EFFECT OF CRACK BLUNTING ON SUBSEQUENT CRACK PROPAGATION

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Abstract

Theories of toughness of materials depend on an understanding of the characteristic instabilities of the crack tip, and their possible interactions. In this paper we examine the effect of dislocation emission on subsequent cleavage of a crack and on further dislocation emission. The work is an extension of the previously published Lattice Greens Function methodology[1, 2, 3]. We have developed a Cavity Greens Function describing a blunt crack and used it to study the effect of crack blunting under a range of different force laws. As the crack is blunted, we find a small but noticeable increase in the crack loading needed to propagate the crack. This effect may be of importance in materials where a dislocation source near the crack tip in a brittle material causes the crack to absorb anti-shielding dislocations, and thus cause a blunting of the crack. It is obviously also relevant to cracks in more ductile materials where the crack itself may emit dislocations.

Introduction

When a sharp crack in a material is loaded until it deforms plastically at the crack tip, two fundamentally different modes of deformation can occur. The crack may propagate (possibly leading to cleavage of the specimen), or it may emit a dislocation. In the first case the material is said to be intrinsically brittle, in the second it is intrinsically ductile. Even for single crystals, many other aspects of the micro-structure of the material influence the behavior of the material, such as dislocation activity in the material surrounding the crack and shielding of the stress fields by the dislocations present in the vicinity of the crack. In this paper we will however concentrate on the intrinsic behavior of the crack.

The intrinsic behavior of the crack can be predicted by comparing the critical stress intensity factors necessary for cleavage and for dislocation emission. The cleavage is well described by the Griffith criterion[4], but several criteria have been proposed for the dislocation emission. Rice[5] has proposed an emission criterion given by a well-defined solid-state parameter, the unstable stacking fault energy (γ_{us}), characterizing the barrier to displacement along the slip plane. In this model the emission criterion becomes a "balance" between two energies: The surface energy (γ_s) and the unstable stacking energy. Zhou *et al.*[2, 6] extended this model to include the energy of the small ledge at the end of the crack, and showed that for most physically realistic force laws this term dominates the energetics, leading to an emission criterion containing both γ_s and γ_{us} and a ductility criterion that is independent of γ_s.

These ductility criteria all assume that the crack is sharp at the atomic level. However, emission of a dislocation will change the local geometry of the crack, possibly changing both the emission and cleavage criteria. Furthermore, a crack may *absorb* a dislocation, coming from sources in the neighborhood of the crack tip. This may also lead to blunting of the crack. In the following we will discuss the effects such blunting may have on the dislocation emission and cleavage of the crack.

Methodology

Ordinary molecular dynamics (MD) simulations of cracks are very difficult, due to the extremely slow decay of the stress fields ($\sigma \propto r^{-1/2}$). This makes it necessary to use very large systems to minimize the effects of boundary conditions; millions of atoms may be required even for two-dimensional simulations. On the other hand all of the interesting phenomena will be concentrated near the crack tip, and most of the atoms are just propagating the elastic field. This leads to a very inefficient use of computer resources.

Our solution is to model the elastic response of the surrounding media by a Green's function. The atoms are divided in two classes. The atoms near the crack tip interact with each other through a non-linear force law (the *non-linear zone*), whereas the atoms far from the crack tip interact only through linear forces. This *linear zone* can then be fully described by a lattice Green's function $G_{ij}(\mathbf{r}, \mathbf{r}')$, describing the response of the atom at $\mathbf{r}$ to a force acting on the atom at $\mathbf{r}'$. One needs only the Green's function elements involving the nonlinear zone and a defect zone. The Green's function can be calculated in a computationally efficient way. The procedure for calculating the Green's function, and for introducing a defect (a crack in this case) has been discussed by Zhou *et al.*[1]. The total energy of the system can then be described as the sum of the energy in the elastic far field (calculated from the Green's function) and in the non-linear interactions. In this way the total energy of the system is described as a function of a much reduced number of degrees of freedom (the positions of the 10^2–10^3 atoms in the non-linear zone, compared to the 10^6–10^7 atoms in the full problem). The problem can then be treated with conventional minimization techniques[3].

