

On the elastic energy invariance of crystal twins

R. GLÜGE

*Institut für Mechanik
Otto-von-Guericke-Universität Magdeburg
Postfach 4120
D-39106 Magdeburg, Germany
e-mail: gluege@ovgu.de*

AN ANALYSIS BY ZANZOTTO (1992, 1996) showed that, if crystal twinning is considered as a material symmetry operation, the symmetry groups of many crystals that form twins correspond to the unimodular group, which is the symmetry group of elastic fluids. It is therefore evident that an elastic modelling based on an elastic energy that includes any possible combination of twin system activation must fail. However, one may try to construct an elastic energy which includes only the stress-free configurations of the parent and the first order twins. It is known that, even under this restriction, many twinning modes exhibit an elastic energy invariance, which renders them indistinguishable in terms of the elastic energy. In this article, it is demonstrated that this energy invariance holds for all compound twins. The implications of the latter are discussed. It is suggested to distinguish between crystallographically equivalent and crystallographically distinct compound twins, since different implications regarding the elastic energy invariance emerge.

Key words: type 1, type 2, compound twinning, pseudoelasticity, nonconvex elastic energy, energy invariance.

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1. Introduction

MANY MATERIALS UNDERGO SOLID to solid phase changes upon thermal or mechanical loading, which induces, e.g., the shape memory effect (SMA), the transformation-induced plasticity effect (TRIP) or the twinning-induced plasticity effect (TWIP). In this work, the focus is on the isothermal and mechanically induced deformation twinning. Deformation twinning can be understood as a special deformation mode available in crystals. A crystal that undergoes twinning reorients its lattice, but unlike to martensitic transformations, does not change the lattice structure, which motivates the term “twinning”. For shuffle-free twinning modes, the twin lattice is obtained by applying a homogeneous shear deformation to the parent lattice, while for twinning modes including shuffling, the homogeneous shear deformation leaves only the atoms of a sub-lattice in their proper twin configuration, while the remaining atoms undergo a shuffling displacement (CHRISTIAN and MAHAJAN, 1995). In both cases, a regular reordering

of the atomic bonding is observed. Although from a chemical point of view one might not want to speak about a phase change, some characteristic ingredients of phase changes are displayed. Twinning produces sharp interfaces, at which the material properties that depend on the crystal orientation undergo a jump.

In contrast to crystallographic glide, twinning enables a crystal to accommodate rapid deformations at low temperatures, which may be exploited to expand the range of application of a material. However, twinning alters strongly the material properties, which is not always beneficial. The twins form as plates inside of grains (Fig. 1), and can alter significantly the morphological and the crystallographic texture, both influencing the yield locus and the elastic anisotropy, while the additional interfaces have an impact on the strain hardening. The interfaces contribute as well to the internal energy. Typical twin interface energies are found in a range from practically zero up to 500 mJ/m². They are mostly determined by molecular dynamic simulations (SERRA and BACON, 1986), since the experimental determination is difficult. Furthermore, the twinning mechanism is polar, which can cause a pronounced differential effect on the strength of the material and on the forming limit, depending on the crystallographic texture. For many materials, these effects are not negligible. Especially the ductile TWIP steels and the lightweight hcp metals, magnesium and titanium, which are interesting for engineering applications, display extensive twin formation at room temperature. Therefore, one is interested in the proper modelling of deformation twinning.

1.1. The pseudoelastic approach

Following the suggestions of ERICKSEN (1984b), one modelling approach could be the framework of elasticity. There are some objections to such an approach. First, the twin formation depends strongly on the specific twinning mode. Distinct twinning modes may display very different characteristics, e.g. the $\{011\bar{2}\}$ and the $\{011\bar{1}\}$ twinning in the hcp crystals. This is due to the underlying propagation mechanism, which may be shuffling dominated as for $\{011\bar{2}\}$ twinning (LI and MA, 2009a), or rely on the movement of pronounced partial dislocations, i.e. steps at the interface (as for $\{011\bar{1}\}$, LI and MA (2009b)). The interface propagation mechanism determines the dissipation due to the interface movement. If the interface movement depends on partial dislocations, the properties of these, like mobility, availability and producibility determine the characteristics of the interface energy and the interface mobility (SERRA and BACON, 1991). These differences can not be accounted for in a purely elastic framework. Moreover, the elastic modelling does not account for any kinetic aspect of twinning, which is too simplistic in many cases (ABEYARATNE and KNOWLES, 2006). E.g., there is no way to account for a strain path dependence. One should also note that an elastic energy which contains several twin configurations must

be nonconvex, which renders the pseudo-elastostatic boundary value problem ill posed (BALL and JAMES, 1987; CARSTENSEN, 2005). Finally, twinning induces a strain energy invariance, which may be considered as the result of additional material symmetry operations, which arises from the isomorphy of the twin and parent lattice (ERICKSEN, 1984b; ZANZOTTO, 1992).

The most crucial flaw, namely the ill-posedness of the pseudoelastic boundary value problem, may be overcome by introducing a kinetic relation or by a relaxation procedure, i.e. a convexification of the strain energy.

Convexification. There are basically two convexification strategies. Firstly, one may construct and use a convex hull from the nonconvex strain energy. By eliminating the nonconvex branches of the strain energy, the latter represents a special homogenisation scheme. Secondly, since the convexity of the strain energy is determined by the dependence on the highest strain gradient (SIDI AMMI and TORRES, 2008), one may add a convex strain gradient dependence to the internal energy. Physically, the latter corresponds to a penalisation of sharp strain gradients, and can therefore be interpreted as the energetic incorporation of regularised interfaces.

Kinetisation. CHRISTIAN (1975); ABEYARATNE and KNOWLES (1991) state that the missing part of the pseudoelastic boundary value problem is a nucleation criterion plus a kinetic relation for the phase boundaries. By this, the mathematical problem is shifted from nonconvex energy minimisation to evolution tracking. In order to avoid the tracking of the interfaces, one may introduce a general kinetic relation. If one wants to incorporate specific interface dynamics, the explicit interface tracking is unavoidable. This is a list of possible augmentations for the pseudoelastic material behaviour:

- convexification of the strain energy (time-independent)
 - construct and use a convex hull (also termed as relaxation, corresponds to a homogenisation)
 - add a convex elastic energy contribution from the strain gradient (capillarity, corresponds to an energetic incorporation of regularised interfaces)
- kinetisation
 - general kinetic relation
 - viscosity (with a convex elastic energy contribution, this corresponds to the incorporation of regularised interfaces, which are equipped with an energy and a specific kinetic relation (ABEYARATNE and KNOWLES, 1991))
 - dynamics (shocks and phase-boundaries, propagation of phase boundaries not completely determined (HOU *et al.*, 1999))

- kinetic relation for interfaces, nucleation criterion (sharp interface theory, explicit interface kinetics).

In particular, the viscous regularisation enjoys some popularity. It is often applied to single out solutions when strain softening, strain rate softening, damage or phase changes occur (DIAS DA SILVA, 2004; BÖHLKE *et al.*, 2009; CHABOCHE *et al.*, 2001; GLÜGE *et al.*, 2010). It is as well used to overcome the Taylor problem in crystal plasticity (HUTCHINSON, 1976), and to transform the algebraic differential equations governing ideal plastic material behaviour to ordinary differential equations (SIMO and HUGHES, 1998). It is also simple to implement, and compliant with thermodynamic considerations.

Phase boundaries. Mostly, interfaces are modelled by a phase field parameter, which is used for the smearing of the interface, in order to avoid a discontinuity. The latter method has coined the term “phase field method” (WANG *et al.*, 2004). It has some similarities to the level set method (HOU *et al.*, 1999). There are also approaches which use discrete interfaces. The latter treatments are quite challenging from a practical point of view. However, they lead, by incorporating the interface properties, to a physically better modelling.

Due to the interface energy, there exists a minimum twin thickness, given by an equilibrium between the twin thickness-dependent elastic energy reduction and the additional interface energy (KHACHATURYAN, 1983; PETRYK *et al.*, 2003). If the elastic properties of a material are known, one may even estimate the interface energy by measuring the characteristic twin thickness (DEMCZYK, 1990). Therefore, the interface energy rules out an infinite fine twin layering, as it is observed in the pseudoelastic boundary value problem (CARSTENSEN, 2005). Moreover, the interface energy is linked to the interface orientation. A deviation from the coherent interface orientation is not only penalised by an increased elastic misfit strain, but as well by an increase of the interface energy. Considering only the elastic misfit, one finds that so-called “kink twins” (FOREST and PARISOT, 2000; GLÜGE and KALISCH, 2008) are admissible. These kink twins form interfaces perpendicular to the twinning shear, which is not observed experimentally. By accounting for the interface energy, these twins can be excluded.

