recall that $(\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \cdot \mathbf{d})$ can be calculated by inspection through (14) and (15) from the experimental data on the elements K_1 and η_2 of the observed twins.

Remark. Because the shear amplitude is small in experimentally observed twinning shears, for any twin-connected elements as in (16) the following is observed to hold:

$$(\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \cdot \mathbf{d}) = \operatorname{tr} \mathbf{H}_1\mathbf{H}_2 + \mathbf{1} \in [\mathbf{0}, \mathbf{4}] \tag{17}$$

and we discuss the features of H under this assumption.

Owing to the general properties of the trace of a matrix, it is clear that if either alternative (ii) or (iii) in §4.2 is to hold for H, the trace $\operatorname{tr} \mathbf{H}_1\mathbf{H}_2$ must be in $\mathbb{Z}$ rather than in $\mathbb{Q}$ ($\mathbb{Z}$ denotes the set of integral numbers):

$$(\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \cdot \mathbf{d}) = \operatorname{tr} \mathbf{H}_1\mathbf{H}_2 + 1 \in \mathbb{Z}; \tag{18}$$

in fact, this is also a sufficient condition for (ii) or (iii) to be true, for instance due to a result by Maxwell (1977). Fig. 1 illustrates two (two-dimensional) twinning modes verifying (18). This condition gives a quick criterion to check whether the Born rule applies, at least in the weak sense, for any couple of twinning modes of a material. Under (17), it can be also seen if (18) holds the group H is conjugate to one of the finite crystallographic groups, with 2, 4, 6, 8 or 12 elements.

We only mention here that the problem is more complex when we consider more than two $\mathbf{H}$'s (see

Vinberg, 1971, lemmas 11 and 12, and Zanzotto, 1992).

4.4. *Elasticity theory cannot be used if the Born rule does not hold*

As we have seen, cases (ii) and (iii) in §4.2 are decided on the basis of (18) and are favorable in the sense that elasticity theory can be applied. If (18) does not hold, which algebraically is the most likely case, then the group H is as in point (iv) of §4.2. In other words, 'generically' the Born rule should not be expected to apply to twinning. In this case, an analysis of the features of the twinning group H shows that elasticity *cannot* provide an appropriate model: the energy invariance becomes too large for a crystal.

This is a consequence of the fact that, if the parameter $(\mathbf{b}\cdot\mathbf{c})(\mathbf{a}\cdot\mathbf{d}) = \operatorname{tr}\mathbf{H}_1\mathbf{H}_2 + 1$ is rational and between 0 and 4 but *not* in $\mathbb{Z}$ [*i.e.* if (17) holds but (18) does not], the element $\mathbf{H}_1\mathbf{H}_2$ is always conjugate to a rotation and its period p is always infinite. Consequently, the topological closure of the subgroup $C = \{(\mathbf{H}_1\mathbf{H}_2)^r, r \in \mathbb{Z}\}$ of H is a topological cyclic Lie group conjugate to a one-dimensional continuous group of rotations [one-parameter subgroup of the proper orthogonal group $SO(3)$]. This means that the material symmetry of an elastic crystal exhibiting two twinning modes is 'generically' *larger than transverse isotropy*.

If also the point-group symmetry of the crystal is taken into account, or if several twin-connected elements $\mathbf{H}$ are considered, it is not difficult to see that the situation gets even worse (Zanzotto, 1992). The one-parameter subgroups generated by aperiodic elements such as the product $\mathbf{H}_1\mathbf{H}_2$ and their crystallographic equivalent elements make the invariance group G a high-dimensional Lie subgroup of the eight-dimensional unimodular group. Thus, for crystals with large point groups, *i.e.* whose lattices have rather high geometrical symmetry like tetragonal and higher, generic experimental data giving even only one aperiodic product $\mathbf{H}_1\mathbf{H}_2$ can be enough to force G to invade the whole unimodular group, which classically describes the material symmetry of elastic fluids (Truesdell & Noll, 1965).

5. Some relevant experimental data

Although the theoretical considerations predict that this should be a quite rare occurrence, the analysis of relevant experimental data indicates that the validity of the Born rule does occur in practice: shape-memory alloys and crystals whose structure is described by one simple Bravais lattice appear to share the very remarkable characteristic of nongeneric behavior in which the validity of the rule is not violated. This section summarizes some of the results of a careful analysis of the experimental literature on mechanical twinning.

5.1. *Macroscopic shear data*

Only part of the abundantly reported experimental results is significant for our purposes because in order to establish the twin-connected elements $\mathbf{H}$ we need data regarding the actual *macroscopic* twinning shear; thus, the elements K_1 and η_2 must be determined by means of macroscopic measurements. However, it is common in the experimental literature to obtain such data by means of geometric considerations when the macroscopic measurements are not precise enough. While the geometric estimates are certainly correct in many cases, even the most careful ones could sometimes be wrong and examples of this can be found in the literature. For this reason, we chose data on twinning that rely on direct macroscopic measurements for their determination. The cases of Rapperport (1959) and Reed-Hill (1960), for instance, are remarkable from this point of view in that the authors estimated the shear elements only by optical means. The case of Cahn (1953) seems more typical: a geometric analysis (based on an assumption of a reasonably 'small' amount of shear) allowed identification of some candidate macroscopic shears, among which the choice of the correct one was made by means of macroscopic measurements.

