Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Equilibrium phase diagrams of alloys using nested sampling NOAM BERNSTEIN, Naval Research Laboratory, ROBERT J N BALDOCK, LIVIA BARTÓK-PARTÁY, GÁBOR CSÁNYI, Cambridge University —
Temperature-pressure-composition phase diagrams describe the structures of materials in thermal equilibrium, and are an essential tool in understanding material properties. Predicting phase diagrams is challenging, even given a description of the interatomic interactions, because of the need to sample a very large configuration space. Nested sampling (NS) has been shown to be an efficient tool for calculating the partition function, and therefore all thermodynamic properties and ensemble averages, by systematically sampling the configuration space of isolated and periodic systems. Its effectiveness comes from sampling starting from high energy, where barriers are relatively low and equilibration is relatively fast, and iteratively eliminating a fixed *fraction* of the remaining configuration space. We present an application of NS at constant pressure to the phase diagram of a model binary alloy, CuAu, using an embedded atom method potential. We identify phase transitions indicated by peaks in the calculated specific heat, and the dominant phase at each temperature from ensemble-averaged structural ordering, as represented by quantities such as the radial distribution function. These results demonstrate the power of NS as a method for calculating complete phase diagrams.

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Date submitted: 05 Nov 2015 Electronic form version 1.4