Despite of the problems listed above, elasticity appeals by its simplicity. And even for a more complex modelling, it is a basic ingredient. Therefore, it should be examined, which is the topic of this work. Here, the elastic strain energy invariance of first order twins is examined in detail, and the implications for the different twinning modes (type 1, type 2, compound and crystallographically equivalent, compound and crystallographically distinct) are discussed. It is found that, even with the restriction to first order twins, only in case of crystallographically equivalent compound twins and non-compound twins the purely elastic modelling is not *a priori* prohibitive. In any other situation, the strain

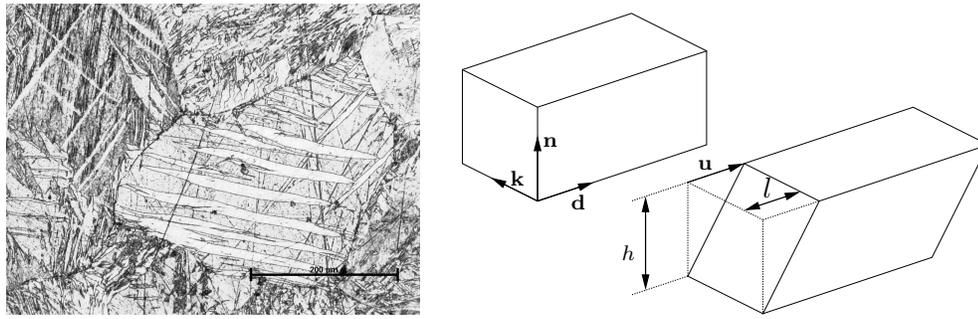


Fig. 1. Light microscope photograph of a polished magnesium sample (left). The twins appear as plates, which are aligned approximately coplanar to the shear plane. Simple shear deformation of a cuboid (right).

energy invariance connects different twin systems, or even a twinning mode with a lattice invariant shear. It is also discussed how the latter problem may be surmounted by the incorporation of an interface energy.

1.2. Notation

Throughout the text a direct tensor notation is preferred. If an expression cannot be represented in the direct notation without introducing new conventions, its components are given with respect to orthonormal base vectors \mathbf{e}_i , using the summation convention. Vectors are symbolised by lowercase bold letters, second order tensors by uppercase bold letters $\mathbf{T} = T_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$. The second order identity tensor is denoted by \mathbf{I} . The dyadic product is defined as $(\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{c} = (\mathbf{b} \cdot \mathbf{c})\mathbf{a}$. Orthogonal tensors are denoted by $\mathbf{Q} = \tilde{\mathbf{e}}_i \otimes \mathbf{e}_i$, mapping one orthonormal basis \mathbf{e}_i into another one $\tilde{\mathbf{e}}_i$, and interpreted as rotations. The special two-fold rotations of amount π are denoted as $\mathbf{R}_{\mathbf{v}} = -\mathbf{I} + 2\mathbf{v} \otimes \mathbf{v}$, with \mathbf{v} being the normalised axial vector. Tensor groups are denoted by calligraphic letters. \mathcal{O}^+ denotes the proper orthogonal group, \mathcal{U}^+ stands for the unimodular group, the elements of which are restricted to have the determinant 1. To indicate directions and planes in crystal lattices, the usual Miller indices are used, $\langle xyz \rangle$ for directions and $\{xyz\}$ for planes, refer also to the Appendix. The signed integer numbers are denoted by \mathbb{G} .

1.3. Two-fold rotations, reflections and self-inverseness

$\mathbf{R}_{\mathbf{v}} = -\mathbf{I} + 2\mathbf{v} \otimes \mathbf{v}$ are referred to as two-fold rotations, with the normalised axial vector \mathbf{v} . They are orthogonal and symmetric, i.e. $\mathbf{R}_{\mathbf{v}} = \mathbf{R}_{\mathbf{v}}^T = \mathbf{R}_{\mathbf{v}}^{-1}$. $-\mathbf{R}_{\mathbf{v}}$ has the same properties, but represents a reflection on the plane normal to the axial vector of the rotation. Therefore, a lattice basis undergoes a central inversion if mapped by $-\mathbf{R}_{\mathbf{v}}$ instead of $\mathbf{R}_{\mathbf{v}}$, which does not affect the lattice

generated by that basis. Note that

$$(1.1) \quad \mathbf{R}_{\mathbf{e}_1} \mathbf{R}_{\mathbf{e}_2} \mathbf{R}_{\mathbf{e}_3} = \mathbf{I},$$

which allows us in conjunction with the self-inverseness to write

$$(1.2) \quad \mathbf{R}_{\mathbf{e}_1} = \mathbf{R}_{\mathbf{e}_2} \mathbf{R}_{\mathbf{e}_3},$$

or, using mirror operations,

$$(1.3) \quad -\mathbf{R}_{\mathbf{e}_1} = -\mathbf{R}_{\mathbf{e}_2} \mathbf{R}_{\mathbf{e}_3}$$

$$(1.4) \quad \mathbf{R}_{\mathbf{e}_1} = (-\mathbf{R}_{\mathbf{e}_2})(-\mathbf{R}_{\mathbf{e}_3}).$$

Mirror symmetries give rise to the Coxeter groups, although not all Coxeter groups can be described using only reflections. It is pointed out that from the viewpoint of application to lattices, the use of reflections or two-fold rotations is equivalent. Further, $\mathbf{R}_{\mathbf{v}} = \mathbf{R}_{-\mathbf{v}}$ holds, i.e. only the direction of the axial vector, but not the sense of direction matters.

REMARK. Note that a tensor which is orthogonal and symmetric is self-inverse, but not all self-inverse tensors must be symmetric. Let \mathbf{M} be a self-inverse tensor. Its eigenvalues can only take the values ± 1 . Its projector representation is given by $\mathbf{M} = \mathbf{P}_1 - \mathbf{P}_2$, with $\mathbf{P}_1 = \frac{1}{2}(\mathbf{I} + \mathbf{M})$ and $\mathbf{P}_2 = \frac{1}{2}(\mathbf{I} - \mathbf{M})$. Note that $\mathbf{P}_i \mathbf{P}_i = \mathbf{P}_i$, and $\mathbf{P}_1 + \mathbf{P}_2 = \mathbf{I}$. In case of the two-fold rotations, one obtains $\mathbf{P}_1 = \mathbf{v} \otimes \mathbf{v}$ and $\mathbf{P}_2 = \mathbf{I} - \mathbf{v} \otimes \mathbf{v}$. Motivated by $\mathbf{M}^2 = \mathbf{I}$, self-inverse tensors are sometimes referred to as tensors of period two (PITTERI and ZANZOTTO, 2002).

1.4. Simple shear deformation

Since simple shear deformations play the leading part when twinning is examined, some explanations regarding shear deformations should be given. Consider Fig. 1 (right), where the shear deformation of a cuboid is sketched. The shear deformation can be imagined as a deck of cards that glide along each other. Thus, the characteristic measures are the card deck normal \mathbf{n} , which is called a shear plane, and the glide direction \mathbf{d} , which is perpendicular to \mathbf{n} and called shear direction. Usually, \mathbf{n} and \mathbf{d} are normalised, which is why a measure for the amount of shear, the shear number $\gamma = l/h$ is introduced (see Fig. 1). The amount of glide of a plane parallel to the shear plane is proportional to the distance from the base plane. E.g., the displacement of the upper plane in the example is $\mathbf{u}(h) = \gamma h \mathbf{d}$, with h denoting the distance from the base plane. The displacement gradient is therefore

$$(1.5) \quad \mathbf{H}_{\text{ss}} = \frac{\partial \mathbf{u}}{\partial \mathbf{X}} = \gamma \mathbf{d} \otimes \frac{\partial h}{\partial \mathbf{X}} = \gamma \mathbf{d} \otimes \frac{\partial (\mathbf{X} \cdot \mathbf{n})}{\partial \mathbf{X}} = \gamma \mathbf{d} \otimes \mathbf{n},$$

where \mathbf{X} is the position vector of a material point before the deformation, i.e. in the reference placement. Commonly, γ is put into \mathbf{d} , at cost of the convenience of working with a normalised \mathbf{d} . In this work, γ and \mathbf{d} are kept separated. Then the tensor $\mathbf{d} \otimes \mathbf{n}$ can be referred to as the Schmid tensor or slip system tensor. Further, it is made use of the plane of shear, denoted by the normal vector $\mathbf{k} = \mathbf{n} \times \mathbf{d}$ (not to be confused with the shear plane \mathbf{n} , PITTERI and ZANZOTTO (2002)). Note that $(\mathbf{n}, \mathbf{d}, \mathbf{k})$ form a positively oriented orthonormal basis. The tensor \mathbf{H}_{ss} is a rank-one tensor, which can be denoted by only one base dyad. The corresponding deformation gradient is given by $\mathbf{S} = \mathbf{I} + \mathbf{H}_{\text{ss}}$. In the sequel, deformation gradients that describe a simple shear deformation are denoted by \mathbf{S} .

