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Ledge effects on dislocation emission from a crack tip: a first-principles study for silicon

By YU-MIN JUAN†, YUEMIN SUN† and EFTHIMIOS KAXIRAS†‡

†Division of Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA
‡Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

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ABSTRACT

Extensive recent efforts to understand the intrinsic brittleness or ductility of materials have focused on crack-blunting mechanisms using the Peierls stress concept. So far, the effects due to newly created ledge surface during crack propagation have been either ignored or included within some semiempirical approximation. Using silicon as a prototypical brittle solid, we show that the energy associated with a newly created ledge surface at a crack tip can be obtained from first-principles calculations. We incorporate these results into a continuum theory of critical loading of cracks by assuming an evanescent force law for the surface effects. Our results indicate that inclusion of surface ledge effects can change the values of the critical load by up to 20%.

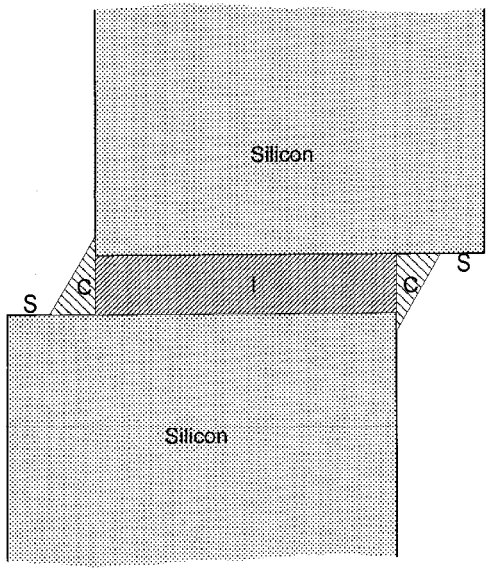
One of the most important macroscopic properties of materials is their intrinsic ductility or brittleness. Determining the ductile or brittle nature of a material from its microscopic structure is a challenging proposition. One approach to this very complex problem is to consider how a crack in the solid will propagate under external loading conditions. Dislocation nucleation at a crack tip causes the crack to blunt, a process associated with ductile behaviour. Thus the external loading is absorbed by the blunting and deformation of the crack tip, preventing propagation of the crack. Brittle behaviour can then be attributed to direct crack propagation through cleavage. Accordingly, the brittle versus ductile issue can be analysed by comparing the criterion for dislocation emission from the crack tip with the Griffith's (1920) criterion for cleavage. Within this picture, the question of how dislocations are emitted from a crack tip becomes of central importance. A recent theoretical breakthrough due to Rice (1992) analyses dislocation emission from the crack tip based on the Peierls stress concept. By assuming a periodic relation between the shear traction τ and the slip displacement δ along a crystal plane emanating from the crack tip, Rice identified the unstable stacking fault energy γ_{us} which controls the critical loading condition for dislocation nucleation at the crack tip. This quantity represents the lowest-energy barrier encountered when one half of the crystal is sliding with respect to the other half on a slip plane. Thus γ_{us} corresponds to a saddle point in the generalized stacking-fault (GSF) energy surface.

The effects due to the surface which is created during the dislocation emission process were neglected in Rice's approach, by assuming that the created surface is traction free. Since the surface created at the crack tip is *not* equivalent to a free surface, including these effects is not trivial. A step toward this goal is the recent

work of Thomson and Carlsson (1994) and Zhou, Carlsson and Thomson (1994). These studies are illuminating, but they are restricted to phenomenological atomistic calculations in two dimensions which do not necessarily correspond to real physical systems. A different approach was pursued by Xu, Argon and Ortiz (1995), within continuum elasticity theory, where surface effects are taken into account by approximating the energy of the ledge surface as the energy of a free surface. In the present paper, we shall show that, using silicon as an example, an accurate description of the surface energy associated with the newly created ledge surface during dislocation emission can be obtained through first-principles quantum mechanical calculations. The ledge energy can then be incorporated into Rice's model by assuming an evanescent force law for the surface effects. The resulting critical loading for the dislocation emission is determined within continuum mechanics.

