

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Phonon mode and Breakdown of a Au nanowire between electrodes LIQIN KE, MARK VAN SCHILFGAARDE, School of Materials, Arizona State University, Tempe, AZ, 85287-8706 — The deformation behavior of an atomic Au wire placed between Au electrodes, was investigated by using a generalization of the method of linear muffin-tin orbitals (LMTO) within the local-density approximation (LDA). We studied the dynamical motion of the atoms in the wire. Soft phonon modes were studied. It has been found that the lowest phonon eigenstate are associated with motions of atom in the middle of the chain. Atomic motion of this mode was studied by solving the nuclear wavefunction of this atom. The quantum and classical effects are compared. At certain stages of the wire breaking process, atomic fluctuations become very large. We also show that the wire conductance is sensitive to the details of the deformation, which implies that the intrinsic noise in the conductance is of the order as the conductance itself. Large displacements which resulted in wire breakage were also studied. The energy barrier associated with this process has been calculated.

Mark Van Schilfgaarde
School of Materials, Arizona State University, Tempe, AZ, 85287-8706

Date submitted: 05 Dec 2007

Electronic form version 1.4