Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A study of the structure and dynamics of the interface between a nanoparticle and a surface: the case of Cu and Ag JAMES BORRELLI, JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We performed a Molecular Dynamics study using the Embedded Atom Method for interatomic potentials for silver and/or copper nanoparticles projectiles incident on Ag and/or Cu (100) surfaces. Nanoparticles in the range of 1 to 2 nm in diameter were used with incident energies ranging from 50 to 500 meV/atom; while the surface temperature is kept at a temperature ranging between 300 and 700K. After collision and thermalization, distributions of nearest neighbor distances show a variety of values that reflect the strength of the local bonding. Using a Real Space Green's Function approach, we have determined the vibrational densities of states and the corresponding thermodynamical functions for a limited number of cases. Results for the vibrational dynamics show a strong effect at the high frequency end of the densities reflecting the stiffness of the bond at the interface. Results for the vibrational enery, entropy, lattice heat capacity as well as Debye temperatures will be presented.

Abdelkader Kara
University of Central Florida

Date submitted: 08 Dec 2010 Electronic form version 1.4