MSE SEMINAR

March 23, 2018
113 McBryde Hall
3:30 – 4:30 PM
Refreshments at 3:00 PM

Ryo Yamada

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"Phase Separation and Ordering in FCC Solid Solutions Using Steepest-Entropy-Ascent Quantum Thermodynamics"

Abstract:

Phase separation and ordering are decomposition processes observed in many metallic alloy systems. The states of a system during decomposition are usually modeled with temperature-dependent state functions, like free energy, despite the fact that temperature is not strictly defined for systems far from equilibrium. An intriguing approach for exploring non-equilibrium phenomena is Steepest-Entropy-Ascent Quantum Thermodynamics (SEAQT), in which a kinetic path from an initial non-equilibrium state to a stable equilibrium is determined from an equation of motion and the postulate that the state of a system follows the direction of steepest-entropy-ascent. In this work, the SEAQT model is applied to decomposition processes in an FCC solid solution. An interesting feature of the SEAQT approach is that it describes both continuous and discontinuous decomposition mechanisms within the same framework. In addition, for some interaction energies and initial conditions, it predicts kinetic pathways that have characteristics of both phase separation and ordering.

Biosketch:

Ryo Yamada is a PhD student in the Materials Science and Engineering Department 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 expansion in various alloy systems using Density Functional Theory, Cluster Variation Method, and Path Probability Method. Now he is working on applications of Steepest-Entropy-Ascent Quantum Thermodynamics to solid-state systems.