On the energy of terminated stacking faults

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Abstract

The equilibrium of dissociated dislocations is discussed in terms of intrinsic material properties such as the ideal stacking fault energy (ideal SFE) and the stacking fault (SF) strain. The ideal SFE is defined as the energy per unit area of an infinitely extended SF in an ideal infinite crystal. The effective SFE is defined as the energy per unit area of a terminated SF. The terminated SF is associated with a strain field. The strain field is modelled in terms of conventional and Somigliana dislocations. It is found that the effective SFE significantly overestimates the ideal SFE if the ideal SFE is low and the SF strain is large. A numerical example is given for austenitic stainless steel.

§ 1. Introduction

The dissociation of a perfect dislocation into partials (with a stacking fault (SF) in between) severely affects the deformation characteristics, which are planar glide, wavy glide, deformation twinning and stress-induced martensite formation. The separation width of the dislocations thereby plays a dominant role. The equilibrium separation of the dissociated dislocation is controlled by the minimum of the total stored energy $E_{\text{tot}}$, which corresponds to a force balance at the partial dislocations:

$$F_{\text{tot}} = -\frac{\partial E_{\text{tot}}}{\partial r} = 0,$$

where $r$ is the shift of the dislocation line perpendicular to itself.

One might now ask the question, what are the intrinsic material properties controlling the force equilibrium? In order to answer this question, we have to analyse the different contributions to the total energy. The SF can be considered as a planar defect or as a volume defect with a constant thickness $d$. There are several arguments that favour the volume approach (e.g. the bonding changes due to a change in the stacking sequence (Hirth and Lothe 1968a, Hirth 1970)). Thus a SF may be considered as a plate-like precipitate or a special martensitic lath. We shall call it a stacking fault phase (SFP).

It has been found experimentally that the SFP may have a distorted lattice, that is distorted with respect to the matrix (Holsworth and Louthan 1968, Lecroyse 1971, Brooks, Loretto and Smallman 1979a, b, Zummer and Janko 1979). Thus elastic strains are introduced and the strain energy $E_{\text{strain}}$ contributes to the defect energy. An attempt has been made to include the strain energy term into the stacking fault energy (SFE) (Olson and Cohen 1976). We shall call this entity the effective

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SFE $\gamma_{\text{eff}}$. Frequently, the strain energy term has been neglected by analysing dislocation configurations assuming that the lattice distortions are very small.

Furthermore, it has been discussed that, in the case of small separation width, the equilibrium separation is affected by the finite width of the dislocation cores and their interaction (Esterling, McGurn, Boswarva and Arsenault 1984, Duesbery and Vetek 1985, Esterling and Arsenault 1985, Kroupa 1994). However, for low-SFE materials, and thus wide separation distances, this effect can be neglected.

The aim of the present letter is to discuss the roles of the strain energy term and of the effective SFE. The analysis is based on the assumption of isotropic elasticity. The effect of dislocation cores will not be considered, thereby restricting the results to materials where the separation distance is large compared with the Burgers vector. It will be shown that the effective SFE is not an intrinsic material property. It is proposed to describe stacking faults by two entities: the ideal SFE which is the SFE of an infinitely extended SF and the stacking fault contraction $\varepsilon$ which is associated with the lattice distortions of the SF. A procedure is suggested to determine the ideal SFE.

§ 2. THE IDEAL STACKING-FAULT ENERGY

Let us consider an infinite and perfect single crystal. We choose a glide plane and cut the crystal along that plane. We call this plane the fault plane. We translate one half-crystal rigidly along the glide plane whereby the translation vector is an element of the glide plane but not a lattice vector. We now let the system relax. Since the translation vector is not a lattice vector, the stacking sequence is disturbed. Consequently, the atomic interaction changes across the fault plane. Thus, the relaxation will establish a new bonding length and the $d$ spacings of planes parallel to the glide plane will change. The system is now an infinite single crystal containing one infinitely extended SF; we call it an ideal SF. The ideal SF is associated with a defect energy. We define the ideal SFE $\gamma_{\infty}$ as the difference $E_{\infty}$ between the potential energies of the faulted and the perfect crystal per unit area SF:

$$\gamma_{\infty} = \frac{\partial E_{\infty}}{\partial A}.$$  \hspace{1cm} (2)

