Kosuke Nagashio
The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8654, Japan

nagashio@material.t.u.tokyo.ac.jp

Full energy spectra of interface states density for *n*- and *p*-type MoS_2 field effect transistors

Two-dimensional (2D) layered materials are promising for replacing Si to overcome the scaling limit of recent ~5 nm-length metal-oxide-semiconductor field-effect transistors (MOSFETs). However, the insulator/2D channel interface severely degrades the performance of 2D-based MOSFETs, and the origin of the degradation remains largely unexplored. Although the dangling-bond-free surface of the layered channel is expected to ideally provide an electrically inert interface, there are many reports on the wide range of interface state densities (D_{it}) from 10^{11}~10^{13} $eV^{-1}cm^{-2}$ for high-*k* top gate MoS_2 FET in reality, which must be reduced to improve the device performance. To date, several physical origins for D_{it} have been proposed, which are summarized in **Figure 1a**. First, trap (I) represents the defects and impurities in the MoS_2 channel. Sulfur vacancies (V_S) with the high density of ~10^{13} cm^{-2} are widely recognized in mechanically exfoliated (ME) and chemically vapor deposited (CVD) MoS_2 [1]. These introduce defect states in the band gap, as shown in **Figure 1b**, which has been evaluated by density functional theory (DFT). Second, trap (II) represents the traps in the high-*k* insulator. In general, the back SiO_2 oxide is formed by thermal oxidation with well-controlled quality, which usually shows an extremely low trap site density inside (~10^{10} cm^{-2}). On the other hand, the top high-*k* oxide is typically formed on the inert MoS_2 surface by atomic layer deposition (ALD) at a relatively low temperature with the aid of a buffer layer, which may introduce many traps inside. The traps close to the interface serve as quick traps while the traps inside the oxide serve as slow traps, as discussed in several reports [2]. Third, trap (III) represents the strain in MoS_2 induced externally. One of the interesting properties of 2D materials is that they can be scaled down to atomic thickness. Strain is easily induced in a thin MoS_2 channel by both substrate surface roughness and/or the high-*k* deposition process, resulting in Mo-S bond bending [3,4] Since the conduction and valence bands of MoS_2 are mainly composed of the energy splitting of the Mo *d* orbital, the band tail states will be easily introduced, as schematically illustrated in **Figure 1b**.

Although several issues on interface properties are discuseed as described above, a common understanding of the origin for the interface states has not yet been obtained. Here, we present a systematical study of the interfacial properties of both *n*- and *p*- MoS_2 FETs with a wide thickness range, from monolayer to bulk, and various gate stack structures, including a 2D heterostructure with *h*-BN as well as typical high-*k* top gate structure. Full energy spectra of the interface state densities (D_{it}) are extracted by modeling *I*-*V* characteristics with including carrier statistics through quantum capacitance and carrier transport through the Drude model, as shown in **Figure 1c**. For *n*-MoS_2, D_{it} around the mid gap was drastically reduced to 5×10^{11} $cm^{-2}eV^{-1}$ for the heterostructure FET with *h*-BN from 5×10^{12} $cm^{-2}eV^{-1}$ for the high-*k* top-gate MoS_2 FET. It is elucidated that the strain induced externally through the high-*k* deposition process is the dominant origin of the interface degradation which is further enhanced in response to the degree of initial surface roughness. Therefore, the strategy to obtain the sharp switching for *n*-MoS_2 FETs is to develop stress-free high-*k* deposition while maintaining the atomic flatness for the substrate surface. On the other hand, for *p*-MoS_2, a niobium (Nb)-doped *p*-type MoS_2 crystal was studied here, since the substitution of Mo site by Nb (Nb_{Mo}) is thermodynamically stable. Even for the heterostructure FET, D_{it} remained high, ~10^{13} $cm^{-2}eV^{-1}$, for *p*-MoS_2.

Although Nb_{Mo} also introduces shallow defect states on the VB side in *p*-type MoS_2, as shown in **Figure 1b**, the density of V_s (~10^{13} cm^{-2}) is much larger than that of Nb_{Mo} (~10^{12} cm^{-2}) in atomically thin MoS_2, which indicates that V_S could be the dominant origin of the degraded hole transport. To improve the hole transport, continued efforts to improve the crystallinity are required. Finally, based on the recent understanding, the perspective on 2D electronics will be discussed.

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References

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Figures

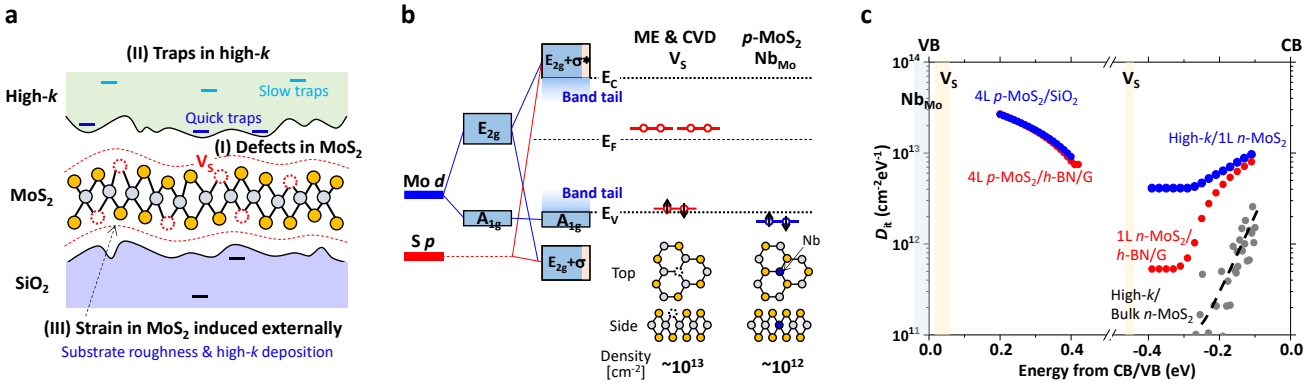

Figure 1: (a) Schematic illustration of different origins of interface states in high-*k*/MoS_2/oxide structures. (b) Schematic bonding diagram showing how the local orbitals on Mo and S interact to form CB, VB, and interface states in MoS_2. V_S and Nb_{Mo} indicate the sulfur vacancy and the substitution of Mo site by Nb, respectively. (c) The full energy spectra of D_{it} for different gate stack structures. Notice that the band gaps of 1L, 4L, and bulk MoS_2 are different. Therefore, the transverse axis for the D_{it} - energy distribution is shown as the energy from the CB/VB edge. For the high-*k*/bulk *n*-MoS_2 interface, D_{it} is extracted from frequency dispersion-free *C*-*V* curves by the Terman method. The bulk MoS_2 thickness is ~ 58 nm, which is larger than W_{Dm}, supporting the availability of the *C*-*V* measurement.