

M.Sc. Defense

Timothy Leisti

DATE: Tuesday, November 24, 2009

TIME: 1:00 p.m.

**PLACE: MacNaughton Room 222
University of Guelph**

THESIS TITLE:

**Modelling Gold Nanoparticles Using the Second Moment Approximation
to the Tight-Binding Model Potential**

ABSTRACT:

An investigation of the temperature and size dependant structural properties of gold nanoparticles was performed. Using a molecular dynamics simulation and the second moment approximation to the tight-binding model potential, a series of nanoparticles ranging in diameter from 1.0 nm to 5.3 nm were simulated over a range of temperatures. A new set of potential parameters had to be derived to accurately model the nearest neighbour distances within the nanoparticle. The results showed significant contraction of the nearest neighbour distances with decreasing nanoparticle size, as well as a dependence on the radial distance from the centre of the nanoparticle. Thermal expansion coefficients of the nanoparticles were calculated and observed to be fairly constant over the range of sizes studied. Most sizes showed expansion greater than the thermal expansion of simulated bulk gold. These results indicated both the abilities and limitations of the tight-binding potential for use on nano-scale systems.

EXAMINING COMMITTEE:

Chair : Paul Garrett

Internal Examiners: Stefan Kycia and deTong Jiang