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Generating Energy Landscapes for Quantum Thermodynamic Applications

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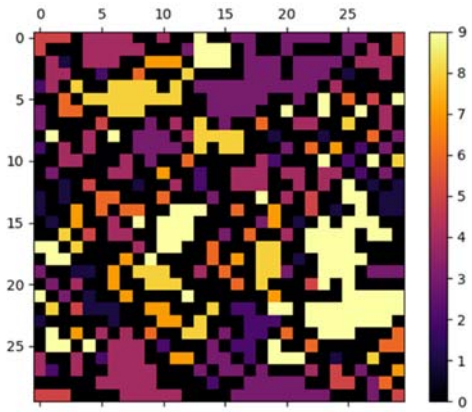
Abstract

Kinetic Monte Carlo and similar models are widely used in the discipline of computational material science, though the models are not without their downsides. Specifically, the Monte Carlo models can require significant computational time to reach equilibrium and necessitate recalculation for the slightest changes in temperature. Intrinsic Quantum Thermodynamics stands as an intriguing method to model non equilibrium phenomena to determine the kinetic path of a Monte Carlo model from an initial non equilibrium state to the stable equilibrium state of the system. However, to obtain the necessary information for each individual state of the discrete system, rigid and time-consuming techniques like Monte Carlo sampling would need to be employed. Recent advancements have seen the rise in Wang Landau and Replica Exchange Wang Landau as efficient methods of calculating the necessary parameters of a multitude of discrete systems, also. Thus, in this work the prior mentioned algorithms will be used to model the thermodynamic state evolution of sintered systems. Additionally, several characteristic descriptors will be calculated for each state: grain size, # of grain boundaries, and # of surface boundaries, in order to chose representative lattices to directly tie the state space evolution to a modeled lattice.



Biography

Jared McDonald received his bachelor's degree in Material Science and Engineering from Virginia Tech in 2018. He is currently working towards his Ph.D. in Material Science and Engineering with Dr. William Reynolds in tandem with Dr. Michael von Spakovsky from the Mechanical Engineering Department and is expected to graduate in 2023. He is currently working on applying Dr. von Spakovsky's Steepest Entropy Ascent Quantum Thermodynamic Framework to a variety of material systems. Specifically, to model sintering of metallic and ceramic materials using models derived from Kinetic Monte Carlo systems.