Abstract Submitted
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Calculating the titanium α to β transition using tight-binding molecular dynamics: a comparison of methods[1] JON WILLIAMS, DANIEL FINKENSTADT, U.S. Naval Academy, A. SHABAEV, George Mason University, N. BERNSTEIN, S.G. LAMBRAKOS, M.J. MEHL, U.S. Naval Research Laboratory — In this we analyze the Titanium phase transition between HCP and BCC structures. Tight-Binding Molecular Dynamics Simulations were run with 64 and 216 atom lattices over temperatures ranging from 50 to 1500 K. Analysis of the data included the phonon Density of States, time evolution of the lattice structure and temperature, and the Vibrational Free Energy of the system. We also develop a theoretical model of the transition based on a perturbation in the Harmonic Oscillator using the coherent states representation. In addition to the tight-binding simulations, we use density functional theory with variable cell shape molecular dynamics at a range of temperatures to study the transition. Direct simulations shows the transition between the two structures, and we investigate the use of constrained simulation to calculate their free energy differences.

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