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Full Length Article

Study of interfacial strain at the α-Al_2O_3/monolayer MoS_2 interface by first principle calculations

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ABSTRACT

With the advances in two-dimensional (2D) transition metal dichalcogenides (TMDCs) based metal–oxide–semiconductor field-effect transistor (MOSFET), the interface between the semiconductor channel and gate dielectrics has received considerable attention due to its significant impacts on the morphology and charge transport of the devices. In this study, first principle calculations were utilized to investigate the strain effect induced by the interface between crystalline α-Al_2O_3 (0001)/h-MoS_2 monolayer. The results indicate that the 1.3 nm Al_2O_3 can induce a 0.3% tensile strain on the MoS_2 monolayer. The strain monotonically increases with thicker dielectric layers, inducing more significant impact on the properties of MoS_2. In addition, the study on temperature effect indicates that the increasing temperature induces monotonic lattice expansion. This study clearly indicates that the dielectric engineering can effectively tune the properties of 2D TMDCs, which is very attractive for nanoelectronics.

1. Introduction

The semiconductor electronics industry is now facing serious challenges in promoting further down-scaling of device sizes and reduction of power consumption. In response to these challenges, alternative semiconductor materials have been proposed and developed to overcome the limitations of Si [1–5]. Low-dimensional nanostructures are attractive for applications in device channel in future ultimately small transistors since their atomic scale thickness offers efficient electrostatic control to suppress the short channel effects [6,7]. Graphene was known to have remarkable electrical and mechanical properties [7], including high carrier mobility high thermal conductance [8], and excellent stiffness [9]. However, the absence of intrinsic energy bandgap obstructs its further application in logic and memory devices which require high on-off ratio and low off-state current [10,11]. The monolayer of hexagonal MoS2 (h-MoS_2), as a typical member of TMDCs, has the intrinsic direct bandgap (Eg ~ 1.8 eV) [12,13]. This is very promising for application in future field-effect transistors (FETs) with excellent current on/off ratio (>10^8) [13,14]. Logic circuits and amplifiers based on monolayer MoS_2 have also been demonstrated recently [15,16], as well as saturation and high breakdown currents [17]. Also, the broken inversion symmetry induced by monolayer TMDCs endows itself with natural piezoelectricity, rendering it a promising candidate for applications in mechano-electric converter [18,19]. In addition, the ultrasensitive monolayer MoS_2 photodetector was further demonstrated with high photoresponsivity [20]. The novel and exciting field of MoS_2, which includes applications in quantum spin hall (QSH) effect and in the design of devices possessing both finite band-gap and high carrier mobility, are under study [21–23].

Although MoS_2 is promising for many applications, it is still facing challenges in industrially applicable devices. MoS_2 monolayer has low carrier mobility, about several tens of cm^2/Vs, in comparison to the conventional semiconductor silicon (~10^3 cm^2/Vs) [24] and 2D semimetal graphene (~10^4 cm^2/Vs) [7] at room temperature (RT). This inevitably limits its application in high-performance FETs [25,26]. Also, the carrier transport in these 2D monolayers is heavily affected by the scattering of the acoustic phonon via intra- and inter-valley deformation potential coupling [27,28]. This further reduces the electrical conductance at room temperature (RT). In addition, the large variation in electrical properties induced by doping and strain in MoS_2 monolayers can affect its applications in

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nanoelectronics [12]. Strain effect can be engineered to effectively improve the carrier mobility of MoS_2 monolayer [28]. Since MoS_2 can endure large strains before breaking, the modification of the MoS_2 band gap by applying strain becomes an important strategy to enhance the performance of nano-devices made from MoS_2 [29].

Large bandgap modulation of MoS_2 monolayer was theoretically predicted by h-BN/MoS_2 interface (0.5-0.8 eV) [30] and by MoS_2/WSe_2 hetero-stacking structure (0.30-0.89 eV) [31–34]. Although the amorphous Al_2O_3/MoS_2 interface only allows limited effect on bandgap of MoS_2, we expect that the crystal Al_2O_3/MoS_2 interface is capable of much larger bandgap modification. In this first principle calculation study, we thoroughly explore the strain effect and bandgap modification induced by the interface between α-Al_2O_3 (0001)/MoS_2 monolayer with the dielectric layers of various thickness. The study first investigates the interface with Al_2O_3 in 1.3 nm thickness in terms of the separation distance between Al_2O_3/MoS_2, the lattice parameter and the induced strain effect. Secondly, the study investigates the effect of various Al_2O_3 thickness on the electronic properties, i.e., electronic band structure and density of states (DOS). Lastly, the temperature effect that induces the thermal expansion is evaluated. Our study demonstrates the strain engineering of the dielectric interface on the 2D TMDCs semiconductor, which can significantly improve the carrier mobility and enhance the performances in MOSFET.

