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**Twinning in minerals and metals: remarks on the comparison of a thermoelastic theory with some experimental results. Generalities and mechanical twinning**

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**Fisica matematica.** — *Twinning in minerals and metals: remarks on the comparison of a thermoelastic theory with some experimental results. Generalities and mechanical twinning.* Nota I di GIOVANNI ZANZOTTO (\*) presentata (\*\*) dal Corrisp. A. BRESAN.

ABSTRACT. — In the present Note I and in a following Note II (Zanzotto 1988), we discuss, taking into account some available experimental data, the results of a thermoelastic theory of twinning in crystalline solids. Various noteworthy problems emerge, some of which involve the hypotheses that are at the very basis of the theory.

KEY WORDS: Crystals; Thermoelasticity; Twinning.

RIASSUNTO. — *La geminazione nei minerali e nei metalli. Osservazioni sul confronto di una teoria termoelastica con alcuni risultati sperimentali. Generalità e geminazione meccanica.* Nella presente Nota I ed in una seguente Nota II (Zanzotto 1988) si discutono, alla luce dei dati sperimentali ora disponibili, i risultati di una teoria termoelastica della geminazione meccanica nei solidi cristallini. Emergono vari problemi degni di nota, alcuni dei quali riguardano le stesse ipotesi di base della teoria.

#### INTRODUCTION

In nature, crystalline edifices do not usually appear in the form of well individualized single crystals. Rather, they often come in complex associations in which many homogeneous and congruent parts intergrow, either in a parallel fashion or with one penetrating into another, with individuals reoriented in typical and characteristic ways for each crystalline species.

These formations are called «twins», with a broad general interpretation of the word, and the rigid transformations taking one individual into another are called «twin operations» or «twins laws».

Of course, these kinds of aggregates have been known and studied for a long time, and are considered to have a particular significance in crystal mechanics. Yet, neither in the mineralogical nor in the metallurgical literature is there a common agreement on what exactly constitutes a twin, and there is no precise definition which is generally accepted. Each author seems to express a personal point of view that others would be likely to share in the general outlines, but probably not in the details. About this, see for instance the introductory remarks written by Buerger for the «Symposium on Twinning» held in Madrid in 1960, where he states: «The reader will find a divergence of views on certain points, and no attempts has been made to force any uniformity into the treatments or results ...». As he then explains in more detail, «one point of divergence concerns the kind of symmetry which can relate the individuals of a twin pair ... The disagreement appears to arise from a different *definition* a twin ...» (see Buerger 1960).

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Definitions of twinning are given for instance by: Barrett and Massalski 1966, Buerger 1945, 1960, Cahn 1954, Bilby and Crocker 1965, 1968, Dana 1962, vol. 3 p. 75, Donnay 1960, Elliss and Treuting 1951, Evans 1912, Friedel 1926, pp. 421-7 pp. 479-83, Friedel 1933, Hall 1954, Hartman 1956, Holser 1958, Kelly and Groves 1970, Klassen-Nekliudova 1964, Mathewson 1928, Santoro 1974, Zoltai and Stout 1984 and many others. We report here only the definition by Dana, which gives an example of the standard attitude:

«A twin is a geometrical position of intergrowth of two or more crystals of the same species with which is associated a frequency of occurrence greater than that of chance».

This covers the phenomenon in general. Two main categories of twins can then be distinguished, depending on the physical origin of the polycrystals: «mechanical» twins and «growth» twins. As we shall see, a basic distinction between them arises in the theory, since they show some distinctive features that are certainly worth noting.

Indeed, workers in the field require that various different but rather broad features are to be exhibited by crystalline aggregates in order that they be actually judged twins, and not random events or «twins of the imagination» (see Friedel 1926, p. 422, and Cahn 1954, pp. 262 and 415). For instance, when mechanical twinning is considered, the reorientations have to be obtained through a shearing deformation of a homogeneous parent crystal, and this provides a definite condition to determine the allowed twinning operations.

On the other hand, in the case of growth twins the requirements are less definite and precise. Only in some points does the literature seem to be rather in accord and assertive: what is demanded is that the same reorientations have to be found in a great number of specimens, frequency and «reproducibility» of a given pattern being key features. Also, interfaces of comparatively low or very low energy seem to be an important feature that twins certainly possess, according to the crystallographer's point of view (for references, see sect. 2 of Note II: Zanzotto 1988).

Nevertheless, there is not yet a clear understanding of the phenomenon, and it is not known what is the best way to set some definite conditions restricting the possible twin reorientations so that they give the configurations usually described as genuine «twins» by the experts (see Zanzotto 1990).

Along with the problem of defining true twins as opposed to random intergrowths, there is the question of their classification, which is tackled in different ways, the same being true for the great variety of twinning mechanisms proposed to explain the experimental observations.

One of the problems with the theories proposed in the past (like the well known one by Friedel on coincidence-site lattices for instance, see also Cahn 1954, Santoro 1974) seems to be that the general «rules» are too broad, in that they allow for many *a priori* possibilities that have never been actually observed (see Buerger 1945, p. 475, and Cahn 1954, pp. 378-9). In a sense, this is also the case with the thermoelastic theory of mechanical twinning proposed and elaborated by various authors in recent years, as explained in detail in sect. 2.

With regard to this, a great deal of work has been done in trying to understand

which further rules, besides the general necessary ones, have to be given to complement the general theories. This in order to tighten them to better agree with the observations, and render them precise enough to give an understanding, for instance, as to why some configurations occur much more often than others, or why certain possibilities have never been observed.

Among the rules reported in the literature are for instance the following:

a) Minimum or «small» shear hypotheses (see for instance Friedel 1926, p. 487, Hall 1954, Bevis *et al.* 1968, and others).

b) Finite period for the relative orientations of the various individuals: generally 2, 3, 4 or 6 (see for instance Friedel 1926, Barrett and Massalski 1966). The occurrence of periods other than 2 is denied by some authors, originating a sort of prejudice according to which true twins can only exhibit the «conventional» orientations given in (3.1) below (see Buerger 1960). Indeed, only the latter are considered in many elementary mineralogy textbooks which treat twinning.

c) Various hypotheses of «rationality» for the interfaces and for other shear elements (see Buerger 1945 among others).

Some further, less common rules can be found in the literature; some assume for instance that the mean adjustments of atoms in twinning deformations should be minimized, others that all the atoms should move roughly the same distance (see Hall 1954, p. 85). Other conditions are stated by Cahn 1954, p. 381, and for growth twins by Evans 1912, Hartman 1956, Holser 1958, for instance.

There is no agreement among the workers regarding the range of validity of the above hypotheses. Anyway, their role, rather than purely theoretical, is that of helpful criteria which are used in practice to select one twinning mode among the various that would possibly fit the observe experimental data collected analyzing twinned specimens of crystals.

On the basis of some of the available literature on the subject, we try in the present Note I, and in the Note II quoted above, to assess the validity of these assumptions, and at the same time to compare with known experimental results some of the hypotheses and predictions of the thermoelastic theory of twinning briefly summarized in sect. 2.

