ATOMISTIC SIMULATION OF THE DUCTILE/BRITTLE TRANSITION*

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INTRODUCTION

Many materials are inherently brittle at very low temperatures in the sense that cleavage cracks can propagate without absorbing plastic work. However, with increasing temperature these inherently brittle solids generally pass through a transition in which plastic processes at the tip of a propagating crack become increasingly important, and energy absorption correspondingly increases. This "ductile to brittle transition" is often a critical design limitation for structural steels, and the well established Charpy test and associated specifications exemplify the recognition of this phenomenon.

In commercial materials such as steels, the transition behaviour is complicated by the complex microstructures normally present. There has been extended debate on the relative importance of crack nucleation and propagation, and the role played by carbides and internal interfaces. However, it is evident that a necessary condition for fully brittle cleavage is that no generation or motion of dislocations in the vicinity of the crack tip occur during propagation. There can be energy absorption and even crack blunting due to motion of pre-existing dislocations, the extent of which will depend on the dislocation density. However, if dislocation nucleation can occur at the tip of a crack, this will result in crack blunting and energy absorption even if the density of pre-existing dislocations is very low. Pre-cleaved single crystals of materials such as silicon exhibit a very sharp transition from brittle to ductile behaviour with increasing temperature, and it seems likely in cases such as this that the transition is due to the onset of dislocation nucleation.

In the present paper, a test will be presented of our ability to treat quantitatively the processes occurring at the crack tip. A comparison will be made between theoretical predictions and experimental studies by computer simulation, with the ultimate goal being the treatment of the effect of thermal activation on crack tip plasticity. Attention will be restricted to the tensile opening mode I.

NUCLEATION OF PLASTIC FLOW AT CRACK TIPS

The stress field near a crack tip in a linearly elastic medium is of the form [1] $\sigma_{ij} = K(2\pi r)^{-1/2} b_{ij}(\theta)$, where K is the stress intensity factor, and (r, θ) are polar coordinates with origin at the crack tip. At the crack tip itself where $r \to 0$ a nonlinear treatment is required as the interatomic bonds are stretched beyond the region of harmonic behaviour. As the stress intensity increases, lattice failure will eventually occur

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at the crack tip in the nonlinear region. Failure can occur by bond rupture in either tension or shear, which will determine whether the behaviour is inherently brittle or ductile.

Two treatments have been presented in the literature to predict the failure mode from known material properties. Kelly, Tyson and Cottrell (KTC) proposed that inherently brittle failure would be observed if $(\sigma/\tau)_{id} < (\sigma/\tau)_{max}$ where the subscripts "id" and "max" refer to the ideal properties of a perfect lattice and to the maximum values attained at a crack tip respectively. Rice and Thomson (RT) [3], on the other hand, have argued that a necessary criterion for brittle fracture is stability against the emission of dislocations from the crack tip and have treated this nucleation process within the approximation of linear elasticity and the Peierls model of a dislocation core.

Both treatments require approximations in their quantitative development. The stress analysis of linear elasticity is used to evaluate $(\sigma/\tau)_{max}$ and the forces on dislocations near the crack tip, and plausible models of the nonlinear and atomistic behaviour of materials are required to evaluate $(\sigma/\tau)_{id}$ and dislocation core structure. Since it is essential to have a clear description of crack tip processes and energetics in order to understand the effects of temperature, it is important to test the predictions of these treatments in order to gauge the validity of the approximations used.

Such a test has become possible with the publication of results of computer simulation studies of the atomistic behaviour at crack tips. Tyson and Alfred [4], Gehlen and Kanninen [5], and Weiner and Pear [6] have studied the modes of bond rupture at crack tips, which should be predictable by the treatments outlined above. The latter two papers also include information on the effects of thermal vibration.

The relevant data is shown in the Table, along with the criteria for ductile behaviour. The observed behaviour at absolute zero is also reported, and the nature of the ductile failure in the TA model is shown in Figure 1. In evaluating ξ_c, it has been assumed that shear failure occurs in a direction normal to the crack, on a plane containing the crack tip and perpendicular to the crack plane. Values of ξ_o have been deduced from the literature, from references [7], [8], and [9] for the three models respectively.

EFFECT OF TEMPERATURE

At temperatures above 0°K, thermal fluctuations enable the nucleation of dislocation loops which can expand in the stress field of the crack tip, and the energetics of this process have been treated by Rice and Thomson [3]. The behaviour then becomes truly three dimensional. However, thermal nucleation of dislocations is also possible in a two-dimensional model, which can be more easily studied atomistically and which allows a simplified treatment of the RT calculations. It is easily shown, following [3], that the energy of a dislocation U generated at the crack tip and moved to a distance ξb from it is given by

$$\frac{U}{\mu b^2} = a_1 \ell n \frac{\xi}{\xi_o} + a_2 \tan^{-1} \frac{2\xi}{e^{3/2}\xi_o} - a_3 \left[\left(\frac{\xi}{\xi_o} \right)^{1/2} - 1 \right] \qquad (1)$$

where

$$a_1 = \frac{1}{4\pi} \frac{1-\nu\sin^2\psi}{1-\nu}$$

$$a_2 = \frac{2}{\pi} \cdot \frac{1}{\eta^2 \beta'}$$

$$a_3 = \frac{2}{\eta\beta} \left[\frac{1}{2\pi(1-\nu)} \right]^{1/2} \xi_o^{1/2}$$

and

$$\eta = \sqrt{\mu b/\gamma}$$

β, β' are geometrical parameters equal to $\sqrt{2}$ and 1 for the geometry described above.