1.5. Usual twin description

In the literature, twins are mostly described by the twinning elements \mathbf{k}_1 , \mathbf{k}_2 , $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$ (Fig. 2, left). \mathbf{k}_1 and \mathbf{k}_2 should not be confused with \mathbf{k} introduced in Sec. 1.4. \mathbf{k}_1 represents the shear plane, also referred to as the invariant

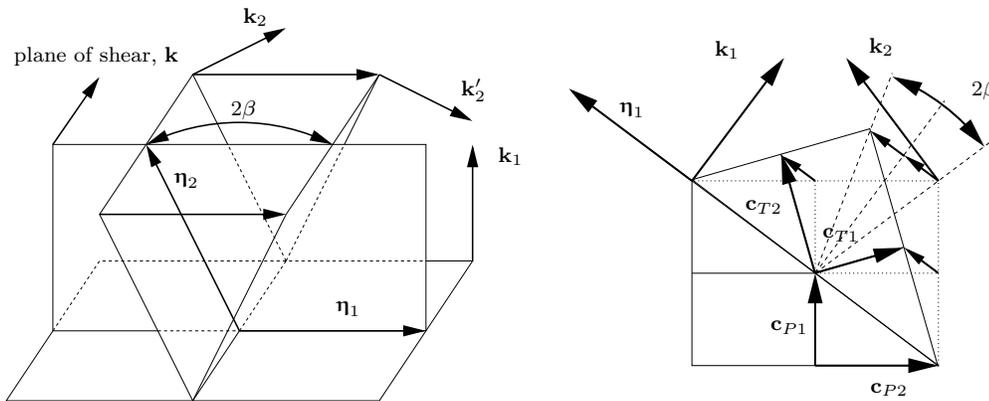


Fig. 2. The commonly used twin elements (left). In compound twins, the lattice vectors of the twin can be introduced such that they differ by a rotation of π around \mathbf{k}_1 or $\boldsymbol{\eta}_1$ from the parent lattice basis (right). The associated deformation is a simple shear deformation.

plane, while $\boldsymbol{\eta}_1$ indicates the shear direction. \mathbf{k}_2 represents the one plane that is, under the simple shear deformation, simply rotated by 2β around \mathbf{k} , but not stretched, therefore also referred to as the second undistorted plane. In this work, the vectors \mathbf{k}_i and $\boldsymbol{\eta}_i$ are always normalised, which is why a shear number γ is needed to uniquely identify the shear deformation. γ is connected to the angle β by

$$(1.6) \quad \gamma = 2 \tan \beta.$$

With β on hand, we can express the $\boldsymbol{\eta}_2$ and \mathbf{k}_2 in terms of $\boldsymbol{\eta}_1$ and \mathbf{k}_1 ,

$$(1.7) \quad \mathbf{k}_2 = \cos \beta \boldsymbol{\eta}_1 + \sin \beta \mathbf{k}_1$$

$$(1.8) \quad \boldsymbol{\eta}_2 = -\sin \beta \boldsymbol{\eta}_1 + \cos \beta \mathbf{k}_1,$$

which is needed later on. The twin lattice is obtained by mirroring the parent lattice at the shear plane \mathbf{k}_1 (type 1 twinning) or at the plane normal to the shear direction $\boldsymbol{\eta}_1$ (type 2 twinning). If \mathbf{k}_1 and \mathbf{k}_2 are rational (or crystallographically embedded), i.e. they can be represented exactly by integer Miller indices (ZHANG and KELLY, 2009), one speaks of compound twins. In that case, both orientation relations hold. For example, for the compound twin depicted in Fig. 2 (right), the orientation relations $\mathbf{c}_{T1} = \mathbf{R}_{\mathbf{k}_1} \mathbf{c}_{P1}$, $\mathbf{c}_{T2} = \mathbf{R}_{\mathbf{k}_1} \mathbf{c}_{P2}$ (type 1 twinning) and $\mathbf{c}_{T1} = -\mathbf{R}_{\boldsymbol{\eta}_1} \mathbf{c}_{P1}$, $\mathbf{c}_{T2} = -\mathbf{R}_{\boldsymbol{\eta}_1} \mathbf{c}_{P2}$ (type 2 twinning) hold. The term “compound twin” has been introduced by CAHN (1953). If \mathbf{k}_1 , \mathbf{k}_2 , $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$ are crystallographically embedded, they may characterise two different twin systems, namely shearing parallel to \mathbf{k}_1 in direction of $\boldsymbol{\eta}_1$, with the second undistorted plane \mathbf{k}_2 , or shearing parallel to \mathbf{k}_2 in direction of $\boldsymbol{\eta}_2$, with the second undistorted plane \mathbf{k}_1 . These two twin systems are said to be conjugate. In many cases, \mathbf{k}_1 and \mathbf{k}_2 are even crystallographically equivalent, exemplified in Fig. 2 (right) and Fig. 3 (right). Then the pairs \mathbf{k}_1 , $\boldsymbol{\eta}_1$ and \mathbf{k}_2 , $\boldsymbol{\eta}_2$ denote shearing in crystallographically equivalent twin systems. In Fig. 4 (left), a type 2 twin is depicted.

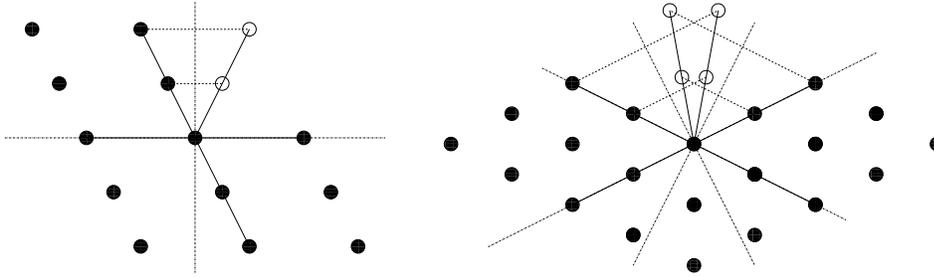


FIG. 3. A compound twin (left), crystallographically equivalent compound twins (right).

The type 1, type 2 and compound twinning modes are the so called “classical” twinning modes (CHRISTIAN and MAHAJAN, 1995), for which one (type 1 or type 2 twinning) or two two-fold rotations (compound twinning) hold as orientation relations. Although there exist solutions (\mathbf{Q} , \mathbf{S} and A_{ab}) to the twinning equation (2.4) which display a non-two-fold \mathbf{Q} , these are apparently of no practical relevance.

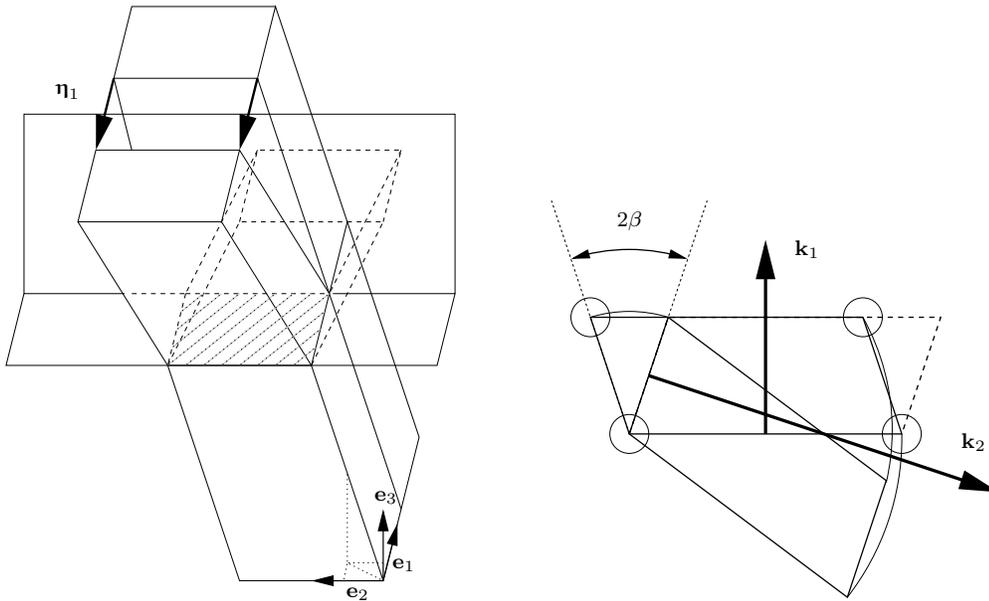


Fig. 4. A type 2 twin in a triclinic unit cell. Shearing occurs in direction η_1 . The plane normal to η_1 serves as a mirror plane, while the plane normal to \mathbf{k}_1 does not (left). Conjugate shear systems of compound twins (right). Consecutive twinning results in a rotation by 2β of the unit cell. Note that the lattice and the body undergo the same rotation.

2. Elastic energy

ERICKSEN (1975, 1980) firstly proposed to expand the applicability of the elasticity theory to phase transition problems. As twinning is regarded as an isothermal process, any temperature dependence is blanked out for convenience. The elastic energy contained in a crystal can be noted as $\phi(\mathbf{l}_i)$, where the crystal lattice is constructed from a set of base and shift vectors \mathbf{l}_i . With the given lattice \mathbf{l}_i and a suitable atomic potential on hand, one can sum up the energies contained in an embedded unit cell to calculate the energy density.