This is the place to notice that some problems related to the so-called Type 1 and Type 2 twins and about «irrational» twins remain open. For instance, the reasons are not clear why Type 1 and Type 2 twins seem to cover the totality of the observations of *mechanical* twinning in metals and in minerals, whereas the theory allows for other orientations to be predicted. We show by an example that two different definitions of Type 1 and Type 2 twins which are common in the literature are *not* equivalent, and we illustrate why the conjecture put forward by Pitteri 1986 about irrational twins seems ill posed, in that the description of the particular type of twins he produces as an example tends to obscure its actual nature.

Some other questions also arise; for instance the one already mentioned of a definite theoretical distinction between growth and mechanical twins. Moreover, a fundamental problems is pointed out, concerning the validity of the Born rule, an hypothe-

sis about the movements of atoms (or of lattice points) in a crystal undergoing a macroscopic change of shape. This is a point of major importance, in that a definite connection between the molecular and continuum descriptions is necessary for applying macroscopic models, like thermoelasticity theory, to crystal mechanics, and in particular for trying to assess correctly the material symmetry group of crystalline substances, on the basis molecular considerations (see Zanzotto 1991).

Some experimental observations suggest that it is *not* safe to use thermoelasticity to describe the behaviour of bodies whose structure is not given by a simple Bravais lattice. On the contrary, it does seem rather safe to use it for the latter. The reasons are unclear.

We try to identify some of the main features exhibited by reported growth twins concerning the question of the energies at twin boundaries. An analysis of this kind is useful for giving some first suggestions for a thermoelastic theory of interfacial energies in crystalline bodies. As already mentioned above, this, together with the study of stability of polycrystals under changes of the environmental pressure and temperature, prove to be important issues in the analysis of mechanical and growth twins that are actually observed.

MOLECULAR AND CONTINUUM PICTURES. THE CAUCHY-BORN HYPOTHESIS.  
«MOTIF» AND «STRUCTURAL» SHUFFLES. MATERIAL SYMMETRY FOR CRYSTALS

In general, a crystalline configuration can be described by means of a multi-lattice, *i.e.* by means of a number of interpreting Bravais lattices, the position of each atom being given by (here and in the sequel, the summation convention will be understood):

$$(1.1) \quad X = M^a E_a + p_k, \quad a = 1, 2, 3, \quad M^a \text{ integers,}$$

where  $E_a$  are lattice vectors and  $p_k$  «shift» vectors,  $k$  ranging from zero to a suitable integer  $N$  (see Pitteri 1985*b*). Nevertheless, in many cases the crystalline structure can be described with enough precision as a simple Bravais lattice  $L$  whose points are

$$(1.2) \quad X = M^a E_a \quad \text{with} \quad M^a \text{ integers,}$$

any such point giving the position of a «motif» of atoms rather than of a single atom. This greatly simplifies the description of atomic movements, because in this way we choose not to deal with the effective atomic movements about the lattice points (1.2), a phenomenon that we here call «motif» shuffling of atoms.

In general, «motif» shuffles are involved in the twinning modes of structures which are not holohedral, that is, in which some of the symmetry operations restoring the skeletal lattice (1.2) do not restore the multi-lattice (1.1). In these cases, it is very common to observe twinning modes which relate the parent and twinned phases by one of the symmetry operations belonging to the holohedral group of the structure but not to its actual crystallographic point group (see for instance Miller 1972 for the theory of crystallographic groups and related topics).

This is the case of Dauphiné and Brazil twins in quartz, where the twinned phase is characterized by a different, symmetry-related, disposition of atoms about the same fundamental lattice as the parent crystal. These twinning modes are called «merohe-

dreal» by Friedel 1926 and Cahn 1954<sup>(1)</sup>. A kinematic theory of shuffle movements in twinning is given by Pitteri 1985a.

We are not interested here in this otherwise physically important phenomenon, and this is the reason for assuming that we can describe also multi-lattices in terms of lattice vectors only, as in (1.2).

Nevertheless, as it will become clear later, the description we are adopting allows for the discussion of another common and important kind of shuffling in mechanical twinning shears, that we shall call «structural». It involves movements of individual atoms in such a way that the final result is equivalent to a shearing of only a given fraction of the *lattice points*, i.e. of only a part of the *main structure*, and to a shuffling of the rest, accompanied in general by some further shuffling in the motif.

As can be easily seen, one given multi-lattice can be described by an equation of the type (1.1) in various ways, depending on the number of shift vectors  $p_k$  chosen. This ambiguity is avoided if we assume, as we do, and as is understood in the very definition of lattice vectors, that they generate a *maximal* group of translational isometries of the crystal (see Ericksen 1984), or equivalently, that the unit cell has minimum volume. Then the number of shifts necessary to describe the crystal is no longer arbitrary, and the distinction between «motif» and «structural» shuffling becomes unequivocal.

The same structure of (1.2) is generated by new lattice vectors  $E'_a$  whenever the mapping  $H$  defined by

$$(1.3) \quad H: E_a \mapsto E'_a = h_a^b E_b = H E_a$$

is a bijection of the lattice  $L$ . This happens when the matrix  $h_a^b$  belongs to  $GL(3, \mathbf{Z})$ , the group of three-dimensional matrices with integral entries such that

$$(1.4) \quad \det h_a^b = \pm 1.$$

The collection of all the the transformations  $H$  defined via (1.3-4) forms a group  $\overline{G}$  which is conjugate to  $GL(3, \mathbf{Z})$  and leaves the lattice  $L$  invariant. Ericksen 1977 proposed  $\overline{G}$  as material symmetry group for elastic crystalline media (see below).

Among the elements of  $\overline{G}$  of great importance in the study of crystal symmetry and in the theory of twinning are the «point group operations» and the «lattice invariant shears». They can be defined as the solutions of the equations

$$(1.5) \quad Q E_a = q_a^b E_b \quad \text{and} \quad S E_a = s_a^b E_b,$$

<sup>(1)</sup> We notice that, from the point of view of constitutive equations, elasticity theory applied to crystals as it is briefly described in sect. 1 can distinguish Dauphiné twinned configurations in quartz. In fact, the two individuals in a Dauphiné twin are connected by a rotation of  $\pi$  about the optic axis of the crystal, an operation which does not belong to the point group of quartz. The two «phases» are modelled as possessing a multi-valued strain-energy function (see for instance James 1987).

On the contrary, elasticity theory fails to identify Brazilian twins. This happens because the twin law is in this case the central inversion  $-1$ , an operation which is also missing from the point group of quartz. As is well known, material symmetry groups in elasticity always contain the operations  $-1$ , so that Brazilian twinned configuration turn out to have the same elastic response: thus, they cannot be distinguished from the point of view of elasticity theory. It is interesting that this probably correspond to the fact that, whereas Dauphiné twins can be mechanically produced and removed, this is known to be impossible for Brazilian twins (see Dana 1962, vol. 3, p. 90, Klassen-Nekliudova 1964, p. 9).

where  $Q$  is an orthogonal tensor and  $S$  a simple shear and where  $q_a^b$  and  $s_a^b$  are matrices in  $GL(3, \mathbf{Z})$ .

