Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Uniaxial compression of group-IV nanoparticles from ab-initio molecular dynamics simulations PRASANJIT SAMAL, MATTEO COCOCCIONI, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 - 0132, U.S.A. — Uniaxial compressions of isolated systems from ab-initio molecular dynamics are made possible through the extension of the electronic enthalphy method [Phys. Rev. Lett. 94, 145501 (2005)] previously introduced for finite systems under hydrostatic pressure. Through this novel approach experimental settings with nanoparticles indented between parallel plates can be reproduced and simulated more realistically, thus allowing for more reliable comparisons between experimental data and simulation results. Molecular dynamics simulations for some group-IV nanoparticles under uniaxial compression have been performed using this extended scheme. Comparison with the deformation of the same systems under hydrostatic loads will elucidate the differences and similarities in the nucleation events of structural transformations and in their kinetic pathways.

Prasanjit Samal
Dept of Chemical Engineering and Materials Science,
University of Minnesota, Minneapolis, MN 55455 - 0132, U.S.A.

Date submitted: 02 Jan 2008 Electronic form version 1.4