In elasticity, to connect the motion of the body with the lattice, it is usually assumed that the lattice undergoes the same deformation as the body. The latter is referred to as the Cauchy Born rule (BORN and HUANG, 1954), which is so fundamental in the theory of elasticity that it is mostly adopted intuitively and without explicit declaration (ERICKSEN, 1984b). The rearrangement of the atoms connected to twinning implies that the lattice vectors do not behave like material vectors. This has to be regarded as a violation of the Cauchy–Born rule. The consequences have been analysed by ZANZOTTO (1992, 1996), in order to determine the limitations of a theory that models deformation twinning by means of elasticity, and are topic of this article as well.

In the theory of elasticity, the use of a special placement called “reference placement” simplifies things considerably. With respect to the reference placement, strains are defined. The basic proposition in elasticity is that the current elastic energy depends only on the current placement of the atoms, but not on former configurations. Elastic mediums are said to have no memory. Therefore, it is convenient to denote the current elastic energy in terms of a deviation from the reference placement, i.e. in terms of strains. A natural choice for the reference placement is the equilibrium state under zero loading, i.e. the stress free configuration. Assuming this, we can write

$$(2.1) \quad \mathbf{l}_i = \mathbf{F}\mathbf{l}_i^R,$$

where \mathbf{F} denotes the deformation gradient and \mathbf{l}_i^R are the lattice base vectors in the stress-free reference placement. The deformation gradient is a second order tensor, mapping line elements from the reference placement to the current placement. As \mathbf{l}_i^R are constant in the reference placement, we may now write $\phi(\mathbf{F})$ instead of $\phi(\mathbf{l}_i)$. Further, we demand the Galilean invariance and the invariance on material symmetry operations. Galilean invariance implies that a rotation of the body does not alter the elastic energy, while the invariance on material symmetry operations demands the invariance of the elastic energy under a mapping of the reference lattice onto itself. Thus, we write

$$(2.2) \quad \phi(\mathbf{F}) = \phi(\mathbf{Q}\mathbf{F}\mathbf{H}),$$

with $\mathbf{Q} \in \mathcal{O}^+$ and \mathbf{H} being an element of the symmetry group \mathcal{G} of the lattice. Together with the polar decomposition of $\mathbf{F} = \mathbf{Q}_F\mathbf{U}$, it has to be concluded that one may write $\phi(\mathbf{U}) = \phi(\mathbf{U}\mathbf{H})$. For convenience, the strain energy is often expressed in terms of $\mathbf{C} = \mathbf{U}^2 = \mathbf{F}^T\mathbf{F}$ rather than \mathbf{U} , i.e. $\phi(\mathbf{U}\mathbf{H}) = \hat{\phi}(\mathbf{H}^T\mathbf{C}\mathbf{H})$.

2.1. Material symmetry operations

The equivalence of two lattice bases \mathbf{l}_a and $\tilde{\mathbf{l}}_b$ is expressed by

$$(2.3) \quad \mathbf{l}_a = A_{ab}\tilde{\mathbf{l}}_b, \quad A_{ab} \in \mathbb{G}, \quad a, b = 1 \dots 3$$

i.e. each lattice base vector \mathbf{l}_a can be constructed from an integer linear combination of the lattice base vectors $\tilde{\mathbf{l}}_b$. With $\tilde{\mathbf{l}}_b = \mathbf{H}\mathbf{l}_b$, \mathbf{H} is a symmetry operation on the lattice \mathbf{l}_a if Eq. (2.3) has a unique solution for A_{ab} . For a solution of Eq. (2.3), the integer values of A_{ab} depend on the specific choice of the basis that is used to describe the simple lattice.

2.1.1. Rotational symmetry. The material symmetry group \mathcal{G} contains at least the symmetry operations which map the crystal lattice by a rotation onto itself. Depending on the lattice type, this is the cubic, hexagonal, tetragonal, rhombohedral, orthorhombic, monoclinic or triclinic symmetry group.

2.1.2. Lattice invariant shear. Further, one can find non-orthogonal symmetry operations. Since all symmetry operations must be volume preserving, the largest possible material symmetry group is the unimodular group \mathcal{U}^+ . Lattice invariant shears have been examined by ERICKSEN (1984a,b). As an example, by shearing a face-centred or a body-centred cubic lattice (the edges aligned parallel to the orthonormal basis \mathbf{e}_i) with $\gamma = 2$, $\mathbf{d} = \mathbf{e}_1$ and $\mathbf{n} = \mathbf{e}_2$, one generates a lattice which is identical to the starting lattice, i.e. the element $\mathbf{S} = \mathbf{I} + 2\mathbf{e}_1 \otimes \mathbf{e}_2$ must be considered as a material symmetry operation. If we interpret \mathbf{S} as a deformation, we would consider it as crystallographic glide.

2.1.3. Twinning. It may occur that the lattice obtained from a shearing differs from the starting lattice by a rotation, such that the overall symmetry operation \mathbf{H} consists of a consecutive shearing and rotation. This is what is usually considered as twinning. The famous “twinning equation” is obtained by stating that after applying a shear to the lattice generated by \mathbf{l}_i , one obtains a rotated version of the lattice generated by \mathbf{l}_i , i.e.

$$(2.4) \quad \mathbf{Q}\mathbf{l}_a = A_{ab}\mathbf{S}\mathbf{l}_b.$$

Transferring \mathbf{Q} to the other side shows that the symmetry operations due to twinning are of the form $\mathbf{H} = \mathbf{Q}^{-1}\mathbf{S}$ (ZANZOTTO (1992), Eq. 2.3). \mathbf{Q} is usually referred to as the orientation relation between the twin and parent lattice.

ZANZOTTO (1992) showed that the additional symmetry elements due to twinning can cause \mathcal{G} to expand to \mathcal{U}^+ , which is the symmetry group of elastic fluids. In other words, any unimodular deformation can be accommodated by a combination of twin formations such that the material is stress free. This comes from the fact that consecutive twinning on the same plane of shear may culminate in any symmetry operation from the transverse isotropic group. This is the case if two conjugate twinning operations can be replaced by a rotation of period ∞ . An illustration is given in Fig. 4 (right). Then, together with the rotational symmetry operations, \mathcal{G} invades the whole unimodular group. This appears to be the “generic” case.

Therefore, ZANZOTTO (1992, 1996) doubted that the elastic modelling of twinning was appropriate. However, the approach of respecting all possible series of twin combinations in one elastic energy is questionable at all, even if \mathcal{G} is finite. Such an elastic energy includes twin configurations which may be only accessible by a specific series of twinning operations. The arrival at such a configuration depends clearly on the strain path, which cannot be accounted for by a purely elastic modelling.

One may therefore restrict the elastic energy to respect only first order twins, as done by GLÜGE and BÖHLKE (2007). Even though, one may encounter an

elastic energy invariance, firstly pointed out by ERICKSEN (1984b). Here, it is shown that all compound twins exhibit this elastic energy invariance. This affects practically all relevant twinning modes, since non-compound twins seem to appear far less frequently, usually in low-symmetry lattices like the monoclinic and the orthorhombic lattice (PITTERI and ZANZOTTO, 2002). Examples for the occurrence of non-compound twins are α -uranium (CAHN, 1953) and sapphire (CLAYTON, 2009).

The equivalence of the material symmetry elements generated by conjugate twins is known for some time (PITTERI, 1986; ZANZOTTO, 1992), but did not receive much attention. For his main conclusion, ZANZOTTO (1992) considers non-conjugate twins (the three lines above Eq. 3.2). Although one can find in his work already the clear statement that conjugate twin systems yield identical symmetry operations, the implications for the elastic modelling are not discussed. The connection of compound twins to a specific rotational symmetry of the lattice, which plays a crucial role in this matter, is not new as well (STARK, 1988).

In this work, the equivalence of the material symmetry operations of conjugate twins is derived. For the derivation, the use of a specific lattice basis is strictly avoided, as the findings should be independent on the choice of the latter. Instead, it is argued by using the symmetry operations that hold for the lattice. Afterwards, the implications for the elastic modelling are discussed.

2.2. Lattice symmetry connected to a compound twin

We may examine the difference between lattice bases that undergo type 1 and type 2 twinning by introducing the tensor \mathbf{A} , mapping the type 2 twinned basis on the type 1 twinned basis,

$$(2.5) \quad \mathbf{R}_{\mathbf{k}_1} \mathbf{l}_i^R = \mathbf{A} \mathbf{R}_{\boldsymbol{\eta}_1} \mathbf{l}_i^R,$$

where \mathbf{l}_i^R is the parent lattice basis. With $\mathbf{R}_{\mathbf{k}_1} = \mathbf{R}_{\mathbf{k}_1}^T = \mathbf{R}_{\mathbf{k}_1}^{-1}$ one can write

$$(2.6) \quad \mathbf{l}_i^R = \mathbf{R}_{\mathbf{k}_1} \mathbf{A} \mathbf{R}_{\boldsymbol{\eta}_1} \mathbf{l}_i^R,$$

which holds only if $\mathbf{R}_{\mathbf{k}_1} \mathbf{A} \mathbf{R}_{\boldsymbol{\eta}_1} = \mathbf{I}$. Therefore, \mathbf{A} is evaluated to

$$(2.7) \quad \mathbf{A} = \mathbf{R}_{\mathbf{k}_1} \mathbf{R}_{\boldsymbol{\eta}_1} = \mathbf{R}_{\mathbf{k}}.$$

It has to be concluded that, if $\mathbf{R}_{\mathbf{k}}$ is in the symmetry group of the lattice generated by \mathbf{l}_i^R , both, the type 1 and type 2 orientation relation hold. Or, in the other direction, if both orientation relations hold, $\mathbf{R}_{\mathbf{k}}$ is an element of the symmetry group of the lattice. To summarise: If \mathbf{k}_1 , \mathbf{k}_2 , $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$ are crystallographically

embedded, we speak of a compound twins, for which the orientation relations $\mathbf{R}_{\mathbf{k}_1}$ and $\mathbf{R}_{\boldsymbol{\eta}_1}$ hold (CAHN, 1953). If both orientation relations hold, $\mathbf{R}_{\mathbf{k}}$ is in the lattice symmetry group of the parent lattice. This means that every compound twin has to come along with a lattice symmetry operation, namely a rotation by π inside the common plane of shear. The same has been found by STARK (1988).