According to molecular calculations (see for instance Ericksen 1977 and Eftis *et al.* 1971), at a given temperature  $\theta$  the internal energy  $\varepsilon$  per unit volume of the crystal depends upon the lattice configuration through the lattice vectors only:

$$(1.6) \quad \varepsilon = \bar{\varepsilon}(\mathbf{E}_a, \theta),$$

Since a transformation  $H$  in  $\bar{G}$  yields new vectors  $\mathbf{E}'_a = H\mathbf{E}_a$  but does not change the lattice  $L$  it is physically clear that the basic invariance of  $\varepsilon$  is related to eqs. (1.3-4), in the sense that

$$(1.7) \quad \varepsilon = \bar{\varepsilon}(\mathbf{E}_a, \theta) = \bar{\varepsilon}(\mathbf{E}'_a, \theta) = \bar{\varepsilon}(h_a^b \mathbf{E}_b, \theta),$$

for every matrix  $b$  in  $GL(3, \mathbf{Z})$ .

In addition, Ericksen 1977 shows that the internal energy of a crystal depends upon the lattice vectors only through the matrix  $C_{ab} = \mathbf{E}_a \cdot \mathbf{E}_b$ , so

$$(1.8) \quad \varepsilon = \bar{\varepsilon}(\mathbf{E}_a, \theta) = \bar{\varepsilon}(C_{ab}, \theta) = \bar{\varepsilon}(C, \theta),$$

for all  $\theta$ ; this expresses Galilean invariance for  $\varepsilon$ .

Since

$$C'_{ab} = \mathbf{E}'_a \cdot \mathbf{E}'_b = H\mathbf{E}_a \cdot H\mathbf{E}_b = h_a^j h_b^k C_{jk}, \quad \text{or shortly} \quad C' = hCb^t,$$

we deduce from (1.7-8) that the constitutive function  $\bar{\varepsilon}$  for the energy density of the lattice satisfies the invariance property

$$(1.9) \quad \bar{\varepsilon}(C, \theta) = \bar{\varepsilon}(hCb^t, \theta),$$

for every symmetric, positive-definite matrix  $C$  and every matrix  $b$  in  $GL(3, \mathbf{Z})$ .

So far, crystalline configurations have been introduced through the «molecular» description given in terms of lattice vectors, and this to the macroscopic continuum point of view via the Cauchy-Born hypothesis, which we now briefly discuss.

Let us choose a reference configuration  $R$  for the crystalline body. Its macroscopic deformation is given by an invertible function  $\chi: R \rightarrow R^3$ , which is assumed to be continuous, 1-1, piecewise differentiable and to have a gradient  $F(X) = D\chi(X)$  such that  $j = \det F > 0$ .

As usual, we denote by  $C$  the symmetric, positive-definite right Cauchy-Green tensor given by  $C = F^t F = U^2$ ,  $U$  being the right «stretch» tensor appearing in the polar decomposition  $F = RU$  of  $F$ .

To introduce thermoelasticity theory into the molecular framework outlined above, it is necessary that we correlate atom movements to gross movement, *i.e.* we need to establish how the lattice points of the crystalline structure move when the macroscopic body experiences a *homogeneous* deformation  $\mathbf{x} = \chi(X) = F\mathbf{X}$  of a reference configuration generated by lattice vectors  $\mathbf{E}_a$ . Following the classical rule due to Cauchy and Born, as interpreted for instance by Ericksen 1984, we assume that the vectors  $\mathbf{e}_a$  defined by

$$(1.10) \quad \mathbf{e}_a = F\mathbf{E}_a,$$

constitute a possible set of lattice vectors for the (homogeneously) deformed configuration.

This enables us to get macroscopic constitutive function from the molecular one (1.6):

$$(1.11) \quad \tilde{\varepsilon}(\mathbf{F}, \theta) = \bar{\varepsilon}(\mathbf{F}\mathbf{E}_a, \theta) = \bar{\varepsilon}(\mathbf{e}, \theta),$$

$\mathbf{E}_a$  being here considered as fixed.

Then (1.7-9) immediately give

$$(1.12) \quad \tilde{\varepsilon}(\mathbf{F}, \theta) = \hat{\varepsilon}(\mathbf{C}, \theta),$$

the functions  $\tilde{\varepsilon}$  and  $\hat{\varepsilon}$  exhibiting the properties

$$(1.13) \quad \tilde{\varepsilon}(\mathbf{F}, \theta) = \tilde{\varepsilon}(\mathbf{Q}\mathbf{F}\mathbf{H}, \theta), \quad i. e. \quad \hat{\varepsilon}(\mathbf{C}, \theta) = \hat{\varepsilon}(\mathbf{H}'\mathbf{C}\mathbf{H}, \theta),$$

for any rotation  $\mathbf{Q}$ , any symmetric, positive-definite tensor  $\mathbf{C}$  and any  $\mathbf{H}$  in  $\bar{\mathbf{G}}$ .

#### MECHANICAL TWINS VS. GROWTH TWINS

Twinning, as the term is interpreted in the theory developed by Ericksen, Pitteri, James, Parry, Gurtin, Kinderlehrer (see the references), is considered as a continuous piece-wise homogeneous deformation  $\chi$  of a given homogeneous reference configuration  $R$  of a crystal such that, in the typical case of two phases, the following conditions are true:

*a)*  $\chi$  is a minimizer of the Helmholtz free energy functional of the body for zero loads;

*b)*  $\chi$  is specified by constant deformation gradients  $\mathbf{F}_1$  and  $\mathbf{E}_2$  defined on the two sides of a plane in  $R$  of normal  $\mathbf{F}_1'\mathbf{n}$  (called the «composition» plane), and solving the equations

$$(2.1) \quad \mathbf{F}_2 = \mathbf{Q}\mathbf{F}_1\mathbf{H} = (\mathbf{1} + \mathbf{a} \otimes \mathbf{n})\mathbf{F}_1,$$

with  $\mathbf{H}$  in the material symmetry group  $\mathbf{G}$  of the body,  $\mathbf{Q}$  a rotation not in  $\mathbf{G}$  and  $\mathbf{a}$  a suitable vector. At this stage,  $\mathbf{G}$  is still left unspecified, and  $\mathbf{H}$  need not be orthogonal, nor belong to  $\bar{\mathbf{G}}$ . In any case, we assume  $\det \mathbf{H} = \det \mathbf{Q}$ ; then  $\det(\mathbf{1} + \mathbf{a} \otimes \mathbf{n}) = 1$ , so that  $\mathbf{a} \cdot \mathbf{n} = 0$ , and  $\mathbf{1} + \mathbf{a} \otimes \mathbf{n}$  turns out to be a simple shear,  $S$  say.

Notice that the condition that  $\mathbf{H} \in \mathbf{G}$  is very important for the deformation  $\chi$  to be a stable equilibrium state of the body under zero dead loads. Indeed, by (2.1)<sub>1</sub> and (1.13)<sub>1</sub>, in this case the two twinned phases reach the same (minimum) value of the free energy. Such minimizers are called «symmetry-related», for obvious reasons; in principle, there is the possibility that non-symmetry-related minimizers of the free energy also exist.

Nevertheless, it is commonly assumed that this happens only at isolated values of the temperature  $\theta$ , and we do not consider these cases here. Thus, the condition that the tensor  $\mathbf{H}$  appearing in (2.1) belong to the material symmetry group  $\mathbf{G}$  of the crystal, becomes necessary to the stability of the twin. As we shall see in Remark III of Note II, this is a point of great importance when trying to assess the most suitable  $\mathbf{G}$  for crystalline solids, see also Ericksen 1987.

