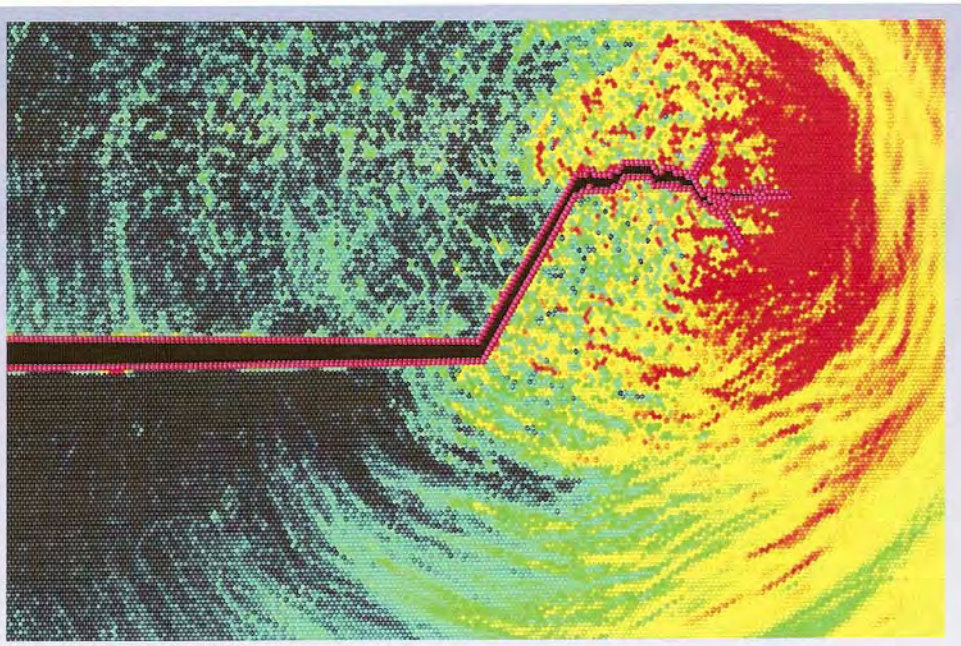
Volume 3 • Number 5 October 2006

www.aspbs.com/ctn

Journal of Computational and Theoretical NANOSCIENCE

For all Theoretical and Computational Aspects of Nanotechnology in Science, Engineering, and Biology



A Special Section on

THEORETICAL AND COMPUTATIONAL CHEMISTRY OF COMPLEX SYSTEMS

GUEST EDITOR: GuanHua Chen

Editor-in-Chief: Wolfram Schommers, Germany

ASP

AMERICAN SCIENTIFIC PUBLISHERS

Journal of
Computational and Theoretical Nanoscience
www.aspbs.com/ctn

VOLUME 3, Number 5
OCTOBER 2006

599–863 (2006)
ISSN: 1546-1955, EISSN: 1546-1963

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.

REPORT

REVIEWS

RESEARCH ARTICLES