Atomic Crack Simulation in Fracture Mechanics

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This paper describes our efforts to connect the macroscopic toughness of materials to lattice structure and relevant atomic properties by simulating the interactions of a large number of atoms on a computer. Parallel work has been reported by Chang[1], Tyson and Alfred[2], and Sinclair[3].

The material being considered is a model of α-iron; i.e., a bcc structure with a lattice parameter of 2.86 Å held together by two-body axial forces extending over first and second nearest neighbors, according to the Johnson I potential.[4] The model reproduces experimentally observable quantities with good accuracy*. We have considered cracks formed by partly separating two adjacent (100) planes with a crack front in the [001] direction. (A clear distinction between "cracked" and "uncracked" regions can be made because the interatomic force-separation law that is used has a finite out-of-range separation distance associated with it.) Attention has been focused on what is known in macroscopic fracture mechanics as plane strain crack extension under mode I (opening mode) loading. The results are compared with $K_G = 0.77\ MNm^{-3/2}$, the critical value of the stress intensity factor derived from linear elastic continuum Griffith Theory, the elastic constants, and the (100) surface energy of the model[5].

Our initial crack tip simulation calculations[5] employed about 200 movable atoms in two adjacent (001) planes. The boundary

* Of particular importance in this study are the surface energies on (100) and (110) planes. They are 1.3 and 1.2 J/m^2, respectively; the corresponding Young's moduli are $1.3\ 10^{12}$ and $2.2\ 10^{12}\ dy/cm^3$.

atoms --the atoms on the periphery of the computational cell--were held fixed in the positions given by the linear elastic continuum displacement field for the specified K level. Periodicity conditions were imposed in the direction parallel to the crack front, thus making the model quasi-three dimensional, and forcing the crack line to remain infinitely long and straight. Thermal vibrations were not included so that, in effect, a near $0^{\circ}K$ temperature was simulated.

The computations performed under these conditions produced no crack extension or dislocation generation at the crack tip even when K was in excess of $3K_G$. Isolated bonds were observed to rupture, however, which suggests that catastrophic crack growth was prevented by one or more of the constraints on the model. These are, (i) the absence of thermal fluctuations, (ii) the inability of the computational cell to generate and propagate (laterally) a kink, and (iii) the failure of the rigidly imposed linear elastic boundary conditions to compensate for nonlinear behavior in the vicinity of the crack tip. These constraints have been removed in succeeding models.

Calculations simulating crack tips at temperatures of $25^{\circ}K$ and $250^{\circ}K$ have been performed[6] employing a model otherwise similar to the one described above. Temperature effects were incorporated by considering each atom to be a classical harmonic oscillator, then injecting the appropriate amount of kinetic energy into the system. After a very short relaxation time, the velocity distribution closely approximated the theoretically expected distribution with many vibrational modes being activated. However, while the temperature simulation was deemed to be successful, crack extension was not observed even at the highest temperature level simulated.

The second constraint was removed from the model by employing a fully three-dimensional computational cell containing about 800 mov-

able atoms.[7] By introducing a [010] jog to the crack line, crack extension by localized bond rupture was observed to occur. This contrasts with the initial quasi-three dimensional computation in which bond rupture, if it was to occur, could only do so simultaneously all along the crack front. In the full three-dimensional model, the jog was observed to move at a critical stress intensity level close to K_G. In fact, the jog moves either to close up the crack or to extend it, depending on whether K is smaller or greater than the critical value.

To remove the final major constraint, we have instituted a scheme whereby the boundary atoms are permitted to adjust their positions (from the linear elastic continuum theory positions) consistent with the nonlinear behavior of the atoms close to the crack tip[8]. This technique provides a way for the discrete region and the continuum region to interact[9] and, in so doing, permits bond rupture to occur in a quasi-three-dimensional model. As shown in Figure 1, "flexible" boundary conditions have made it possible to observe crack extension by large-scale bond rupture. The critical K level was found to be about triple K_G and the crack propagated on a (110) plane, rather than the (100) plane. The latter observation is surprising, not only because the (100) plane coincides with the original crack, but because the (100) plane is predicted for this model by linear elastic continuum Griffith Theory and is also the observed cleavage plane for α-iron.

There are a number of shortcomings still present in our atomic crack tip model. These include the approximate way in which the flexible boundary conditions are presently being handled (see Reference 8), the absence of imperfections such as vacancies and impurity atoms, and the overly simple interatomic force law used. Of particular importance may be the fact that the force law does not presently account for a non-axial force.

In addition to abolishing these discrepancies, the next stage of our work must employ fully three-dimensional models with flexible boundary conditions that can simulate the generation and motion of different kinds of kinks. Subsequently, extension to consider the presence of more than one kind of atom will be undertaken to deal with problems of stress corrosion cracking and alloying. These activities obviously will require much further work so that a completely acceptable model is still far in the future. It is nevertheless clear that computer simulation is providing an important new tool for studying the metallurgical contributions to fracture toughness.

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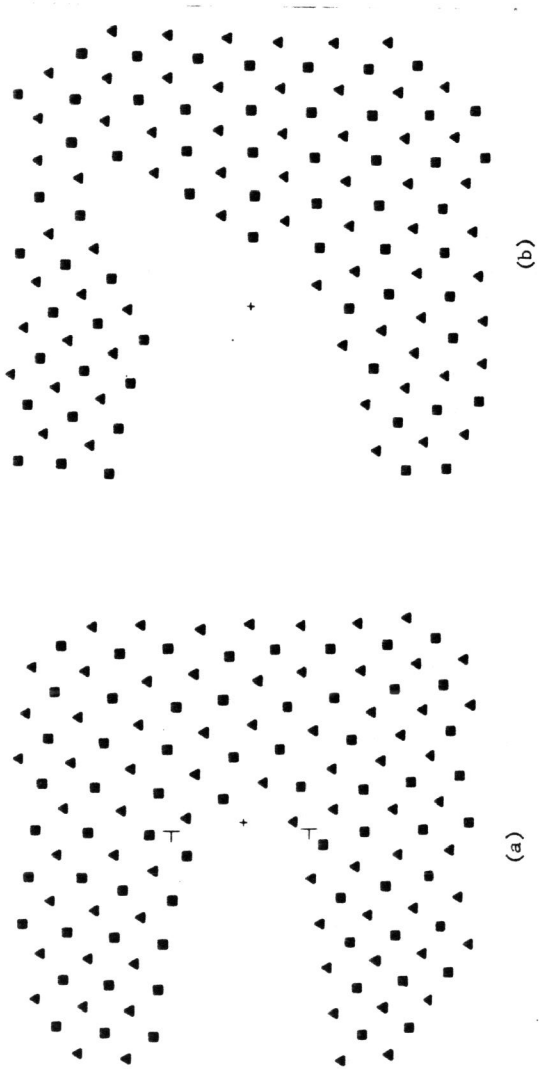

Figure 1. Crack tip behaviors at two stress field intensity levels, K. The calculations were performed at nomially 0°K in a quasi-three-dimensional model of bcc iron using the Johnson potential I(1). The crack plane is parallel to a (100) plane and the crack front is in a [001] direction. The atoms in two consecutive (001) planes parallel to the plane of the figures are represented by ■ and ▲. The + locates the position of the crack tip given by linear elasticity.

Figure (a) represents the crack tip configuration for K/K_G = 2.1 (with flexible boundaries); although there are signs of dislocation generation at the tip, the crack has not extended. Figure (b) is for K/K_G = 3.1 (with flexible boundaries); the array has become unstable and ruptures