First-principles study on atomic and electronic structures of graphene/SiC interfaces

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Graphene is in the limelight as a post-silicon material in next-generation devices due to its unique electronic and mechanical properties and conductivity. In recent years, the epitaxial growth in the silicon carbide (SiC) pyrolysis method has attracted attention as one of useful methods for producing large-scale and high-quality graphene. However, in the pyrolysis method, the bottom graphene layer is covalently bonded to the Si atom of the SiC substrate. To separate the bottom layer from the substrate, atomic intercalation technique is employed. As the result, the bottom layer becomes an ideal single-layer graphene, and the Dirac cone appears in the electronic band structure. On the other hand, atomic vacancies are formed in the graphene during the epitaxial growth process. Since the intercalants can be bonded to the dangling bonds, which are affected on the energy band structure and the position of the Dirac point of graphene.

In this study, fluorine atoms are adopted as intercalants, and the effect of the bond between a fluorine atom and a dangling bond on the electronic state of graphene is investigated using the first-principles calculation code: RSPACE[1, 2]. We investigate the difference in the effects of the number of fluorine atoms adsorbed on the single vacancy in the graphene on the electronic state. It is found that, in the model where two fluorine atoms are bonded to the defect, the dangling-bond state is hybridized with the conduction band bottom of SiC substrate. Moreover, the conjugated π state of graphene is extended over the energy range in which the bandgap of SiC substrate is located (Fig. 1). On the other hand, in the system produced by hydrogen intercalation, the dangling bond state is in the middle of the band gap of the SiC substrate and extends to the inside of the substrate, which can cause a large leakage current.

This work has been performed on System B of the Supercomputer Center, the Institute for Solid State Physics, the University of Tokyo.

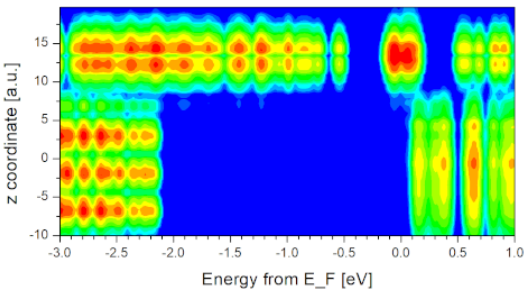

Figure 1: Local density of states of graphene with single vacancy on fluorine-intercalated SiC substrate. Two of dangling bonds are terminated by fluorine atoms.

References

[1] K. Hirose *et al.*: First-principles calculations in real-space formalism (Imperial College Press, 2005).

[2] Y. Egami, S. Tsukamoto and T. Ono: Phys. Rev. Res. **3**, 013038 (2021).