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Change in Electronic Properties of Hetero-Interface Systems by Applied Bias Voltage

The change in electronic properties of hetero-interface systems by an applied bias has been extensively investigated because of the interest in developing electronic devices such as transistors and diodes. Recently, novel electronic devices are gradually being produced with hetero-integrated systems consisting of 2-dimensional materials such as graphene, boron nitride (BN), and transition metal dichalcogenide [1, 2]. For sophisticatedly controlling device functions, it is required to obtain atomic-scale insights into electronic structure changes in the interface region by an applied bias. Thus, we have developed a theoretical approach for describing the electronic properties of hetero-interface systems under an applied bias [3]. In this approach, the finite-temperature density functional theory [4] is applied to the interfacial region in which the electronic functions are performed, whereas dielectrics and electrodes are approximated as continuum models. Furthermore, the approach is implemented in our original first-principles computational program named GCEED [5], which is applicable to nanostructures because of its high efficiency in massively parallel calculations. Thus, the developed approach is capable of revealing electronic structure changes in hetero-interface systems by an applied bias that are practically useful for experimental studies. By using this approach, we calculate the electronic structure of a SiO_2–graphene–BN system (Fig. 1) where an electrode bias is applied between the graphene layer and electrode 1. Figure 2 shows the band energy variations, E_F-E_D and E_C-E_F, in the graphene–BN interface region (the pink area in Fig. 1), where E_F, E_D, and E_C are the Fermi level, Dirac point energy, and conduction-band energy in BN, respectively. As the electrode bias is applied, E_F-E_D increases and E_C-E_F decreases because the graphene layer is electronically charged. Experimental studies also reported the variations in E_F-E_D and E_C-E_F analogous to the present computational result [2]. The variations in E_F-E_D and E_C-E_F decrease on changing the BN film thickness from 900 nm to 3 nm. It is also found that the absolute values of the variations in E_F-E_D and E_C-E_F are different from each other by using the 3-nm BN film. Fig. 3 shows the surface excess electron densities by an applied bias of 60 V. By changing the BN film thickness from 900 nm to 3 nm, the density in the interfacial region decreases, and that of electrode 2 (see Fig. 1) significantly increases. The electronic charging of electrode 2 is attributed to the quantum capacitance effect of graphene; the density of states of graphene is so low that the electric field generated by electrode 1 is not fully screened by the graphene layer and induces the electronic charging of electrode 2. Because of the electronic charging by an applied bias, an electric field is generated and alters the electronic structure. In particular, when the BN film thickness is 3 nm, the electric field from electrode 2 is crucially radiated on the BN layer. This is the origin of the band energy variations depending on the BN film thickness.

References

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Figures

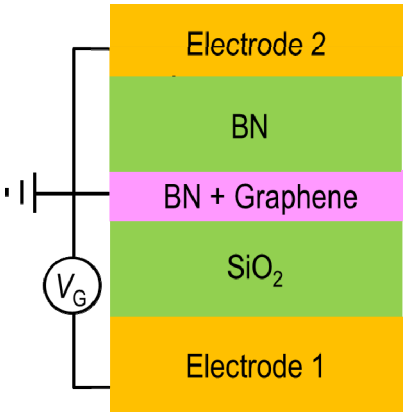

Figure 1: Schematic of the employed system in this study.

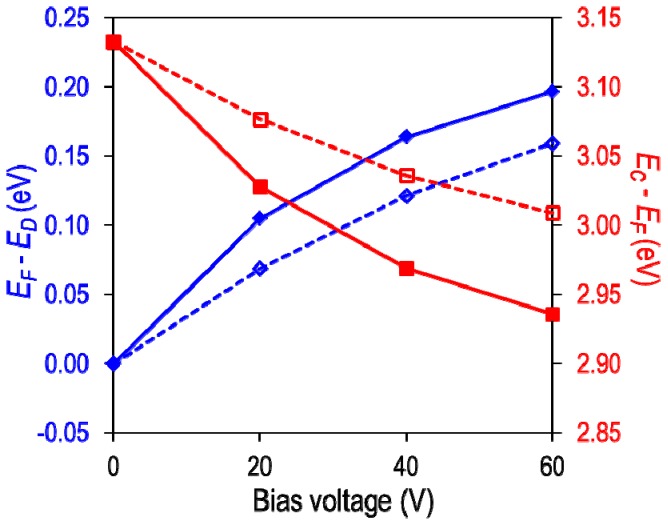

Figure 2: Band energy variations in the SiO_2-graphene-BN system due to an applied bias with the 900-nm BN layer (solid line) and the 3-nm BN layer (dashed line).

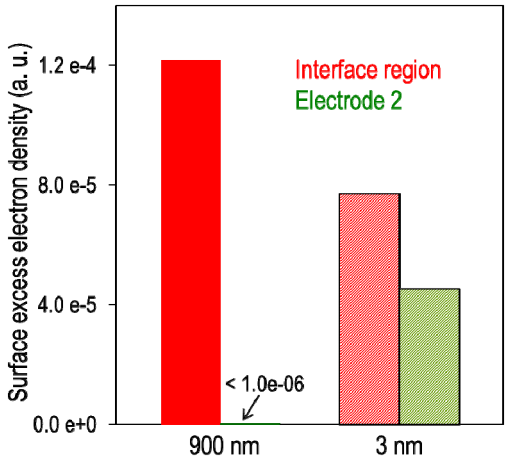

Figure 3: Surface excess electron densities (in atomic unit) in the interface region (red) and electrode 2 (green) due to an applied bias of 60 V with the 900-nm BN layer (left hand side) and the 3-nm BN layer (right hand side).