We use this method to study the deformation modes of blunt cracks with up to seven atomic layers of blunting, for a range of force laws. Figure 1a show a typical initial configuration. We have a region in front of the crack where the atoms are allowed to move freely, and two spurs are added, alog which dislocations generated at the crack tip can move away from the crack. Since bonds cannot be broken and reformed in the linear zones, dislocations will be unable to leave the non-linear zone.

The inter-atomic interactions in the non-linear zone are described by the UBER pair potential:

$$F(r) = -k(r - r_0)\exp\left(\frac{r - r_0}{\beta}\right) \tag{1}$$

where r is the inter-atomic separation, r_0 is the separation in equilibrium, and β is a range parameter. We cut off the interactions so that only nearest-neighbor interactions are included, and shift the potential slightly to avoid

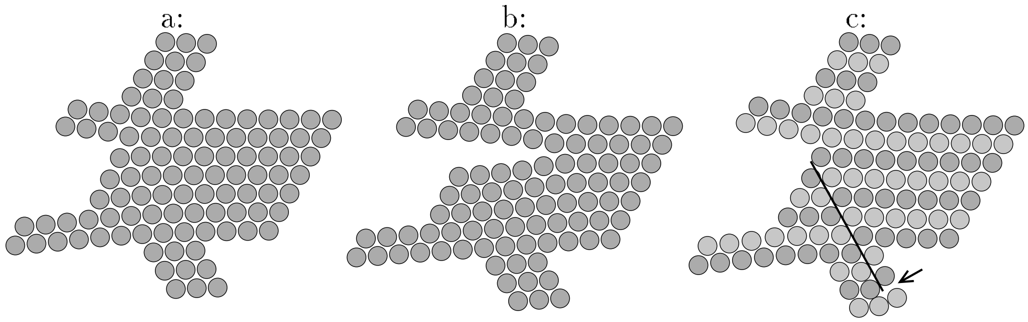

Figure 1: The two deformation modes. (a) shows the configuration before plastic deformation. The crack, three atomic layers thick, extends out of the left of the picture. Only atoms in the non-linear zone are shown, see text. (b) shows the crack propagating by cleavage. (c) shows the crack emitting a dislocation. The dislocation has traveled along the black line. Since it cannot leave the non-linear zone, it has been pinned at the bottom (indicated by the arrow). To make the path of the dislocation visible, the atoms were given two different colors. Prior to emission the atoms were lined up in rows of the same color. Where the dislocation has traveled lines of atoms of different color meet.

a step in the force law. Further, a small scaling of the force law is used to preserve the elastic constants, thus enabling us to use the same Green's function for all the force laws. The force law thus becomes

$$F(r) = C\left[-k(r-r_0)\exp\left(\frac{r-r_0}{\beta}\right) - F_0\right] \tag{2}$$

where $F_0 = -k(r_{\text{cutoff}} - r_0)\exp\left((r_{\text{cutoff}} - r_0)/\beta\right)$ assures that the force is zero at the cutoff distance r_{cutoff} (in this work $1.7r_0$). This is only a slight perturbation of the force law as the scaling factor C only differs from unity by a few percent. Since this work does not study specific materials, no attempt is made to use realistic many-body potentials.

Results

When we load the cracks until plastic deformation occur, two different deformation modes are observed: cleavage and dislocation emission, see figure 1. The dislocation emission always occurs in the downwards direction, as shown

