Dislocation Nucleation Versus Cleavage in Ni_3Al and Ni

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ABSTRACT

Recent advances in the modelling of dislocation nucleation from a crack tip are used here to compare the critical energy release rate associated with emission in Ni_3Al and Ni. The method for analyzing nucleation makes use of a Peierls-type stress versus displacement relation ahead of the crack tip. It has been shown recently by Rice [1] that the energy release rate for emission scales with γ_{us}, the "unstable stacking" energy associated with the sliding of atomic planes past one another. The advantage of this approach is that it allows for an extended dislocation core during nucleation, thus eliminating the need for a core cutoff radius. Preliminary calculations which take into account only the shear stress on a slip plane show that it is more difficult to emit a dislocation in Ni_3Al than in Ni. Working within the framework of the competition between atomic decohesion and blunting by dislocation emission, the implications for explaining the brittleness of Ni_3Al are also discussed.

INTRODUCTION

The Rice-Thompson model [2] further advanced Kelly, Tyson, and Cottrell's proposition [3] that the brittle versus ductile response of a crystal or grain boundary should be put in the context of the competition between cleavage versus dislocation nucleation, and considered the detailed dislocation processes at an atomistically sharp crack. Recent treatments of that model have evolved to posing the question of which happens first: (1) cleavage, i.e., atomic decohesion; or (2) blunting of the crack tip by dislocation nucleation.

The condition for the cleavage process is well established by the Griffith concept:

$$G = 2\gamma_{int}, \tag{1}$$

where G is the crack extension force (the energy release rate for crack extension) and is based on the local plastically screened stress field at the crack tip, and $2\gamma_{int}$ is the work required to cleave and create the two free surfaces.

A new approach by Rice [1] to the analysis of dislocation nucleation and emission from a crack tip incorporates the Peierls-type [4] shear stress versus relative atomic displacement relation for the incipient "dislocation" core, with the assumption of continuum elasticity in the medium surrounding the crack tip and a slip plane emerging from it. By solving a simple version of the mechanical problem of a traction free crack with the Peierls-type stress versus slip relation being satisfied as a boundary condition along the slip plane, Rice shows that a dislocation is emitted unstably when G reaches a critical value G_d which scales with a physical quantity, γ_{us}, i.e., the *unstable stacking* energy. The advantage of this approach is that it incorporates the nonlinear atomic force field at the crack tip and allows a core of variable size found as part of the analysis, and thus eliminates the need of the dislocation core cutoff radius, which is not well defined.

The shear stress versus relative atomic displacement relation in the new approach by Rice [1] is analogous to that discussed in the context of the theoretical shear strength of crystal by Frenkel [5]. The potential function for such a shear stress, with the relative atomic displacement

as the independent variable, is the free energy of the generalized stacking fault created when one half of a crystal is translated uniformly in shear relative to the other half, along a slip plane. The potential is periodic with period the same as the atomic spacing in the slip plane (examples are shown later). Most importantly, the potential of such a shear stress must pass through a maximum, which is termed by Rice as γ_{us}, i.e., the unstable stacking energy, since it corresponds formally to an equilibrium state, requiring zero shear stress, but an unstable one.

This work concentrates on the cleavage versus dislocation nucleation competition as a source for understanding the ductile versus brittle behavior of Ni_3Al and Ni, and thus sheds some light on the key physical properties which control their ductile versus brittle behavior.

ENERGETICS OF CRYSTAL SLIP

The energy γ of a generalized stacking fault, i.e., the free energy excess due to having the planar fault, can be calculated by splitting the crystal along a slip plane, and translating the upper half relative to the lower half by a vector **D**. Such type of calculations were carried out by Yamaguchi *et al.* [6] on Ni_3Al and Cheung [7] on Fe. In the current work, we use the embedded atom method with functions for Ni_3Al taken from Foiles and Daw [8] and functions for Ni from Foiles *et al.* [9]. We take the two atomic blocks to be rigid, allow no relaxation of normal separation between the two halves, and perform the calculations at 0 K.

On the <111> directions there are three types of layers, named *a, b, c*. Let us choose a slip plane which splits the crystal into two halves between *a* and *b* layers. Then we translate the upper half relative to the lower one in the slip plane, as shown in Fig. 1a for slip on (111). We can mark the path of one atom in the *a* layer in order to trace the slip route. For the sake of argument, we choose $[\bar{1}10]$ as the slip direction.

