Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Structural determination of metal nanoparticles from their vibrational (phonon) density of states[1] IGNACIO GARZON, Universidad Nacional Autonoma de Mexico, HUZIEL SAUCEDA, Univeridad Nacional Autonoma de Mexico — The vibrational (phonon) density of states of metal nanoparticles with size between 2-6 nm can be measured using nuclear resonant inelastic x-ray or plasmon resonance Raman scattering. In this work, we present atomistic calculations, based on a semiempirical tight-binding many-body Gupta potential, of the vibrational density of states (VDOS) for FCC, decahedral, and icosahedral (ICO) gold and silver nanoparticles with sizes $\sim$ 4 nm ($\sim$ 2000 atoms). The calculated VDOS are compared with experimental data, recently published for gold and silver nanoparticles of similar size, obtained through plasmon resonance Raman scattering. The best agreement between the calculated and measured VDOS's is obtained for the ICO morphology for both metal nanoparticles. These results indicate that most of the nanoparticles in the experimental samples should have icosahedral structures. The present study also shows that, as in the case of molecular systems and small clusters, vibrational spectroscopy of metal nanoparticles with few nanometers in size, together with theoretical calculations, are powerful tools for their structure determination. with your abstract body.

[1]Work supported by CONACYT-Mexico under Project 177981.

Ignacio Garzon
Universidad Nacional Autonoma de Mexico

Date submitted: 13 Nov 2014 Electronic form version 1.4