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In situ Materials Characterization of 2-Dim Materials at High Energy and Spatial Resolution

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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.

Figure 1 show several HAADF images of $Mo_{1-x}W_xS_2$, where the heavier W atoms can be clearly identified as the brighter image contrast. The shift of the plasmon peak is then measured as a function of temperature in these materials, while the corresponding shift as a function of lattice parameter is calculated using DFT calculations in the random phase approximation (RPA). Combining the experimental and modeling data, we can now predict the TEC for the $Mo_{1-x}W_xS_2$ alloys, as show in Figure 2. It is interesting to note here that the thermal expansion coefficient appears to be largest in the $Mo_{0.5}W_{0.5}S_2$ samples and appears independent of the structural model used.

We will also explore the thermal stability and thermal expansion behavior of other TMD alloys, such as $Mo_{1-x}V_xS_2$. First-principles modeling suggests that the formation of an alloy requires moderate synthesis temperatures. The phase stability, structural stability as well as the atomic structure of 2-d particles edges in $Mo_{1-x}V_xS_2$ will be explored during in-situ heating experiments and compared to our DFT models. These results will lead to more accurate model for predicting stable TMD alloy structure with novel electronic and electro-chemical properties [4].

References:

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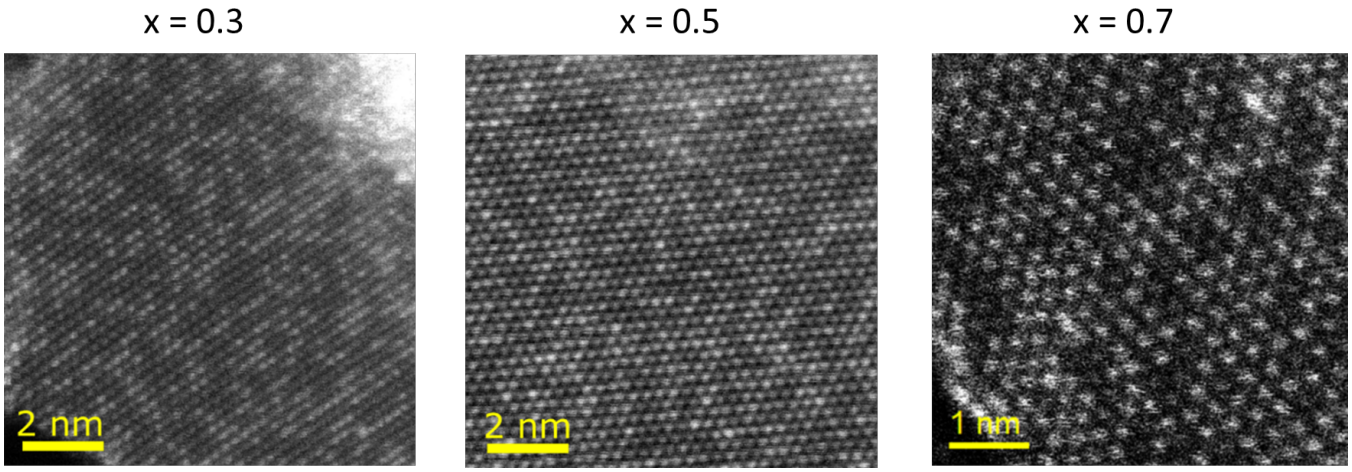

Figure 1. Atomic-resolution images of monolayer $Mo_{1-x}W_xS_2$ at 300 K.

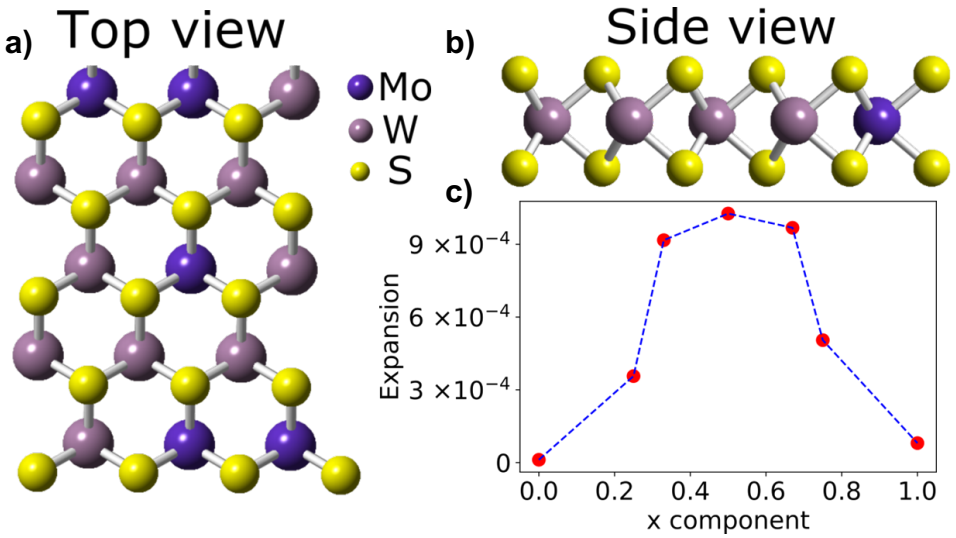

Figure 2. Special quasi-random structure a) top view and b) side view used to calculate the thermal expansion coefficient in $Mo_{1-x}W_xS_2$ below 700 K.

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