

Electronic Structure Modulation of Graphene Adsorbed by Metal Pillars

Yoshiteru Takagi^{1,2} and Susumu Okada^{1,2}

¹University of Tsukuba.

Graduate School of Pure and Applied Sciences, University of Tsukuba,
1-1-1 Tennodai, Tsukuba 305-8571, Japan

²CREST,

Japan Science and Technology Agency, CREST, 5 Sanbancho, Chiyoda-ku,
Tokyo 102-0075, Japan

Phone: +81-29-853-5600-8233 E-mail: ytakagi@comas.frsc.tsukuba.ac.jp

1. Introduction

Graphene is considered to be one of emerging materials for the constituent of the electronic devices in the post-silicon era. Since the exfoliation of graphene from bulk graphite [1], much theoretical and experimental effort has been devoted to elucidate the fundamental properties and to fabricate the device structures. One of the fascinating properties is the remarkable carrier mobility which comes up to 2,000,000 cm²/Vs [2,3]. However, every experimental works do not reach such high carrier mobility under any conditions [4-6]. These unexpected results are now considered to arise from the electronic structure modulation of graphene caused by the structural undulation, insulating substrates, and metal electrodes. Therefore, for the realization of the graphene based electronic devices, it is now urgent to investigate the fundamental properties of hybrid structures of graphene with other conventional materials. In particular, the interfaces between graphene and metal electrodes are essential for the graphene-based metal-oxide semiconductor devices in any structures [7,8].

The aim of our paper is to investigate electronic structure of graphene adsorbed by metal pillars to uncover the effect of metal electrodes on the fundamental properties of graphene by performing the first-principles total-energy calculations in the framework of the density functional theory. The electronic structure of graphene is modulated by forming interfaces with metal electrode. We focus on special modulation of electronic structure of graphene which partially forms interfaces with metal pillar. In particular, we uncover the penetration depth of the electrode-induced effect on the electronic structure of graphene and give a theoretical insight to the gate length limit of graphene based electronic devices.

2. Calculation method

We performed first-principle total-energy calculations based on the density of functional theory [9,10] to investigate electronic structures of graphene hybrid structure with the metal pillars. We used the local density approximation to express the exchange-correlation energy between interacting electrons with a functional form fitted to the Monte-Carlo results [11] for a homogeneous electron

gas [12]. Ultrasoft pseudopotentials were used to describe the electron-ion interaction [13]. The valence wave functions were expanded in terms of the plane-wave basis set with a cutoff energy of 408 eV. Actual calculations were done by TAPP code [14,15]. The lattice parameters and atomic position were fixed. Integration over the two-dimensional Brillouin zone was carried out using four k points.

3. Structural model

Figure 1 shows a structural model used in this work. In our model, graphene partially forms interface with the metal pillars, i.e. Pd, Pt, Ag, and Au pillars with FCC structure, that simulate electrodes in graphene based electronic devices. The pillar forms interface with graphene through the (111) surface of FCC structure. We imposed a commensurability condition between the periodicity of the graphene and the that of the metal pillars. The commensurability condition leads to the elongation of the lattice constant of the graphene by about 3%. We apply the periodic boundary condition in which the unit cell is represented by the rectangular in Fig. 1(a): The lattice parameter along x-direction is about 7.5 nm and the distance between edges of metal pillar is about 7 nm. We take 1nm vacuum region along the normal to graphene.

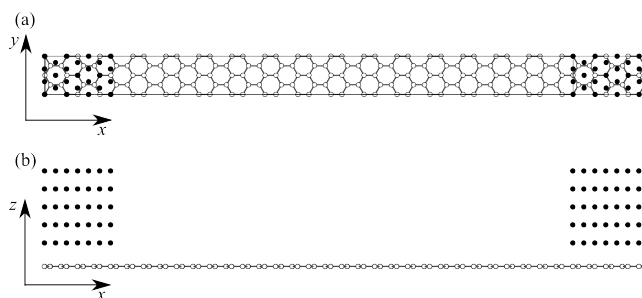


Fig. 1 A structural model of graphene hybrid structure with metal pillars. (a) Top view. (b) Side view. Open circles and closed circles represent carbon atoms and metal atoms, respectively. The rectangular in (a) represents a unit cell.

