

The Department of Mechanical Engineering presents:

The Ph.D. Dissertation Defense of Qingan Cai

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Effects of Temperature and Pressure on the Lattice Dynamics in Tungsten Diselenide

Doctor of Philosophy, Graduate Program in Mechanical Engineering University of California, Riverside, September 2022 Dr. Chen Li, Chairperson

Tungsten Diselenide (WSe₂), one valuable member of transition metal dichalcogenides, has attracted intensive attentions and emerged as promising candidates for advanced applications as field-effect transistors and light-emitting diodes. Understanding the microscopic lattice dynamics is essential for regulating the thermal properties of WSe₂ to enhance the functionality and stability of WSe₂-based devices. Here, by combining inelastic X-ray scattering and first-principles calculations, the lattice dynamics of WSe₂ was investigated comprehensively. We performed the first measurements of the temperature-dependent phonon dispersions and the mode Grüneisen parameters of bulk WSe₂, which are found to be in better agreement with the calculations on the monolayer system than those of the bulk. This observation indicates that lattice dynamics in bulk WSe₂ hold the characterization of monolayers. We also performed the high-pressure IXS measurements on acoustic phonon in bulk WSe₂ and observed the significant pressure-induced phonon stiffening. The pressure-dependent lattice dynamics are very useful to study the strain effects on the van der Waals interactions and anisotropic thermal conductivity in layered materials.