Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Computation of Microcanonical Entropy Differences in Atomistic Computer Simulation[1] SERGIO DAVIS, Departamento de Física, Facultad de Ciencias, Universidad de Chile — In this work, two alternative methods to compute thermodynamic entropy differences $\Delta S = S(E_2) - S(E_1)$ between two microcanonical states (produced via atomistic computer simulation, either deterministic or stochastic) at total energies E_1 y E_2 are presented. The first method is straightforward to implement, as it only needs potential energy samples from both simulations; however, it requires that fluctuations of potential energy are similar in magnitude to the energy difference ΔE between the states. It is therefore best suited for simulations in small systems (hundred of atoms). The second method, based on Bayesian probability and information theory, removes this limitation: it allows the computation of the entropy curve $S(E)$ for a wide range of energies and therefore is a viable alternative to methods such as Wang-Landau Monte Carlo. It is based on inferring the configurational density of states (CDOS) from potential energy samples. A simple model for the CDOS of embedded atom metals is presented and tested in Au and Cu by computing entropy and free energy differences.

[1]SD Acknowledges FONDECYT grant 3110017

Sergio Davis
Departamento de Física, Facultad de Ciencias, Universidad de Chile

Date submitted: 10 Dec 2012 Electronic form version 1.4