Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Surface Stress and Energy of Metal Nanoclusters[1] IGOR VASILIEV, BHARAT MEDASANI, YOUNG HO PARK, New Mexico State University — We combine first-principles and empirical computational methods to study the surface energy and surface stress of silver and aluminum nanoparticles. The structures, cohesive energies, and lattice contractions of Ag and Al nanoclusters over a broad size range are analyzed using two theoretical approaches: an *ab initio* density functional pseudopotential technique combined with the generalized gradient approximation and the embedded atom method. Our calculations predict the surface energy of Ag and Al nanoclusters to be in the region of $1.0-2.2$ J/m^2 and $0.9-2.0$ J/m^2, respectively. The surface stress is evaluated from the average lattice contraction by considering the hydrostatic pressure on the surface of a spherical particle. A comparison of the calculated surface energies and stresses indicates a greater degree of surface reconstruction in Al nanoclusters than in Ag nanoclusters.

[1]Supported by NSF DMR-0505270 and by the IRG program of New Mexico State University.

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Date submitted: 26 Nov 2007 Electronic form version 1.4