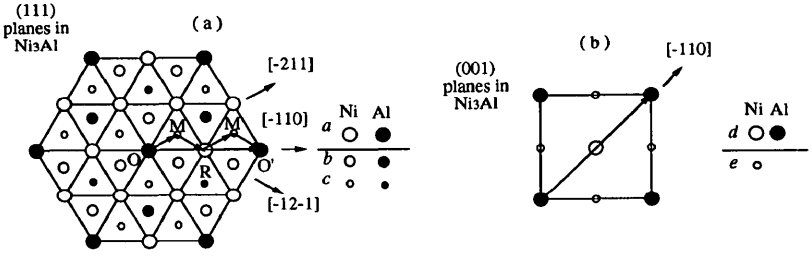

Fig. 1. The Ni_3Al (111) (Fig. 1a) and (001) (Fig. 1b) planes. Open and filled circles represent the Ni and Al atoms. Large, medium, and small circles in Fig. 1a represent the *a, b,* and *c* planes layers, respectively. Large and small circles in Fig. 1b represent the *d* and *e* layers, respectively.

When the displacement $\mathbf{D} = \mathbf{b} = 1/2\,[\bar{1}10]$, for a simple FCC like Ni, the crystal regains crystallinity identical to the original, as if no such slip displacement had occurred. There is a maximum, which is γ_{us}, i.e., the unstable stacking energy, of the generalized stacking fault energy exactly at half the slip displacement **b** (Fig. 2a). The calculation gives $\gamma_{us} = 1163\ mJ/m^2$. The position of this maximum is a consequence of the periodicity and mirror symmetry in the slip direction. However, the *b* layer immediately below the slip plane has interstitial spaces (Fig. 1 a), which accommodate the *a* layer atoms with much lower energy, and advantage is taken of this by the partial slip route $O \rightarrow M \rightarrow R$. At slip displacement $\mathbf{D}=\vec{OM}$, a stable intrinsic stacking fault is formed. This EAM calculation gives a result $\gamma_{sf} = 14.5\ mJ/m^2$ (Fig. 2b) for the

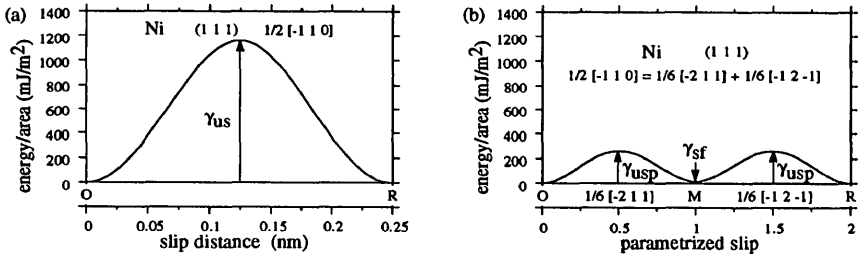

Fig. 2. The energy of a generalized stacking fault on (111) plane in Ni as a function of the slip distance in the straight route Fig. 2a and the partial route Fig. 2b.

stable intrinsic stacking fault, which is rather small compared to the experimental result of 125 mJ/m^2 [10] or a theoretical value of 180 mJ/m^2 based on a quantum mechanical one electron calculation [11]. The unrealistically low value of the stable stacking fault energy is inherent in the EAM functions, which were not well constrained for such configurations as dominated by non-nearest-neighbor interactions. Most importantly, the unstable stacking energy γ_{us} = 260 mJ/m^2 encountered along the partial route is only about one fifth of that for the straight slip route.

For the $L1_2$ structure such as Ni_3Al, however, for the same displacement **D** = **b** = 1/2[$\bar{1}$10], the crystal would not regain the original crystallinity because of the different chemical elements, but instead forms a planar fault called an antiphase boundary (APB). The free energy of the APB is a measure of ordering energy of Ni and Al. As a result, the maximum does not occur at a displacement of half of **b**, but at slightly larger displacement (Fig. 3a). The crystal

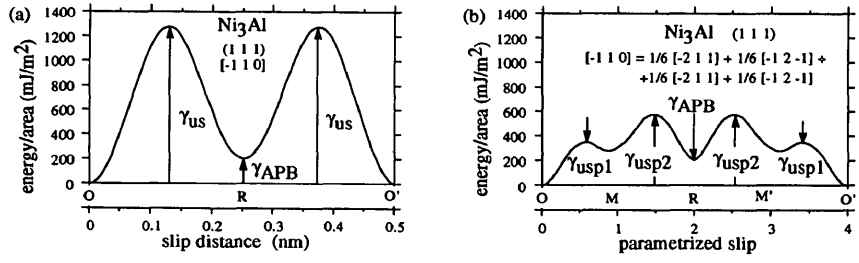

Fig. 3. The energy of a generalized stacking fault on (111) plane in Ni_3Al as a function of the slip distance in the straight route Fig. 3a and the partial route Fig. 3b.