2.3. Composition of conjugate twins

Taking the twinning equation (2.4), we find that

$$(2.8) \quad \mathbf{H} = \mathbf{Q}^{-1}\mathbf{S}.$$

Since the focus is on a pair of conjugate, compound twins here, for twinning in direction $\boldsymbol{\eta}_1$ parallel to \mathbf{k}_1 , we may take the two-fold rotations $\mathbf{R}_1 = \mathbf{R}_{\mathbf{k}_1}$ or $\mathbf{R}_1 = \mathbf{R}_{\boldsymbol{\eta}_1}$ as orientation relations, and $\mathbf{R}_2 = \mathbf{R}_{\mathbf{k}_2}$ or $\mathbf{R}_2 = \mathbf{R}_{\boldsymbol{\eta}_2}$ for twinning parallel to \mathbf{k}_2 in direction of $\boldsymbol{\eta}_2$. The twinning shears \mathbf{S}_1 and \mathbf{S}_2 are given by $\mathbf{S}_1 = \mathbf{I} + \gamma\boldsymbol{\eta}_1 \otimes \mathbf{k}_1$ and $\mathbf{S}_2 = \mathbf{I} + \gamma\boldsymbol{\eta}_2 \otimes \mathbf{k}_2$. With the self-inverseness of the \mathbf{R}_i , the symmetry relations for both twin systems emerge to

$$(2.9) \quad \mathbf{H}_1 = \mathbf{R}_1\mathbf{S}_1,$$

$$(2.10) \quad \mathbf{H}_2 = \mathbf{R}_2\mathbf{S}_2.$$

One can review that, independently on whether $\mathbf{R}_{\mathbf{k}_i}$ or $\mathbf{R}_{\boldsymbol{\eta}_i}$ is taken as orientation relation, the \mathbf{H}_i display the remarkable property of self-inverseness. This implies that double twinning on the same twin system results in a recovery of the parent.

In the remainder of this section, the symmetry operation $\mathbf{H}_{12} = \mathbf{H}_1\mathbf{H}_2$ is analysed. For now, the orientation relations $\mathbf{R}_{\mathbf{k}_1}$ and $\mathbf{R}_{\mathbf{k}_2}$ are used. Afterwards, it is discussed what happens when $\mathbf{R}_{\boldsymbol{\eta}_1}$ and $\mathbf{R}_{\boldsymbol{\eta}_2}$ or a mixture ($\mathbf{R}_{\mathbf{k}_1}$ and $\mathbf{R}_{\boldsymbol{\eta}_2}$) are applied. With $\mathbf{R}_{\mathbf{k}_i} = -\mathbf{I} + 2\mathbf{k}_i \otimes \mathbf{k}_i$ and $\mathbf{S}_i = \mathbf{I} + \gamma\boldsymbol{\eta}_i \otimes \mathbf{k}_i$, one obtains

$$(2.11) \quad \mathbf{H}_1 = -\mathbf{I} - \gamma\boldsymbol{\eta}_1 \otimes \mathbf{k}_1 + 2\mathbf{k}_1 \otimes \mathbf{k}_1,$$

$$(2.12) \quad \mathbf{H}_2 = -\mathbf{I} - \gamma\boldsymbol{\eta}_2 \otimes \mathbf{k}_2 + 2\mathbf{k}_2 \otimes \mathbf{k}_2,$$

which results in

$$(2.13) \quad \mathbf{H}_{12} = (-\mathbf{I} - \gamma\boldsymbol{\eta}_1 \otimes \mathbf{k}_1 + 2\mathbf{k}_1 \otimes \mathbf{k}_1)(-\mathbf{I} - \gamma\boldsymbol{\eta}_2 \otimes \mathbf{k}_2 + 2\mathbf{k}_2 \otimes \mathbf{k}_2).$$

To summarise further, we have calculate the remaining product, summarise the coefficients belonging to each base dyad, and employ the relations (1.7) and (1.8)

$$\begin{aligned}
(2.14) \quad \mathbf{H}_{12} &= \mathbf{I} + \gamma \boldsymbol{\eta}_2 \otimes \mathbf{k}_2 - 2\mathbf{k}_2 \otimes \mathbf{k}_2 \\
&\quad + \gamma \boldsymbol{\eta}_1 \otimes \mathbf{k}_1 + \gamma^2 (\mathbf{k}_1 \cdot \boldsymbol{\eta}_2) \boldsymbol{\eta}_1 \otimes \mathbf{k}_2 - 2\gamma (\mathbf{k}_1 \cdot \mathbf{k}_2) \boldsymbol{\eta}_1 \otimes \mathbf{k}_2 \\
&\quad - 2\mathbf{k}_1 \otimes \mathbf{k}_1 - 2\gamma (\mathbf{k}_1 \cdot \boldsymbol{\eta}_2) \mathbf{k}_1 \otimes \mathbf{k}_2 + 4(\mathbf{k}_1 \cdot \mathbf{k}_2) \mathbf{k}_1 \otimes \mathbf{k}_2
\end{aligned}$$

$$\begin{aligned}
(2.15) \quad &= \mathbf{I} + \gamma \boldsymbol{\eta}_2 \otimes \mathbf{k}_2 - 2\mathbf{k}_2 \otimes \mathbf{k}_2 \\
&\quad + \gamma \boldsymbol{\eta}_1 \otimes \mathbf{k}_1 + (\gamma^2 \cos \beta - 2\gamma \sin \beta) \boldsymbol{\eta}_1 \otimes \mathbf{k}_2 \\
&\quad - 2\mathbf{k}_1 \otimes \mathbf{k}_1 + (-2\gamma \cos \beta + 4 \sin \beta) \mathbf{k}_1 \otimes \mathbf{k}_2.
\end{aligned}$$

In order to interpret the result it should be denoted with respect to an orthonormal basis, where we choose $(\mathbf{k}_1, \boldsymbol{\eta}_1, \mathbf{k})$. To shorten the intermediate expressions, the abbreviations $c = \cos \beta$ and $s = \sin \beta$ are used,

$$\begin{aligned}
(2.16) \quad \mathbf{H}_{12} &= \mathbf{I} + \gamma(-s\boldsymbol{\eta}_1 + c\mathbf{k}_1) \otimes (c\boldsymbol{\eta}_1 + s\mathbf{k}_1) - 2(c\boldsymbol{\eta}_1 + s\mathbf{k}_1) \otimes (c\boldsymbol{\eta}_1 + s\mathbf{k}_1) \\
&\quad + \gamma \boldsymbol{\eta}_1 \otimes \mathbf{k}_1 + (\gamma^2 c - 2\gamma s) \boldsymbol{\eta}_1 \otimes (c\boldsymbol{\eta}_1 + s\mathbf{k}_1) \\
&\quad - 2\mathbf{k}_1 \otimes \mathbf{k}_1 + (-2\gamma c + 4s) \mathbf{k}_1 \otimes (c\boldsymbol{\eta}_1 + s\mathbf{k}_1).
\end{aligned}$$

The last step is to summarise all coefficients, which yields

$$\begin{aligned}
(2.17) \quad \mathbf{H}_{12} &= \mathbf{I} + [\gamma s c - 2s^2 - 2 - 2\gamma s c + 4s^2] \mathbf{k}_1 \otimes \mathbf{k}_1 \\
&\quad + [-\gamma s c - 2c^2 + \gamma^2 c^2 - 2\gamma s c] \boldsymbol{\eta}_1 \otimes \boldsymbol{\eta}_1 \\
&\quad + [-\gamma s^2 - 2s c + \gamma + \gamma^2 c s - 2\gamma s^2] \boldsymbol{\eta}_1 \otimes \mathbf{k}_1 \\
&\quad + [\gamma c^2 - 2s c - 2\gamma c^2 + 4s c] \mathbf{k}_1 \otimes \boldsymbol{\eta}_1.
\end{aligned}$$

