New Approaches to Relating Structure and Function using Analytical Transmission Electron Microscopy

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Two-dimensional materials, including graphene, BN and transition metal dichalcogenides (TMDs), exhibit great potential for a variety of applications, such as transistors, spintronics, or photovoltaics. [1-2] When 2-dim materials are used in electronic devices, the potential for miniaturization offers remarkable improvements in electrical performance. Yet, controlling the heat flow across a hetero-structure will be crucial to developing high-speed electronic devices based on 2-dim materials. We have recently shown that the thermal expansion coefficient (TEC) dramatically increases in 2-dim materials when the thickness of the material shrinks from bulk to a few monolayers.[3] Therefore, the TEC mismatch of 2-dim materials becomes an additional concern in designing electronic nano-devices. More specifically, we need to develop methods that enable us to control and tailor the TEC of TMDs through alloying or defect engineering.

In this contribution, we will utilize atomic-resolution imaging and electron spectroscopy in an aberration-corrected scanning transmission electron microscope (STEM) to characterize the thermal properties of 2D materials, including pristine and allowed transition-metal dichalcogenides. Specifically, we will use the aberration-corrected JEOL ARM200CF at the University of Illinois at Chicago, equipped with a cold-field emission electron source and a Gatan Continuum GIF. Specifically, we will measure the thermal expansion coefficient of monolayer $Mo_{1-x}W_xS_2$ materials with $0 \leq x \leq 1$ using our plasmon-EELS based approach.[3] Various 2D materials are heated up to 700 K in our ProtoChips Aduro double-tilt stage and high-resolution imaging and EEL spectroscopy are performed on single layer particles. The experimental data is then compared to our first-principles modeling results, based on special quasi-random structures, as well as structures directly extracted from the high-angle annular dark-field (HAADF) images of alloyed TMDs. In-situ heating experiments will also be conducted to test the effects of temperature and strain on phase separation in alloyed TMDs.

We will further highlight other examples where atomic-resolution in-situ, multi-modal characterization and first-principles modeling are used to unravel the fundamental structure-property relationships of materials with potential applications in high-efficiency photovoltaic, rechargeable batteries or high-power/frequency electronic devices.

References:

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[4] This work was supported by the National Science Foundation (EFMA-1542864 (EFRI), DMREF CBET-1729420) and DMR-1831406).