Mechanical Engineering Thesis Defense

Atomic-Scale Simulations of Si-Ge-Sn Alloys Using Deep-Learning-Based Interatomic Potentials

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Abstract

Accurate knowledge and understanding of thermal conductivity is very important in a wide variety of applications both at microscopic and macroscopic scales. Estimation, however, varies widely with respect to scale and application. At a lattice level, calculation of thermal conductivity of any particular alloy require very heavy computation even for a relatively small number of atoms. This thesis aims to run conventional molecular dynamic simulations for a particular supercell and then employ a machine learning based approach and compare the two in hopes of developing a method to greatly reduce computational costs as well as increase the scale and time frame of these systems. Conventional simulations were run using interatomic potentials based on density function theory-based ab initio calculations. Then deep learning neural network based interatomic potentials were used run similar simulations to compare the two approaches.

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Zoom Link: https://asu.zoom.us/j/89187086932