5.2. *Some h.c.p. metals*

Magnesium shares, with a number of other h.c.p. metals (see, for instance, Barrett & Massalski, 1966, p. 415; Klassen-Nekliudova, 1964, p. 168; Kelly & Groves, 1970, p. 303; Yoo, 1981), a twinning mode that gives the element $\mathbf{H}_1$ below. Among the other data on twinning modes in magnesium, those collected by Reed-Hill (1960) are now commonly accepted in the literature (see also Reed-Hill & Robertson, 1963). All in all, these results give, by (14) and (15), the following $\mathbf{H}$'s:

$$\begin{aligned}\mathbf{H}_1 &= \mathbf{1} - \tfrac{1}{2}(2\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3)\otimes(\mathbf{E}^1 + 2\mathbf{E}^3),\\ \mathbf{H}_2 &= \mathbf{1} - \tfrac{1}{4}(6\mathbf{E}_1 + 3\mathbf{E}_2 + 2\mathbf{E}_3)\otimes(\mathbf{E}^1 + \mathbf{E}^3),\\ \mathbf{H}_3 &= \mathbf{1} - \tfrac{1}{4}(2\mathbf{E}_1 + \mathbf{E}_2 + 2\mathbf{E}_3)\otimes(\mathbf{E}^1 + 3\mathbf{E}^3),\end{aligned} \qquad (19)$$

where the usual lattice vectors for hexagonal crystals are used.* Very interesting experimental data are also available for zirconium, which besides the common mode of h.c.p. metals connected with $\mathbf{H}_1$ also exhibits three other mechanical twins. These yield

* For hexagonal lattices, the use of the four-index notation is rather common. However, in this section we use a three-index notation, referring for further information and transformation formulae to Otte & Crocker (1965).

$$\begin{aligned}
\mathbf{H}_1 &= \mathbf{1} - \tfrac{1}{2}(2\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + 2\mathbf{E}^3),\\
\mathbf{H}_2 &= \mathbf{1} - \tfrac{1}{3}(2\mathbf{E}_1 + 2\mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + \mathbf{E}^2 + 2\mathbf{E}^3),\\
\mathbf{H}_3 &= \mathbf{1} - \tfrac{2}{17}(8\mathbf{E}_1 + 8\mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + \mathbf{E}^2 + \mathbf{E}^3),\\
\mathbf{H}_4 &= \mathbf{1} - (\mathbf{E}_1 + \mathbf{E}_2) \otimes (\mathbf{E}^1 + \mathbf{E}^2 + \mathbf{E}^3).
\end{aligned} \tag{20}$$

The first three **H**'s are obtained from data by Rapperport (1959), while the mode connected with $\mathbf{H}_4$ was subsequently determined by Reed-Hill, Slippy & Buteau (1963). All of the data utilized in (20) were obtained by means of purely macroscopic measurements.

For both magnesium and zirconium, the twin-connected **H**'s and the reflections in the point group of the crystal violate (18) in pairs, so that the discussion in §4.4 applies. Even in the weak sense, the Born rule does not apply and their twinning groups are generic. Twinning makes their energy invariance much too large for thermoelasticity theory to give a useful description of their behavior as crystalline materials.

The conclusions above regarding zirconium and magnesium are likely to apply to titanium as well, which has the same h.c.p. structure and exhibits, among others, the same twinning planes as both zirconium and magnesium. However, regarding titanium, only geometric determinations of the shear elements other than K_1 appear to be available in the literature, with the exception of very few partial studies (see, for instance, Paton & Backofen, 1969). The foregoing analysis confirms the statement by Kelly & Groves (1970, p. 300): 'It will be evident that physically, twinning in hexagonal metals is not well understood.'

5.3. *Uranium*

Situations similar to that of the h.c.p. metals occur also in the case of lower-symmetry metals. A clear example is given by orthorhombic uranium, for which some interesting data are available. The experimental literature reports five twinning modes, two of which are conjugate (see Cahn, 1953; Lloyd & Chiswik, 1955; Daniel, Lesage & Lacombe, 1971; Crocker, 1965). These modes are now well accepted in the literature (see Klassen-Nekliudova, 1964, p. 168; Barrett & Massalski, 1966, p. 415; Kelly & Groves, 1970, p. 303). Explicitly, the elements **H** we obtain from (14) and (15) are

$$\begin{aligned}
\mathbf{H}_1 &= \mathbf{1} - \tfrac{1}{2}(\mathbf{E}_1 + \mathbf{E}_2) \otimes (\mathbf{E}^1 + 3\mathbf{E}^2),\\
\mathbf{H}_2 &= \mathbf{1} - \tfrac{1}{4}(3\mathbf{E}_1 + \mathbf{E}_2 + 2\mathbf{E}_3) \otimes (\mathbf{E}^1 + \mathbf{E}^2 + 2\mathbf{E}^3),\\
\mathbf{H}_3 &= \mathbf{1} - \tfrac{1}{3}(3\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + 2\mathbf{E}^2 + \mathbf{E}^3),\\
\mathbf{H}_4 &= \mathbf{1} - \tfrac{1}{4}(5\mathbf{E}_1 + \mathbf{E}_2 + 2\mathbf{E}_3) \otimes (\mathbf{E}^1 + \mathbf{E}^2 + \mathbf{E}^3),
\end{aligned} \tag{21}$$

in terms of orthorhombic lattice vectors. In this case, too, the elements **H** above and the reflections in the point group of the crystal violate (18) in pairs, so that the discussion in §4.4 applies and the conclusions are the same as for the h.c.p. metals.

