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A study of the stress state associated with twin nucleation and propagation in anisotropic materials

By R. A. LEBENSOHN and C. N. TOMÉ

Instituto de Física Rosario (Consejo Nacional de Investigaciones Científicas y Técnicas–UNR), 27 de Febrero 210 bis, 2000 Rosario, Argentina

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ABSTRACT

In this work we are concerned with the study of the stress state associated with the activation of twinning in elastically anisotropic materials, in an attempt to achieve a better understanding of the contribution that twinning makes to plastic deformation and to texture development during forming operations. The assumption usually made is that twinning is activated by a critical resolved shear stress on the twinning plane and in the twinning direction, although the experimental evidence suggests that twinning depends in a more complex way upon the other stress components present in the medium.

Here we use a continuum approach to model the twin lamella as a flat inclusion of elliptic section embedded in an elastically anisotropic medium being acted upon by externally applied stresses. We calculate the Gibbs free energy of the system as the sum of an elastic term associated with size and inhomogeneity effects, and a surface energy term, associated with the twin–matrix interface. The minimization of the total energy with respect to the dimensions of the lamella is relevant both to twin nucleation and to twin propagation; in the former case, it gives the condition for when twin nucleation is energetically favourable with respect to a homogeneously strained matrix. In the latter case, it gives the condition of instability of an existing twin embryo, much the same as the Griffith's criterion does for crack extension.

We derive explicit results for the twinning systems active in silicon-iron, calcite and hexagonal zirconium, titanium and zinc. We find that, although the critical condition for twin activation depends on all six independent stress components, the resolved shear dominates and the influence of the other stress components is about two orders of magnitude weaker. We conclude that any substantial dependence of twinning upon stress components other than the resolved shear must come from the dependence of the twin-boundary energy upon stress. Possible atomistic mechanisms which may be influenced by a general stress field are discussed qualitatively.

§ 1. INTRODUCTION

Twinning is an important deformation mechanism in some cubic and in most non-cubic materials. In h.c.p. crystals, where deformation by slip along some directions either is not possible or at least requires very high stresses, twinning plays a predominant role in maintaining the ductile behaviour of the polycrystal. Our interest in twinning stems from the necessity of modelling the elastoplastic and large plastic deformation of non-cubic materials. In a recent paper (Tomé, Lebensohn and Kocks 1991) we addressed the problem of accounting properly for the contribution to texture

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of the twinned fractions in each grain. Here we address another aspect of twinning which is also relevant to modelling, namely the stress state required to nucleate and propagate twinning.

It is widely acknowledged that slip is activated by means of a critical resolved shear stress (CRSS) in the slip plane and in the slip direction. This CRSS can, to a large extent, be regarded as independent of the other stress components and of the hydrostatic pressure. For the case of twinning, although a CRSS in the twinning plane κ_1 and in the shear direction η_1 seems to be a necessary condition for activation, the experimental evidence indicates that the value of the CRSS depends upon the other stress components present in the material. In an early review, Cahn (1954) concludes, after analysing compression experiments done on rutile, dypside and baride, that twinning is favoured by the superposition of hydrostatic stress. Turner, Griggs and Heard (1954), on the other hand, find that pressure tends to inhibit the twinning activity in calcite single crystals. Priestner and Louat (1963) performed tensile tests in coarse-grained silicon steel samples cut from a sheet with a strong (110)⟨001⟩ texture and observed that the CRSS for activating $\{2\bar{1}1\}\langle 111\rangle$ twins is a function of the orientation of the tensile axis with respect to the texture component. Compressive tests performed by Blahovec (1972) on single crystals of silicon–iron also provide evidence of a dependence of the CRSS on the orientation of the crystals.

Less direct evidence of the dependence of twinning activation upon stress components other than the resolved shear is given by careful measurements of the evolution of internal stresses during mechanical loading of Zircaloy bar reported by MacEwen *et al.* (1988); at a stage of deformation that coincides with the initiation of twinning, they observe a marked relaxation of the stress normal to the basal planes. One way to explain such relaxation is to assume that twinning activation relaxes not only the resolved shear but also the stress component normal to the twinning plane. Atomistic simulations of twin boundaries performed by Serra and Bacon (1986) indicate that there is a variation in lattice spacing of the order of 0·3% across and within a few atomic planes parallel to the twin boundary. If twinning tends to distort the plane spacing, then the logical conclusion is that twinning may be enhanced or inhibited by superimposing a normal stress to the shear component.

A better understanding of twinning and its related mechanisms, at both the continuum and the atomistic levels, is required in order to interpret the evidence presented previously. We concentrate in what follows on the study of the elastic aspects of the problem and, specifically, on the 'size' and 'inhomogeneity' effects associated with the volumetric contributions of the twin to the free energy of the system. The size effect is due to the plastic shear strain associated with twinning and the inhomogeneity effect, which is included by the elastic anisotropy of the crystal, originates in the difference between the elastic constants of the matrix and of the twinned region. The criterion that we use to minimize the energy is equivalent to that used by Lee and Yoo (1990) and Yoo and Lee (1991) for dealing with the problem. By using a numerical (as opposed to an analytical) formulation we derive an explicit relation between the stress components and the critical dimensions of the twin lamella, valid for nucleation and for propagation. No attempt is made here to describe accurately the free energy of the twin–matrix interface or its dependence on the stress components.

Yoo (1979a, b) was the first to address the size and the inhomogeneity effects in an approximate way. He proposed to treat the twin lamella as if it were a slit crack in an elastically anisotropic medium, being activated by a mode II shear state. Using the formal treatment of Stroh (1958), Yoo replaced the 'misfit strain' by a continuum

distribution of dislocations and derived explicit expressions for the free energy of such a system subjected to externally imposed stresses for the case of hexagonal symmetry. The condition for twin propagation is obtained applying the Griffith's criterion of energy extrema to the slit crack, which leads to the following relation between the critical stress components:

$$\sigma_{12}^0(B_{11}\sigma_{12}^0+B_{12}\sigma_{22}^0)=\frac{G_t^I}{\pi a_1}, \tag{1}$$

where a_1 is the width of the twin lamella, regarded as an infinite slit parallel to the twinning plane κ_1, σ_{ij}^0 are the critical values of the stress components, B_{ij} is the symmetrical compliance tensor defined by Stroh (1958) and G_t^I is the 'twin extension force per unit length', analogous to the 'crack extension force per unit length' for a mode II crack. Since eqn (1) is formally derived from the interaction between a crack and a stress field, Yoo mentioned two important differences which may invalidate the twin-crack analogy: (a) while the free boundary of the crack is unable to withstand shear stresses, it is possible to transmit stress across the 'welded' twin crystal interface. In other words, while the lamella is represented as an inclusion with elastic stiffness C_{ijkl}^* of the same order as that of the crystal, the crack is equivalent to a void with $C_{ijkl}^*=0$; (*b*) although twin lamellae exhibit a lens shape of low aspect ratio, they are not infinitely flat in one dimensions and infinitely long in the other, as implied by the assumption of the slit crack. As a consequence, it may not be realistic to model it as an infinite flat cylinder, and an oblate ellipsoid seems to be closer to the actual shape for modelling purposes.