must undergo an additional displacement **b** to regain the original crystallinity. The two energy maxima are equal in the straight slip route, and give γ_{us} = 1276 mJ/m^2, which is only slightly higher than the γ_{us} in the straight route for Ni. Yamaguchi *et al.* [6] gave γ_{us} = 950 mJ/m^2, based on pairwise potentials. For Ni_3Al, the partial route is O → M → R → M' → O', and is energetically favorable. There are four maximum γ values. Due to the chemical difference between Ni and Al, these occur at displacements offset from those for a simple FCC. The first maximum at γ_{us} = 348 mJ/m^2 is about one third of that for straight slip (Fig. 3b), and the second at γ_{us} = 575 mJ/m^2 is about one half of that for straight slip. From the mirror symmetry at half of the full slip route, the third is equal to the second and the fourth to the first. The crystal must be forced over all these energy barriers for full slip.

The partial slip route in Ni_3Al gives a much higher value of γ_{us} than the partial route in Ni, so that it is correspondingly more difficult to nucleate dislocations from a crack tip in Ni_3Al than in Ni.

Slip on (001) planes for Ni_3Al, which is shown on Fig. 1b, experiences a significantly higher energy barrier. The $\gamma_{us} = 2253$ mJ/m^2, and is about twice that for (111) on the straight route (Fig. 4). (In this case, Yamaguchi *et al.* [6] gave $\gamma_{us} = 1040$ mJ/m^2.) The high γ_{us} value means that it is more difficult to slip, which is consistent with this slip system being active only at high temperature. The full slip is $[\bar{1}10]$, and at half the full slip an APB is formed. The APB energy in this calculation is 32 mJ/m^2 (Yamaguchi *et al.* [6] gave $\gamma_{APB(001)} = 43$ mJ/m^2. Foiles and Daw [8] gave 28 mJ/m^2). These results can be understood in terms of crystallography. The stacking layers are of two types along [001], one type is half Ni and half Al (labeled *d* type) and the other all Ni (labeled *e* type). The stacking sequences goes like *dede* along [001]. Suppose slip is imposed between a *d* layer and an *e* layer. The (001) is not a slip plane for simple FCC structures because it is not close packed. Therefore, a higher energy barrier is expected. It is clear that the APB on (001) is locally stable from symmetry considerations based on the crystallography. Also, the APB energy on the (001) is much lower than that on the (111) plane, because it is only from the second-nearest neighbor chemical element difference. Once the slip on (001) planes is activated, it would tend to dissociate into two superpartials which are separated by the stable APB.

DISLOCATION NUCLEATION VERSUS CLEAVAGE: CRYSTAL LATTICES

We analyze the cleavage versus dislocation nucleation competition for the crack configuration shown in Fig. 5. The crack plane has a normal **y** and crack front **z**. The slip plane, having a normal **n**, is inclined away from the crack plane by an angle θ. The slip direction, which is parallel to **b**, makes an angle ϕ to **r**, where **r** is in the slip plane and perpendicular to the crack front **z**. Suppose that this crack system is under tensile loading K_I.

Fig. 4

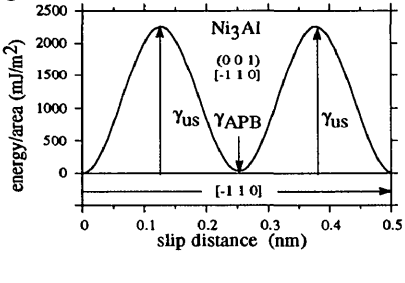

Fig. 5.

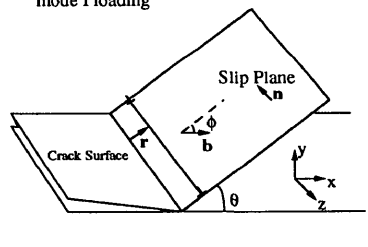

Fig. 4. The energy of a generalized stacking fault on (001) plane in Ni_3Al as a function of the slip distance in the straight route.

Fig. 5. The crack system with crack surfaces of normal **y** and crack front **z**, slip system with slip plane normal **n** and slip vector **b**; the crack is under mode I loading.