Let  $R$  be generated as usual by some reference lattice vectors  $\mathbf{E}_a$ . When the Cauchy-Born rule applies, *i.e.* when (1.10) holds, then by (1.3) equation (2.1) is easily seen to be equivalent to

$$(2.2) \quad b_a^b \mathbf{Q}\mathbf{e}_b = \mathbf{S}\mathbf{e}_a \quad \text{with} \quad b \in GL(3, \mathbf{Z}),$$

where the vectors  $e_a = F_1 E_a$  play the role of lattice vectors on one side of the composition plane in the deformed configuration  $\chi(R)$ , whose normal is  $n$ .

Equations (2.1) and (2.2) can be referred to as the «twinning equations»: (2.2) implies that both  $S e_a$  and  $Q e_a$  are possible sets of lattice vectors generating the twinned lattice on the other side of the interface. The twinned lattice is hence obtained from the parent one *either* by a simple shear  $S$  (the «twinning shear») *or* by a rotation  $Q$  (the «twinning operation»). Relation (2.2)<sub>2</sub> implies that the tensor  $H$  in (2.1) belongs to the group  $G$  introduced in sect. 1.

REMARK I: Notice that, if only the lattice structure of a twin pair is known, without any further information concerning the actual macroscopic deformation that possibly took place, as is usually the case after X-ray inspection of the twinned specimens, then many different descriptions of the same crystalline configuration are possible. In fact,  $Q$  and  $S$  are determined as solutions of any equation of the type (2.2) only up to point group operations, and to lattice invariant shears with same composition plane, respectively.

Indeed, let equation (2.2) hold, and  $\bar{S}$  and  $\bar{Q}$  satisfy (1.5): then we immediately see that  $\bar{S}\bar{S}$  and  $\bar{Q}\bar{Q}$  solve an equation of the type (2.2) with  $\bar{b} = s^{-1} b q \in GL(3, \mathbf{Z})$ . This leaves open a wide range of possibilities that are used in trying to match macroscopic changes of shape with X-ray observations (see for instance Nishiyama 1978).

Similarly, it can be seen that the twinning equations are independent of the set of lattice vectors  $E_a$  chosen.

Equations (2.1-2) which give rise to the «simple shear condition» described above, are well known consequences (see for instance Truesdell and Toupin 1960, eq. (175.9)<sub>1</sub>) of the supposed *continuity* of the deformation  $\chi$  bringing the homogeneous configuration  $R$  to the deformed one «containing» the twin.

Now, such continuity seems always to hold for what workers consider to be *mechanical* twinning: a continuous, macroscopic shearing deformation is actually observable in *all* the twinning deformations mechanically induced from a homogeneous parent crystal.

Indeed, the question of existence of *mechanical* twins *not* involving any shearing deformation of an originally homogeneous crystal was raised long ago, see Friedel 1926, pp. 488-89, for instance (who gave what appears to be a wrong example in his well known textbook, as is discussed in the Appendix to Note II).

Nevertheless, it seems now pretty well agreed that all mechanical twins actually involve a shearing deformation; in fact, there is quite a common consent for instance to the statement by Cahn 1954, pp. 367 and 376: «It is an empirical fact that mechanically induced twins always occur in this way», *i.e.* «with a part of the parent crystal transformed undergoing a macroscopic change of shape which can be described exactly as a simple shear»<sup>(2)</sup>.

Hence, a deformation  $\chi$  meeting all the conditions stated with equation (2.1), with all

(<sup>2</sup>) Dauphiné twinning in quartz is an example of mechanical twins with no macroscopic change of shape, and hence with no homogeneous shear involved. Indeed it is the only of this kind known to Cahn 1954, p. 367, p. 433. However, as already mentioned in sect. 1, this is a type of twinning we do not consider here.

the subsequent crystallographic implications of equation (2.2) whenever the Born rule applies, seems to give an appropriate formal description of *mechanical* twinning.

On the contrary, in dealing with growth twins, there is no need to presume that the twinned crystal has ever experienced a continuous deformation from a homogeneous (reference) state. Actually, some instances of twinned crystals reported in literature lead to the conclusion that the continuity assumption above could not be sound in many cases. We give here one of these examples: a growth twin in alum which is carefully described in by Shalkolsky and Schubnikow 1933 and Friedel 1933.

Small cubic crystal sprinkled onto the horizontal face of a large octahedron immersed into a saturated solution were found to adhere to the octahedral face either in parallel or twinned positions. The twin mutual orientation was determined by the sole condition of parallelism in the two individuals of the closest packed rows belonging to the interface.

The lattice is in this case face-centered-cubic, with lattice vectors  $E_a$  such that

$$(2.3) \quad E_a \cdot E_b = \begin{bmatrix} 1/2 & 1/4 & 1/4 \\ 1/4 & 1/2 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{bmatrix}$$

The cubic cell edge hence is of unit length. The twinning operation is the following rotation  $Q$ :

$$(2.4) \quad QE_a = q_a^b E_b, \quad \text{with} \quad q_a^b = \begin{bmatrix} \sqrt{3}/2 & -\sqrt{3}/2 & 1/2 \\ \sqrt{3}/2 & \sqrt{3}/6 & (3-2\sqrt{3})/6 \\ 0 & 0 & 1 \end{bmatrix}$$

It brings the  $\langle E_3, E_2 - E_1 \rangle$  cubic face onto the  $\langle E_2, E_3 \rangle$  octahedral face through a rotation about the axis  $E_3$ . With the given data, equation (2.2) cannot be solved, in the sense that it is not possible to find a matrix  $h$  in  $GL(3, \mathbf{Z})$  and a simple shear  $S$  (with amplitude parallel to the interface indicated above) such that equation (2.2) holds with the rotation  $Q$  defined in (2.4). The proof is obvious once it is seen that the two individuals meet at lattice planes which do *not* share congruent nets of lattice points, this being a necessary condition for equation (2.2) to hold, in the case of rational interfaces<sup>(3)</sup>. Notice also

<sup>(3)</sup> *Crystallographic* (or *rational* or *lattice-*) planes are planes containing two dimensional sub-lattices («nets») of a given lattice. They are characterized by integral indices, that is, the normal directions can be expressed as integral combinations of the reciprocal lattice vectors  $E^a$ .

Two rational planes of a lattice are said to be crystallographically equivalent when they can be brought into coincidence by a point group operation, so that they have the same indices relative to suitable congruent sets of lattice vectors. We remark that, whereas two crystallographically equivalent planes in a lattice of course carry congruent nets of atoms, the converse is not true. We also see that, in the case of a rational interface, the twinning equation implies that the net of atoms on the contact plane is common to the two individuals; this follows immediately from the fact the points on the interface are fixed points for the twinning shear. This necessary condition is not satisfied by the structure of the alum twin analyzed in the text.

that the twinning operation is not of order 2, 3, 4 or 6. These and other related features of twins are discussed in some detail in sect. 2 of Note II.

