

# INVESTIGATING MATERIALS FAILURE USING LOTS OF ATOMS AND BIG COMPUTERS

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During the last decade, we have been simulating the dynamic failure of brittle and ductile solids at the atomic level using lots of atoms and some of the world's fastest computers. Our computer experiments have included crack dynamics in brittle fracture, crack blunting in ductile failure, and multiple dislocation entanglement in work-hardening, all of which have given new and exciting insights into the failure processes of solids. Most important, these simulations are based on an "ab initio" description of materials failure where atomic systems as large as one billion atoms are employed.

One of our most intriguing findings is a dynamic instability of the crack tip in rapid brittle fracture which prevents a crack from achieving its theoretical steady-state speed equal to the Rayleigh wave speed. Continuum fracture theory typically assumes that cracks are smooth and predicts that they accelerate to a limiting velocity equal to the Rayleigh speed. In contrast, experiment tells us that, in a common fracture sequence, an initially smooth and mirror like fracture surface begins to appear misty and then evolves into a rough, hackle region with a limiting velocity of about six-tenths the Rayleigh speed. All of these features are unexplained using conventional continuum theory. Our atomistic simulations duplicate these experimental features and yield physical explanations for the dynamic crack instability.

If a crack is constrained to propagate straight, theory suggests that crack speeds beyond the Rayleigh speed be forbidden. However, recent experiments, for shear dominated crack growth, report evidence to the contrary. To understand this phenomenon, we have performed molecular dynamics simulations of crack propagation along a weak interface joining to strong crystals and show that a mode I tensile crack is indeed limited by the Rayleigh wave speed, consistent with the classical theories of fracture. However, a mode II shear dominated crack can accelerate to the Rayleigh wave speed and then nucleate an intersonic daughter crack which quickly accelerates to the longitudinal wave speed. Furthermore, crack speeds can even surpass the longitudinal wave speed, becoming supersonic, in materials exhibiting elastic stiffening behavior. This phenomenon is totally contradictory to predictions of classical theories.

For ductile failure, we discovered that an fcc solid can fail by brittle cleavage even though we are taught that this atomic packing is intrinsically ductile. But this brittle character is very "fragile." At a certain speed a dynamic brittle-to-ductile transition occurs, immediately leading to the initiation of plastic failure, crack arrest and the spontaneous proliferation of dislocations. Most recently, we have simulated work-hardening on the 12-teraflop ASCI White computer at Lawrence Livermore National Laboratory. This investigation simulates ductile failure using over one billion atoms where the true complexity of the creation and interaction of hundreds of dislocations are revealed for the first time.

All of these phenomena are governed by the "hyperelasticity" of the solid. The elasticity of a solid clearly depends on its state of deformation. Metals will weaken, or soften, and polymers may stiffen as the strain approaches the state of materials failure. It is only for infinitesimal deformation that the elastic moduli can be considered constant and the elasticity of the solid linear. However, many existing theories model fracture using linear elasticity. Certainly, this can be considered questionable since material is failing at the tip of a dynamic crack because of the extreme deformation. Our large-scale atomistic simulations show that hyperelasticity, the

elasticity of large strains, plays the governing role in the dynamics of failure in materials and that linear theory is incapable of capturing all phenomena.

However, a complete treatment of materials failure based solely on atoms is not computationally possible and not necessary. Only near the crack tip do we need atoms and, maybe, quantum electrons for the snapping of chemical bonds. Indeed, a challenging paradigm in the computational sciences is the coupling of the continuum, the atomistic and the quantum descriptions of matter for a unified dynamic treatment of a physical problem. This requires the simultaneous use of the tools of engineering, physics and chemistry in a seamless formalism. We report such an accomplishment for the study of the brittle fracture of silicon, though our approach has general applicability. In a single concerted simulation of dynamic fracture comprising the finite-element method, classical molecular dynamics and quantum tight-binding dynamics, we demonstrate that "spanning the length scales" with dynamical bridges between the different physical descriptions is feasible.

Multimedia versions of our atomistic simulation studies of fracture are available via the World Wide Web:  
<http://www.almaden.ibm.com/st/Simulate/Fracture>.