Doctoral Dissertation Defense

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Atomic Scale Study of Thermal Properties using STEM/EELS and First-Principles Calculations

As predicted by Moore's Law, the density of transistors has doubled every two years which was contributed significantly to the miniaturization of electronic devices. When the dimensions of a transistor approach the single-atom limit, as in devices consisting of two-dimensional materials, including graphene, transition metal dichalcogenides (TMDs) and their heterostructures, such miniaturization offers remarkable improvements in electrical performance. However, heat dissipation and thermal expansion mismatch can cause problems in designing electronic devices based on two-dimensional materials. Therefore, the nanoscale thermal properties are an important subject of current research in two-dimensional materials, and, correspondingly, new methods are needed for temperature measurements and thermal property measurements at nanometer scale. In my thesis, I have developed a novel method for measuring local temperature and the thermal expansion coefficient of two-dimensional materials, using a combination of scanning transmission electron microscope (STEM), electron energy loss spectroscopy (EELS) and first-principles calculations.

During my Ph.D. research, I have explored the temperature-dependent plasmon energy shift as measured by low-loss EELS and utilized it to predict the local temperature in combination with atomic-resolution STEM images. These experimental results are used to perform first-principles calculations to determine the thermal expansion coefficients of different two-dimensional materials (graphene, MoS_2, $MoSe_2$, WS_2, WSe_2) in different thickness were determined. I also utilized alloying engineering of TMDs to explore the effects of defects to control the thermal expansion behavior of materials. Using the same thermal expansion measurement methods performed on pure TMDs, the thermal expansion coefficients of the TMD alloys ($Mo_{1-x}W_xS_2$) in different alloying concentrations were determined. I find that the thermal expansion coefficients of alloyed TMD are reduced due to the interference from the additional substitutional atoms on the lattice expansion. This provides a control over the thermal expansion coefficients and presents great potential to eliminate the thermal expansion mismatch problem in the electronic devices. The future research on thermal expansion and thermal transport properties across the in-plane hetero-interface of TMDs will be discussed.