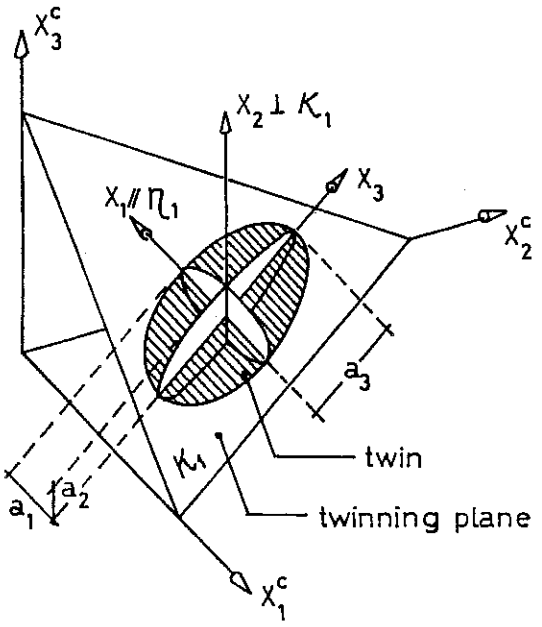
In the present work we improve upon the twin-crack analogy and treat the lamella as an elastic inclusion of ellipsoidal shape embedded in the elastically anisotropic medium represented by the crystal. Making use of results valid for inclusions in elastic media, we calculate the stress in the inclusion and the free energy of the system when a general stress field is externally imposed on the crystal. From these expressions we derive conditions for twin nucleation and twin propagation.

§2. Modelling the twin lamella

The twin lamella is a region of the grain which has undergone a plastic shear characteristic of the twin system under consideration and which has reoriented with respect to the parent crystal. As a consequence, the elastic constants of the twinned region differ from those of the matrix when both are referred to the same set of axes. In this work we assume that the lamella is a flat ellipsoid and use the standard Eshelby formalism for elastic inclusions to analyse the elastic response of such a system. The main axes of the ellipsoid are taken as a_1 parallel to the shear direction η_1, a_2 perpendicular to the twinning plane κ_1 and a_3 perpendicular to the other two axes (see fig. 1). We shall characterize the ellipsoid by the length a_1 of the main axis and by the aspect ratios $\gamma_2=a_2/a_1$ and $\gamma_3=a_3/a_1$. The experimental evidence and the results derived in this work indicate that $\gamma_2\ll 1$. As for the third aspect ratio, although the derivation that follows is completely general, for the calculations presented here it is given the value $\gamma_3=1$, which corresponds to a lamella with the shape of an oblate spheroid, and $\gamma_3=\infty$, which defines an infinite elliptic cylinder and allows us to test the twin-crack analogy.

In what follows we shall use the main axes of the ellipsoid, defined by the unitary vectors associated with the twinning system, as in the reference system (see fig. 1). We

Fig. 1



Position of the twinning plane κ_1, the twinning direction η_1 and the axes of the ellipsoid representing the twin lamella, with respect to the crystal axes.

shall denote by C^*_{ijkl} and C_{ijkl} the elastic constants of the lamella and of the parent crystal respectively, referred to this set of axes. When expressed in this system, the plastic deformation associated with the twin adopts the simple form

$$\epsilon^{\mathrm{p}}_{mn} = \tfrac{1}{2}s(\delta_{m1}\delta_{n2} + \delta_{m2}\delta_{n1}), \tag{2}$$

where s is the characteristic shear of the twinning system under consideration and δ_{ij} is Kronecker's delta. Since our interest is to analyse the effect of stress upon twin activation, we shall assume a uniform stress σ^0 applied to the crystal, which would induce a uniform strain $\epsilon^0_{ij} = C^{-1}_{ijkl}\sigma^0_{kl}$ if the medium were homogeneous. The presence of the lamella modifies the otherwise homogeneous stress and strain and induces the size effect, associated with the plastic transformation ϵ^{p}, and the inhomogeneity effect, associated with the difference between the elastic constants of the domain occupied by the lamella and of the medium.

Although the elastic treatment of an inhomogeneous inclusion of ellipsoidal shape is standard and can be found in textbooks (Mura 1987), it will help in understanding what follows to review the main results. The total stress inside the inclusion is uniform and given by

$$\sigma^0_{ij} + \sigma^{\mathrm{i}}_{ij} = C^*_{ijkl}(\epsilon^0_{kl} + \epsilon^{\mathrm{i}}_{kl} - \epsilon^{\mathrm{p}}_{kl}), \tag{3}$$

where $-\epsilon^{\mathrm{p}}$ is the elastic strain necessary to bring the inclusion back to the original shape and ϵ^{i} is the relaxation strain. The stress σ^{i} and the strain ϵ^{i} are, by definition, the deviations with respect to σ^0 and ϵ^0 induced by the inclusion. The standard way of solving this problem is to replace the inhomogeneous inclusion by a homogeneous inclusion having the same shape and supporting the same stress as the former. That is

achieved by defining a fictitious transformation $\epsilon_{kl}^{**}=\epsilon_{kl}^{p}+\epsilon_{kl}^{*}$ and imposing the condition

$$\sigma_{ij}^{0}+\sigma_{ij}^{i}=C_{ijkl}(\epsilon_{kl}^{0}+\epsilon_{kl}^{i}-\epsilon_{kl}^{**}). \tag{4}$$

The relaxation term is related to the fictitious transformation strain through the equation

$$\epsilon_{kl}^{i}=S_{klmn}\epsilon_{mn}^{**} \tag{5}$$

where S_{klmn} is the Eshelby tensor, a key element in the calculation and a function of the ellipsoid shape and the elastic constants of the matrix. Although explicit expressions exist which give S for isotropic media and particular inclusion shapes, for the purpose of this work we need to evaluate S for inclusions of general shape embedded in a medium with low symmetry elastic constants (when expressed in the inclusion axes the constants C_{ijkl} frequently exhibit orthotropic symmetry). In the Appendix we describe a simple numerical method that permits one to evaluate S for the most general conditions. From eqns (3–5) and using the relation $\epsilon=C^{-1}\sigma$ the following system of equations is obtained:

$$(\Delta C_{ijkl}S_{klmn}+C_{ijmn})\epsilon_{mn}^{**}=-\Delta C_{ijkl}C_{klmn}^{-1}\sigma_{mn}^{0}+C_{ijkl}^{*}\epsilon_{kl}^{p}, \tag{6}$$

where $\Delta C=C^{*}-C$. After calculating S the system (6) can be inverted to obtain ϵ^{**}, which depends upon the imposed stress σ_{ij}^{0}. Replacing ϵ^{**} and S in eqn. (4) gives the internal stress σ_{ij}^{i} in the lamella as a function of σ_{ij}^{0}:

$$\sigma_{ij}^{i}=C_{ijkl}(S_{klmn}\epsilon_{mn}^{**}-\epsilon_{kl}^{**}). \tag{7}$$

§ 3. Energetic considerations

The elastic energy W of a medium undergoing a transformation strain ϵ^{p} and being acted upon by external stresses is given by the general expression (Mura 1987)

$$W=\frac{1}{2}\int_{D}(\sigma_{ij}^{0}+\sigma_{ij}^{i})(u_{i,j}^{0}+u_{i,j}^{i}-\epsilon_{ij}^{p})\,\mathrm{d}D-\int_{S}F_{i}(u_{i}^{0}+u_{i}^{i})\,\mathrm{d}S, \tag{8}$$

where F_i are the components of the applied surface traction, σ_{ij}^{i}, $u_{i,j}^{i}$ and u_{i}^{i} are the stress, the distortion and the displacement respectively induced by the inclusion, and D and S are the volume and the external surface respectively of the medium. An inclusion-free homogeneous medium would have associated a Gibbs free energy W^{0} given by

$$W^{0}=\frac{1}{2}\int_{D}\sigma_{ij}^{0}u_{i,j}^{0}\,\mathrm{d}D-\int_{S}F_{h}u_{i}^{0}\,\mathrm{d}S, \tag{9}$$