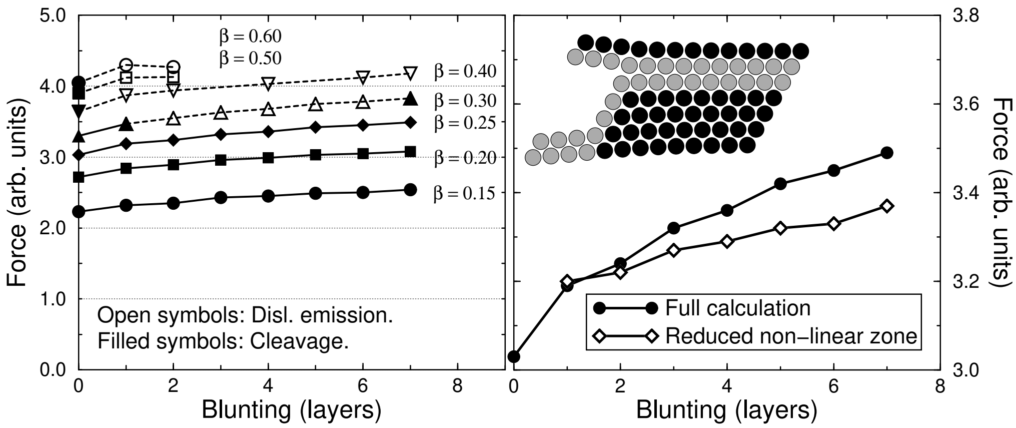

Figure 2: Left: The force required for cleavage or dislocation emission as a function of the blunting, for seven different force laws. Right: The effect of reducing the non-linear zone at the crack tip. When the atoms shown in black are removed from the non-linear zone (i.e. they are restricted to interact through linear forces), the effect of the blunting is reduced. The range parameter in the force law is $\beta = 0.25$.

in the figure, except for the case of a single layer of blunting, where the crack geometry is symmetric. Furthermore, the emission occurs in such a way that the asymmetric crack geometry is preserved. This means that further dislocations can be expected to be emitted in the same direction, provided that the dislocation can move so far away that its effect on the local stress field at the crack tip is small. When a sufficient number of dislocations have been emitted, their combined screening may prevent further emission, and cause the crack to propagate by cleavage or begin emitting in the opposite direction. This may have been observed experimentally[7, 8].

Figure 2 (left) shows the force required for cleavage or dislocation emission as a function of the blunting, for seven different force laws. All force laws result in cleavage in the case of a sharp crack, but for a range of force law parameters dislocation emission becomes favored as soon as the crack is blunted. In all cases the required force for cleavage increases slightly with increasing blunting. When dislocation emission occur the force also increases slightly with the blunting as soon as any blunting occurs, but for these force laws the force required to emit a dislocation from the sharp crack is *larger* that for the blunt crack. The tendency for the sharp crack to propagate is so large that it is difficult to measure the dislocation emission criterion accurately.

Using a conformal mapping technique, we have been able to calculate the stress field around a blunt crack (to be published elsewhere), but only in anti-plane strain (mode III loading). The result is as could be expected: far from the crack the stress field is unperturbed by the blunting, and decays as for the sharp crack ($\sigma \propto r^{-1/2}$), but near the crack tip the stress singularity is similar to what is found near a wedge-shaped crack[9]:

$$\sigma \propto r^{\alpha}, \qquad \alpha = \frac{\pi}{2\pi - \theta} - 1 \tag{3}$$

i.e. $\alpha = -2/5$ for the given configuration, a $60°$ wedge, as opposed to $-1/2$ for a sharp crack ($\theta = 0$). This leads to a reduction of the stresses near the crack tip, and thus to an increase in the crack loading needed to break the bonds. However, this leads us to expect an increase in the load of approximately 25–50% over the range of blunting investigated here, versus the observed increase of only $\sim 10\%$. This is caused by the difference between the mode I and mode III configurations. Williams[10] has solved the mode I wedge configuration and the stress singularity is significantly different. He finds $\alpha = -0.478$ for this geometry, leading to a stress singularity that is indistinguishable from the sharp crack. This would lead us to expect that there should be no effect from the blunting. So we have to seek the explanation of the observed effect elsewhere than in linear elasticity.

Figure 2 (right) shows the result of reducing the number of atoms interacting through non-linear forces. This strongly suppresses the effect of the blunting, indicating that it is mostly a non-linear effect. When the crack is loaded the bonds at the blunt end of the crack are stretched into their non-linear regime. They are thus stretched more than they would have been if the bonds had been purely linear, and the bonds at the corner where the crack appear do not have to stretch as much, and therefore do not break as early. As the blunting increases, more non-linear bonds become available for relieving the stress concentration at the corner.

Conclusions

We have shown that blunt cracks have a stronger tendency to emit dislocations than do sharp cracks. This may be important in intrinsically brittle materials, where the natural tendency for a sharp crack is to propagate by cleavage rather than to emit dislocations. In these materials a dislocation may be blunted by *absorbing* a dislocation from a nearby source, and thereby be turned into an emitting crack, preventing further cleavage.

We also observe, that dislocation emission from an asymmetric blunt crack preferentially occurs to one side, and that the emission preserves the shape of the crack. This leads to emission of multiple dislocations to the same side, even in situations where emission on two symmetrical slip planes should be equally favorable, and where a simple shielding argument would result in emission of every second dislocation on alternate planes.

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