

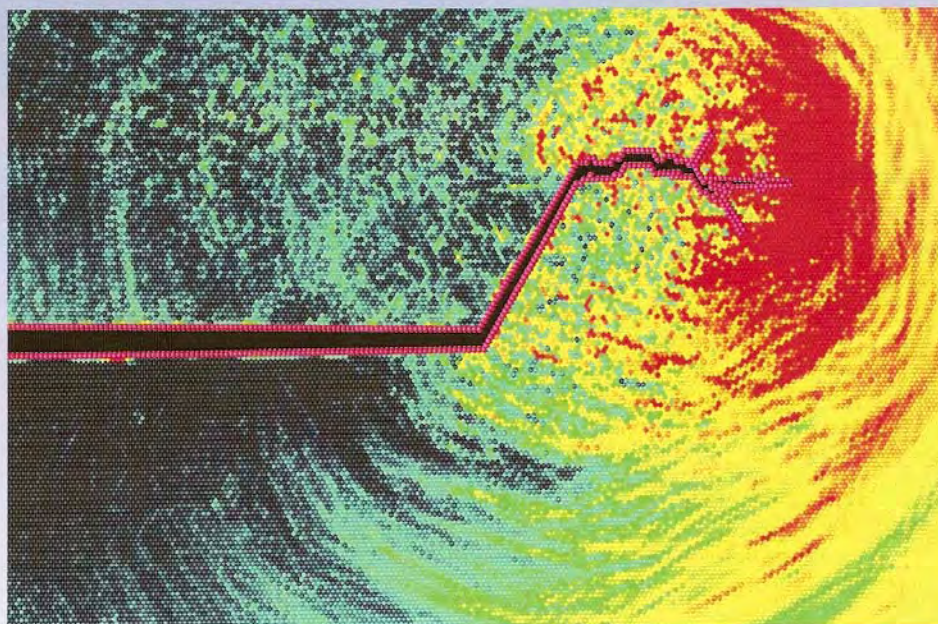
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**NANOSCIENCE**

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**THEORETICAL AND COMPUTATIONAL**  
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## ON THE COVER:

Atomistic view of the dynamics of crack propagation through a brittle material. The motion of atoms is modeled using a large-scale molecular dynamics scheme, featuring a total system size of up to 70 million atoms. The atoms are colored according to their potential energy. Surface atoms are rendered as red particles. The figure shows the atoms near a rapidly propagating crack shortly after the dynamical crack tip instability has set in. Experiment has shown that cracks start out slow while forming a straight, clean flat-as-a-mirror surface. As the crack gains speed, at a certain point it starts to change direction, leaving in its wake an increasingly rough, uneven surface that eventually creates a chaotic branching pattern as the crack spreads out further. This phenomenon happens in many different classes of brittle materials, including glasses, ceramics, polymers, and semiconductors. Large-scale atomistic modeling and theoretical analyses indicate that a change of material properties under large deformation, close to the breaking of bonds, is responsible for these instabilities. (Credits: M. J. Buehler, MIT, image prepared using the OpenDX Data Explorer.) More details are given in the review "Large-Scale Hierarchical Molecular Modeling of Nanostructured Biological Materials" by Markus J. Buehler, pp. 603–623, of this issue.

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