For the analysis that follows, what matters is to compute the variation in free energy associated with the presence of the inclusion and defined by $\overline{\Delta W}=W-W^{0}$. Mura (1987) demonstrates that

$$\overline{\Delta W}=-\frac{1}{2}\int_{\Omega}\sigma_{ij}^{i}\epsilon_{ij}^{p}\,\mathrm{d}D-\int_{\Omega}\sigma_{ij}^{0}\epsilon_{ij}^{p}\,\mathrm{d}D, \tag{10}$$

where Ω is the volume occupied by the inclusion. According to the classical nucleation theory, the first term in eqn. (10) corresponds to the 'elastic strain energy' induced by the inclusion in the absence of externally applied stress (W^{*} in the book by Mura (1987)), while the second term corresponds to the 'driving force' and gives the interaction energy between the inclusion and the applied stress (ΔW in the book by Mura (1987)).

For the case of inhomogeneous inclusions, ϵ^p has to be replaced in eqn. (10) by the equivalent transformation strain ϵ^{**}. However, when solving eqn. (6) it turns out that $\epsilon_{12}^{**}=\epsilon_{21}^{**}\approx\frac{1}{2}s$ and $\epsilon_{ij}^{**}\ll\epsilon_{12}^{**}$ if $ij\neq 12$, provided that σ_{ij}^0 remains below the relatively high bound of 10^4 MPa. As a consequence, the inhomogeneity effect is relatively small in this case and ϵ^p, instead of ϵ^{**}, can be used to compute the energy variation. Replacing eqn. (2) in eqn. (10) and using the fact that the stress is uniform within the ellipsoidal inclusion, we obtain

$$\overline{\Delta W}\approx -\Omega s(\tfrac{1}{2}\sigma_{12}^i+\sigma_{12}^0). \tag{11}$$

Our calculation indicate that the induced stress given by eqn. (7) is, for a parametric value of γ_3, a linear function of the externally imposed stress and of the aspect ratio γ_2. In particular, the component

$$\sigma_{12}^i=F_{12kl}\sigma_{kl}^0-\beta\gamma_2. \tag{12}$$

The coefficients F_{12kl} and $\beta>0$ are calculated numerically by linear regression, which requires the solving of eqns (6) and (7) for several values of σ_{kl}^0 and γ_2. The linearity expressed by eqn. (12) is valid only for a lamella of low aspect ratio ($\gamma_2<0{\cdot}1$) and stress components σ_{kl}^0 not exceeding 10^4 MPa. Equation (12) is an important result because it allows one to write an analytical expression for the free energy in terms of the stress components and the physical dimensions of the lamella. One may, in turn, derive analytical expressions for the critical parameters that minimize the energy.

Up to now, only the elastic contribution to the Gibbs free energy has been accounted for. Since the twin lamella has a different crystallographic orientation from the crystal in which it is embedded, a term has to be added to the free energy to account for the presence of the twin–matrix interface. This term is associated with interactions on the atomic scale and, as will be discussed later, we believe that it plays a dominant role in controlling the conditions for twin nucleation and propagation. A proper calculation of this contribution would require detailed calculations of the atomic configurations of the twin boundaries, which is beyond the scope of this work. Fortunately, the contribution of the interface to the energy can be treated independently from the volumetric contribution associated with the elastic interactions. As a consequence, in what follows we shall concentrate in properly describing the latter, while for the former we shall assume that the boundary energy per unit area Γ_t is constant. Within this assumption, no distinction is made between the coherent and the incoherent parts of the interface, and Γ_t has to be interpreted as an average characteristic energy per unit area. The total free energy is $G=W+T$, with

$$T=2\pi a_1^2\gamma_3\Gamma_t \tag{13}$$

where $\gamma_2\ll 1$ is assumed for calculating the area of the ellipsoid. The variation in Gibbs free energy induced by the lamella is given by eqns. (11)–(13) as

$$\begin{aligned}\Delta G&=G-W^0\\&=\overline{\Delta W}+T\\&=\tfrac{4}{3}\pi a_1^3\gamma_2\gamma_3 s(\tfrac{1}{2}F_{12kl}\sigma_{kl}^0-\tfrac{1}{2}\beta\gamma_2+\sigma_{12}^0)+2\pi a_1^2\gamma_3\Gamma_t.\end{aligned} \tag{14}$$

Equation (14) gives the difference between the free energy of a medium containing a lamella of a given dimension and shape and subjected to a stress σ^0, and that of the same medium without the inclusion. Since an elastic system will tend to minimize its

Gibbs free energy G in a form compatible with the conditions externally imposed, in what follows we investigate the stability conditions for a twin lamella in the shape of an ellipsoid being acted upon by a stress σ^0. Since W^0 is independent of the parameters a_1, γ_2 and γ_3 that characterize the lamella, stability is defined by the extrema condition on the free energy variation at constant stress and temperature:

$$\mathrm{d}(\Delta G)_{\sigma_{ij}^0, T}=0. \tag{15}$$

As will be discussed later, eqn. (15) is relevant both to twin nucleation and to twin propagation.

For a lamella of fixed a_1 and γ_3 in equilibrium with a stress σ^0 there is a critical value of γ_2 which minimizes the free energy, given by the conditions

$$\left.\frac{\partial(\Delta G)}{\partial\gamma_2}\right|_{a_1,\gamma_3}=0, \quad \left.\frac{\partial^2(\Delta G)}{\partial\gamma_2^2}\right|_{a_1,\gamma_3}>0. \tag{16}$$

When the free energy is given by eqn. (14), this condition leads to a critical aspect ratio

$$\gamma_2^{\mathrm{cr}}=\frac{\frac{1}{2}F_{12kl}\sigma_{kl}^0+\sigma_{12}^0}{\beta}$$

$$\approx\frac{(F_{1212}+1)\sigma_{12}^0}{\beta}=J\sigma_{12}^0, \tag{17}$$

where J is a positive constant which depends on the crystallographic orientation of the twin system, its characteristic shear s and the eleastic constants of the crystal. Our calculations indicate that J is mildly dependent on the aspect ratio γ_3 *but is independent of the absolute size* a_1. Because of the simple form of the surface energy assumed here, the critical aspect ratio turns out to be independent of Γ_t for a flat lamella. In writing the approximate form of eqn. (17) we take into account that, according to the results of the numerical regression, $F_{1212}\gg F_{12kl}$ for $kl\neq 12$. The relation (17) between applied stress and aspect ratio has been deduced previously by Venables (1973) for elastically isotropic f.c.c. crystals using energetic considerations and dislocation theory. A related calculation was presented recently by Mitchell and Hirth (1991); they treated the interface as a distributed array of straight dislocations and calculated their equilibrium distribution under the action of a shear stress, showing that to a first order in the stress the equilibrium shape is a flat ellipse. In their case, however, the dimensions of the lamella are fixed and the stresss only has a sharpening or blunting effect upon the tip.

