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Nanoscale Thermometry for 2D Materials

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Two-dimensional materials, including graphene, transition metal dichalcogenides (TMDs) and their heterostructures, exhibit great potential for a variety of applications, such as transistors, spintronics, and photovoltaics.[1-3] While the miniaturization offers remarkable improvements in electrical performance, heat dissipation can be a problem in designing electronic devices based on two-dimensional materials. Therefore, the thermal properties of these materials are an important subject of current research in two-dimensional materials, and, correspondingly, new methods are needed for temperature measurements at nanometer scale. Here, we present a method for measuring local temperature in two-dimensional materials, using a combination of scanning transmission electron microscope (STEM) and electron energy loss spectroscopy (EELS).

Specifically, we prepared a set of different free-standing two-dimensional material samples including graphene, MoS_2, $MoSe_2$, WS_2, and WSe_2, through a liquid phase exfoliation and drop casting method. In-situ heating experiments are combined with low-loss EEL acquisition at 8 different set temperatures (T=373K, 423K, ..., 723K at 50K per step) for each sample and the shift in the plasmon peak is correlated to the sample temperature. A typical TMD nanoflake (WS_2) on a holey-carbon support is presented in Fig. 1A. This nanoflake has regions of several different thicknesses, labelled (I-V), and is suspended over vacuum. As the thickness must be taken into account when computing the plasmon peak shift, the relative thicknesses are calculated using the low-loss EELS signal log-ratio method. The resulting distribution of the thickness is shown in Fig. 1B. The thickness distribution was fitted using Gaussian functions, and five distinct peaks are identified representing the number of layers in each region. The strong linear relationship between the peak centers and the relative ratios in Fig. 1C shows that the five areas (I-V) are 2-6 layers thick.

The temperature is extracted from the low-loss EELS spectra after accounting for the sample thickness. A representative low-loss EEL spectrum for single layer MoS_2 suspended over vacuum at 373 K is shown in Fig. 2. The plasmon peak for 2D materials is more complicated compared to bulk metals. We identified two distinct peaks *a* and *b* (around 7 eV and 20 eV) which stem from the π and $\pi + \sigma$ bonding. The second peak can be deconvoluted into two peaks (a main peak *b* near 20 eV and a shoulder *c* near 13 eV). Since fitting the main peak provides better accuracy than the shoulder peak, we mainly consider the major peak. As the temperature of the MoS_2 sample is increased, a redshift occurs for the main peak. This temperature dependent plasmon energy shift can be used to map the temperature by tracking the plasmon peak center. Similar phenomena are observed and applied for other TMDs. However, graphene behaves quite differently, with a blueshift in the center of the main peak. Since the plasmon energy shift can be explained by the change of density of valence electron from the thermal expansion, this confirms that the plasmon peak energy shift is tied to the thermal expansion, which is negative for graphene. We apply density functional theory (DFT) with the random phase approximation (RPA) using the Vienna Ab-initio Simulation Package (VASP) to explore the relation between the plasmon energy shift and thermal expansion. Using first-principles calculations in conjunction with our measurements, we are able to measure both temperatures and the thermal expansion coefficients of graphene and single-layer TMDs. Using theory and extrapolating from the single layer measurements, we find a good agreement with the literature data for bulk TMDs[4] [5].

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Figure 1:

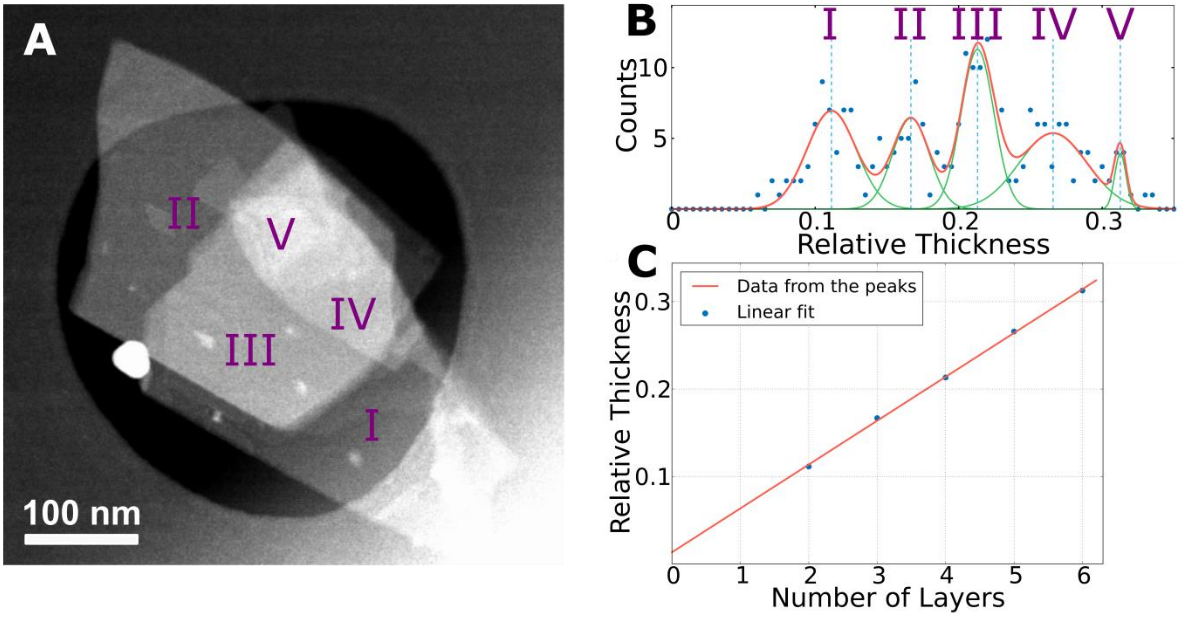

Figure 1. A) Z-contrast image of a WS_2 nanoflake consisting of five regions (I-V) of different thickness. B) The distribution of the thickness with fit curve fits for each location. C) A linear fit of the peak centers confirming the number of layers.

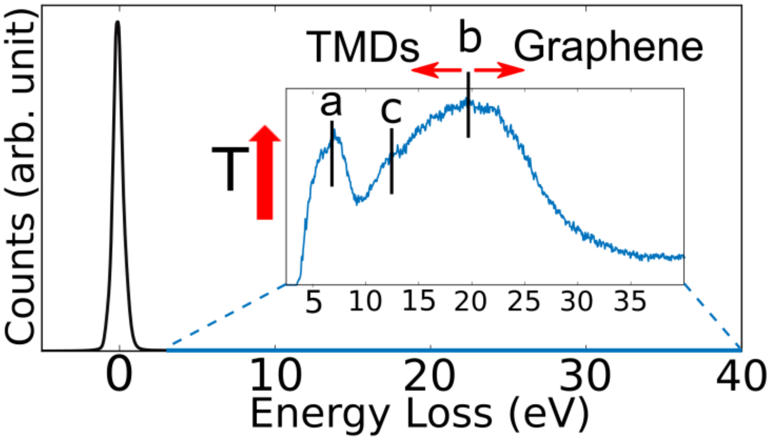

Figure 2. A low-loss EELS of single layer MoS_2 presenting the zero-loss peak and plasmon peaks (*a*-*c*). When temperature (T) increases, for the plasmon mode *b*, there is a redshift for TMDs and a blueshift for graphene.