MSE SEMINAR

March 31, 2017
113 McBryde Hall
3:30 – 4:30 PM
Refreshments at 3:00 PM

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"Calculated thermal expansion from intrinsic quantum thermodynamics"

ABSTRACT

Mechanics and equilibrium thermodynamics are powerful scientific disciplines that overlap in computational materials science. However, there are well-known conceptual incompatibilities between the two frameworks that arise from their different origins. Intrinsic Quantum Thermodynamics (IQT) is one intriguing approach to reconcile the incompatibilities. We demonstrate the use of IQT to estimate the thermal expansion of face-centered-cubic silver not only at stable equilibrium states but also along a path from non-equilibrium to stable equilibrium states. The eigenstructures (eigenvalues and eigenfunctions) of anharmonic oscillators determined from band calculations were employed to determine the temperature dependence of the lattice parameter of Ag. The thermal expansion of Ag calculated using two different exchange-correlation functionals was in good agreement with experimental values. Analysis of the pair interaction potential derived from the band calculations allowed us to infer the origin of errors in the thermal expansion calculation.

BIOSKETCH

Ryo Yamada is a PhD student in Materials Science and Engineering at Virginia Tech. He received a B.S. in Materials Science and Engineering from Hokkaido University in 2013 and an M.S. in Materials Processing from Tohoku University in 2015. In his bachelor's program he worked on experimental determination of ternary phase equilibria in the Mg-Zn-Y system, and his master's program he studied theoretical calculations of phase equilibria, phase transformations, and thermal expansions in various alloy systems using Density Functional Theory, Cluster Variation Method, or Path Probability Method. Now he is working on applications of Intrinsic Quantum Thermodynamics to solid-state systems.