Inserting $\gamma = 2s/c$ and employing $s^2 + c^2 = 1$ allows to summarise the first two squared brackets to -2 and both the remaining brackets to 0 . With $\mathbf{I} = \mathbf{k}_1 \otimes \mathbf{k}_1 + \boldsymbol{\eta}_1 \otimes \boldsymbol{\eta}_1 + \mathbf{k} \otimes \mathbf{k}$, one sees that the result can be simplified to

$$(2.18) \quad \mathbf{H}_{12} = \mathbf{I} - \mathbf{k}_1 \otimes \mathbf{k}_1 - \boldsymbol{\eta}_1 \otimes \boldsymbol{\eta}_1 = -\mathbf{I} + 2\mathbf{k} \otimes \mathbf{k} = \mathbf{R}_{\mathbf{k}}.$$

This holds also if $\mathbf{R}_{\boldsymbol{\eta}_1}$ and $\mathbf{R}_{\boldsymbol{\eta}_2}$ are the preferred orientation relations, since $\mathbf{R}_{\boldsymbol{\eta}_i} = \mathbf{R}_{\mathbf{k}_i} \mathbf{R}_{\mathbf{k}} = \mathbf{R}_{\mathbf{k}} \mathbf{R}_{\mathbf{k}_i}$, which, by using the self-inverseness of $\mathbf{R}_i \mathbf{S}_i$ and the latter result, allows to write

$$(2.19) \quad \mathbf{H}_{12} = \mathbf{R}_{\boldsymbol{\eta}_1} \mathbf{S}_1 \mathbf{R}_{\boldsymbol{\eta}_2} \mathbf{S}_2 = \mathbf{R}_{\mathbf{k}} \mathbf{R}_{\mathbf{k}_1} \mathbf{S}_1 \mathbf{S}_2^{-1} \mathbf{R}_{\mathbf{k}_2} \mathbf{R}_{\mathbf{k}} = \mathbf{R}_{\mathbf{k}}^3 = \mathbf{R}_{\mathbf{k}}.$$

If one employs $\mathbf{R}_{\boldsymbol{\eta}_1}$ and $\mathbf{R}_{\mathbf{k}_2}$ as orientation relations, one obtains

$$(2.20) \quad \mathbf{H}_{12} = \mathbf{R}_{\boldsymbol{\eta}_1} \mathbf{S}_1 \mathbf{R}_{\mathbf{k}_2} \mathbf{S}_2 = \mathbf{R}_{\mathbf{k}} \mathbf{R}_{\mathbf{k}_1} \mathbf{S}_1 \mathbf{R}_{\mathbf{k}_2} \mathbf{S}_2 = \mathbf{R}_{\mathbf{k}}^2 = \mathbf{I}.$$

The same result emerges if $\mathbf{R}_{\mathbf{k}_1}$ and $\mathbf{R}_{\boldsymbol{\eta}_2}$ are employed. Since we are free to choose any combination of valid orientation relations, the properties of the result \mathbf{H}_{12} should be independent of this choice. Since either \mathbf{I} or $\mathbf{R}_{\mathbf{k}}$ emerges, and \mathbf{I} is trivially an element of the rotational symmetry group, one has to conclude that $\mathbf{R}_{\mathbf{k}}$ is as well in the rotational symmetry group of the parent lattice. This is a more subtle argumentation for the result of Sec. 2.2.

3. Discussion

Suppose one wants to construct a multi-well elastic energy which respects the parent configuration and the first order compound twins of a twinning mode given by $\mathbf{k}_1^i, \boldsymbol{\eta}_1^i, \mathbf{k}_2^i, \boldsymbol{\eta}_2^i$, where $i = 1 \dots n$ indexes possible twin variants. Let the shearing along $\boldsymbol{\eta}_1^i$ parallel to \mathbf{k}_1^i be the twinning modes of interest. Since multiple twinning should be avoided, one cannot treat the \mathbf{H}_1^i as material symmetry operations, but use them as plastic transformations (BERTRAM, 1999), which map the convex, well behaving quadratic strain energy of the parent ϕ_p to the n different twinning configurations ϕ_i . The overall elastic energy may be obtained by a combination of all elastic energies, for example by the Ball and James (BALL and JAMES, 1987, 1992) approach $\phi = \min(\phi_p, \phi_1 \dots \phi_n)$, or by the partition function (ROUBÍČEK, 2004).

The formal mathematical treatment of the \mathbf{H}_1^i does not differ, whether interpreted as material symmetry operations or as plastic transformations. Since the $\mathbf{R}_{\mathbf{k}}^i = \mathbf{R}_{\boldsymbol{\eta}_1^i \times \mathbf{k}_1^i} = \mathbf{R}_{\boldsymbol{\eta}_2^i \times \mathbf{k}_2^i}$ must be in the rotational symmetry group of the parent crystal (see Sec. 2.2), and $\mathbf{H}_2^i = \mathbf{R}_{\mathbf{k}}^i \mathbf{H}_1^i$ holds (see Sec. 2.3), the elastic energies $\phi_1, \phi_2 \dots \phi_n$ may represent twinning along $\boldsymbol{\eta}_1^i$ parallel to \mathbf{k}_1^i , or the conjugate twinning mode, $\boldsymbol{\eta}_2^i$ and \mathbf{k}_2^i . Therefore, one enables automatically, wanted or not, the conjugate twinning mode to the twinning mode which is intended to be modelled. Depending on whether the pairs $(\mathbf{k}_1, \boldsymbol{\eta}_1)$ and $(\mathbf{k}_2, \boldsymbol{\eta}_2)$ are crystallographically equivalent or not, different conclusions have to be drawn.

3.1. Crystallographically equivalent compound twins

In the case that the pairs $(\mathbf{k}_1, \boldsymbol{\eta}_1)$ and $(\mathbf{k}_2, \boldsymbol{\eta}_2)$ are crystallographically equivalent, the conjugate twinning modes belong to a set of crystallographically equivalent twin systems. Practical examples are the $\{112\}\langle\bar{1}\bar{1}1\rangle$ twinning in the bcc, $\{111\}\langle 11\bar{2}\rangle$ twinning in the fcc, $\{01\bar{1}2\}\langle 0\bar{1}11\rangle$ twinning in hcp, $\{101\}\langle 10\bar{1}\rangle$ twinning in the bct and orthorhombic and $\{100\}\langle 00\bar{1}\rangle$ twinning in the orthorhombic lattice. E.g., for the $\{01\bar{1}2\}\langle 0\bar{1}11\rangle$ twin systems in the hcp lattice (Fig. 5), $\mathbf{k}_1, \boldsymbol{\eta}_1, \mathbf{k}_2, \boldsymbol{\eta}_2$ are $\{01\bar{1}2\}, \langle 0\bar{1}11\rangle, \{01\bar{1}\bar{2}\}, \langle 01\bar{1}1\rangle$, respectively. This implies that the conjugate twin to the $\{01\bar{1}2\}, \langle 0\bar{1}11\rangle$ twin system is crystallographically equivalent, i.e. one has six crystallographically equivalent twin systems. These

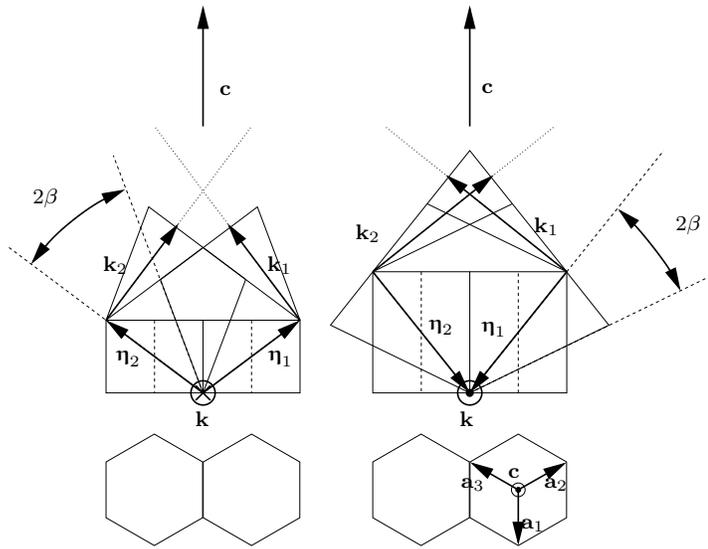


FIG. 5. $\{01\bar{1}2\}\{0111\}$ twin systems in the hexagonal unit cell, with $c/a < \sqrt{3}$ (left) and $c/a > \sqrt{3}$ (right), and $\gamma = 2\tan(\beta)$.

are pairwise energetically invariant, which means that from the viewpoint of an elastic modelling, one can only distinguish three possible twinning modes. FE Simulations (GLÜGE and BÖHLKE, 2007) have shown that, despite the pairwise energy invariance, the conjugate twins can be identified by relating the interface that establishes to the lattice basis. This is, however, only possible by looking at finite section of the model. At a single material point, due to the elastic energy invariance, no conclusion regarding which of the conjugate twin systems has been activated, can be drawn. However, the spatial lattice orientations of conjugate twin systems differ, which is problematic if one intends to model, e.g., double twinning or slip system activity inside the twin. This is not possible without knowing the crystal orientation, which is due to the energy invariance not uniquely determined.