Next, if the size a_1 is also left free to adopt a value compatible with the imposed stress, the lamella will evolve to a critical size a_1^{cr} defined by the conditions

$$\left.\frac{\partial(\Delta G)}{\partial a_1}\right|_{\gamma_2^{\mathrm{cr}},\gamma_3}=0, \quad \left.\frac{\partial^2(\Delta G)}{\partial a_1^2}\right|_{\gamma_2^{\mathrm{cr}},\gamma_3}<0. \tag{18}$$

Equations (16) and (18) define the coordinates of a saddle point in the surface $\Delta G(a_1,\gamma_2)$ for parametric values of γ_3 and σ^0. In the previous analysis we use the aspect ratio γ_2 and the dimension a_1 as independent variables. It can be shown that our approach is equivalent and leads to the same critical conditions as the formulation by Yoo and Lee (1991) who, following Johnson and Cahn (1984), minimized the energy with respect to the aspect ratio γ_2 and the volume V of the lamella. The equivalence is easily demonstrated if the numerically obtained relations given by equations (12) and (17), are replaced in the formulation of Yoo and Lee (1991).

Substituting the Gibbs free energy given by eqn. (14) into eqn. (18) and using the aspect ratio given by eqn. (17) lead to the condition for being at the saddle point:

$$-a_1 sJ\sigma^0_{12}(D_{mn}\sigma^0_{mn})+\Gamma_t=0, \tag{19}$$

where the dimensionless tensor **D** is defined as

$$D_{mn}=\tfrac{1}{2}[F_{12mn}+I_{12mn}(1+F_{1212})]. \tag{20}$$

Equation (19) gives the relation between stress, size and aspect ratio for a twin in the shape of an oblate ellipsoid to be in equilibrium under the action of an applied stress. It is evident that shear stress σ^0_{12} acting on the twinning plane is a necessary condition for stability. We analyse in what follows the implications of the previous formulation upon twin nucleation and growth. Numerical calculations are presented for the following materials: zirconium, titanium, zinc, Fe–Si and calcite. The commonly observed twinning systems and the elastic constants of these materials are listed in tables 1 and 2

Table 1. Elastic constants and c/a ratio for the materials studied in this work. (After Simmons and Wang (1971).)

Material	Structure	c/a	C_{11} (10^{11} Pa)	C_{12} (10^{11} Pa)	C_{13} (10^{11} PA)	C_{33} (10^{11} Pa)	C_{44} (10^{11} Pa)	C_{14} (10^{11} Pa)
Zr	h.c.p.	1·593	1·43	0·73	0·65	1·65	0·32	0
Ti	h.c.p.	1·588	1·62	0·92	0·69	1·81	0·47	0
Zn	h.c.p.	1·856	1·64	0·36	0·53	0·63	0·39	0
Fe–3·2 wt% Si	b.c.c.	—	2·38	1·36	1·36	2·38	1·20	0
Calcite	Trigonal	3·418	1·46	0·60	0·51	0·85	0·34	−0·72

Table 2. Observed twinning systems and associated twin shear s for the materials studied in this work.

Material	System	System	s
Zr	tt1	$(10\bar{1}2)\langle\bar{1}011\rangle$	0·167
	ct1	$(2\bar{1}\bar{1}2)\langle 2\bar{1}\bar{1}3\rangle$	0·225
	tt2	$(11\bar{2}1)\langle\bar{1}\bar{1}26\rangle$	0·628
	ct2	$(10\bar{1}1)\langle 10\bar{1}2\rangle$	0·104
Ti	tt1	$(10\bar{1}2)\langle\bar{1}011\rangle$	0·174
	ct1	$(2\bar{1}\bar{1}2)\langle 2\bar{1}\bar{1}3\rangle$	0·219
	tt2	$(11\bar{2}1)\langle\bar{1}\bar{1}26\rangle$	0·630
	ct2	$(10\bar{1}1)\langle 10\bar{1}2\rangle$	0·099
Zn	tt1	$(10\bar{1}2)\langle 10\bar{1}\bar{1}\rangle$	0·138
	ct1	$(2\bar{1}\bar{1}2)\langle 2\bar{1}\bar{1}3\rangle$	0·519
	tt2	$(11\bar{2}1)\langle\bar{1}\bar{1}26\rangle$	0·539
	ct2	$(10\bar{1}1)\langle 10\bar{1}2\rangle$	0·372
Fe–3·2 wt% Si	—	$(2\bar{1}\bar{1})\langle 111\rangle$	0·707
Calcite	e^+	$(01\bar{1}8)\langle 0\bar{4}41\rangle$	0·694

Table 3. Proportionality constant J between the applied shear σ^0_{12} and the lamella aspect ratio γ_2; non-zero dimensionless coefficients D_{ij} coupling the applied shear σ^0_{12} with the other stress components (eqn. (19)) are also shown. These are for the case $\gamma_3 = 1$.

Material	System	J (10^{-11} Pa^{-1})	D_{11} (10^{-2})	D_{22} (10^{-2})	D_{33} (10^{-2})	$2 \times D_{12}$	$2JsD_{12}$
Zr	tt1	8·57	−0·16	−0·30	0·35	0·501	1·434
	ct1	6·35	0·56	−0·14	−0·32	0·502	1·434
	tt2	2·31	−0·54	0·28	0·20	0·502	1·456
	ct2	14·34	0·60	−0·21	−0·29	0·503	1·497
Ti	tt1	7·11	−0·32	−0·35	0·70	0·504	1·245
	ct1	5·19	0·36	0·25	−0·65	0·503	1·434
	tt2	1·84	−0·26	−0·13	0·41	0·501	1·161
	ct2	11·65	0·35	0·22	−0·61	0·503	1·160
Zn	tt1	12·33	−1·96	−1·64	1·46	0·531	1·807
	ct1	3·42	−2·45	−0·40	1·15	0·528	1·874
	tt2	3·36	1·78	−0·11	−0·68	0·511	1·851
	ct2	4·83	−2·39	−0·21	−1·05	0·525	1·887
Fe–3·2 wt% Si	—	0·96	0	1·20	−1·20	0·511	0·693
Calcite	e^+	2·29	0·96	0·99	−1·08	0·506	1·608

respectively. The calculated value of the components D_{mn} are listed in table 3 for all the materials and twinning systems, assuming a lamella in the shape of an oblate spheroid ($\gamma_3 = 1$). It can be seen that, for all materials, D_{12} is much larger than the other D_{ij} components. Furthermore, $D_{23} = D_{32} = D_{13} = D_{31} = 0$ for all the twinning systems because of the orthotropic symmetry of the elastic constants expressed in the system of the ellipsoid axes.

