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Spanning the continuum to quantum length scales in a dynamic simulation of brittle fracture

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Abstract. – We have coupled the continuum, the atomistic, and the quantum descriptions of matter for a unified treatment of the dynamic fracture of silicon. We have devised schemes for handshaking between the finite-element, molecular dynamics and semi-empirical tight-binding representations. We illustrate and validate the methodology for brittle crack propagation in silicon.

A challenging objective in computational physics is the coupling of the continuum, the atomistic and the quantum descriptions of matter for a *unified dynamic* treatment of a physical problem. We report such an accomplishment for the simulation of brittle fracture in silicon. 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. Our approach maps naturally onto scalable computer architectures.

Rapid brittle fracture dynamics may be considered an application where the three mechanics may be required. The traditional approach is to adopt continuum mechanics [1, 2]. In this case material lengths go to zero, and there is no natural small-length cut-off, such as the size of an atom. Hence, a failure mechanism describing the loss of local material cohesion does not arise naturally from this macroscopic description. At the finer level of description of classical atoms interacting through empirical force laws, material decohesion does arise naturally [3, 4]. We choose to label the atomic length scale the mesoscopic regime. We can even go one level finer. Treating bond breaking with an empirical potential may be questioned, and a quantum-mechanical treatment may be desired. This *ab initio* level of description we call the microscopic regime. And if the crack is moving, a unified macroscopic, atomistic, *ab initio* dynamics (MAAD) description must be brought together into a compatible union.

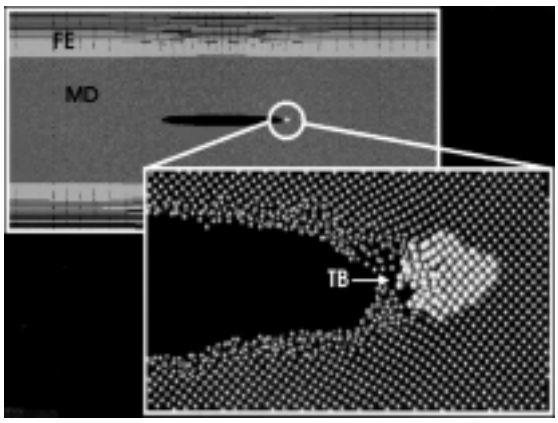

Fig. 1

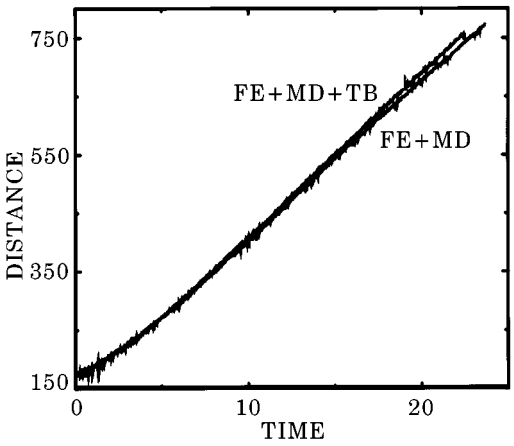

Fig. 2

Fig. 1. – The geometrical decomposition of the silicon slab into the five different dynamic regions of the MAAD simulation: the continuum finite-element region (FE) which is not shown in its entire extent; the atomistic molecular dynamics region (MD); the quantum tight-binding region (TB); the FE-MD "handshaking" interface; and the MD-TB "handshaking" interface. The image is the simulated silicon slab, with expanded view of the TB region surrounded by MD atoms. Note that the TB region surrounds the crack tip with broken-bond MD atoms trailing behind this region.

Fig. 2. – The distance *vs.* time history of the two crack tips, one having the TB atoms always centered at the immediate failure region. The distance is in angstroms, and the time is in picoseconds.

Our MAAD simulation is composed of computational procedures formulated in terms of a spatial decomposition of the system and has an obvious applicability for parallel processing. Our study is the rapid brittle fracture of a silicon slab flawed by a microcrack at its center and under uniaxial tension. The silicon slab is partitioned into five dynamic regions of the simulation, see fig. 1. In the "far-field" region, we have a continuum treated by the well-known finite-element (FE) procedure [5]. This macroscopic description merely needs the constitutive law for the material. One processor is used for each of the two FE regions. Around the crack, with large strain gradients but with no bond rupture, we use the classical molecular dynamic (MD) method to treat the highly nonlinear deformation on the atomic scale. Molecular dynamics predicts the motion of the atoms governed by their mutual interatomic interactions and requires the numerical integration of Newton's classical equations of motion. The Stillinger-Weber (SW) potential [6] is taken to represent the empirical force law between the silicon atoms. Because MD has a large computational burden, we partition this region spatially onto several processors (16 in the present example). Lastly, in the region of bond failure at the crack tip, we use the tight-binding (TB) formalism which is a semiempirical electronic structure description of matter. It is one of the fastest numerical quantum methods containing electronic information. For this silicon study, we employ the nonorthogonal TB scheme due to Bernstein and Kaxiras [7]. The nuclei are treated as point objects. The TB region is the most computationally demanding part of the overall code, and small TB regions must be used so as to allow overall load balancing. We track the path of the crack and place the center of the TB region at the apex of the crack where the bond breaking occurs. For extended regions of bond rupture, we use overlapping TB regions taken to be a "clover leaf" of (eight) overlapping TB regions, each being cylindrical and distributed to a different processor.