We thus conclude that growth twins are in general materially uniform bodies that can be found in configurations not homeomorphic to any homogeneous one: hence they possibly contain dislocations, according to the theory developed by Noll 1967 and Wang 1967. In a sense, we can say they do not have a homogeneous reference configuration at all; as a matter of fact, polycrystals do not experience such configurations while growing. The example given here is not the only one known; for others, see sect. 2 of Note II.

The discussion above makes it clear that a basic distinction arises between *mechanical* and *growth* twins, and that the thermoelastic theory developed by the authors quoted at the beginning of the section can only account for the former. We will take this a *definition* of mechanical twinning. A comprehensive treatment of growth twinning is not yet available (see sect. 2 of Note II and Zanzotto 1990).

We keep this basic distinction explicit throughout this work, noting that a classification of twins according to their origin is of course very common also in mineralogical and metallurgical literature, where *growth*, *deformation* and *transformation* twins are distinguished. The last named are obtained as the effect of the variations of temperature and, together with deformation twins, fall in the class of mechanical twins defined here.

Let us mention incidentally that, although the actual «physical» origin of a twin is usually known, there are nevertheless cases in which this origin is not clear (see Kelly and Groves 1970, p. 290). When this happens, the distinction introduced in the theory can help, in the sense that it can at least exclude the mechanical origin of given twins if equations (2.1-2) are not satisfied.

#### MECHANICAL TWINS: «TYPE 1», «TYPE 2» AND «RATIONAL» TWINS.

##### VALIDITY OF THE BORN HYPOTHESIS

As emerges from the works of Pitteri 1985*a*, 1986, 1987, Ericksen 1985, 1986, one class of solutions of (2.1) (or equivalently of (2.2)) is pretty well understood: the one with  $H$  (or  $b \in GL(3, \mathbf{Z})$ ) of period two. As is stated by Pitteri, these solutions correspond to what are often referred to as Type 1 and Type 2 twins in mineralogical and metallurgical literature, in that the two individuals in a twin pair can be related by either one of the following rotations:

$$(3.1) \quad Q = D(\mathbf{1} - 2\mathbf{n} \otimes \mathbf{n}) \quad \text{or} \quad \bar{Q} = D[\mathbf{1} - 2(\mathbf{a} \cdot \mathbf{a})^{-1} \mathbf{a} \otimes \mathbf{a}] \quad D \pm 1,$$

where the same notations are used as in sect. 2. Of course, by Remark I, other descriptions are possible if the point group is not trivial: see Remark VI in Note II.

We will call «conventional» the orientations above; they represent, respectively, a rotation of  $\pi$  about the normal  $\mathbf{n}$  to the composition plane  $S$  (or equivalently, in the simple Bravais lattices we are considering here, a mirror symmetry relation across  $S$ ), and a rotation of  $\pi$  about the direction of the amplitude  $\mathbf{a}$  (or equivalently a mirror symmetry relation across the plane orthogonal to  $\mathbf{a}$ ).

Twins in which the twin law can be interpreted either way are termed «compound».

Now, two different definitions of Type 1 and Type 2 (and of compound) twins are common in the literature, and are considered equivalent by widespread consent.

To be precise, let us introduce the elements  $K_1$ ,  $K_2$ ,  $\eta_1$ ,  $\eta_2$ ,  $S$  and  $s$  of a given shear  $S = \mathbf{1} + \mathbf{a} \otimes \mathbf{n}$ . As usual,  $K_1$  is the invariant plane of  $S$ , which is orthogonal to the vector  $\mathbf{n}$ ; the direction of the vector  $\mathbf{a}$  is indicated by  $\eta_1$  and is called the «shear direction»; the «plane of shear»  $S$  is the plane containing  $\mathbf{a}$  and  $\mathbf{n}$ , and  $K_2$  is the «second undistorted plane».  $K_1$  is neither rotated nor distorted while  $K_2$  is only rotated. The intersection of  $S$  with  $K_2$  is the direction  $\eta_2$ , and finally  $s = \sqrt{\mathbf{a} \cdot \mathbf{a}}$  is the «amount of shear». The shear  $S$  is determined either by  $K_1$  and  $\eta_2$  or  $K_2$  and  $\eta_1$ .

Whereas we defined Type 1 and Type 2 twins by means of the orientations (3.1), following for instance Pitteri 1985a, 1986, 1987, Crocker 1962, p. 1902, Bilby and Crocker 1965, p. 241, Bevis 1968, in most of the classical references in mineralogy or metallurgy another definition is adopted, according to which Type 1 are modes which can be described by a twinning shear whose elements  $K_1$  and  $\eta_2$  are rational, while  $K_2$  and  $\eta_1$  are irrational; the converse is true for Type 2 twins. Furthermore, «compound» twins are those in which all the four shear elements are rational, see for instance Barret and Massalski 1966, Cahn 1954, Hall 1954, Kelly and Groves 1970, Klassen-Nekliudova 1964.

The common understanding is that the two points of view are equivalent.

We prove now with an example that, *if the Born rule as stated in sect 1 applies, then the two definitions above are actually not equivalent.*

Accordingly, we will call here «Type 1» and «Type 2» the twins whose law is given by (3.1)<sub>1,2</sub> respectively, and «Rational of Type 1» and «Rational of Type 2» those mechanical twins in which the twinning shear elements  $K_1$ ,  $K_2$ ,  $\eta_1$  and  $\eta_2$  have the rationality properties stated above; we will generically call «conventional» the above assumptions on rationality.

Let us consider lattice vectors  $E_a$  such that

$$(3.2) \quad E_a \cdot E_b = \begin{bmatrix} 1 & 0 & \alpha \\ 0 & 1 & \beta \\ \alpha & \beta & 1 + \alpha^2 + \beta^2 \end{bmatrix},$$

where  $\alpha$  and  $\beta$  are suitable rational (non integral) numbers, with  $\alpha \neq \beta$ , and let us introduce the shear

$$(3.3) \quad S = \mathbf{1} + [(\beta - \alpha)E_1 - (\alpha + \beta)E_2] \otimes E^3,$$

where  $E^a$  are reciprocal lattice vectors:  $E_a \cdot E^b = \delta_a^b$ .

It is not difficult to prove that the above shear  $S$  is indeed a twinning shear for the lattice generated by vectors (3.2), in that it solves the twinning equation (2.2) with lattice generated by vectors (3.2), in that it solves the twinning equation (2.2) with matrix  $b_a^b$  and rotation  $R$  as follows:

$$(3.4) \quad b_a^b = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R = \mathbf{1} - (E_2 + E_1) \otimes E_1 - (E_2 - E_1) \otimes E_2.$$

Here,  $b$  has period four; also,  $R$  has period four and axis  $E^3$ . Furthermore,

it can be proved that none of the operations (3.1) can account for the twin orientation in this case.

This shows that, if *all* the lattice points follow the path dictated by the shear  $S$ , that is, if the Born rule applies, then the final reorientation of a rational *compound* twin can be different from the conventional laws indicated in (3.1), see also Remarks V and VI in Note II.

Hopefully, this issue will be completely clarified elsewhere. Nevertheless, the question is raised, which is of great interest in itself, of whether the Born hypothesis truly holds in general, that is, whether the relationship between the macroscopic and molecular descriptions is given by equation (1.10) also in the range of «large» deformations.

It is known that in some types of phase transitions there are problems with the validity of Born's assumption (Ericksen 1982, 1984, Parry 1981).

