ABSTRACT

Title of Dissertation: PHONON MEDIATED THERMAL TRANSPORT IN TRANSITION METAL DICHALCOGENIDES

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Transition metal dichalcogenides (TMDCs) have attracted extensive interests due to outstanding electronic, optical, and mechanical properties, thus are highly promising in nanoelectronic device applications. However, comprehensive understanding of phonon mediated thermal transport in TMDCs is still lacking despite the important roles they play in determining the device performance. The topics requiring further explorations include the full Brillouin zone (BZ) phonons, temperature dependence of thermal properties, and structural-thermal relations of TMDCs. In determining above phonon transport characteristics, the anharmonic effect plays a central role.

In this thesis, we present studies on the phonon properties of two TMDC materials, namely MoS_2 and HfS_2. In the first study, effect of folding on the electronic and phonon transport

properties of $SLMoS_2$ are investigated. The atomic structure, ground state electronic, and phonon transport properties of folded $SLMoS_2$ as a function of wrapping length are determined. The folded structure is found to be largely insensitive to the wrapping length. The electronic band gap varies significantly as a function of the wrapping length, while the phonon properties are insensitive to the wrapping length. The possibility of modulating the gap values while keeping the thermal properties unchanged opens up new exciting avenues for further applications of MoS_2.

In the second study, we examine the temperature dependent phonon properties of HfS_2 under two different assumptions - the quasi-harmonic approximation (QHA) and fully anharmonic approximation (FAA). Under the QHA, the commonly known 1T phase is considered and full BZ phonon properties are investigated. We show that ZA phonons alone are responsible for 80% of the thermal transport - both in-plane and c-axis. The cause is the uncommonly strong c-axis VDW interactions relative to its in-plane interactions. Under the FAA, a new lattice configuration ABC - which is featured by a different staking order between adjacent layers compared to the 1T phase - is discovered. As a result, all the temperature coefficients of lattice parameters and phonon frequencies change at room temperature. These results are validated by good agreement with the experimentally measured temperature dependent out-of-plane (A_{1g}) and in-plane (E_g) frequencies, and lattice parameters. The anharmonic effect is the dominant mechanism leading to the phase change at room temperature.