3.1. *Twin nucleation*

Twin nucleation differs from the more familiar second-phase or precipitate nucleation in that there is no difference between the intrinsic energy per unit volume of each phase, a feature which can tip the energetic balance and induce spontaneous nucleation. Instead, ΔG gives the energy to be provided either by local fluctuations or by some other mechanism if nucleation of a twin of a given size and shape is to take place under the presence of a stress σ^0. The condition for stability of the nucleated lamella is given by eqn. (19), which for a fixed value of σ^0 defines the minimum size of the twin lamella that can nucleate as being

$$a_1^{cr} = \frac{\Gamma_t}{Js\sigma^0_{12}(D_{mn}\sigma^0_{mn})}. \tag{21}$$

Equation (21) indicates that, the smaller the applied shear, the larger has to be the twin lamella for it to be stable, and the feasibility of such nucleation is measured by the amount of energy required. After substituting eqn. (21) in eqns (14) and (20), we obtain

$$\Delta G(a_1^{cr}, \sigma^0) = \tfrac{2}{3}\pi(a_1^{cr})^2\gamma_3\Gamma_t, \tag{22}$$

which is exactly one third of the twin interface energy given by eqn. (13). An estimate of the critical dimensions and the nucleation energy for the two compressive twin systems

$(2\bar{1}\bar{1}2)$ and $(10\bar{1}1)$ in titanium can be obtained using typical values of $\gamma_3=1$, $\sigma^0_{12}=10^3$ MPa, the values of J, $2D_{12}$ and s listed in tables 2 and 3, and the values of surface energy $\Gamma_t=0{\cdot}266\,\mathrm{J\,m^{-2}}$ and $\Gamma_t=0{\cdot}765\,\mathrm{J\,m^{-2}}$ respectively reported by Yoo and Lee (1991) from their atomistic simulations. The following values are then obtained: $a_1=0{\cdot}047\,\mu\mathrm{m}$, $\gamma_2=0{\cdot}052$ and $\Delta G=1{\cdot}23\times10^{-15}\,\mathrm{J}$ (or $2{\cdot}97\times10^5 kT$ at $T=300\,\mathrm{K}$) for the $(2\bar{1}\bar{1}2)$ system, and $a_1=0{\cdot}131\,\mu\mathrm{m}$, $\gamma_2=0{\cdot}117$ and $\Delta G=27\times10^{-15}\,\mathrm{J}$ (or $65\times10^5 kT$ at $T=300\,\mathrm{K}$) for the $(10\bar{1}1)$ system. The immediate conclusion is, as Yoo and Lee (1991) pointed out, that the first system is more likely to be active than the latter, as the experimental evidence confirms.

Such high energies cannot be provided by thermal fluctuation, which eliminates the likelihood of inducing homogeneous nucleation. It should be borne in mind that we are modelling a simple system, formed by an inclusion in an infinite homogeneous matrix, while the real situation is far more complex. However, if the previous results are combined with this complexity, they provide a clue for the mechanisms that may facilitate twin nucleation. To start with, the linear dependence on γ_3, expressed by eqn. (22), indicates that the required energy is reduced if the lamella nucleates adopting a 'needle' (instead of a 'disc') shape. Also, dislocation pile-ups could provide stress concentrations high enough to lower the critical size a_1 of the stable twin (given by eqn. (21)) and, consequently, the energy required for nucleation. Grain boundaries or dislocation jogs can be envisaged as 'pre-existent' defective zones that may act as a 'seed' and provide part of the energy ΔG required for nucleation, so reducing the energy to be provided by the elastic term. Dislocation pile-ups at grain boundaries would combine two of the previous mechanisms and would be likely candidates for triggering nucleation. In principle, according to the previous arguments, any microstructural feature acting as a stress concentrator or having an associated extra energy improves the chances of inducing twin nucleation in the grains.

The stresses involved in the nucleation process would be of a local short-range type and, once the lamella has been created, it is conceivable that the configuration will become unstable; the lamella will go 'over the top', grow beyond the critical size and, in the process, will relax the stress that induced nucleation. As a result, the critical value for nucleation given by eqn. (21) represents a lower bound and the final size of the lamella may be expected to be within the range of the stresses being relaxed.

3.2. *Twin growth*

The fact that twins can form, as single-crystal experiments show, under conditions of suddenly falling stress, implies that the stress for propagation is different from the stress for nucleation. To analyse twin propagation, one has to assume that a previously nucleated lamella of size a_1 is already present in the material. As the imposed stress increases, the energy G will eventually reach a maximum, after which any further increase in stress will destabilize the lamella and make it grow, much the same as a crack does. In this respect, the theory of twin growth is formally equivalent to the Griffith's theory of crack propagation. The condition of instability is given by the maximum of the free energy $G=W^0+\Delta G$ but, since W^0 is independent of the twin parameters, the problem reduces to find the extremum of ΔG, which has been done in the previous section. For a lamella of size a_1 the stress state that will make the system overcome the energy barrier is given by eqn. (19) as

$$\sigma^0_{12}(D_{mn}\sigma^0_{mn})=\frac{\Gamma_t}{a_1 Js}, \tag{23}$$

which indicates that a shear component is a necessary condition for twin propagation. However, the precise value of such component depends on the values that the other components adopt, and their influence upon σ_{12}^0 is measured by the coupling coefficients D_{mn}. As is evident from table 3, for all the cases studied, D_{12} is much larger than the other D_{mn} values and, as a consequence, eqn. (23) can be written in the approximate form

$$\sigma_{12}^{02} \approx \frac{\Gamma_t}{2D_{12}Jsa_1} = \frac{\Gamma_t}{D'_{12}a_1}, \tag{24}$$

provided that none of the other stress components is much larger than σ_{12}^0. Equation (24) is important because it justifies the assumption of a CRSS associated with twin activation. Such CRSS depends on crystallographic parameters and physical constants of the material through $D'_{12} = 2D_{12}Js$, listed in table 3. It also shows that, the smaller the interface energy per unit area or the larger the size of the existing lamella, the smaller is the CRSS required to propagate it. A lower bound for the CRSS is set by the grain dimension, which limits the maximum size achievable and may explain why twinning is not observed in fine-grained polycrystals.

3.3. *The case of a flat elliptic cylinder*

We analyse in this section the saddle point-configuration of the free energy for the case of lamella having the shape of a flat elliptic cylinder ($\gamma_2 \ll 1$; $\gamma_3 = \infty$) subjected to a stress σ^0. Although such morphology may be unrealistic, the case is useful for showing that the assumption of a lenticular lamella ($\gamma_3 = 1$) is not restrictive and that similar results are obtained at the other extreme of the interval $1 < \gamma_3 < \infty$. Also, the cylindrical morphology will permit us to test the validity of the twin-crack analogy used by Yoo (1979a, b) to study the effect of stress upon twin activation.

For an infinite lamella the relevant magnitudes are the interface energy per unit length given by

$$T^1 = 4a_1\Gamma_t \tag{25}$$

the volume per unit length given by

$$\Omega^1 = \pi a_1^2 \gamma_2 \tag{26}$$

and the free-energy variation per unit length given by

$$\Delta G^1 = -\pi a_1^2 \gamma_2 s(\tfrac{1}{2}F_{12kl}\sigma_{kl}^0 - \tfrac{1}{2}\beta\gamma_2 + \sigma_{12}^0) + 4a_1\Gamma_t. \tag{27}$$

The search for the energy extrema (eqns (16) and (18)) leads to a condition of the same form as eqn. (19):

$$-\pi a_1 sJ\sigma_{12}^0(D_{mn}\sigma_{mn}^0) + 2\Gamma_t = 0, \tag{28}$$

where J and D_{mn} have to be calculated for $\gamma_3 = \infty$ (see Appendix). As before, eqn. (28) gives the minimum size for a stable twin lamella to nucleate under the action of a stress σ^0. The corresponding change in free energy required for such nucleation is

$$\Delta G^1(a_1^{cr}, \sigma^0) = 6a_1^{cr}\Gamma_t = \tfrac{3}{2}T^1. \tag{29}$$

Table 4. Proportionality constant J between the applied shear σ^0_{12} and the lamella aspect ratio γ_2; non-zero dimensionless coefficients D_{ij} coupling the applied shear σ^0_{12} with the other stress components (eqn (19)) are also shown. These are for the case $\gamma_3=\infty$.