Now we can obtain the dislocation nucleation condition by the approximation that dislocation nucleation is governed by the effective shear stress intensity factor K_{II}^e in the slip plane. Define $K_{II}^e = K_I f(\theta)$, where $f(\theta) = \cos^2(\theta/2) \sin(\theta/2)$. This geometric factor comes from the stress field solution near a crack under Mode I loading by writing stress $\sigma_{\theta r} = K_{II}^e / \sqrt{2\pi r}$. Rice [1] showed in the new approach using Peierls-type stress, for a crack

coplanar with the slip plane, under mode II loading, edge dislocation nucleation happens when the shear stress intensity K_{II} reaches a critical value which corresponds to the crack extension force $G_d = (1-\nu)\, K_{II}^2/ 2\mu = \gamma_{us}$. When the Burgers vector makes a general angle ϕ with the normal to the crack tip, the corresponding result is [1] $G_d = (1-\nu)\, K_{II}^2/ 2\mu = [1+(1-\nu)\tan^2 \phi]\, \gamma_{us}$. The dislocation nucleation condition for the mode I crack of interest here, with slip plane inclined at angle θ to the crack plane, is then estimated by assuming that K_{II}^e obeys the same criterion. Thus

$$G_d \doteq \frac{\gamma_{us}\,[1+(1-\nu)\tan^2 \phi]}{f^2(\theta)} \,. \qquad (2)$$

The dislocation nucleation condition is compared against the cleavage condition $G_c = 2\gamma_{int}$, from which we can conveniently define a dimensionless measure of brittleness q to be the ratio of G_d to G_c:

$$q = G_d / G_c \doteq \frac{\gamma_{us}\,[1+(1-\nu)\tan^2 \phi]}{2\gamma_{int}\, f^2(\theta)} \,. \qquad (3)$$

The results of this dimensionless measure of brittleness q are tabulated in Table I. For the sake of comparison, we consider only the G_d corresponding to emission of the first Schockley partial, for which $\phi = 0°$ for {001} crack planes. When we consider the {011} planes as crack surfaces, $\phi = 30°$. This gives $[1+(1-\nu)\tan^2 \phi] = 1.233$ by taking the Poisson's ratio $\nu = 0.3$. Considering only the first Schockley tends to bias the q values shown in favor of ductility, since, for full dislocation emission, the second partial must be considered too. This involves complications of (1) repulsion between the partials, (2) attraction due to the planar stacking faults that separate them, and (3) screening by the previously emitted partial. All of these effects are important because the partials are always coupled in pairs. Of course, there may be many possible slip systems in operation relative to the crack geometry; we have chosen only the ones with the lowest G_d, which may be degenerate.

Our model predicts that Ni_3Al is more brittle than Ni in single crystal form. We suggest that the reason is mainly that it is more difficult to emit dislocations to blunt crack tips in Ni_3Al than in Ni (γ_{us} for Ni_3Al is more than twice that for Ni along the partial routes), not of

Table I. Dislocation nucleation vs. cleavage extension in Ni_3Al and Ni.

material	crack system	slip system	γ_{us} (mJ/m^2)	$2\gamma_{int}$ (mJ/m^2)	$f^2(\theta)$	G_d/G_c
Ni	(001)[110]	1/6[$\bar{1}$12](1$\bar{1}$1)	260	3160[a]	0.131	0.628
Ni_3Al	(001)[110]	1/6[$\bar{1}$12](1$\bar{1}$1)	348	3505[b]	0.131	0.758
Ni	(1$\bar{1}$0)[11$\bar{2}$]	1/6[$\bar{1}$2$\bar{1}$](111)	260	3460[a]	0.125	0.741
Ni_3Al	(1$\bar{1}$0)[11$\bar{2}$]	1/6[$\bar{1}$2$\bar{1}$](111)	348	3650[b]	0.125	0.941

a: $2\gamma_{int}$ from Foiles, Baskes, and Daw [9].

b: $2\gamma_{int}$ from Foiles and Daw [8].

differences in Griffith cohesion, which actually predict the opposite trend ($2\gamma_{int}$ for Ni_3Al is slightly greater than that for Ni). We suggest that this may be the source of the intrinsic brittleness of polycrystals of Ni_3Al [12,13,14]. We predict also that (011) planes are more brittle than (001) planes in Ni_3Al.

In this work, we consider only the shear stress in the slip plane to govern the dislocation nucleation from a crack tip. Beltz and Rice [15] take into account the role of the stress component normal to the slip plane in dislocation nucleation from a crack tip by a nonlinear coupling of the shear stress with the normal stress in the slip plane in the context of the new approach [1] to nucleation.

SUMMARY

The ductile versus brittle behavior of crystals or grain boundaries may be in part understood in the context of the competition between dislocation nucleation versus cleavage. While the Griffith energy $2\gamma_{int}$ determines the crack extension, the dislocation nucleation is controlled by γ_{us}, the unstable stacking energy, i.e., the energy barrier that would be encountered in a process of homogeneous slip.

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