However, away from such changes of symmetry, the behaviour of crystal structures in this regard is not very well understood.

As a matter of fact, the Born hypothesis is tacitly assumed true in most of the experimental literature where it is used in connection with the relatively «small» macroscopic deformations that a crystal undergoes in compression or in thermal expansion as a consequence of changes in the environmental conditions. For a brief discussion on this, see footnote (<sup>4</sup>).

Experimental evidence indicates that, in the case of single lattice structures, the Born hypothesis does hold even in the range of large twinning deformations, a clear example being given by crystalline mercury (see Crocker *et al.* 1966, Guyoncourt and Crocker 1968). In these cases, the actual observed twinning modes always involve a macroscopic shear deformation that is capable of restoring the whole lattice structure of the new reoriented individual, with no need of «structural» shuffling as it is meant in sect. 1. In other words, the macroscopic shear, which is described by the tensor  $S = 1 + a \otimes n$  appearing in equation (2.1), is such that equation (2.2) holds, with  $Q$  the twinning operation. Hence, all the lattice points in the parent configuration generated by  $e_a$ , are effectively sheared to new positions in such a way to restore a twinned lattice generated by lattice vectors  $Qe_a$ , as discussed below equation (2.2).

However, this does not always happen in the shear deformations involved in many of the mechanical twinning modes for crystals whose structure is *not* a simple Bravais lattice, such as the hexagonal close-packed metals, for instance. In these cases, the restoration in shear of a 3-dimensional sub-lattice appears to suffice, so that the remaining lattice points have to undergo some additional shuffle movement («struc-

(<sup>4</sup>) Some interesting experimental observations, performed by Balzer and Sigvaldson 1979a, 1976b, show that the Born rule sometimes does not even apply to the kind of «small» deformations mentioned in the text. Indeed, these authors measured the thermal expansion of tetragonal Tin and hexagonal Zinc, simultaneously in the lattice parameters and in the length of macroscopic specimens. The results agreed very well only for Tin, Zinc showing considerable divergence in the two length changes measured. The authors opine that this is associated with defects of the crystal structure, namely vacancies.

The experiments show that, independent of the actual causes which we do not discuss here, it is not always safe to use the Born hypothesis to relate the gross and microscopic deformations, not even in the cases in which this appears to be a most natural possibility.

tural» shuffling) to reach the correct twinned positions. About this, see for instance Cahn 1953, 1954, Crocker and Bevis 1970, Hall 1954, Kelly and Groves 1970.

It is to be noticed that in these and other works, a great number of twinning modes in metals involving structural shuffling is reported. Yet, the common practice for finding the shear elements is to determine only a part of them through actual measurements of twinned specimens. Typically, the indices of the contact plane  $K_1$ , and sometimes of the shear direction  $\eta_1$ , are evaluated by means of X-ray diffraction. Then geometrical considerations are employed to estimate the other elements of the shear, following some *a priori* guidelines, such as the «minimum shear» rule mentioned in the Introduction, to help eliminate some of the various possibilities that are allowed in estimating the macroscopic deformation, see Remark I. A clear example of this common procedure is given by Hall 1954, pp. 74 and 79.

It follows that in these cases, since the actual macroscopic deformation is unknown and only estimated, it is impossible to effectively check the validity of the Born rule.

There are exceptions. Rapperport 1959 and Reed-Hill *et al.* 1963, for instance, carefully investigated various twinning modes in Zirconium, using X-ray techniques for establishing the crystal orientations and macroscopic measurements to determine the elements of the shearing deformation. Their observations seem to establish beyond doubt that the Born rule, as stated by Ericksen 1984, fails to apply to these metals.

Indeed, the experimental results of the kind mentioned above can be described by the statement that the Born hypothesis applies to a suitable sub-lattice, which is different for each different observed twinning mode, rather than to the whole lattice of the crystal; this means that eq. (1.10) should be replaced by

$$(3.5) \quad \mathbf{v}_a = F\mathbf{V}_a$$

with  $\mathbf{v}_a$  [ $\mathbf{V}_a$ ] appropriate sub-lattice vectors (see Ericksen 1982) in the twinned [reference] configuration, different from the actual lattice vectors. Since we can always write  $\mathbf{V}_a = m_a^b \mathbf{E}_b$  with  $m_a^b$  integers and  $\det m_a^b > 1$ , equation (2.1) becomes, with the aid of (3.5):

$$(3.6) \quad k_a^b \mathbf{Q} \mathbf{e}_b = \mathbf{S} \mathbf{e}_a \quad \text{with} \quad k_a^b = (m^{-1})_a^i h_i^r m_r^b \quad \text{and} \quad h \in GL(3, \mathbf{Z}),$$

so that  $k_a^b$  is not in  $GL(3, \mathbf{Z})$ , because it has rational entries. Hence, in these cases, the twinning elements  $\mathbf{Q}$  and  $\mathbf{S}$  satisfy an equation like (3.6), in which the matrix  $m_a^b$  varies for each twinning mode in an unpredictable way, rather than (2.2).

The works by Rapperport 1959 and Reed-Hill *et al.* 1963 constitute a direct confirmation that, among the aforementioned various geometrical estimates of the twinning shear elements in metals and minerals, there are certainly cases in which the Born rule fails to apply in the many twinning modes actually observed in crystals whose structure is *not* a simple lattice; see for some clear examples Cahn 1953, commented on by Crocker 1965 and Bevis 1968, or Crocker and Bevis 1970. Some authors indeed express the opinion that in certain material shuffles are unavoidable, see Crocker *et al.* 1966, pp. 1202-3; see also Remark IV in Note II.

Let us notice that this also confirms the results of the measurements reported by the German mineralists of the early 1900's, like Johnsen, Mügge, Niggli, which are

credited by Klassen-Nekliudova 1964, pp. 10-12, for first pointing out the problem. On this question, see also Friedel 1926, pp. 486-7, where the example of calcite is considered. This is a case in which, even though the crystal is a multi-lattice, the Born rule works. In fact, the twinning shear restores correctly the whole fundamental lattice without structural shuffling; motif shuffling of the cluster of atoms at the centre of the unit cell is then necessary in order to correctly restore the microstructure. This is clearly exemplified by fig. 8 in Klassen-Nekliudova 1964.

Structural shuffles in mechanical twinning are discussed in detail by Bilby and Crocker 1965, Bevis and Crocker 1967, Bevis and Crocker 1969.

Some further comments on the foregoing observations are made in sect 1 of Note II.