The relaxation will affect a certain number of planes. However, we approximate the situation by considering the SF as a plate-like precipitate of the SFP with the thickness being two atomic layers (Hirth 1970, Olson and Cohen 1976). In this approach, the ideal SFE is the sum of the specific Gibbs free-energy difference $\Delta G_{\text{SFP,M}}$ between the SFP and matrix and twice the specific interfacial energy $\sigma_1$ (Olson and Cohen 1976):

$$\gamma_{\infty} = d \Delta G_{\text{SFP,M}} + 2\sigma_1.$$ \hspace{1cm} (3)

§ 3. THE TERMINATED STACKING FAULT

In reality, of course, there are no infinitely extended SFs, that is SFs are terminated. A SF may terminate at the crystal surface (this situation is the closest to the ideal situation), but mostly it terminates within the crystal. Thus the SF has to be bounded by a partial dislocation which carries the shift across the fault plane. Figure 1 depicts a cross-section of the terminated SF.
Since the \(d\) spacing in the fault is different from the rest of the crystal, there are elastic strains present additional to that of the terminating dislocation. The SF now in fact is a coherent plate-like precipitate.

With this, the total energy \(E_{\text{tot}}\) of a terminated SF in an infinite crystal is

\[
E_{\text{tot}} = E_{\text{disl}} + E_{\text{\infty}} + E_{\text{strain}},
\]

where \(E_{\text{disl}}\) is the total energy of the dislocation (line energy plus interaction energy) and \(E_{\text{\infty}}\) is proportional to the ideal SFE and the area of the SF.

With eqn. (1) it is found that the ideal SFE acts as an attractive force, being independent of the size and shape of the SF. Thus, although the ideal SFE is a virtual property, it can be considered as an intrinsic material property. The force due to the interaction energy of the dislocations depends strongly on the dislocation character, on the dislocation path and on the SF size. The force contribution of the strain energy term depends on the shape of the SF (Khachaturyan 1983). Thus, the strain energy cannot be expressed in terms of a product of an intrinsic material property and the SF size.

§ 4. THE EFFECTIVE STACKING FAULT ENERGY

With eqns. (1) and (4), the equilibrium is given by

\[
F_{\text{tot}} = - \frac{\partial E_{\text{disl}}}{\partial r} - \frac{\partial E_{\text{\infty}}}{\partial r} - \frac{\partial E_{\text{strain}}}{\partial r} = 0.
\]

The first contribution (that of the dislocation energy) depends on the geometry of the dislocation arrangement only. It can be determined straightforwardly in many situations. The contribution of the strain energy term, however, requires measurement of the lattice distortion in the fault plane. This is not trivial and therefore the effect of the lattice distortion is often neglected, assuming that it is small.

Thus, in practice it is usually not the ideal SFE which is determined, but rather an effective SFE which can be written as
It should be pointed out that the effective SFE is not an intrinsic material property because $E_{strain}$ depends on the shape, on the presence of other defects and on the specimen dimensions. Therefore the values of the effective SFE obtained by different methods (e.g. by measuring the size of isolated nodes, the size of nodes in dislocation networks, or the separation of straight dissociated dislocations) and also by measurement in samples with different thicknesses may differ.

§ 5. STRAIGHT DISSOCIATED DISLOCATIONS

For the particular situation of straight dissociated dislocations, the strain energy per unit length, that is $E_{strain}/L$, can be obtained by modelling the SFP in terms of continuous defects (Kroupa 1970, Müllner 1995). Figure 2 illustrates the model.

The dislocation lines of the partials are parallel to the $z$ axis. The line sense is that of the positive $z$ direction. The partials are called $SP_1$ and $SP_2$ and are located at $P_1(\sqrt{2}, 0)$ and at $P_2(-\sqrt{2}, 0)$ respectively (fig. 2(a)). The strain due to the contraction of close-packed planes can be described by two opposite edge dislocations $M_1$ and $M_2$ at $P_1$ and at $P_2$ respectively (fig. 2(b)). These dislocations (we call them M dislocations) have a different physical origin from the usual Volterra dislocations.

The exact stress field of an M dislocation is that of a distribution of infinitesimal dislocations. In that sense, it can be compared with an in-plane edge Somigliana dislocation dipole of type A (Müllner 1995). However, since the thickness $y_d$ of the compressed zone is small compared with the separation width ($x \gg d$), the approximation of a finite dislocation is valid. The vectors $m_1$ and $m_2$ of $M_1$ and $M_2$ are

$$m_1 = -m_2 = -m_\epsilon y,$$

$$m = \left(1 - \frac{d_1}{d_0}\right)\Delta y = -\epsilon_y d_0$$

where $\epsilon_y = \epsilon$ is the strain in the $y$ direction. For the case of contraction, $m$ is positive.

