Quantum-mechanical effects in atomically thin MoS_2 FET

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1. Introduction

C-V measurement is the powerful tool to gain further insight into the device physics of 2D materials. We have successfully measured quantum capacitance (C_Q) in monolayer MoS_2 FET[1]. C_Q is originally derived from the finite DOS of a 2D electron gas and Fermi distribution. With increasing channel thickness, the electron distribution in the finite channel thickness should contribute to the total capacitance (C_{total}). Here, we discuss thickness dependence of quantum-mechanical effects in MoS_2 FET.

2. Results & Discussion

ALD-Al_2O_3 (10 nm) top gated MoS_2 FET with different channel thickness are fabricated through the mechanical exfoliation on the quartz substrate. **Fig. 1** shows the experimental C_{total}-V_{TG} curves at 1 MHz of monolayer, trilayer, 10-nm and 84-nm thick MoS_2, respectively.

2.1 Accumulation region Two distinct features are observed by increasing the MoS_2 thickness. Monolayer *C-V* shows higher saturation capacitance and sharper change than thicker MoS_2 case. To understand these behaviors, the quantum-mechanical model was considered by solving Poisson equation and Schrödinger equation self-consistently. Calculated square modulus of wave functions $|\psi|^2$ for lowest subband with different MoS_2 thickness are shown in **Fig. 2**. At thick MoS_2 (>tetralayer), the centroid of wave function is confined in the triangle potential formed in the channel by electrical field, which leads to the negligible thickness dependence. While at MoS_2 (<tetralayer) thinner than the triangle potential, the centroid of wave function is confined in the potential wall formed by the atomic channel thickness itself. This quantum-mechanical effect forces electron distribution to locate away from Al_2O_3/MoS_2 interface. This reduces C_{total} at strong accumulation region because C_{total} is expressed as $1/C_{ox} + l/\varepsilon_{MoS2}$, where l is the distance between centroid wave function and interface. Calculated C_{total} at strong accumulation as a function of MoS_2 thickness is shown in **Fig. 3**. When EOT = 1 nm, the decrease of C_{total} is as high as 20 % in multilayer case. The use of monolayer MoS_2 is highly demanded in order to increase accumulation C_{total} especially at low EOT case.

2.2 Depletion region Since the parasitic capacitance is totally removed by using the quartz substrate, the minimum capacitance plateau observed for 84-nm thick MoS_2 results from the contribution of depletion capacitance (C_D) with the maximum depletion width (W_{Dm}). W_{Dm} is determined to be ~48-55 nm by thickness dependence measurement[2]. As a result, the undepleted MoS_2 layer will always remain, which results in residual conductance and low I_{ON}/I_{OFF} in *I-V*. N_D is determined to be 2~3×10^{17} cm^{-3} from W_{Dm}, which indicates the intrinsically-existed S vacancy concentration.

W_{Dm} for various 2D materials are summarized here as a function of N_D (N_A), as shown in **Fig. 4**. At high N_D (N_A) region (>10^{19} cm^{-3}), W_{Dm} will decrease substantially, resulting in a small thickness window for "fully controlled band transport". Full control of channel will be lost when the 2D thickness become greater than W_{Dm}. This explains why well-controlled FETs with high I_{ON}/I_{OFF} are difficult to achieve in recent heavily doped 2D materials such as PtS_2, $PtSe_2$, SnS, and SnSe. From the above analysis, well controlled doping approaches on 2D crystals are in great demand for positive control of FET performance.

Acknowledgements This research was partly supported by the JSPS Core-to-Core Program, A. Advanced Research Networks, & JSPS KAKENHI, Japan. **References** [1] N. Fang *et al.*, J. Phys. D 2018, **51,** 065110. [2] N. Fang *et al.*, ACS Appl. Mater. Interfaces 2018, **10,** 32355.

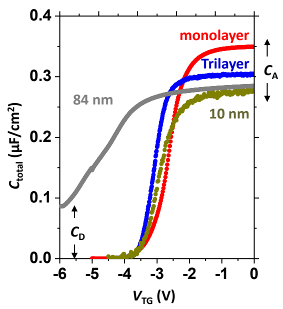

Fig. 1 C_Q-V_{TG} curves.

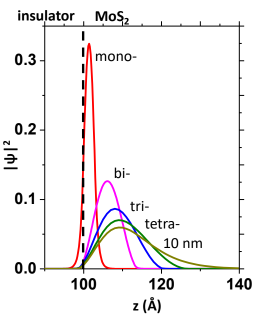

Fig. 2 Calculated $|\psi|^2$ of lowest subband .

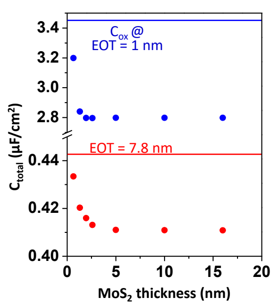

Fig. 3 Calculated accumulation C_{total} of MoS_2.

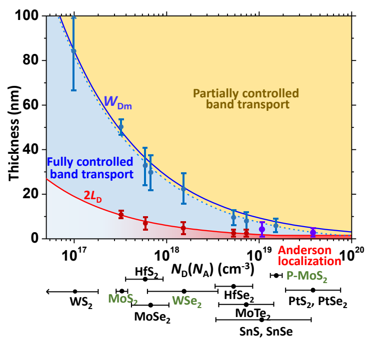

Fig.4 Thickness scaling rule of 2D-FETs. 2D in green are studied here.