Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Global and local properties used as analyses tools for molecular-dynamics simulations[1] MARTINA E. BACHLECHNER, West Virginia University, Physics Department, JONAS T. ANDERSON[2], DENG CAO, ROBERT H. LEONARD, ELI T. OWENS, JARROD E. SCHIFFBAUER, West Virginia University, Physics Department, MELISSA R. BURKY[3], Chemistry Department, Davis & Elkins College, Elkins, West Virginia 26241, SAMUEL C. DUCATMAN, ERIC J. GUFFEY[4], University High School, Morgantown, West Virginia 26505, FERNANDO SERRANO RAMOS2, Department of Computer Science, Metropolitan University, San Juan, Puerto Rico 00928 — Molecular dynamics simulations have been used to study mechanical failure in realistic interface materials. Averaging over the individual atoms' contributions yields local and global information including displacements, bond angles, strains, stress tensor components, and pair distribution functions. A combined analysis of global and local properties facilitates detailed insight in the mechanisms of failure, which will eventually guide on how to prevent failure of interfaces.

[1]Supported in parts by NASA.
[2]NSF (Virtual Environments REU at WVU)
[3]Undergraduate Research Experience (SURE) Program funded by WV EPSCoR
[4]NASA Independent Verification and Validation Facility Science and Engineering Apprenticeship Program

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Date submitted: 06 Dec 2005 Electronic form version 1.4