2. Methodology

In this study, first principle calculations were carried out by using the Virtual Nanolab Atomistix ToolKit (ATK) package with the density functional theory (DFT) [35]. The localized density approximation (LDA) exchange correlation with a double zeta polarized (DZP) basis was used with a mesh cut-off energy of 150 Ry [36]. All the atomic positions and lattice parameters were optimized by using the generalized gradient approximations (GGA) with the maximum Hellmann-Feynman forces of 0.05 eV/Å, which is sufficient to obtain relaxed structures [37]. The Pulay-mixer algorithm was employed as iteration control parameter with tolerance value of 10^5 [38]. The maximum number of fully self-consistent field (SCF) iteration steps was set to 1000 [36]. The electronic temperature is set to 300 K for our simulations before considering the temperature effect. The periodic boundary condition was employed along all the three directions in the hexagonal lattice [39]. The distance between neighboring interface is set to be 30 Å to minimize the interaction between them. Due to the large vacuum between the layers, the boundary condition no longer remains periodic along the vertical direction. The self-consistent field calculations were checked strictly to guarantee fully converging within the iteration steps [36].

Fig. 1 demonstrates the schematic of interface between 1.3 nm-Al_2O_3 (0001)and a MoS_2 monolayer. T_{Al2O3} denotes the thickness of the dielectric layer while D_i indicates the separation distance between Al_2O_3 and MoS_2, which is calibrated by the nearest vertical distance between Oxygen and Sulfur. The unit cell of the crystal with the hexagonal lattice is enclosed by the parallelogram shown in Fig. 1(a). This unit cell stems from merging together the unit cell of Al_2O_3 in repetition of 2×2 and MoS_2 monolayer by 3×3 [28,40]. The lattice mismatch between Al_2O_3 and MoS_2 monolayer is 1.2%. In this study, we investigate the strain effect from this interface by following steps: (a) set the thickness of Al_2O_3 to 1.3 nm and investigate the intrinsic separation between Al_2O_3/MoS_2; (b) investigate the evolution of the total energy of the unit cell vs. lattice parameter (L_c) and figure out the intrinsic L_c corresponding to the minimum total energy; (c) calculate the strain effect by comparison of L_c with the lattice parameter of MoS_2 monolayer (L_0): $\varepsilon = (L_c\text{-}3L_0)/3L_0$; and (d) investigate the strain effect by varying the thickness of dielectric layer to 1.3 nm, 2.6 nm, 3.9 nm and 5.2 nm.

3. Results and discussion

Fig. 2 explores the intrinsic lattice parameter of this interface. Fig. 2(a) demonstrates the evolution of the total energy of the unit cell with the separation distance between MoS_2 and Al_2O_3. It exhibits the intrinsic separation distance of 2.4 Å if the thickness of dielectric layer is fixed to 1.3 nm. Fig. 2(b) indicates the evolution of the total energy of the unit cell with L_c. As shown the intrinsic L_c is 9.51 Å in case of 1.3nm-thickness of the dielectric layer. The calculated strain effect from this interface on MoS_2 monolayer is 0.3%. Fig. 2(c) explores the structural stability of the interface. The formation energy for each structure is denoted by the mathematical expression: $E_F = E_{MoS2/Al2O3} - (E_{MoS2} + E_{Al2O3})$. $E_{MoS2/Al2O3}$ denotes the total energy of the interface, E_{MoS2} and E_{Al2O3} represent the structural energy of MoS_2 monolayer and

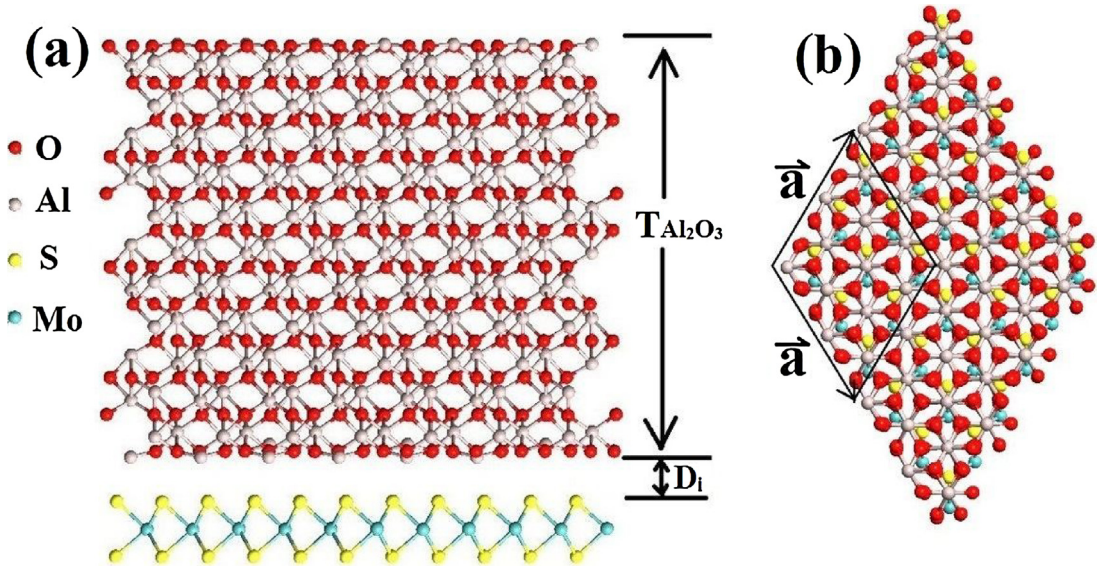

Fig. 1. Schematic of 1.3nm-layer Al_2O_3 (0001) and MoS_2 monolayer interface. TAl_2O_3 represents the thickness of the dielectric layer, while D_i represents the distance between Al_2O_3 and MoS_2 monolayer.