The terms in this expression represent self energy, ledge energy, and interaction energy with the stress field respectively. The variation of $U/\mu b^2$ with ξ/ξ_o for the WP model with $\xi_o = 0.29$ is shown in Figure 2, which is qualitatively similar to the three dimensional results shown by RT [3]. The energy barrier is of height $0.14\ \mu b^2$, at $\xi_c = 2.7$ consistent with the Table. Thermal nucleation of dislocations is expected at a temperature at which thermal fluctuations can supply an energy of this order.

The effect of thermal motion, simulated atomistically by adding kinetic energy to the lattice, has been investigated for models GK and WP (with $\xi_o = 0.29$). The GK model allowed three dimensional atomic motion, although the length of the crack front in the model (about 6b) is considerably less than the diameter of a stable dislocation loop in α Fe, estimated to be $\sim 34b$ [3]. The model is therefore closer to two-dimensional than three. In two dimensions, we find for this model that $\xi_c = 2.7$ (see the Table) and $U_c/\mu b^2 = 0.031$ from equation (1). This energy is equivalent to 0.44 eV per repeat distance along the crack front. Gehlen and Kanninen found that the crack was essentially stable against bond rupture and dislocation nucleation at a temperature of 250°K. At this temperature, the average kinetic energy per atom is $3kT/2 = 0.032$ eV. This is so much less than U_c that the observed stability is expected theoretically.

The WP model is explicitly two-dimensional, and we find for dislocation generation with $\xi_o = 0.29$ that $\xi_c = 2.7$ and $U_c/\mu b^2 = 0.14$. Using $\mu \sim 0.5 \times 10^{12}$ d/cm^2 and $b \sim 2 \times 10^{-8}$cm, this energy is equivalent to $U_c \sim 0.35$ eV per atomic plane. Weiner and Pear simulated a temperature of 800°K in their model, for which kT = 0.069 eV. As in the GK model, this is much less than U_c and so dislocation nucleation is not expected. In agreement with this, the model behaviour remained brittle with increasing temperature.

DISCUSSION AND CONCLUSIONS

The absence of thermally activated plastic flow in the simulations reported above is consistent with the large activation energies calculated theoretically. However, before this confirmation of the theory can be accepted with confidence, it is necessary to check that the correct behaviour is predicted at absolute zero. Here, the situation is not so encouraging. The criterion proposed by RT for ductile behaviour, namely $\xi_c < \xi_o$, is not satisfied for any of the models reported in the Table and yet half of them exhibit ductile behaviour. On the other hand, the KTC criterion predicts

the correct behaviour in all cases.

These observations are strongly reminiscent of the conceptual difficulties surrounding the Griffith criterion for fracture. The KTC approach is based on stresses at the crack tip and requires that the lattice strength be exceeded for failure to occur, which is analogous to requiring that sufficient stress concentration exist to cause bond rupture for cleavage fracture. The Griffith model, however, is based on an energy balance and thereby arrives at a necessary condition for crack growth, although the condition is not sufficient; stress concentration, i.e., a suitably sharp crack, is required as well.

It would appear from the results of the Table that the KTC criterion is both necessary and sufficient, although sufficiency has not been proven. On the other hand, the RT criterion does not seem to be necessary for the two models which fail in ductile fashion. This can only be ascribed to the difficulty of estimating accurately the forces on dislocations in the highly nonlinear region at crack tips. As seen from the Table, ξ_c is only of the order of b, and the application of linear continuum elasticity in this region is an over-simplification, as well understood by Rice and Thomson.

In conclusion, it has been shown that the results of computer simulation of crack motion in the presence of thermal vibrations can be understood on the basis of the theory developed by Rice and Thomson [3] for dislocation nucleation at crack tips. However, this theory is not successful in contrast to that proposed by Kelly, Tyson and Cottrell [2] in predicting the behaviour at absolute zero, pointing to a need for caution in applying the quantitative results of the theory of Rice and Thomson for dislocation nucleation. Further simulation results, particularly for a range of models extending from brittle to ductile behaviour at absolute zero, are needed to resolve the role of the nonlinear effects at the crack tip.