In the continuum formulation that neglects surface effects (Rice 1992), the quantity that controls dislocation emission at a crack tip, γ_{us}, can be calculated by considering the shearing of two infinite size blocks. Such calculations using a first-principles approach have already been reported for silicon (Kaxiras and Duesbery 1993). In order to obtain the energy associated with surface creation during dislocation emission, it is necessary to perform a calculation for a *finite* size block shearing process, as illustrated in fig. 1. In principle, only one ledge is required which could be described by one semi-infinite block being sheared over another. The symmetric geometry of fig. 1 allows for a supercell structure with periodic boundary conditions in each direction, which makes feasible the first-principles calculations described below. In the schematic representation in fig. 1, *I* indicates the interfacial area between two blocks, *S* represents the surface created through the shearing process, and *C* indicates the coupling between the corner and the newly created surface. It is

Fig. 1



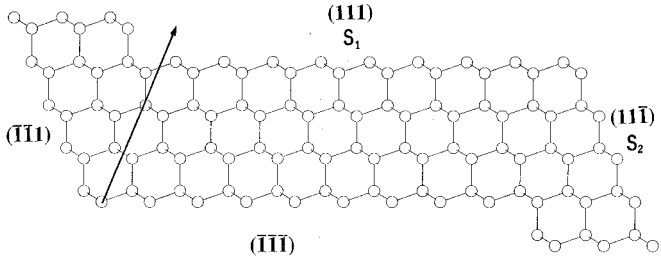
A schematic drawing of the configuration corresponding to finite size block shearing. The symbols *S*, *I* and *C* represent the surface area, interfacial area and corner coupling respectively.

the existence of this coupling term C which causes the energy associated with surface creation during dislocation emission to be different from the energy of a free surface. In order to peform first-principles calculations, a non-trivial supercell which contains all the essential featues has to be adopted. A supercell that meets these requirements is displayed in fig. 2. The advantages of this geometry are the following. First, by simply changing the horizontal component of the supercell vector $\mathbf{a}_1$, one cell is sheared with respect to another and a surface is created. Second, all the surfaces which are exposed through this process are in the {111} crystallographic directions of the diamond lattice, that is the natural cleavage planes for this crystal system.

In terms of computational details, we have adopted the local-density approximation (Perdew and Zunger 1984) to density functional theory (Hohenberg and Kohn 1964, Kohn and Sham 1965), which is a first-principles quantum-mechanical approach known to provide reliable total-energy comparisons for both bulk and surface properties of silicon. We use the iterative scheme of Car and Parrinello (1985) to solve the Kohn–Sham equations, and norm-conserving pseudopotentials (Bachelet, Hamann and Schlüter 1982) in the Kleinman–Bylander (1982) form to represent the ionic cores. We employ a plane-wave basis with cut-off of 8 Ryd and the Γ point for the sampling of the Brillouin zone. The largest supercell we considered corresponds to 144 atomic volumes of silicon.

We have calculated the total energy of the system as a function of the horizontal component of $\mathbf{a}_1$. The distortions that we have considered relative to the ideal structure (bulk silicon) include changes in the horizontal component of $\mathbf{a}_1$ from 0 to $4a_0/2^{1/2}$ at increments of $a_0/2^{3/2}$, where $a_0/2^{1/2}$ is the primitive lattice vector of silicon along the [110] crystallographic direction (a_0 being the cubic lattice constant of silicon; $a_0 = 5{\cdot}43$). In order to simplify the analysis, we separate the total-energy change into the following three terms: the interfacial energy U_I, the surface energy U_S and the coupling energy U_C. U_I is the energy cost associated with the interface during the shearing of the two blocks. This term can be calculated by multiplying the generalized stacking fault energy $\gamma_{GSF}(f)$, which corresponds to shearing of two infinite blocks (taken from the work of Kaxiras and Duesbery (1993)), with the interfacial area A_I. Because of the way that we construct the supercell, the surface energy U_S is composed of two different terms: U_{S_1} and U_{S_2}. U_{S_1} is the energy

