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Ph.D. DISSERTATION DEFENSE

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School/Department: Mechanical Engineering
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Title: THERMAL TRANSPORT IN SOLID MATERIALS FROM PERFECT CRYSTALS TO DISLOCATIONS BASED ON A MACHINE LEARNING METHOD

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ABSTRACT

Thermal transport properties are essential for sustainable energy and thermal management. For solid materials, thermal conductivity is an important property which denotes the ability of heat conduction. Without high cost and tedious preparation for experimental measurements, simulation methods become more and more popular with the development of computing power. However, the simulation of thermal conductivity is still limited by the huge computational cost and accuracy issues. Also, the broad existence of defects reduces thermal conductivity, making it important to thermoelectric applications, whereas accurate simulations of such defective effects are still lacking. This dissertation aims to study the thermal conductivity of materials from perfect crystals to defective structures with the machine learning assisted method. This method achieves a new balance between computational cost and accuracy through machine learning algorithms by combining two most widely used thermal property simulations: first-principles calculation and molecular dynamics (MD) method.

In this dissertation, we constructed potentials using the Gaussian Approximation Potential (GAP) method for cubic boron nitride (cBN). The constructed potential was used to study mechanical and thermal properties of perfect cBN crystal and the effect of isotopic defect. The results matched well with experimental measurements. For linear defects, the similar approach was applied to construct potentials for single screw dislocation and Eshelby twist in silicon nanowires. Equilibrium molecular dynamics (EMD) and non-equilibrium molecular dynamics (NEMD) simulations were applied for the calculation of thermal conductivity in dislocated structures. Reductions on thermal conductivity due to dislocation and twist were shown in results. For planar defects, we studied the phonon scatterings by the grain boundaries using first-principles calculation with empirical equations regarding boundaries as arrays of edge dislocations. The results revealed the dependency of phonon frequency in different regions and the effect of grain size on thermal conductivity. We also conducted experiments to measure the lattice thermal conductivity of nanocrystalline silver selenide using 3ω method. A large reduction in the lattice thermal conductivity was shown.