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Table 1 Material Properties and Observed Model Behaviour at Absolute Zero

Model	$\left(\frac{\sigma}{\tau}\right)_{id}$	$\frac{\gamma}{\mu b}$	ξ_c''	ξ_c	ξ_o	Behaviour (0°K) Observed (Simulation)	Predicted * KTC**	RT
Tyson, Alfred (TA)	3.4	0.14	0.71	1.39	0.35	Ductile	Ductile	Brittle
Gehlen, Kanninen (GK)	0.9+	0.05‡	2	2.7	0.63	Brittle	Brittle	Brittle
Weiner, Pear (WP)	1	0.05	2	2.7	0.29	Brittle	Brittle	Brittle
	2.04	0.02	2	6.5	0.48	Ductile	Ductile	Brittle

+ σ in <100>; τ in <100> on {100} Estimated From Frenkel Approximation

‡ μ, b for <100> {100} Shear

* Criteria for Ductile Fracture: $(\sigma/\tau)_{id} > (\sigma/\tau)_{max}$ (KTC)

$\xi_c < \xi_o$ (RT)

** Using $(\sigma/\tau)_{max} = 2$

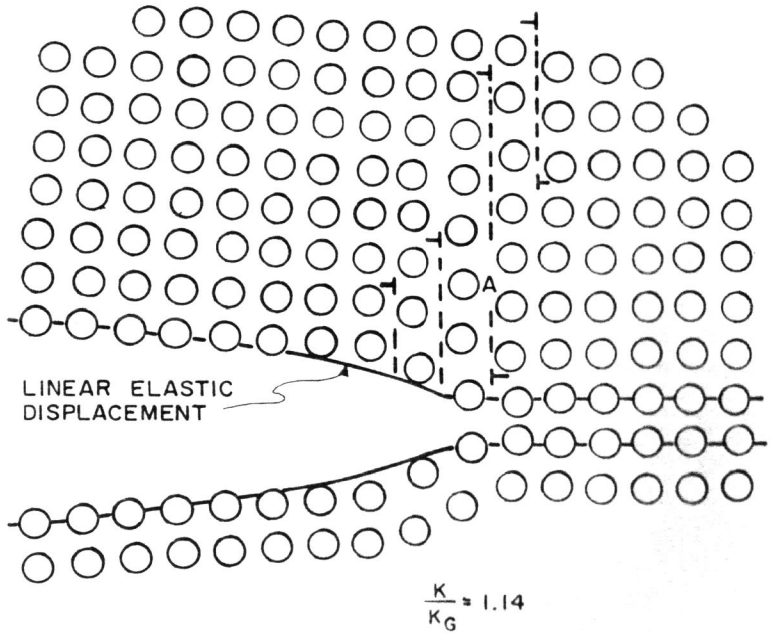

Figure 1 Atomic Positions at a Crack Tip at a Stress Intensity 14% above the Griffith Value. Atoms Have Been Relaxed within a Radius of 14 Lattice Spacings of the Crack Tip

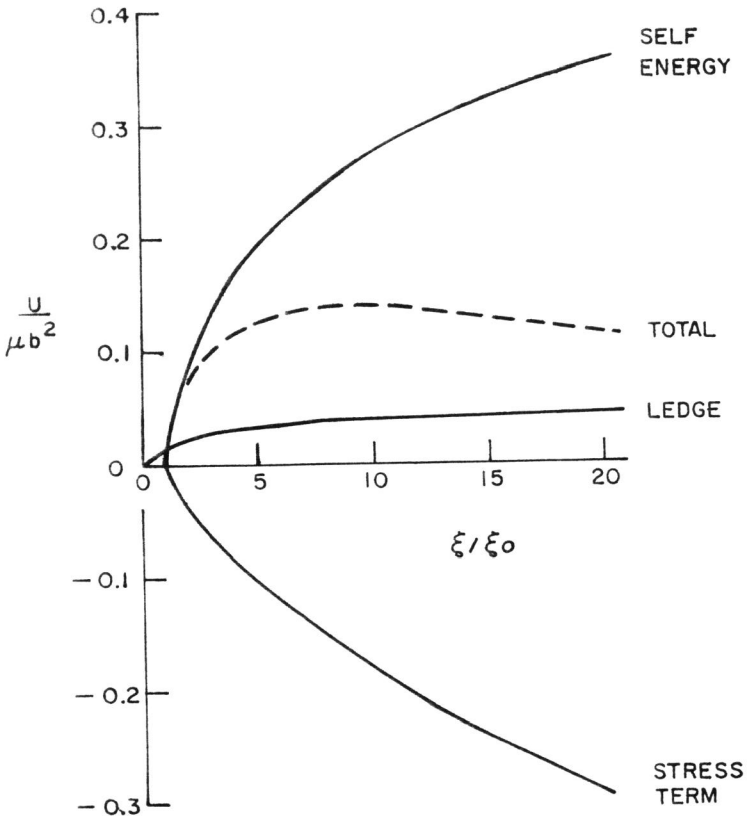

Figure 2 Energy of a Dislocation Near a Crack Tip. Model Parameters: $\gamma/\mu b = 0.05$, $\xi_o = 0.29$