Fig. 2



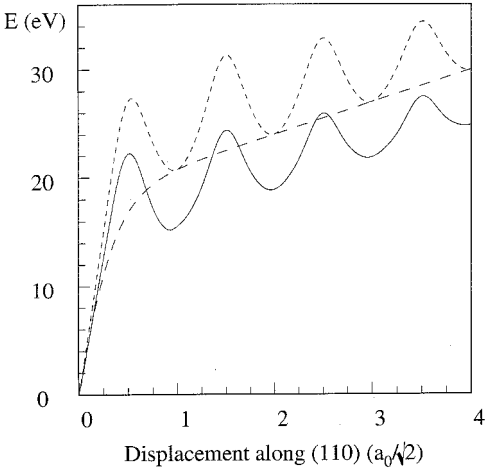
The geometry of the supercell used for the present calculations. One repeat lattice vector is shown, $\mathbf{a}_1$ (arrow), the horizontal component of which is increased to produce shearing. All the exposed surfaces during shearing belong to the {111} set of planes, the natural cleavage plane of silicon.

associated with the ledge surface, while U_{S_2} is the energy due to the creation of the side surface. We have performed independent calculations for the block separation process to determine the value of the term U_{S_2} as well as the energy of the free surface γ_s. The energy cost for the block separation process was calculated along a direction corresponding exactly to the direction along which the S_2 side surfaces are separated during shearing of the unit cell (see fig. 2). The asymptotic value of that energy cost represents the energy of the free surface γ_s. The value of the surface term U_{S_1} is then determined by taking the simplest linear approximation

$$U_{S_1} = S_1\gamma_s, \tag{1}$$

where S_1 is the exposed surface area at the ledge. Since we have assumed that the term U_{S_1} corresponds to creation of a free surface, all the effects of the ledge are included in the last term, U_C. We define U_C implicitly as the difference between the calculated total energy and the sum of the U_I and U_S terms which are obtained from separate calculations. The results of our calculations are displayed in fig. 3. The broken curve (long dashes) is the surface energy U_S. The broken curve (short dashes) is the sum of the surface energy and the interface energy: $U_S + U_I$. The solid curve is the result that we obtained for the finite-size block shearing process. The coupling energy is simply the difference between the solid curve and the broken curve (short dashes). It is evident that the variation in U_C becomes negligible once the relative displacement is greater than $a_0/2^{1/2}$. This means that the corner-corner interactions are insignificant for the present case and can be neglected at this level of approximation. Therefore we only need to consider the value of this coupling energy at the integral steps of increment of the horizontal component of $\mathbf{a}_1$ in units of $a_0/2^{1/2}$. The difference between the solid curve and broken curve (short dashes) at the integral steps is essentially the difference between the energy for the creation of one area of free surface and one area of ledge surface during dislocation emission from the crack

Fig. 3



The energy forms obtained from the present calculations: (———), total energy; (– – –), surface energy; (- - - - -), sum of the surface energy and the interfacial energy.

tip. From this comparison we extract the crucial quantity, namely the energy for creation of a unit area of ledge surface during dislocation emission, defined as $\tilde{\gamma}_s$. This quantity is equal to $\gamma_s + U_C$. The number we have obtained is $\tilde{\gamma}_s = 0{\cdot}58\gamma_s$. As expected, the energy of the ledge surface is a fraction (58%) of the energy of the free surface, since the coupling between the ledge and the corner is attractive, in other words $U_C < 0$ (see fig. 3).

The effects due to the creation of ledge surface during dislocation emission can then be taken into account within continuum mechanics by assuming a evanescent force law:

$$\tau_s(r) = \frac{\tilde{\gamma}_s}{\Lambda} \exp\left(\frac{-r}{\Lambda}\right), \tag{2}$$

where τ_s is the stress associated with surface creation, Λ is a phenomenological decaying length scale and r is the distance between the crack tip and the point where the stress is evaluated. This expression satisfies the requirement that the integral of the stress equals the ledge surface energy $\tilde{\gamma}_s$. Furthermore, the exponential decay with distance from the crack tip is a reasonable approximation for the case of silicon, since surface effects are expected to decay fast into the bulk, as, for example, in the structural relaxations due to reconstruction of the free surface. A similar expression has been considered by Xu *et al.* (1995) in their analysis of surface effects on dislocation emission. By treating the incipient dislocation as a continuous distribution of infinitesimal dislocations denoted by $\delta(r)$, one can then write down the continuum equation for force balace. For simplicity, consider the case where crack and slip occur on the same plane with a purely shear mode loading, where we obtain:

$$\tau_I(r) + \tau_s(r) = \sigma(r) - \int_0^\infty g(r, r') \frac{\mathrm{d}\delta(r')}{\mathrm{d}r'} \mathrm{d}r', \tag{3}$$

with $\tau_s(r)$ defined above, and $\tau_I(r)$ the stress from the misfit across the slip plane given by

$$\tau_I(r) = \frac{\mathrm{d}\gamma_{GSF}[\delta(r)]}{\mathrm{d}\delta(r)} \tag{4}$$