In the approximation of zero volume change between matrix and SFP, and owing to lattice symmetry, the strains in the $x$ and $z$ directions are related to $\epsilon_y$ by

$$\epsilon_x = \epsilon_z = -\frac{\epsilon_y}{2} = -\frac{\epsilon}{2}.$$
The stress field of an in-plane edge Somigliana dislocation quadrupole (SDQ) (Müllner 1995). Since the dislocations are straight and infinite, the stress field vanishes.

(a) Conventional model of a dissociated dislocation: the Shockley partials SP\(_1\) and SP\(_2\) are located at P\(_1\)(x/2, 0) and P\(_2\)(−x/2, 0), in between the stacking fault SF which is considered to be a two-dimensional defect. (b) The M dislocations M\(_1\) and M\(_2\) are also located at P\(_1\) and at P\(_2\); they have opposite Burgers vectors. (c) The SDQ representing the main strain \(\varepsilon_x\); with this, the stacking fault SF becomes a three-dimensional defect with the thickness \(d\); the definition of the symbols are given in the paper by Müllner (1995).

The stress field of \(\varepsilon_x\) is that of an in-plane edge Somigliana dislocation quadrupole (SDQ) (fig. 2(c)) (Müllner 1995). Since the dislocations are straight and infinite, the stress field \(\varepsilon_x\) vanishes.†

The proposed model (fig. 3) results from the superposition of the two Shockley partials SP\(_1\) and SP\(_2\) (fig. 2(a)), the two M dislocations M\(_1\) and M\(_2\) (fig. 2(b)) and the Somigliana dislocation quadrupole SDQ (fig. 2(c)).

The strain energy per unit length of dislocation line is the sum of the self-energies of M\(_1\), M\(_2\) and SDQ and of the interaction energies of these defects with each other.

† The stress field of a strained region of infinite extension can be described by a virtual in-plane edge Somigliana dislocation dipole with infinite arms. The stress field on an in-plane edge Somigliana dislocation dipole vanishes in the midplane of the dipole (Müllner 1995, eqns. (2a)–(2e)). Considering a dipole with infinite arms, any plane that is perpendicular to the direction of infinite extension can be the midplane, and therefore the stress field vanishes everywhere.
and with $SP_1$ and $SP_2$. The derivation is outlined in the Appendix. The attractive force acting due to the strain energy is then

$$-\frac{\partial E_{strain}}{\partial x} = -\frac{\pi D \varepsilon^2}{2}, \quad (9)$$

where $L$ is the unit length of dislocation line, $D = G/2\pi(1-\nu)$, $G$ is the shear modulus and $\nu$ is the Poisson ratio. The effective SFE is related to the equilibrium separation $x_{eq}$ of dissociated dislocations by (Hirth and Lothe 1968b)

$$\gamma_{eff}x_{eq} = B^2 D b^2, \quad (10a)$$

where $B$ is a geometrical factor which, in the fcc structure, is given by

$$B^2_{fcc} = \frac{1}{12}[2-\nu-2\nu \cos(2\alpha)], \quad (10b)$$

where $\alpha$ is the angle between the Burgers vector of the perfect dislocation and its line. With eqns. (6), (9) and (10), the ideal SFE is

$$\gamma_\infty = \gamma_{eff} - \frac{\pi D \varepsilon^2}{2} = \frac{B^2 D b^2}{x_{eq}} - \frac{\pi D \varepsilon^2}{2}. \quad (11)$$

$B$ and $x_{eq}$ can be measured by transmission electron microscopy analysis. The strain $\varepsilon$ can be determined by comparison of SF contrasts in transmission electron micrographs with contrast simulations (Brooks et al. 1979a, b). With this, the ideal SFE, that is the proper entity to compare different materials, can be experimentally determined. Equation (11) demonstrates that the effective SFE overestimates the ideal SFE.

