Experimental and Computational Investigation of Layer Dependent Thermal Conductivities and Interfacial Thermal Conductance of 1- to 3-Layer WSe_2

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Atomically thin materials such as graphene and semiconducting transition metal dichalcogenides (TMDC) have attracted extensive interest in recent years, motivating investigation into multiple properties. In this work, we used the opto-thermal Raman technique to measure the thermal transport properties of a popular TMDC material tungsten diselenide (WSe_2), in single-atomic layer (1L), bi-layer (2L), and tri-layer (3L) forms. We implemented more direct measurements of the 1L-3L WSe_2 under study and discovered WSe_2's absorption coefficient from the measurements. In addition, by comparing the response of 1L-3L WSe_2 using different laser spot sizes, we are able to obtain the lateral thermal conductivity of 1L-3L WSe_2 and the interfacial thermal conductance to the substrate. We also implemented full-atom nonequilibrium molecular dynamics simulations (NEMD) to investigate thermal conductivities of 1L-3L WSe_2 computationally to provide comprehensive evidence and confirm the experimental results. The trend of layer dependent lateral thermal conductivity and interfacial thermal conductance of 1L-3L WSe_2 is discovered. For 1L-3L WSe_2, the room-temperature thermal conductivities are 36 ± 12, 23 ± 11, and 18 ± 5 W/(m·K), respectively. Crucially, the interfacial thermal conductance of 1L-3L WSe_2 is found to be 2.89 ± 0.45, 3.55 ± 0.51, and 3.56 ± 0.46 MW/(m2·K), with a flattened trend starting the 2L, a finding that has important implications for thermal management design and modeling of electronic devices.