#### REFERENCES

- ACTON A. F., M. BEVIS, A. G. CROCKER and D. H. ROSS (1970) – *Transformation strains in lattices*, «Proc. Roy. Soc. Lond.», A 320, 101.
- BALL J. M. and R. D. JAMES (1987) – *Fine phase mixtures as minimizer of energy*, «Arch. Rational Mech. Anal.», 100, 13.
- BALZER R. and H. SIGVALDSON (1979a) – *Equilibrium vacancy concentrations measurements on Zinc single crystals*, «J. Phys. F: Metal. Phys.», 9, 171.
- BALZER R. and H. SIGVALDSON (1979b) – *Equilibrium vacancy concentrations measurements on Tin single crystals*, «Phys. Stat. Sol. (b)», 92, 143.
- BARRETT C. S., and T. B. MASSALSKI (1966) – *The structure of metals*, McGraw-Hill.
- BEVIS M. (1968) – *On the crystallography of deformation twinning in alpha-Uranium*, «J. Nucl. Mater.», 26, 235.
- BEVIS M. and A. G. CROCKER (1968) – *Twinning shears in lattices*, «Proc. Roy. Soc. Lond.», A304, 123.
- BEVIS M. and A. G. CROCKER (1969) – *Twinning modes in lattices*, «Proc. Roy. Soc. Lond.», A 313, 509.
- BEVIS M., P. C. ROWLANDS and A. F. ACTON (1968) – *Deformation and transformation twinning modes in Fe-Ni and Fe-Ni-C martensites*, «Trans. Met. Soc. AIME», 242, 1555.
- BILBY B. A. and A. G. CROCKER (1965) – *The theory of crystallography of deformation twinning*, «Proc. Roy. Soc. Lond.», A 288, 240.
- BUERGER M. J. (1945) – *The genesis of twin crystals*, «J. Min. Soc. Am.», 30, 469.
- BUERGER M. J. (1960) – *Symposium on twinning. Introductory remarks*, in *Cursillos y Conferencias del Instituto «Lucas Mallada»*, Fasciculo VII, C.S.I.C. Madrid, 1960.
- CAHN R. W. (1953) – *Plastic deformation of alpha-Uranium; twinning and slip*, «Acta Metall.», 1, 49.
- CAHN R. W. (1954) – *Twinning crystals*, «Advances in Physics», suppl. of «Phyl. Mag.», 3, 363.
- CROCKER A. G. (1962) – *Double twinning*, «Phyl. Mag.», 7, 1901.
- CROCKER A. G. (1965) – *The crystallography of deformation twinning in alpha-Uranium*, «J. Nucl. Mater.», 16, 306.
- CROCKER A. G. (1982) – *The phenomenological theory of martensite crystallography*, «Journal de Physique, suppl. n. 12», 43, 209.
- CROCKER A. G., M. BEVIS and R. H. RICKMAN (1963) – *Discussion*, «Trans. Met. Soc. AIME», 227, 1471.
- CROCKER A. G., F. HECKSCHER, M. BEVIS and D. M. M. GUYONCOURT (1966) – *A single surface analysis of deformation twins in crystalline Mercury*, «Phil. Mag.», 13, 1191.
- CROCKER A. G. and M. BEVIS (1970) – *The crystallography of deformations twinning in Titanium*, in «The science, technology and application of Titanium» (T. Jaffee and R. Promisel eds.), Pergamon Press.

- CURIEN H. (1960) – *Sur les axes de maclé d'ordre supérieur à deux*, in *Cursillos y Conferencias del Instituto «Lucas Mallada» Fascículo VII*, C.I.S.C. Madrid.
- CURIEN H. and R. KERN (1957) – *Macles par contact et par pénétration. Essai d'interprétation causale*, «Bull. Soc. Franç. Miner. Crist.», 80, 111.
- DANA J. D. (1962) – *The System of Crystallography*, «Seventh edition», Wiley, New York and London.
- DANIEL J. S., B. LESAGE and P. LACOMBE (1971) – *The influence of temperature on slip and twinning in Uranium*, «Acta Met.», 19, 163.
- DONNAY J. D. H. (1952) – *Cryolite twinning*, «Am. Min.», 37, 230.
- DONNAY J. D. H. (1960) – *Twinning*, in «Encyclopaedia Britannica», Vol. 6, p. I-810, K. M. Benton Publisher, Chicago etc.
- DUBERTRET A. and A. LE LANN (1979) – *A development of Kronberg's model for {1, 0, -1, 2} twins in b.c.p. metals*, «Phys. Stat. Sol.», 51, 497.
- DUBERTRET A. and A. LE LANN (1980) – *Development of a new model for atom movement in twinning*, «Phys. Stat. Sol.», 60, 145.
- EFTIS J., D. E. MAC DONALD and G. M. ARKILIC (1971) – *Theoretical calculations on the pressure variations of the 2<sup>nd</sup> order elastic coefficients for alkali metals*, «Mater. Sci. Eng.», 7, 141.
- ELLIS W. C. and R. G. TREUTING (1951) – *Atomic relationship in the cubic twinned state*, «Trans. Amer. Inst. Metall. Engrs.», 200, 53.
- ELLIS W. C. and R. G. TREUTING (1951) – *Atomic relationship in the cubic twinned state; discussion*, «Trans. Amer. Inst. Metall. Engrs.», 200, 1070.
- ERICKSEN J. L. (1970) – *Some topics in Elastostatics*, in «Advances in Applied Mechanics» (C. S. Yih ed.), vol. 17, Academic Press. New York etc.
- ERICKSEN J. L. (1979) – *On the symmetry of deformable crystals*, «Arch. Rational Mech. Anal.», 72, 1.
- ERICKSEN J. L. (1980a) – *Some phase transitions in crystals*, «Arch. Rational Mech. Anal.», 73, 99.
- ERICKSEN J. L. (1980b) – *Changes in symmetry of elastic crystals*, Proceedings of the IUTAM Symposium on Finite Elasticity (D. E. Carlson and R. T. Shield eds.), M. Nijhoff Publishers, The Hague etc.
- ERICKSEN J. L. (1982) – *Crystal lattices and sub-lattices*, «Rend. Sem. Mat. Padova», 68, 1.
- ERICKSEN J. L. (1983) – *The theory of stress-free joints*, «J. Elasticity», 13, 3.
- ERICKSEN J. L. (1984) – *The Cauchy and Born hypotheses for crystals*, in «Phase transformations and materials instabilities in solids» (M. F. Gurtin ed.), Academic Press, New York.
- ERICKSEN J. L. (1985) – *Some surface defects in unstressed thermoelastic solids*, «Arch. Rational Mech. Anal.», 88, 337.
- ERICKSEN J. L. (1986) – *Stable equilibrium configurations for elastic crystals*, «Arch. Rational Mech. Anal.», 94, 1.
- ERICKSEN J. L. (1987) – *Twinning in crystals*, in «Metastability and incompletely posed problems» (S. Antman, J. L. Ericksen, D. Kinderlehrer and I. Müller, eds.), IMA Volumes in Mathematics and Applications, Vol. 3, Springer, New York etc.
- EVANS J. W. (1912) – *The geometry of twinned crystals*, «Proc. Roy. Soc. Edinburgh», 32, 416.
- FRIEDEL G. (1923) – *Sur les macles du quartz*, «Bull. Soc. Franç. Min.», 46, 79.
- FRIEDEL G. (1926) – *Leçons de Cristallographie*, Librairie Scientifique Blanchard, Paris.
- FRIEDEL G. (1933) – *Sur un nouveau type de macles*, «Bull. Soc. Franç. Min.», 56, 262.
- GURTIN M. E. (1983) – *Two-phase deformations of elastic solids*, «Arch. Rational Mech. Anal.», 84, 1.
- GUYONCOURT D. M. M. and A. G. CROCKER (1968) – *The deformation twinning mode of crystalline mercury*, «Acta Met.», 16, 523.
- HALL E. O. (1954) – *Twinning and diffusionless transformations in metals*, Butterworths, London.
- HARTMAN P. (1956) – *On the morphology of growth twins*, «Zeit. fur Krist.», 107, 225.
- HOLSER W. T. (1958) – *Relation of symmetry to structure in twinning*, «Zeit. fur Krist.», 110, 249.
- HOLSER W. T. (1960) – *Relation of pseudosymmetry to structure in twinning*, in *Cursillos y Conferencias del Instituto «Lucas Mallada» Fascículo VII*, C.S.I.C. Madrid.