Two crucial aspects of our MAAD procedure are the handshaking algorithms between the

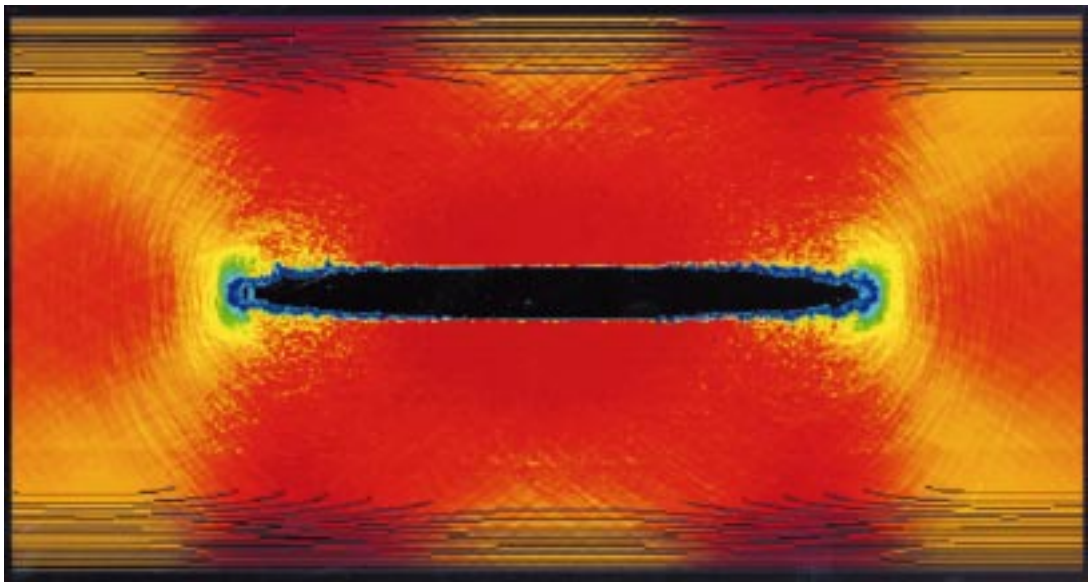

Fig. 3. – The stress waves propagating through the slab using a finely tuned potential energy color scale.

FE and the MD and between the MD and the TB where interface couplings are required [8]. In the FE/MD handshake region, the FE mesh spacing is scaled to atomic dimensions. The FE region has displacements associated with each mesh point which follow a Hamiltonian given by continuum linear elasticity theory. We employ an update algorithm identical to that used in conventional MD so that the displacements now are dynamical variables which follow in lock step with those of their atomic cousins in the MD region. The FE/MD interface is chosen to be far from the fracture region; atoms and the displacements of the FE lattice can be unambiguously assigned to one another. This is accomplished by taking the interactions across the FE/MD boundary to be the mean of the FE Hookian description and the MD interatomic potential description. Moving away from the FE/MD region and deep into the continuum, we can expand the mesh size. Thus we can embed our atomistic simulation in a large continuum solid. For the MD/TB handshake interface, dangling bonds at the edge of the TB region are terminated with pseudo hydrogens; "pseudo" because the matrix elements are carefully constructed to tie off a single bond and ensure no charge transfer when that atom is placed at a position commensurate with the silicon lattice. Thus at the perimeter of the MD/TB region, we have "hydrogens" which sit directly on top of the atoms of the MD simulation. On one side of the TB/MD interface, we imagine that the bonds to an atom are derived from the TB Hamiltonian and on the other side the bonds are derived from the interatomic potential of the MD simulation. As before, the TB code updates atomic positions in lock step with its FE and MD cousins. The entire MAAD procedure is formulated in such a way that the system, in the absence of dynamic TB tracking of the crack front, follows a conservative Hamiltonian. A detailed discussion of the MAAD techniques is in preparation [9].