$g(r, r')$ describes the stress exerted at one point r on the slip plane by the infinitesimal dislocation at another point r', and has been obtained for a line dislocation and crack tip in the elastic medium (Lin and Thomson 1987, Beltz 1992):

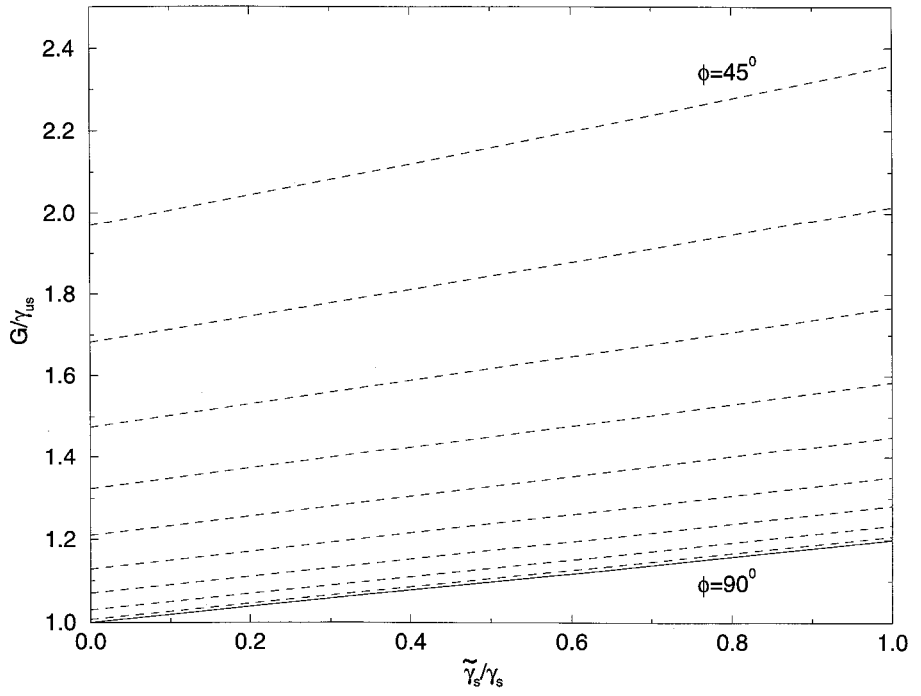
$$g(r, r') = \frac{\mu}{2\pi(1-\nu)} \left(\frac{r'}{r}\right)^{1/2} \frac{1}{r - r'}, \tag{5}$$

where μ and ν are the shear modulus and Poisson's ratio respectively. $\sigma(r)$ is the shearing stress due to the external loading and is equal to $K_{II}/(2\pi r)^{1/2}$, where K_{II} is the stress intensity factor corresponding to mode II loading (pure shear). We solved eqn. (3) numerically to obtain the critical loading for dislocation emission, by increasing the loading continuously until a stable solution no longer exists. The advantage of this approach is that it treats the effects of surface and interface on equal footing based on a simple extension of the original Peierls stress concept. The critical loading condition has been determined for a wide range of $\tilde{\gamma}_s$ and Λ under different loadings (mixture of mode I and mode II loading), assuming that only shearing takes place during the process. A formal justification and details of the numerical calculation results will be published elsewhere. Here we emphasize only

the general trends. The energy release rate G corresponding to the critical loading increases linearly with increasing effective surface energy $\tilde{\gamma}_s$. The results for silicon with $\Lambda = 2^{1/2}a_0$ for different loadings are shown in fig. 4. The reason for choosing this particular value for Λ is that it corresponds approximately to the length scale for surface relaxation of silicon. Incidentally, G does not change much for values of $\Lambda > 2b$. The solid line in fig. 4 represents the results obtained with pure shear loading, that is with phase angle $\phi = 90^\circ$, where ϕ is defined by $\phi \equiv \tan^{-1}(K_{II}/K_I)$. The broken lines are obtained under mixed loading conditions with ϕ ranging from 90° to 45°, the latter corresponding to equal intensities of shear and tension loading. Values of ϕ smaller than 45° would correspond to higher tension than shear, which would seem contradictory to our earlier assumption that the crystal is deformed by shearing only. The coefficient for the linear increase of G with effective surface energy $\tilde{\gamma}_s$ obtained from this figure for the case of pure shear loading is approximately 0·2. For the case of silicon, with $\tilde{\gamma}_s = 0{\cdot}58\gamma_s$ as obtained above, the inclusion of surface effects leads to an increase in the energy release rate of about 12%.