3.2. Crystallographically distinct compound twins

In the case that the pairs $(\mathbf{k}_1, \boldsymbol{\eta}_1)$ and $(\mathbf{k}_2, \boldsymbol{\eta}_2)$ are crystallographically distinct, different conclusions emerge. Practical examples are $\{01\bar{1}1\}\{01\bar{1}2\}$ (Fig. 6) and $\{11\bar{2}2\}\{11\bar{2}3\}$ twinning in the hcp lattice, $\{031\}\{0\bar{1}3\}$ twinning in the bct lattice, $\{100\}\{0\bar{1}\bar{1}\}$ twinning in the rhombohedral lattice, $\{10\bar{1}\}\{1\kappa_11\}$ and $\{130\}\{3\bar{1}0\}$ twinning in the orthorhombic lattice and $\{100\}\{001\}$, $\{110\}\{00\bar{1}\}$, $\{100\}\{0\kappa_2\kappa_3\}$ and $\{011\}\{0\kappa_4\kappa_5\}$ twinning in the monoclinic lattice, where κ_i denotes some lattice constant. E.g., for the $\{01\bar{1}1\}\{01\bar{1}2\}$ twin systems in the hcp

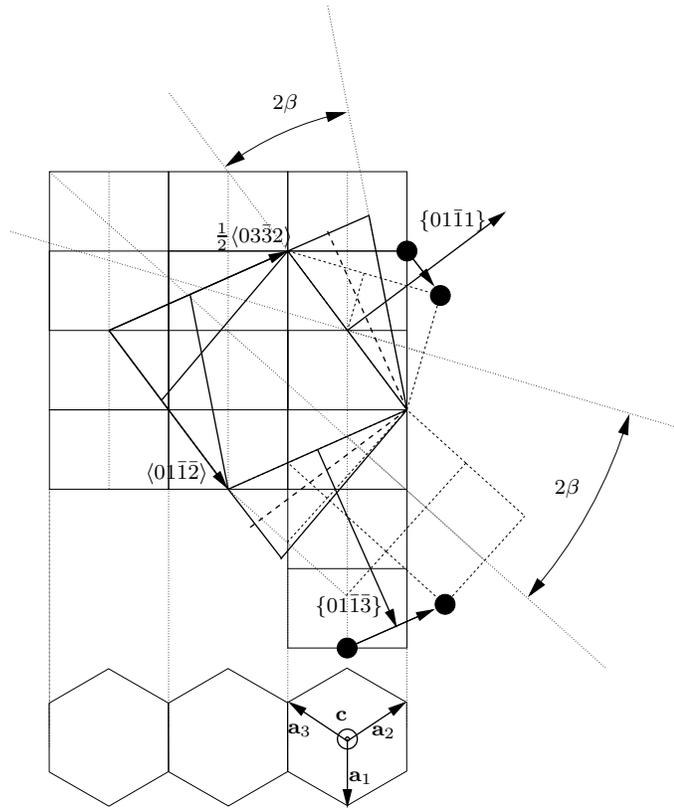


FIG. 6. The $\{01\bar{1}1\}\langle 01\bar{1}2\rangle$ and the $\{01\bar{1}3\}\langle 03\bar{3}2\rangle$ twin system in the hcp lattice.

lattice, $\mathbf{k}_1, \boldsymbol{\eta}_1, \mathbf{k}_2, \boldsymbol{\eta}_2$ as depicted in Fig. 6, are $\{01\bar{1}1\}, \langle 01\bar{1}2\rangle, \{01\bar{1}3\}, \langle 03\bar{3}2\rangle$, respectively. This means that the conjugate twin to the $\{01\bar{1}1\}\langle 01\bar{1}2\rangle$ twin system, which is the $\{01\bar{1}3\}\langle 03\bar{3}2\rangle$ twin system, is crystallographically distinct. Therefore, as mentioned in the introduction, both may display different characteristics, like different critical shear stresses, or one may only be active under exceptional conditions, while the other may be activated easily. In fact, for magnesium and its alloys, the $\{01\bar{1}1\}\langle 01\bar{1}2\rangle$ twins form readily under c -axis compression, while the $\{01\bar{1}3\}\langle 03\bar{3}2\rangle$ twins are hardly reported. Both twin systems are, however, connected by the elastic energy invariance. By introducing an elastic energy which displays the six distinct minima of the $\{01\bar{1}1\}\langle 01\bar{1}2\rangle$ twin variants, one enables automatically $\{01\bar{1}3\}\langle 03\bar{3}2\rangle$ twinning.

3.3. Lattice invariant shear

The strain energy invariance may even connect a twinning mode to a lattice invariant shear, namely to a deformation which one would consider as crystal-

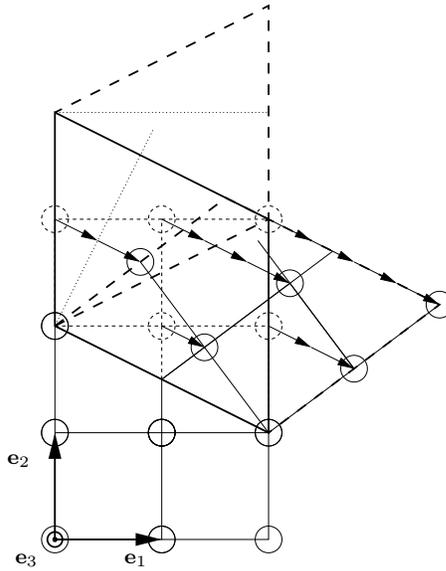


Fig. 7. A lattice invariant shear ($\mathbf{d} \parallel \mathbf{e}_2, \mathbf{n} \parallel \mathbf{e}_1$) and a twinning mode ($\mathbf{d} \parallel (2\mathbf{e}_1 - \mathbf{e}_2), \mathbf{n} \parallel (\mathbf{e}_1 + 2\mathbf{e}_2)$), that are connected by the conjugacy of the shear systems.

lographic glide (ERICKSEN, 1984a). An example hereof is twinning with the elements $\mathbf{k}_1 = \{120\}$, $\boldsymbol{\eta}_1 = \langle 2\bar{1}0 \rangle$, $\mathbf{k}_2 = \{100\}$ and $\boldsymbol{\eta}_2 = \langle 010 \rangle$ in a simple cubic lattice, see Fig. 7 for a sketch. With β being the angle between \mathbf{k}_1 and $\boldsymbol{\eta}_2$, $\gamma = 2 \tan \beta$ is evaluated to $\gamma = 1$. After normalising \mathbf{k}_1 and $\boldsymbol{\eta}_1$, \mathbf{H}_1 and \mathbf{H}_2 are given by

$$(3.1) \quad \mathbf{H}_1 = \mathbf{R}_{\mathbf{k}_1} \mathbf{S}_1 \\ = \left(-\mathbf{I} + \frac{2}{5}(\mathbf{e}_1 + 2\mathbf{e}_2) \otimes (\mathbf{e}_1 + 2\mathbf{e}_2) \right) \left(\mathbf{I} + \frac{1}{5}(2\mathbf{e}_1 - \mathbf{e}_2) \otimes (\mathbf{e}_1 + 2\mathbf{e}_2) \right),$$

$$(3.2) \quad \mathbf{H}_2 = \mathbf{R}_{\mathbf{k}_2} \mathbf{S}_2 = (-\mathbf{I} + 2\mathbf{e}_1 \otimes \mathbf{e}_1)(\mathbf{I} + \mathbf{e}_2 \otimes \mathbf{e}_1).$$

Summarising and representing \mathbf{H}_1 and \mathbf{H}_2 with respect to the base dyads $\mathbf{e}_i \otimes \mathbf{e}_j$ yields

$$(3.3) \quad \mathbf{H}_1 = \begin{bmatrix} -1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \mathbf{e}_i \otimes \mathbf{e}_j \quad \mathbf{H}_2 = \begin{bmatrix} 1 & 0 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \mathbf{e}_i \otimes \mathbf{e}_j.$$

One can check the self-inverseness of \mathbf{H}_1 and \mathbf{H}_2 , the components of which are moreover of the form of “canonical self-inverse integer matrices” (HANSON, 1985). Calculating the composition $\mathbf{H}_1 \mathbf{H}_2$ yields $\mathbf{R}_{\mathbf{e}_3}$, which shows that these two twinning modes are indeed conjugate. However, one notes that a reorientation by a two-fold rotation around \mathbf{k}_2 or $\boldsymbol{\eta}_2$ maps the lattice onto itself, while

a two-fold rotation around \mathbf{k}_1 or $\boldsymbol{\eta}_1$ generates a rotated copy of the lattice. With the classification given in Sec. 2.1, we have to conclude that \mathbf{H}_1 represents the symmetry operation for a twinning mode, while \mathbf{H}_2 should be considered as crystallographic glide. Clearly, both have to be modelled by entirely different methods. In a purely elastic modelling approach, due to the strain energy invariance, one cannot incorporate the $\{120\}\langle 2\bar{1}0\rangle$ twinning without enabling $\{100\}\langle 010\rangle$ twinning, which is not even a valid twin variant.