5.4. *Fe–Ni–C martensites*

The properties of the deformation modes of various ferrous martensites as a function of their carbon content and in a range of conditions allowing for the stability, or at least metastability, of both the austenitic and the martensitic phases, have been investigated by a number of workers. Twinning data, clear enough for our purposes, are reported, for instance, by Richman (1963) (see also Crocker & Bevis, 1963). A kinematical discussion and reappraisal of the above results was made by Bevis, Rowlands & Acton (1968). Rowlands, Fearon & Bevis (1968), after further experimental study of twinning in several Fe–Ni and Fe–Ni–C martensites, reported, in addition to the former ones, a further (type 2) mode to be active, the geometrical appraisal of whose elements was found to be in excellent agreement with experimental data. Taking into account only the three most certain and frequent modes, we get from (14) and (15) the following **H**'s:

$$\begin{aligned}
\mathbf{H}_1 &= \mathbf{1} - \tfrac{1}{2}(\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + \mathbf{E}^2 + 2\mathbf{E}^3),\\
\mathbf{H}_2 &= \mathbf{1} - \tfrac{1}{2}(-\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^2 + 3\mathbf{E}^3),\\
\mathbf{H}_3 &= \mathbf{1} - \tfrac{1}{4}(5\mathbf{E}_1 + \mathbf{E}_2 - 3\mathbf{E}_3) \otimes (\mathbf{E}^1 - \mathbf{E}^3)
\end{aligned} \tag{22}$$

in terms of tetragonal lattice vectors. We notice that $\mathbf{H}_1$ is associated with the common well established (1, 1, 2) mode of b.c.c. materials. Again, it is not difficult to check that, if we consider the above elements **H** and the reflections that belong to the point group of the crystal, they violate (18) in pairs, so that the resulting energy invariance prevents the adoption of an elastic model.

5.5. *Shape-memory alloys*

As an example of these materials, we examine the deformation twinning modes reported by Ichinose, Funatsu & Otsuka (1985) for orthorhombic γ_1' martensite in a Cu–Al–Ni alloy. The twinning elements were all experimentally determined by means of a macroscopic analysis of various single-crystal specimens after transformation from cubic austenite. The skeletal lattice of the crystalline multilattice of the martensite is generated by orthorhombic vectors. Observations led to three twinning modes (two of which are 'reciprocal' and give the same **H**); these modes, on the basis of (14) and (15), yield the following two twin-connected **H**'s:

$$\begin{aligned}
\mathbf{H}_4 &= \mathbf{1} - \tfrac{1}{2}(\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + 2\mathbf{E}^2 + \mathbf{E}^3),\\
\mathbf{H}_5 &= \mathbf{1} - (\mathbf{E}_1 + \mathbf{E}_3) \otimes (\mathbf{E}^1 + \mathbf{E}^3).
\end{aligned} \tag{23}$$

If to the above generalization reflections we adjoin

$$\mathbf{H}_i = \mathbf{1} - 2\mathbf{E}_i \otimes \mathbf{E}^i \quad (i = 1, 2, 3), \tag{24}$$

which are the reflections generating the point group of the orthorhombic martensitic phase, it can be seen that, for the five **H**'s in (23) and (24), condition (18) is always satisfied and that they generate a group conjugate to the cubic holohedral crystallographic group. The latter is the symmetry group of the higher-symmetry phase of this material.

The other shape-memory alloys that we checked behaved similarly to Cu–Al–Ni, at least near their symmetry-breaking phase transitions; their twinning groups always coincide with the point groups of the higher-symmetry phase.

5.6. *Simple lattices*

Crystals whose structure can be described by one simple (monoatomic) Bravais lattice appear always to behave in such a way that the Born rule (3) holds *stricto sensu*. We refer to Zanzotto (1988) for more details, who could not find any data in the literature regarding twinning or other deformations violating (3) in such materials, for whose behavior elasticity theory thus provides a good model. Unlike the case of shape-memory alloys, the twinning subgroups of these crystals are infinite discrete groups. This is what happens, for instance, with the very common $(1, 1, 2)$ twinning mode in b.c.c. materials (see Klassen-Nekliudova, 1964; Kelly & Groves, 1970; and the Fe–Ni–C martensites above) or with the well established '$(-1, -3, 5)$' type 2 twinning mode in crystalline mercury (see Crocker, Heckscher, Bevis & Guyoncourt, 1966; Guyoncourt & Crocker, 1968).

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