Material	System	J (10^{-11} Pa^{-1})	D_{11} (10^{-2})	D_{22} (10^{-2}	D_{33} (10^{-2})	$2\times D_{12}$
Zr	tt1	11·34	−0·12	−0·23	0·26	0·501
	ct1	8·27	0·43	−0·11	−0·24	0·502
	tt2	2·92	−0·42	0·22	0·16	0·502
	ct2	18·54	0·46	−0·17	−0·23	0·504
Ti	tt1	9·12	−0·25	−0·27	0·54	0·502
	ct1	6·68	0·28	0·20	−0·50	0·502
	tt2	2·37	−0·20	−0·10	0·32	0·501
	ct2	14·99	0·27	0·17	−0·47	0·502
Zn	tt1	17·46	−1·37	−1·14	1·02	0·518
	ct1	5·11	−1·62	−0·27	0·77	0·516
	tt2	5·31	1·11	−0·07	−0·42	0·506
	ct2	7·33	−1·55	−0·14	−0·69	0·514
Fe–3·2 wt% Si	—	1·19	0	0·97	−0·97	0·508
Calcite	e^+	3·40	0·65	0·67	−0·73	0·504

For an existing lamella of size a_1, however, eqn. (28) gives the combination of stress components that will destabilize it and make it propagate:

$$\sigma^0_{12}(D_{mn}\sigma^0_{mn})=\frac{4\Gamma_t}{2Js\pi a_1}. \tag{30}$$

Values of J and D_{mn} for all the materials and twinning systems considered here are calculated for $\gamma_3=\infty$ and are reported in table 4, where it can be seen that they are slightly smaller in absolute value but not substantially different from the values reported in table 3, corresponding to $\gamma_3=1$. Although the corresponding values are not reported here, we have verified that both J and D_{mn} show a smooth monotonic decrease when γ_3 varies from 0·5 to ∞. As a consequence, the formulation does not depend critically on the width of the lamella as far as the energy extrema are concerned. The required energy for nucleation given by eqn. (22), however, is directly proportional to such width, which would suggest that narrow lamellae would be favoured in the nucleation process.

§4. Discussion of results

Owing to the crystallographic symmetry of the materials and twinning systems considered in this work, $D_{23}=D_{13}=0$ for all the cases. As a result, the critical stress condition for twin nucleation and propagation (eqn. (19)) can be written explicitly as

$$\sigma^0_{12}(2D_{12}\sigma^0_{12}+D_{11}\sigma^0_{11}+D_{22}\sigma^0_{22}+D_{33}\sigma^0_{33})=\text{constant}, \tag{31}$$

indicating that a shear stress is a necessary condition for destabilizing the lamella, and that its precise value depends on the values adopted by the diagonal stress components.

Of particular interest is the case of a hydrostatic pressure p superimposed on the shear component, which gives a critical condition of the form

$$\sigma_{12}^0[2D_{12}\sigma_{12}^0-(D_{11}+D_{22}+D_{33})p]=\text{constant}. \tag{32}$$

From the results in tables 3 and 4 it is evident that a hydrostatic pressure should have no effect over twinning in cubic crystals, because $D_{11}+D_{22}+D_{33}=0$ for this case.

The fact that $D_{12}\gg D_{mm}$ for all the cases (see tables 3 and 4) indicates that the critical shear is weakly affected by the diagonal components. As a consequence, (*a*) the predicted dependence of twin nucleation and twin propagation with stress components other than the resolved shear in the twinning plane and along the twinning direction is very weak within the present approach and (*b*) it is possible to derive a CRSS in terms of crystal parameters, interface energy and size of the lamella (eqn. (24)).

The experimental evidence available for silicon-iron, although not so clear cut, indicates a stronger coupling between the diagonal and the shear components. The tensile experiments performed by Priestner and Louat (1963) in strongly textured material, show an increase in the critical shear for twinning as the difference $\sigma_{33}^0-\sigma_{22}^0$ decreases. An analysis of their experimental data permits us to estimate the coupling coefficients to be of the order $2D_{12}=0{\cdot}5$ and $D_{33}=-D_{22}=0{\cdot}1$. The latter components differ in sign and absolute value from those calculated here, which are listed in tables 3 and 4. The only way to explain the discrepancy is to ascribe such behaviour to a different mechanism which couples more strongly the stress components and screen completely the inhomogeneity effect. Compressive experiments done by Blahovec (1972) in silicon–iron single crystals, also exhibit a dependence of the CRSS for twinning with the orientation of the twinning plane with respect to the compressive axis. The scatter in his results, however, does not allow reliable estimation of the coupling coefficients.

A case for which our approach predicts the correct order and the correct sign for the coupling is that of calcite subjected to large hydrostatic pressure. According to the classical experiments performed by Turner *et al.* (1954), the critical twinning shear at atmospheric pressure ($p=0{\cdot}1$ MPa) is 1·5 MPa, while at a pressure of 1000 MPa they observed that the critical shear rises to 6 MPa. Replacing the values of D_{mn} from table 3 ($\gamma_3=1$) in eqn. (32) we obtain a relation

$$\sigma_{12}^0(0{\cdot}506\sigma_{12}^0-0{\cdot}0087p)=\text{constant}, \tag{33}$$

from where the constant term can be calculated by replacing the critical stress measured at atmospheric pressure. After doing that, the critical shear predicted for a superimposed hydrostatic pressure of 1000 MPa is 17·1 MPa. If instead the values from table 4 ($\gamma_3=\infty$) are used, a CRSS of 11·9 MPa is obtained. It should be noted that, although the coupling is weak, it is enhanced by a pressure two orders of magnitude larger than the critical shear.

4.1. *The twin-crack analogy*

Yoo (1979a, b) has addressed the competition between twinning and fracture in hexagonal metals using an energy criterion and assuming that the twin lamella reacts to the applied stress in the same manner as a mode II slit crack. By imposing such a twin-crack analogy, Yoo arrived at a criterion for deciding whether twinning or fracture is the dominant mechanism. Such a criterion depends on the ratio of the interface energy associated with the twin to that of the crack, which in turn is a function of the orientation of the slit plane with respect to the crystal axes for the case of elastic

anisotropy. Yoo was aware, however, of the distinction between slit cracks and deformation twins and warned that 'the finite thickness of the twin and the welded boundary condition for twin interfaces' may invalidate the conclusions that he derived through the twin-crack analogy. In this section we assess the validity of such an assumption using the model developed in the previous sections.

