Abstract Submitted
for the 4CF17 Meeting of
The American Physical Society

An EAM Model Comparison of the Alkali Metals in BCC, FCC, and HCP Lattice Structures JAKE CHRISTENSEN, MARCUS JACKMAN, MARK RIFFE, Utah State Univ — The alkali metals (Li, Na, K, Rb, and Cs) form in body-centered cubic (BCC) lattice structure at room temperature. As temperature is lowered, both sodium and lithium undergo a phase transition to a close-packed structure. Previously, we have developed an Embedded-Atom-Method (EAM) model that accurately describes the vibrational properties of the alkali metals in the BCC structure. Here, we use the same model to calculate the vibrational properties of alkalis arranged in the close-packed face-centered cubic (FCC) and hexagonal close-packed (HCP) lattice structures. The goal is to see if the model can account for the fact that, at higher temperatures, BCC is the preferred structure. This will be done by comparing the free energies of the metals in the three different structures.

Jake Christensen
Utah State Univ

Date submitted: 21 Sep 2017 Electronic form version 1.4