

## AN ATOMISTIC MODEL FOR AN EQUILIBRIUM CRACK IN DIAMOND

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An ideally brittle crack extends by progressive stretching and rupture of cohesive bonds at the crack tip. A fundamental understanding of this process therefore requires a description of events on an atomic scale. One approach, which is valuable in providing physical insight into the fracture mechanism, is to consider only atom planes immediately above and below the crack plane, using linear or non-linear spring elements to represent bonds [1,2]. An alternative approach involves the introduction of well-established potential functions to represent interatomic interactions in a small volume surrounding the crack tip [3-7]. Although the second approach involves a large increase in mathematical complexity, which must be handled by computer, it is considered worthwhile because it more closely simulates the behaviour of real materials.

To date all attempts at computer simulation of atomic structures of crack tips have been directed toward metallic materials, in particular  $\alpha$ -iron. Metals do not constitute the most brittle class of solid, however, and the possibility that plasticity effects may be associated with crack extension may cause complication [5-7]. We have accordingly applied computer simulation methods to a crack system in diamond, whose covalent bond structure minimizes the likelihood of dislocation nucleation and propagation [8].

In our model we treat a long plane crack formed by bond rupture across the (111) cleavage plane and held open in an equilibrium configuration by an external tension. A state of plane strain is assumed parallel to (0 $\bar{1}$ 1), and the crack front is taken perpendicular to this plane. Atom relaxation is allowed within a rectangular "core" region (comprising 512 independent point-mass atoms) immediately surrounding the crack tip (Figure 1). Linear anisotropic elasticity theory is taken to provide the boundary conditions for the core region, and a first approximation for the lattice-point displacements within. The critical loading conditions follow from values of the surface energy and elastic constants.

For our relaxation operation the core atoms are assumed to interact through a potential function constructed in accordance with the following: energy dependence on the angles between nearest-neighbour bonds is included, in addition to Morse-law dependence on bond length; for small, uniform strains the elastic behaviour matches the observed elastic constants; the work to separate bonds across the fracture plane provides a reasonable value for the surface energy..

Relaxation to a minimum in the total potential energy was achieved with the well-known method involving integration of the motion of atoms with damping [5]. Figure 2 shows the results for the equilibrium crack in diamond. No shear instabilities in the structure occurred during relaxation. The figure shows bonds "ruptured" behind

the crack tip, and stretched by up to 20% just ahead of it. This degree of stretching is well beyond the "linear" range, and just short of the rupture limit, for the potential used. Also indicated in Figure 2 is the crack profile predicted by continuum theory; the tip radius is only about 0.1 atomic spacings, emphasising the microscopic scale of the crack-tip geometry.

The above procedure makes it possible in principle to relate the fracture properties of a perfectly brittle solid to the strength of the chemical bond. A more detailed description of the calculations will be reported elsewhere.

#### REFERENCES

- [1] J. N. Goodier and M. F. Kanninen, Technical Report no. 165, Division of Engineering Mechanics, Stanford University (1966).
- [2] R. Thompson, C. Hsieh, and V. Rana, *Journal of Applied Physics* 42 (1971) 3154.
- [3] R. Chang, *Fracture 1969*, Chapman & Hall (1969) 306.
- [4] R. Chang, *International Journal of Fracture Mechanics* 6 (1970) 111.
- [5] P. C. Gehlen and M. F. Kanninen, *Inelastic Behaviour of Solids*, McGraw-Hill (1970) 587.
- [6] P. C. Gehlen and M. F. Kanninen, *Interatomic Potentials and the Simulation of Lattice Defects* (1972), (to appear).
- [7] M. F. Kanninen and P. C. Gehlen, *International Journal of Fracture Mechanics* (to appear).
- [8] A. Kelly, W. R. Tyson, and A. H. Cottrell, *Philosophical Magazine* 15 (1967) 567.

25 January 1972

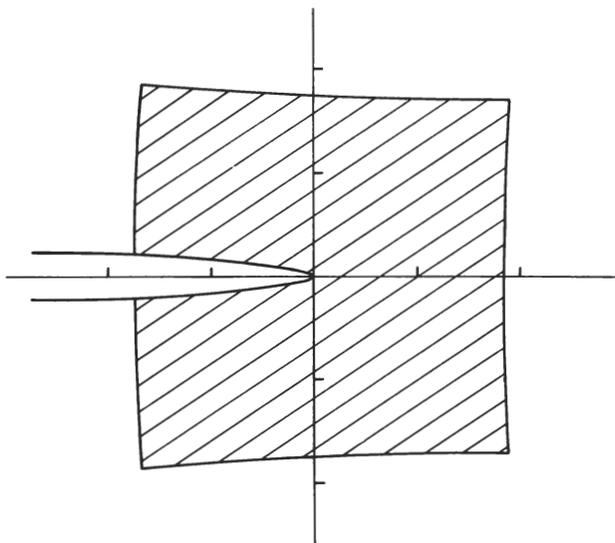


Figure 1. Crack model for relaxation procedure. Shaded rectangular area indicates atomistic core region about tip. The core is large compared with atomic dimensions, but small compared with the crack length. The axis markings have 10Å spacing; the nearest-neighbour distance for diamond is 1.54 Å.

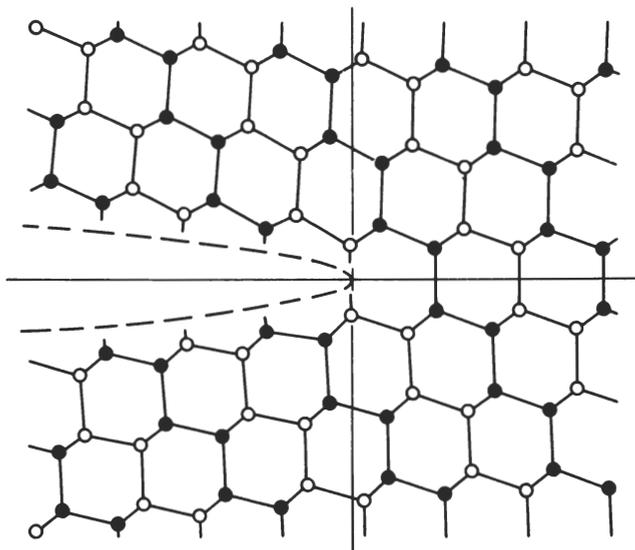


Figure 2. Computer-relaxed atomic configuration for equilibrium crack in diamond. Crack plane is (111), plane of diagram (011). Two consecutive layers are shown, distinguished by open and closed circles. Broken line indicates continuum solution for crack profile.