The linear behaviour of G with $\tilde{\gamma}_s$ can be understood in a simple manner (this line of arguing was pointed out to us by J.R. Rice) by considering the energy release rate which, for the case of pure shear loading is given by

Fig. 4



The critical energy release rate G (in units of γ_{us}) against the effective surface energy $\tilde{\gamma}_s$ (in units of γ_s), which can range from zero to being equal to the energy of a free surface (units on this scale), for different loading conditions denoted by $\phi = \tan^{-1}(K_{II}/K_I)$: (———), pure shear loading ($\phi = 90^\circ$); (- - - -), values of ϕ ranging from 85° to 45°, in increments of 5°.

$$G = -\int_0^\infty [\tau_I(r) + \tau_s(r)]\frac{d\delta}{dr}dr. \tag{6}$$

The integral of the first term is the GSF energy with the displacement equal to δ_{tip} (the position of the crack tip) as described by Rice (1992). Therefore, using eqn. (2) for $\tau_s(r)$:

$$G = \Phi(\delta_{tip}) - \frac{\tilde{\gamma}_s}{\Lambda}\int_0^\infty \exp\left(-\frac{r}{\Lambda}\right)\frac{d\delta}{dr}\,dr \tag{7}$$

By assuming the surface effects on the function $d\delta/dr$ to be small, it is obvious that the second term increases linearly with increasing effective surface energy. No exact analytic solution exists for the integral containing the surface effects. An approximate value can be obtained, based on the following argument. Since both $\exp(-r/\Lambda)$ and $d\delta/dr$ decrease rapidly with increasing distance r from the crack tip, it is reasonable to assume that only the value of $d\delta/dr$ at the crack tip will make important contributions to the integral. We then have

$$G \sim \Phi(\delta_{tip}) + \tilde{\gamma}_s\left.\frac{d\delta}{dr}\right|_{tip}. \tag{8}$$

An approximation for $(dr/d\delta)|_{tip}$ has been given by Rice (1992):

$$\left.\frac{d\delta}{dr}\right|_{tip} \sim 6\frac{(1-\nu)\gamma_{us}}{\mu b}. \tag{9}$$

Substituting this in eqn. (8), we obtain (with $\Phi(\delta_{tip} = b/2) \equiv \gamma_{us}$)

$$G \sim \gamma_{us}\left(1 + \frac{6(1-\nu)}{\mu b}\tilde{\gamma}_s\right). \tag{10}$$

Using the relevant values of μ and ν for silicon, we find a coefficient for linear increase of G (measured in units of γ_s) equal to 0·24. This compares favourably with the value of 0·2 obtained from the numerical solution of eqn. (3) (see above). For the case of mixed loading, since $G = [(1-\nu)(K_I^2 + K_{II}^2)]/2\mu$ and $K_{II}/K_I = \tan\phi$, $G = G_{pure\ shear}/\sin^2\phi$ (Sun, Beltz and Rice 1993). Thus the corresponding linear coefficient of G with respect to $\tilde{\gamma}_s$ under mixed loading should be approximately $0{\cdot}24/\sin^2\phi$, which agrees well with all the numerical values obtained from fig. 4.

In conclusion, we used silicon as an example to show that surface effects due to the ledge when a dislocation is emitted from a crack tip can be obtained from first-principles calculations. For the case of silicon, the energy associated with ledge surface creation is approximately 60% of the energy of the free surface. By assuming an evanescent force law, the ledge effects are incorporated into Rice's original theory within continuum mechanics. The inclusion of surface effects increases the necessary loading for dislocation emission. This increase is linear with the effective surface energy $\tilde{\gamma}_s$ and can be up to 20% for mixed mode I and II loading, depending on the value of $\tilde{\gamma}_s/\gamma_s$. In silicon, the increase in the critical loading due to surface ledge effects is approximately 12%.

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