Understanding High Contact Resistance in MoS_2 FETs Using STEM-EELS

Wu, R.[1] and Mkhoyan, K.A.[2]

[1] University of Minnesota, United States, [2] University of Minnesota, United States

TMDs, with chemical formula MX_2, where M is a group IV, V, or VI transition metal and X is the chalcogenide, is a sub-group of materials with highly tunable properties within the family of van-der-Waals bonded 2D materials [1]. This tunability has led to increasing applications for TMDs, particularly in electronics and optoelectronics devices, most notably MoS_2 as channels in ultra-thin FETs. However, a major obstacle in realizing MoS_2 channel FETs is the high contact resistances measured across the metal contact and semiconducting MoS_2 channel, which severely limits electron injection from the metal [3]. The origins of this resistance continue to be a topic of scientific debate because our understanding of the MoS_2 atomic and electronic structure at and near the metal contact interface remains muddled.

In this work, we report the interactions of the metal-MoS_2 interface within FETs as observed directly using atomic resolution scanning transmission electron microscopy (STEM) and present their effects on FET performance. Following device fabrication and performance measurements, functioning FETs embedded with MoS_2 are thinned using an FEI Helios G4 FIB, and, subsequently, analytical TEM is performed using an aberration corrected FEI Titan G2 60-300 S/TEM.

Annular dark field (ADF)-STEM imaging is used in conjunction with electron energy loss spectroscopy (EELS) to show that strong covalent bonding between Ti, a metal commonly used for FET contacts, and S dramatically alters the atomic and electronic structure of the topmost MoS_2 layer as shown in Figure 1. Furthermore, EELS acquired layer-by-layer also suggest that the electronic structure of MoS_2 layers further from the interface may also be affected by the possible diffusion of metal atoms, a phenomenon further supported and explained by density-functional-based calculations. In contrast, similar analysis on FETs with In/Au alloy contacts show an atomically sharp interface between the contact and MoS_2, as shown in Figure 2, and explains the markedly different contact resistance and overall device performances measured between the two FETs with distinct metals. These results show that the properties of the metal used as the contact can greatly affect the performance of the 2D material device and must be tailored to the specific 2D material in order to optimize device performance.

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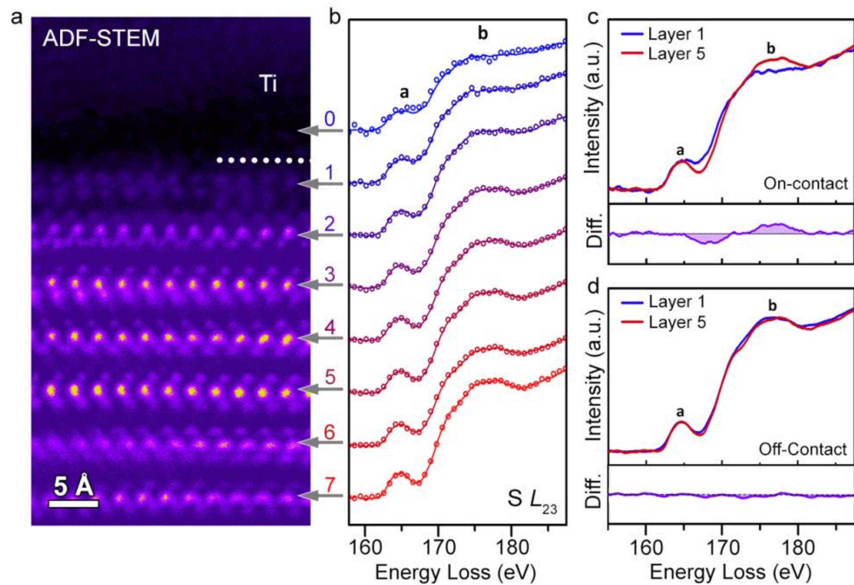

Figure 1:**STEM-EELS of the Ti-MoS_2 interface in a FET**. (a) ADF-STEM image of the Ti-MoS_2 interface within a FET in which the topmost layer of MoS_2 appears visibly altered compared to underlying layers. (b) S L_{23} edge measured using EELS at each layer of MoS_2. Changes in the S partial-DOS can be seen in features a and b. (c) comparison of S L_{23} edge at layer 1 and layer 5 of MoS_2 for a region of MoS_2 in contact with Ti. (d) similar comparison for a region of MoS_2 away from contact with Ti. Differences in the spectra are observable above noise in (c) but not in (d)

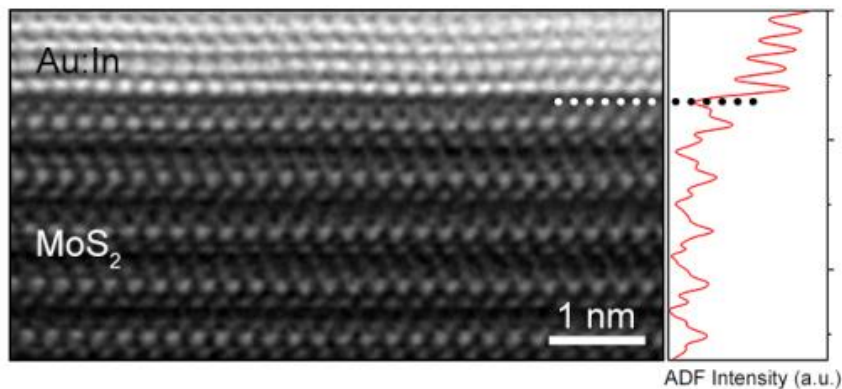

Figure 2: STEM of the Au:In-MoS_2 interface in a FET. (left) ADF-STEM image of the interface between MoS_2 and an Au:In alloy electrical contact in a FET. (right) Line scan of the ADF intensity across the interface. The position of the interface is denoted by the dotted lines.