In order to facilitate comparison with eqn. (1) derived by Yoo (1979a), it is convenient to rewrite eqn. (30) in terms of the compliance factors $D'_{mn}=2JsD_{mn}$ and the twin extension force $G_t^1=4\Gamma_t$ per unit length as

$$\sigma_{12}^0(2D'_{12}\sigma_{12}^0+D'_{11}\sigma_{11}^0+D'_{22}\sigma_{22}^0+D'_{33}\sigma_{33}^0)=\frac{G_t^1}{\pi a_1}. \tag{34}$$

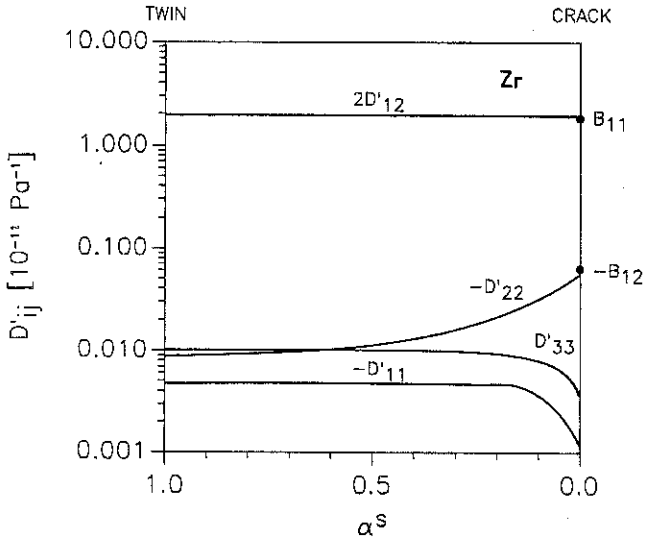
The elastic compliances D'_{mn} are the equivalent, for the twin lamella, to the symmetrical second-order tensor B_{mn} defined by Stroh (1958) for the slit crack. Next, we modify the elastic moduli of the twin lamella by a softening factor α^s:

$$C_s^*=\alpha^s C^* \tag{35}$$

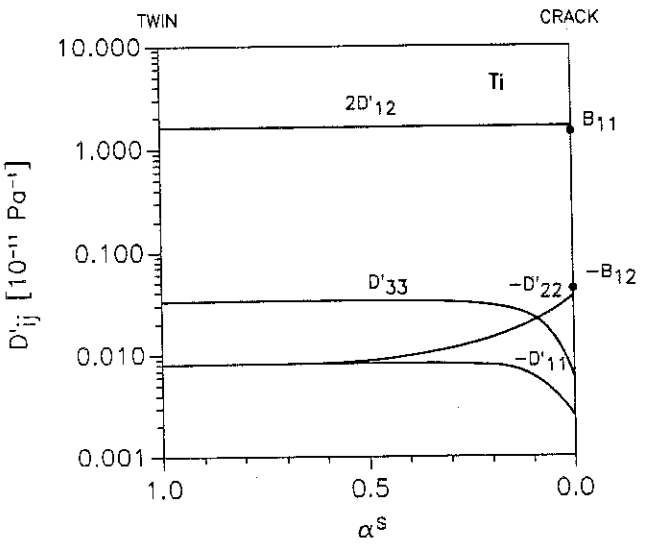
such that, when α^s varies from 1 to 0 we go from the elliptic lamella that represents the twin to an elliptic void of the same shape. Using C_s^* instead of C* in eqns (3)–(7), we compute $D'_{mn}=2JsD_{mn}$ as a function of α^s for the $(10\bar{1}2)\langle 10\bar{1}1\rangle$ twinning system in titanium, zirconium and zinc. Equation (17) giving the proportionality parameter J between the applied shear and the equilibrium aspect ratio γ_2 was not applied because the inclusion tends to adopt a spherical shape as it becomes softer. Instead, the value of J corresponding to $\alpha^s=1$ is enforced throughout the calculation, which corresponds to the assumption of a small but non-zero aspect ratio γ_2. The case $\gamma_2=0$ cannot be treated because our expression for the Eshelby tensor (see Appendix) is not defined at that value.

The non-zero coupling components D'_{mn} are plotted in fig. 2 as a function of α^s and the values corresponding to $\alpha^s=1$ and $\alpha^s=0$ (in fact $\alpha^s\ll 1$) are reported in table 5. For

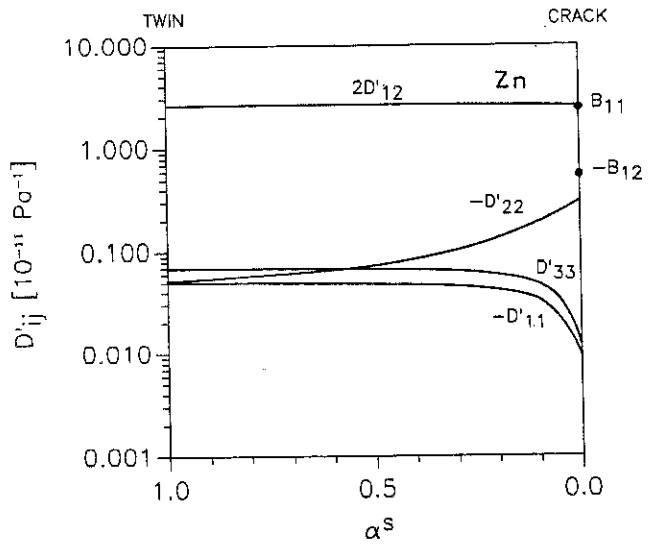
Fig. 2



(a)



(*b*)



(*c*)

Variation in the coupling components D'_{ij} entering eqn. (34), when going from a cylindrical twin lamella ($\alpha^s = 1$) in the $(10\bar{1}2)\langle\bar{1}011\rangle$ system to an ellipsoidal cavity of the same shape ($\alpha^s = 0$) in the same plane. Calculations correspond to (*a*) zirconium, (*b*) titanium and (*c*) zinc.

Table 5. Compliance factors $D'_{ij}=2JsD_{ij}$ calculated for a twin ($\alpha^s=1$) and for a crack ($\alpha^s\approx 0$), together with the Stroh compliance factors B_{11} and B_{12} used by Yoo in eqn. (1).

		$\alpha^s=1$				$\alpha^s\approx 0$					
Material	System	D'_{11}	D'_{22}	D'_{33}	$2\times D'_{12}$	D'_{11}	D'_{22}	D'_{33}	$2\times D'_{12}$	B_{11} (10^{-11}Pa^{-1})	B_{12} (10^{-11}Pa^{-1})
Zr	tt1	−0·0045	−0·0087	0·0098	1·90	−0·0012	−0·055	0·0032	1·90	1·80	−0·062
Ti	tt1	−0·0079	−0·0085	0·0322	1·59	−0·0013	−0·038	0·0052	1·61	1·44	−0·043
Zn	tt1	−0·0662	−0·0549	0·0487	2·50	−0·0115	−0·288	0·0094	2·35	2·38	−0·544

$\alpha^s = 0$ they have to be compared with the values B_{11} and B_{12} which appear in eqn. (1), corresponding to the slit crack. We observe that the leading component, D'_{12}, remains almost constant thoughout the softening process and equal to the value of B_{11} for the slit crack. The component D'_{22}, coupling σ^0_{12} with the normal stress σ^0_{22}, increases by an order of magnitude and falls very close to the corresponding compliance B_{12} for the slit crack. The other two coupling compliances D'_{11} and D'_{33} decrease by an order of magnitude when $\alpha^s \to 0$, in agreement with the response predicted for the slit crack. The difference between our predictions and those for the slit crack arises because, in our calculations, $\gamma_2 \ll 1$ but is still different from zero while, for the slit crack, $\gamma_2 = 0$.

What our results show is that the twin-crack analogy proposed by Yoo (1979a) is valid for calculating the main compliance D'_{12}; on the other hand, it predicts the correct sign for the coupling with σ^0_{22} but overestimated the coupling coefficient D'_{22}. However, the latter is still much smaller than D'_{12} (with the sole exception of D_{22} for zinc) and, as a consequence, the twin-crack analogy provides a reasonable estimate of the effect of stress upon twin activation. It should be borne in mind that only elastic effects are accounted for by this formulation. A qualitative discussion of possible atomistic mechanisms which may show a stress dependence is presented in the following section.