3.4. Non-compound twins

The non-compound twinning modes, type 1 and type 2 twinning, do not exhibit the energy invariance, since $\mathbf{R}_{\mathbf{k}}$ is not an element of the symmetry group of the lattice. This is due to the fact that only one of the orientation relations $\mathbf{R}_{\boldsymbol{\eta}}$ or $\mathbf{R}_{\mathbf{k}}$ holds. Therefore, as long as no improper elastic law is applied, the elastic energy is not invariant under a symmetry transformation with $\mathbf{R}_{\mathbf{k}}$.

4. Conclusion

Since an elastic model of deformation twinning may be used either as a simple material model or be part of a more advanced material model, its limitations are examined.

Firstly, due to the findings of ZANZOTTO (1992) and the intrinsic strain path independence of an elastic material, the purely elastic modelling has to be restricted to first order twins.

Secondly, it has to be noted that an elastic energy invariance between compound twins exists, which are therefore, at the level of a material point, indistinguishable in a pure elasticity framework.

Therefore, one has to ask whether it is important to distinguish these twins. Compound twins can be crystallographically equivalent or distinct. In case of crystallographically equivalent compound twins, one is able to incorporate, by an elastic modelling, a set of crystallographically equivalent twin systems. Each energy minimum, i.e. each phase, corresponds to a pair of potentially active twins. These cannot be distinguished at a single material point, due to the energy invariance. However, it has been found that by solving the boundary value problem, one can clearly decide which of the two twin variants is activated, since the solution displays twin lamellas, and the interfaces of which can be related to the crystal lattice. With an interface-independent kinetic relation, the elastic modelling allows for an examination of twin tip geometries under different loading conditions, the interaction between twinning and crystallographic slip, and the abrupt twin formation (GLÜGE *et al.*, 2010). Moreover, by numerical homogenisation via the representative volume element technique, such a model

is able to predict some important twinning-related characteristics of the effective behaviour of a polycrystal (GLÜGE, 2009).

The situation is different when the twin systems that should be incorporated are compound twins with crystallographically distinct conjugate twins. The energy invariance prevents a priori a distinction, although the characteristics of the twin systems may differ largely. Therefore, the purely elastic modelling cannot be applied. Note that both types of compound twins, crystallographically equivalent and distinct, are of practical interest. It should be mentioned that material models that relate the stress state to the twin system activity, e.g., by a Schmid law (see, e.g., FOREST and PARISOT (2000)), are not problematic with respect to conjugate twin systems, since, in general, different shear stresses in both twin systems are obtained.

The purely elastic modelling is very restricted. To overcome the limitations, additional modelling effort is required. The properties of the twin interface need to be accounted for, which are in particular the interface energy and the interface mobility. The interface kinetic governs the time dependent behaviour (see HOU *et al.* (1999) for a concise outline), while the interface energy induces an internal length to the elastic modelling, namely a minimum twin thickness. Moreover, the interface energy, which depends on the orientation of the interface with respect to the lattice, works as a selection criterion for possible twins. Specifically, kink twins can be excluded by connecting a large interface energy to the corresponding interface orientation (FOREST and PARISOT, 2000). In principle, the same is applicable to the crystallographically distinct compound twins, which can be used to overcome their energetic invariance. Moreover, the modelling of the twin interface allows to account for the vastly varying twin interface mobility (LI and MA, 2009b,a), which is in principal not accessible by a purely elastic modelling with interface-independent kinetics (ABEYARATNE and KNOWLES, 1991; HOU *et al.*, 1999). On the other hand, if interfaces should be respected in the model, the modelling effort increases considerably. However, for the physically sound modelling of twinning, this effort is unavoidable.

Appendix

For a hexagonal lattice, it is convenient to use the Miller–Bravais basis:

$$(A.1) \quad \mathbf{a}_1 = a\mathbf{e}_1,$$

$$(A.2) \quad \mathbf{a}_2 = a \left(-\frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2 \right),$$

$$(A.3) \quad \mathbf{a}_3 = a \left(-\frac{1}{2}\mathbf{e}_1 - \frac{\sqrt{3}}{2}\mathbf{e}_2 \right),$$

$$(A.4) \quad \mathbf{c} = c\mathbf{e}_3,$$

see Fig. 8, NEUMANN (1966); PITTERI and ZANZOTTO (2002). The lattice parameters c and a represent the height of the cell and the edge length of the base hexagon, respectively, and correspond to the norms of \mathbf{c} and \mathbf{a} , $c = \sqrt{\mathbf{c} \cdot \mathbf{c}}$ and $a = \sqrt{\mathbf{a} \cdot \mathbf{a}}$. Although one usually does not appreciate the use of linearly dependent base vectors, this basis has the advantage that it reflects the hexagonal symmetry. Permutations of the components belonging to $\mathbf{a}_{1\dots 3}$, a change of sign of the c -component or a simultaneous change of sign of all $a_{1\dots 3}$ yield crystallographically equivalent directions, which are denoted as $\langle a_1 a_2 a_3 c \rangle$. Usually, negative components are denoted by \bar{x} instead of $-x$. Further, due to the linear dependence of $\mathbf{a}_{1\dots 3}$, the condition $a_1 + a_2 + a_3 = 0$ is imposed, and therefore sometimes the third component a_3 is omitted.

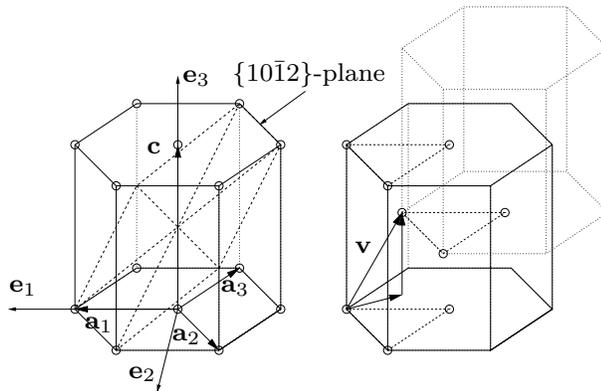


Fig. 8. Simple hexagonal lattice with Miller-Bravais basis (left), hexagonal close packed multilattice constructed from the simple lattice by introducing additional translations in $\mathbf{v} = \langle \frac{1}{3} 0 \frac{1}{3} \frac{1}{2} \rangle$ (right).

To indicate planes, it is advantageous to introduce another basis. This is done by taking the dual basis $(\tilde{\mathbf{a}}_1, \tilde{\mathbf{a}}_2, \tilde{\mathbf{c}})$ of $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{c})$ and defining the base vectors

$$(A.5) \quad \mathbf{a}_1^* = \frac{2}{3}\tilde{\mathbf{a}}_1 - \frac{1}{3}\tilde{\mathbf{a}}_2 = \frac{2}{3a^2}\mathbf{a}_1,$$

$$(A.6) \quad \mathbf{a}_2^* = -\frac{1}{3}\tilde{\mathbf{a}}_1 + \frac{2}{3}\tilde{\mathbf{a}}_2 = \frac{2}{3a^2}\mathbf{a}_2,$$

$$(A.7) \quad \mathbf{a}_3^* = -\frac{1}{3}\tilde{\mathbf{a}}_1 - \frac{1}{3}\tilde{\mathbf{a}}_2 = \frac{2}{3a^2}\mathbf{a}_3,$$

$$(A.8) \quad \mathbf{c}^* = \tilde{\mathbf{c}} = \frac{1}{c^2}\mathbf{c}.$$

This basis again satisfies $\mathbf{a}_1^* + \mathbf{a}_2^* + \mathbf{a}_3^* = 0$, but it is not the dual basis of $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c})$. It also has the advantage that crystallographically equivalent planes are connected by permutations of the components and changes of sign as stated above. Again, the components should be restricted to $a_1^* + a_2^* + a_3^* = 0$. If this is done, several practical simplifications are obtained: If a normal vector is given with respect to the basis $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*, \mathbf{c}^*)$, the reciprocals of its components correspond to the piercing point distances of the plane with the base vectors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c})$. Therefore, the plane $\{10\bar{1}2\}$ can be visualised by considering the points \mathbf{a}_1 , $-\mathbf{a}_3$ and $1/2\mathbf{c}$ (see Fig. 8). Moreover, one can easily see whether direction and normal vectors are perpendicular to each other by calculating the scalar product as if $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c})$ and $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*, \mathbf{c}^*)$ were dual bases. One notes easily that $\langle 10\bar{1}1 \rangle$ and $\{\bar{1}012\}$ are perpendicular to each other:

$$\begin{aligned}
 \text{(A.9)} \quad & (\mathbf{a}_1 - \mathbf{a}_3 + \mathbf{c}) \cdot (-\mathbf{a}_1^* + \mathbf{a}_3^* + 2\mathbf{c}^*) \\
 &= -\mathbf{a}_1 \cdot \mathbf{a}_1^* + \mathbf{a}_1 \cdot \mathbf{a}_3^* - \mathbf{a}_3 \cdot \mathbf{a}_3^* + \mathbf{a}_3 \cdot \mathbf{a}_1^* + 2\mathbf{c} \cdot \mathbf{c}^* \\
 &= -\frac{2}{3} - \frac{1}{3} - \frac{2}{3} - \frac{1}{3} + 2 = -1 - 1 + 2 = 0.
 \end{aligned}$$

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