A numerical example will illustrate the significance of the strain energy term; the values for type 316 austenitic steel are $b = 2\cdot54\ \text{Å}$ (Ledbetter and Austin 1985), $G = 75\ \text{GPa}$ (Ledbetter 1980), $\nu = 0.294$ (Ledbetter 1980), $\alpha = 40^\circ$ (Bampton,
Jones and Loretto 1978), $x_{eq} = 60 \text{Å}$ (Bampton et al. 1978) and $\varepsilon = 0.02$ (Brooks et al. 1979b). Thus, the effective SFE (23.6 mJ m$^{-2}$) overestimates the ideal SFE (19.3 mJ m$^{-2}$) by 22%. The effect of the strain energy term on the ideal SFE in type 316 steel as a function of $\varepsilon$ is depicted in fig. 4. The value for $\varepsilon$ of 2% is certainly vague but not unreasonable. The $c/a$ ratio in hexagonal metals usually deviates from the ideal hexagonal close-packed structure. In cobalt, this deviation is about 0.6% (Nishiyama 1978) which corresponds to a strain normal to the fault plane of about 0.4%. In austenitic steel, the lattice distortion in the fault plane is much stronger than in a Co–6.5% Fe alloy (Brooks et al. 1979b).

§ 6. CONCLUSIONS

1. The ideal SFE is defined in the ideal infinite crystal containing one infinite SF. The ideal SFE is an intrinsic material property.

2. It is found that the strain energy term cannot be included into the SFE without changing the nature of the SFE as an intrinsic material property (§4).

3. The approximation $\gamma_{eff} \approx \gamma_{\infty}$ is valid only if the ideal SFE is large and the strain energy term small, that is the lattice distortions within the SF are small. In that case, the values of the effective SFE obtained by different methods will coincide.

4. In low-SFE materials, however, the strain energy term significantly contributes to the forces acting on the partial dislocations and must not be neglected (eqn. (11) and fig. 4). In particular, the strain energy results in an attractive force, and thus the effective SFE overestimates the ideal SFE. In this case, different methods of measuring the effective SFE will give

Comparison of the effective and the ideal SFE (eqn. (10)) for an austenitic steel type 316 (Brooks et al. 1979b, Ledbetter 1980, Bampton et al. 1978, Nishiyama 1978). With $\varepsilon = 0.02$ (Brooks et al. 1979b), the effective SFE overestimates the ideal SFE by 22%.
different results. The ideal SFE is the proper entity to compare different materials.

(5) A correct description of the dislocation properties requires the analysis of the geometry of the fault as well as the measurement of the lattice distortion. A procedure for determining the ideal SFE at straight dislocations is outlined in §5.

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APPENDIX

THE FORCE OF THE STRAIN ENERGY

The strain energy per unit length $L$ is the sum of the self-energies $E^k$ of $M_1$, $M_2$ and SDQ and of the interaction energies $E^{kl}$ of these defects with each other and with $SP_1$ and $SP_2$:

$$
\frac{E_{\text{strain}}}{L} = 2E^M_L + \frac{E^{SDQ}}{L} + \frac{E^{M_1M_2}}{L} + 2\frac{E^{M_1SDQ}}{L} + 2\frac{E^{M_1SP_1}}{L} + 2\frac{E^{M_1SP_2}}{L} +
$$

(A 1)

$E^M/L$ is independent of the separation distance and thus irrelevant for the equilibrium distance. $E^{SDQ}/L$ can be obtained by integration of the interaction energies of infinitesimal dislocations (the concept has been outlined by Kroupa (1970) and Müllner (1995)). The result is

$$
\frac{E^{SDQ}}{L} = D\varepsilon_x^2 \left\{ \frac{\chi^2}{2} \ln \left( \frac{\chi^2 + d^2}{\chi^2} \right) + \chi \left[ \pi + 2\tan^{-1} \left( \frac{\chi}{d} \right) - 2\tan^{-1} \left( \frac{d}{\chi} \right) \right] + \frac{3\chi^2}{2} \right\}
$$

(A 2)

The interaction energies can be obtained similarly. The non-vanishing components are

$$
\frac{E^{M_1M_2}}{L} = -Dd^2 \varepsilon_x^2 \left[ 1 + \ln \left( \frac{\chi}{R_0} \right) \right],
$$

(A 3)

$$
\frac{E^{M_1SDQ}}{L} = \frac{Dd^2 \varepsilon_x \varepsilon_y}{2} \ln \left( \frac{4\chi^2 + d^2}{d^2} \right).\n$$

(A 4)

The force contribution of the strain energy term is given by its derivation by $\chi$. Using eqn. (8) and the approximation $\chi \gg d$, we obtain

$$
\frac{\partial E_{\text{strain}}}{\partial \chi} / L = \frac{\partial E^{SDQ}}{\partial \chi} / L - \frac{\partial E^{M_1M_2}}{\partial \chi} / L - 2\frac{\partial E^{M_1SDQ}}{\partial \chi} / L \approx -\frac{\pi D\varepsilon_x^2}{2}.
$$

(A 5)
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