- ICHINOSE S., Y. FUNATSU and K. OTSUKA (1985) – *Type II deformation twinning in  $\gamma'$ -martensite in Cu-Al-Ni alloy*, «Acta Metall.», 33, 1613.
- JAMES R. D. (1981) – *Finite deformations by mechanical twinning*, «Arch. Rational Mech. Anal.», 77, 143.
- JAMES R. D. (1982) – *Mechanics of coherent phases in solids*, «Material Research Laboratory Report MRL», E-143, Brown University, Providence.
- JAMES R. D. (1984) – *Stress-free joints and polycrystals*, «Arch. Rational Mech. Anal.», 86, 13.
- JAMES R. D. (1987) – *The stability and metastability of quartz*, in «Metastability and incompletely posed problems» (S. Antman, J. L. Ericksen, D. Kinderlehrer and I. Müller eds.), IMA Volumes in Mathematics and Applications, Vol. 3, Springer, New York etc.
- KELLY A. and G. W. GROVES (1970) – *Crystallography and crystal defects*, Addison-Wesley, Reading etc.
- KERN R. (1961) – *Sur la formation des macles de croissance*, «Bull. Soc. Franç. Min. Crist.», 84, 292.
- KINDERLEHRER D. (1987a) – *Twinning in crystals (II)*, «Metastability and incompletely posed problems» (S. Antman, J. L. Ericksen, D. Kinderlehrer and I. Müller, eds.), IMA Volumes in Mathematics and Applications, Vol. 3, Springer, New York etc.
- KINDERLEHRER D. (1987b) – *Remarks about the equilibrium configurations of crystals*, «IMA Preprint series n. 289», University of Minnesota, Minneapolis USA.
- KLASSEN-NEKLIUDOVA M. V (1964) – *Mechanical twinning of crystals*, Consultant Bureau, New York.
- MATHEWSON C. H. (1928) – *Twinning in metals*, «Amer. Inst. Metall. Engrs., Proc. Inst. Metals. Div.», 78, 5, 554.
- MILLER W. (1972) – *Symmetry groups and their applications*, Academic Press, New York-London.
- NISHYAMA Z. (1978) – *Martensitic transformation*, Academic Press, New York, San Francisco London.
- NOLL W. (1967) – *Materially uniform simple bodies with inhomogeneities*, «Arch. Rational Mech. Anal.», 27, 1.
- OTTE H. M. and A. G. CROCKER (1965) – *Crystallographic formulae for hexagonal lattices*, «Phys. Stat. Solidi», 9, 441.
- PARRY G. P. (1976) – *On the elasticity of monatomic crystals*, «Math. Proc. Camb. Phil. Soc.», 80, 189.
- PARRY G. P. (1981) – *On the phase transitions involving internal strain*, «Int. J. Solids Structures», 17, 361.
- PARRY G. P. (1982) – *On structural phase transitions in perfect crystals*, «Int. J. Solids Structures», 18, 59.
- PITTERI M. (1984) – *Reconciliation of global and local symmetries in crystals*, «J. Elasticity», 14, 175.
- PITTERI M. (1985a) – *On the kinematics of mechanical twinning in crystals*, «Arch. Rational Mech. Anal.», 88, 25.
- PITTERI M. (1985b) – *On  $v + 1$  lattices*, «J. Elasticity», 15, 3.
- PITTERI M. (1986) – *On Type 2 twins*, «Int. J. Plast.», 2, 99.
- PITTERI M. (1987) – *A contribution to the description of natural states for elastic crystalline solids*, in «Metastability and incompletely posed problems» (S. Antman, J. L. Ericksen, D. Kinderlehrer and I. Müller eds.), IMA Volumes in Mathematics and Applications, Vol. 3, Springer, New York etc.
- RAPPERPORT E. J. (1959) – *Room temperature deformation process in Zirconium*, «Acta Met.», 7, 254.
- REED-HILL R. E. and R. D. ROBERTSON (1957) – *Additional modes of deformation twinning in Magnesium*, «Acta Met.», 5, 717.
- REED-HILL R. E., W. A. JR. SLIPPY and L. J. BUTEAU (1963) – *Determination of alpha Zirconium  $\{11\bar{2}1\}$  twinning elements using grain boundary rotations*, «Trans. Met. Soc. AIME», 227, 976.
- RICHMAN R. H. (1963) – *Plastic deformation modes in Fe-Ni-C martensites*, «Trans. Met. Soc. AIME», 227, 159.

- RICHMAN R. H. and G. P. CONARD (1963) – *Mechanical twinning in Fe–5 wt pct Be*, «Trans. Met. Soc. AIME», 227, 779.
- SANTORO A. and A. D. MIGHELL (1973) – *Coincidence-site lattices*, «Acta Cryst. A», 29, 171.
- SANTORO A. (1974) – *Characterization of twinning*, «Acta Cryst. A», 30, 224.
- SHALKOLSKY M. and A. SCHUBNIKOW (1933) – *Über die künstliche Herstellung gesetzmassiger Kristallverwachsungen des Kalkalauns*, «Zeit. für Krist.», 85, 1.
- TAKEDA H., J. H. D. DONNAY and D. E. APPELMAN (1967) – *Djurleite twinning*, «Zeit. für Krist.», 125, 414.
- TERTSCH H. (1949) – *Die Festigkeitsercheinungen der Kristalle*, Springer, Wien.
- TRUESDELL C. (1977) – *A first course in Rational Continuum Mechanics*, vol. 1, Academic Press, New York etc.
- TRUESDELL C. and R. A. TOUPIN (1960) – *The classical field theories*, Handbuch der Physik III/1, Springer-Verlag, Berlin, Heidelberg, New York, 1960.
- WANG C.-C. (1967) – *On the geometric structures of simple bodies. A mathematical foundation for the theory of continuous distributions of dislocations*, «Arch. Rational Mech. Anal.», 27, 33.
- ZANZOTTO G. (1988) – *Twinning in minerals and metals: remarks on the comparison of a thermoelastic theory with some experimental results. Mechanical twinning and growth twinning: Nota II.*, «Atti Acc. Lincei Rend. fis.», 82, 743.
- ZANZOTTO G. (1990) – *Thermoelastic stability of multiple growth twins in quartz and general geobarothermometric implications*, «J. Elasticity», 23, 253.
- ZANZOTTO G. (1991) – *On the material symmetry group of elastic crystals and the Born Rule*, in preparation.
- ZOLTAI T. and J. H. STOUT (1984) – *Mineralogy: concepts and principles*, Burgess, Minneapolis.
- ZYNDEL F. (1914) – *Über Quarzwillinge mit nichtparallelen Hauptaxen*, «Zeit. für Krist.», 53, 15.