Field induced structural modulation of graphene thin films

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Since discovery of graphene, it has gained significant interest in the wide areas of pure and applied sciences due to its excellent physical properties. The field effect on the electronic properties of graphene thin films is one of important issues for practical applications. A perpendicular electric field makes a bilayer graphene with AB stacking a semiconductor whose band gap depends on the field strength [1,2,3]. Although, the electronic properties of graphene thin films have been well elucidated by various experimental and theoretical works, the geometric properties of graphene thin films under the electric field are uncertain. Therefore, in this work, we aim to elucidate the geometric structure of graphene thin films under electric field by using density functional theory with effective screening medium method. The bond length of graphene monotonically increased with increasing the hole doping concentration, while it remained insensitive to electron doping (Fig. 1). Besides, accumulated carriers mostly distributed in the outermost layer located just below the gate electrode (Fig. 2). These results enabled the construction of moiré superlattices in bilayer graphene, possessing different moiré periodicity depending on carrier concentration.

References

[1] J. B. Oostinga, H. B. Heersche, X. Liu, A. F. Morpurgo, and L. M. K. Vandersypen, Nat. Mater. **7** (2008) 151.
[2] M. Otani and S. Okada, J. Phys. Soc. Jpn. **79** (2010) 073701.
[3] N. Sultana, M. Maruyama, Y. Gao, and S. Okada, Jpn. J. Appl. Phys. **62** (2023) 075001.

Figures

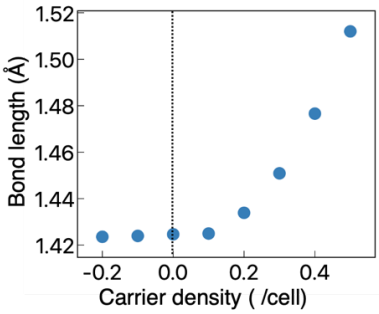

Figure 1: A bond length of monolayer graphene as a function of carrier concentration. A vertical dotted line indicates the neutral position. Positive and negative values correspond with hole and electron doping respectively.

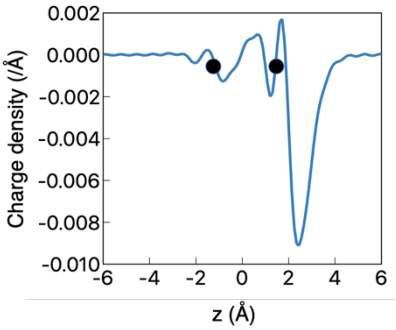

Figure 2: Plane-averaged accumulated electron density along the z axis under the hole doping concentration of 0.1h/cell of bilayer graphene.