§ 5. Concluding remarks

We try in this work to elucidate the influence upon twinning of stress components other than the resolved shear in the twinning plane and in the twinning direction. We adopt for this purpose an elastic continuum approach and treat the twin lamella as an ellipsoidal inclusion embedded in an elastic matrix being acted upon by an externally imposed stress. We express the free energy of the system as the sum of three terms: the internal strain energy associated with the twinning shear, the elastic energy arising from the interaction between the inclusion and the external stress, and a surface energy term associated with the presence of the twin–matrix interface. The latter term is strongly related to the atomistic and crystallographic characteristics of the boundary, but the assumption is made here that this contribution is simply proportional to the area of the interface. Such an assumption amounts to putting the coherent and incoherent parts of the boundary on the same footing and to defining an average energy per unit area which is characteristic of the lamella under study.

Within a continuum approach, the coupling between the resolved shear and the other strees components is related to the inhomogeneity effect and would not show up in an elastically isotropic crystal. For all materials analysed in this work, the elastic anisotropy is not strong enough to give a substantial coupling of the diagonal stress components with the shear component. Only if the diagonal components are orders of magnitude larger than the shear stress does the critical shear show a non-negligible variation, as the experimental evidence for calcite shows.

When the elastic stiffness moduli of the twin lamella are 'softened' artificially in order to derive results for the crack, the inhomogeneity effect is more pronounced but the predicted influence of the diagonal stress components (table 5) remains still low.

An important conclusion of this study is that, from a continuum point of view, the activation of twinning is correctly described by the Schmid criterion of CRSS, independent of the other stress components (and of the hydrostatic pressure in particular) provided that the latter are not much bigger. Also, our calculations show

that the twin-crack analogy proposed by Yoo (1979b) for deciding whether twins or cracks are operative in a given material, depending upon the relative energy associated with the twin and the crack interfaces, is meaningful.

In performing this study, however, we are not accounting for any dependence of the interface energy with the stress components. We would like to close the present discussion with a brief analysis of the atomistic characteristics of the twin boundary and the possible effect of stress upon it.

Twin growth requires the motion of twin dislocations, which shift the atoms in the twinning plane to the perfect lattice positions in the twinned crystal. Such a shift, however, does not take place in every plane but after every n planes (n varies depending on the crystallography of the system). The atoms in intermediate planes have to 'shuffle' in order to recompose the perfect lattice, and in the process they have to overcome the energy barriers created by the interaction with the neighbours. As a consequence, shuffling is a likely candidate when looking for atomistic mechanisms which can affect the dynamics of twinning in low-symmetry crystals. Yoo and Lee (1991) suggest that the enhancement and inhibition of twinning observed in titanium and zirconium alloys respectively, when the content of alloying elements increases, may be due to differences between the shuffling dynamics of solute and matrix atoms. In relation to our problem, it is clear that the presence of a stress field will change the atomic separations in the lattice. As a consequence, shuffling (and so twinning) will be affected because of the induced variations in the atomic interactions and in the energy barriers that the atoms have to overcome.

Another feature of twinning, revealed by atomistic simulations performed by Serra and Bacon (1986), Serra *et al.* (1991), and Yoo and Lee (1991) among others, is a variation in the spacing of the atomic planes close to the twin boundary, with respect to the perfect lattice spacing. Calculations done by those workers for $\{11\bar{2}2\}$ twins in a h.c.p. crystal with an ideal c/a ratio held together by a short-range empirical central potential predict positive distortions of 0·3% and 0·15% in the atomic spacing of the $\{11\bar{2}2\}$ planes close to the twin boundary. Such a distortion, which results from minimizing the configurational energy of the system, suggests that the occurrence of twinning may be enhanced by superimposing externally an elastic distortion of the same sign to the untwinned crystal. Conversely, a superimposed distortion of opposite sign will force the forming twin to perform work against it and will tend to inhibit the occurrence of twinning. This is still another way in which the presence of stress components other than shear can be envisaged to modify the dynamics of twinning.

As for the mechanisms which may be modified by the presence of a stress field in the non-coherent region of the interface one may consider the twin-dislocation pile-up at the tip of the lamella. The energy and shape of such configuration has been studied by Mitchell and Hirth (1991) for screw and edge dislocations as a function of the applied shear. It is evident that the addition of other stress components will modify the configuration of the dislocation cores and, as a consequence, the Peierls stress. What is not clear is in which direction and to what extent the dislocation dynamics will be affected. Such an analysis, and the previous analyses as well, can be carried out only through atomistic calculations.

APPENDIX

THE ANISOTROPIC ESHELBY TENSOR

The Eshelby tensor associated with an ellipsoidal inclusion of main axes a_1, a_2, a_3 embedded in an elastically anisotropic medium can be calculated using the integral expression derived in Chapter 3 of the book by Mura (1987):

$$S_{ijmn}=\Lambda_{ijpq}C_{pqmn}, \tag{A 1}$$

where C_{pqmn} is the tensor of elastic stiffness expressed in the axis of the inclusion and

$$\Lambda_{ijpq}=\frac{1}{16\pi}\int_0^{\pi}\sin\theta\,d\theta\int_0^{2\pi}\lambda_{ijpq}\,d\phi, \tag{A 2}$$

with

$$\lambda_{ijpq}=L_{ip}^{-1}(\bar{\xi})\xi_j\xi_q+L_{jp}^{-1}(\bar{\xi})\xi_i\xi_p+L_{iq}^{-1}(\bar{\xi})\xi_j\xi_p+L_{jq}^{-1}(\bar{\xi})\xi_i\xi_p. \tag{A 3}$$

Here

$$L_{ip}(\bar{\xi})=C_{ijpl}\xi_j\xi_l \tag{A 4}$$

and

$$\xi_1=\frac{\sin\theta\cos\phi}{a_1},\qquad \xi_2=\frac{\sin\theta\sin\phi}{a_2},\qquad \xi_3=\frac{\cos\theta}{a_3}, \tag{A 5}$$

where $0<\phi<2\pi$ are spherical coordinates defining the position of a point in a unitary sphere, referred to the main axes of the ellipsoid. The case of an elliptic cylinder ($\gamma_3=\infty$) corresponds to $\xi_3=0$. It is evident from eqns (A 2) and (A 3) that

$$\Lambda_{ijpq}=\Lambda_{jipq}=\Lambda_{ijqp}=\Lambda_{pqij}. \tag{A 6}$$

The Eshelby tensor given by eqn. (A 1) is evaluated in this work using the previous formulation as follows: the intervals $0<\theta<\pi$ and $0<\phi<2\pi$ are partitioned in 2° increments and $\bar{\xi}$ (eqn. (A 5)), L (eqn. (A 4)) and λ (eqn. (A 3)) are evaluated in that sequence for every pair of angles θ_n, ϕ_m. The tensor Λ given by eqn. (A 2) is integrated straightforwardly using an extended trapezoidal rule in each dimension and, once obtained, is multiplied by C to derive the Eshleby tensor defined by eqn. (A 1). By taking advantage of the general inversion symmetry $\lambda(\bar{\xi})=\lambda(-\bar{\xi})$ it is possible to reduce the domain where the numerical integration has to be performed to $0<\theta<\pi/2$ and $0<\phi<\pi/2$.

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