We give important details of the MAAD simulation of silicon fracture. The exposed notch faces are (x, z)-planes with (100) faces, with the notch pointed in the $\langle 010 \rangle$ direction. For the largest system simulated, there are 25 8048 mesh points in each FE region, 1 032 192 atoms in the MD region, and around 280 unique atoms in the TB region. Each of the eight TB regions

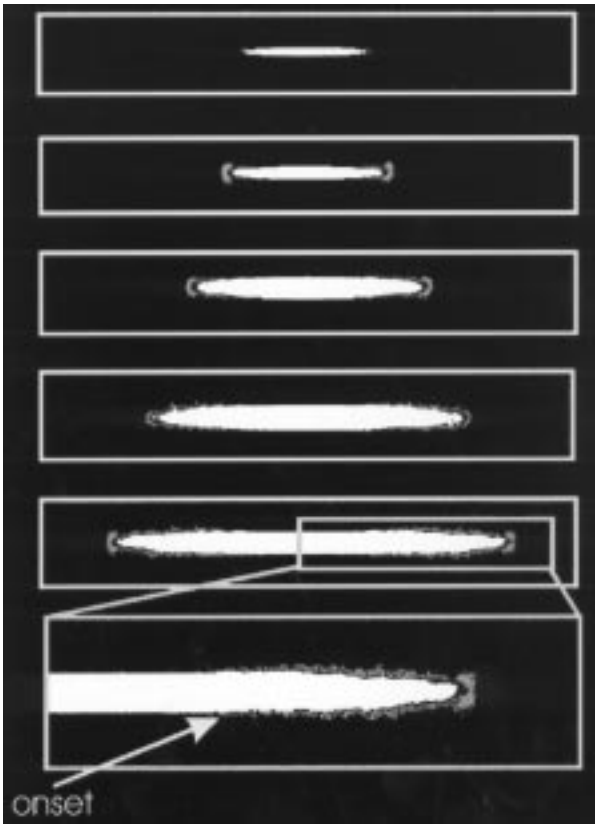

Fig. 4. – An increase roughening of the solid silicon surfaces with growing crack length.

is a cylinder with radius 5.43 Å in the (y, z)-plane. The lengths of the MD region are 10.9 Å (the slab thickness and periodic), 521 Å (before the pull, in the direction of pull), and 3649 Å (the primary direction of propagation and periodic). The full pull length of the FE + MD system is 5602 Å. The entire system including the FE represents 11 093 376 atoms. The time for a TB force update is 1.5 seconds, that for the MD update was 1.8 seconds and that of the FE was 0.7 seconds. We could thus afford to double the size of the FE region in order to accomplish complete computational load balancing but without any sacrifice of wall-clock time. The TB region was relocated every 10 time steps. The slab is initialized at zero temperature, and a constant strain rate is imposed on the outermost FE boundaries defining the opposing horizontal faces of the slab. A linear velocity gradient is established across the slab, and an increasing strain with time occurs in the solid slab. The solid fails at the notch tip when the solid has been stretched by $\sim 1.5\%$. The imposed strain rate is set to zero at the onset of crack motion. Figure 2 presents the distance *vs.* time history of the two crack tips, one having the TB atoms dynamically centered at the immediate failure region. The propagating cracks rapidly achieve a limiting speed equal to 85% of the Rayleigh speed, the sound speed of the solid silicon surface. The two distance-time histories are very similar. In hindsight, this might have been expected since the elastic modulus of silicon calculated from the empirical SW potential and from TB are very similar up to the mechanical stability limit of the bulk solid [10]. More importantly, this indicates that the handshaking between the MD region and

the TB region is reliable. In fig. 3, we note that the stress waves are passing from the MD region to the FE regions with no visible reflection at the FE-MD interface; *i.e.* the coupling of the MD region with the FE region appears transparent. In fig. 4, we see that the straight-ahead brittle cleavage of the silicon slab leaves behind surfaces that show an increasing roughening with crack distance. The origin of this observed surface roughening may be consistent with a suggestion by Rice [11] that silicon should show dislocation nucleation from a crack tip but the low dislocation mobility condemns Si to a brittle response. We speculate that the spawning of dislocations with very low mobility on the time-scale of the crack motion could result in surface disorder.

In conclusion we have studied the physics of brittle fracture in silicon as an illustration of our simulation approach to *spanning length scales*. Future studies may likely apply more sophisticated computational techniques for the three mechanics, invent more robust procedures for interfacing the three mechanics, and address physical problems very different from this present study. The concurrent spanning of the continuum to the quantum should prove to be a powerful approach in computational physics.

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[10] For small deformations, overall consistency was ensured by making sure that the linear elastic constants in all three regions are the same. We also found from calculation that the elastic modulus of silicon using the empirical SW potential is almost identical to the prediction of TB for strains up to the mechanical stability limit of the bulk solid [9].
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