4. Results and discussion

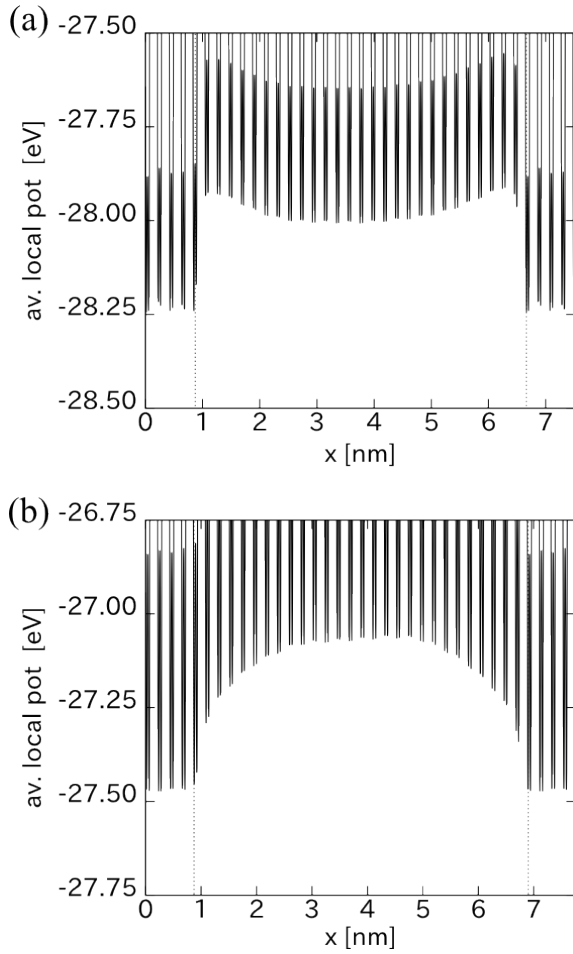


Fig 2. Plane-averaged local potential profile of graphene with (a) Pd pillar and (b) Ag pillar. The broken lines represent an edge of metal electrode. x-axis is illustrated in Fig 1(a). The origin of local potential is set at the vacuum level.

Figures 2(a) and 2(b) show local potential of graphene partially adsorbed by Pd pillars and Ag pillars, respectively. On the both pillars, the potential is strongly modulated by underneath metal pillars. However, in the uncovered region, the potential modulation is not substantial and disappears with increasing the distance from the metal pillar. The penetration depth of the metal-induced electron-states modulation is about 2 nm for both metals. It should be noted that the penetration depth suggests the narrowest limit of the gate length of the graphene-based device utilizing the unperturbed electronic structure of graphene as channel is a few nanometers irrespective the electrode metal species. Although the penetration depth is independent to the metal species, the local potential as a function of the distance between the metal pillars substantially depends on the metal species: the bottom of the potential gradually decrease with increasing the distance from the Pd pillar, while in contrast, the potential bottom gradually increase

with increasing the distance from the Ag pillar. This metal species dependence in the local potential profile is ascribed to the difference in work function of metal pillars. Furthermore, according to this potential modulation, Dirac point of graphene is also modulated depending on the position from the electrodes.

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References

- [1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, *Science* **306**, (2004) 666.
- [2] E.H. Hwang, S. Adam, and S.D. Sarma, *Phys. Rev. Lett.*, **98** (2007) 186806.
- [3] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Rev. Mod. Phys.* **81**, (2009) 109.
- [4] X. Du, I. Skachko, A. Barker, and E. Y. Andrei, *Nat. Nanotech.* **3**, (2008) 491.
- [5] K.I. Bolotina, K.J. Sikesb, Z. Jianga, M. Klimac, G. Fudenberg, J. Honec, P. Kima and H.L. Stormer, *Solid State Commun.* **146**, 351 (2008).
- [6] C. R. Dean, A. F. Young, I. Meric, C. Lee, L. Wang, S. Sorgenfrei, K. Watanabe, T. Taniguchi, P. Kim, K. L. Shepard, and J. Hone, *Nat. Nanotechnology* **5**, (2010) 722.
- [7] B. Huard, N. Stander, J. A. Sulpizio, and D. Goldhaber-Gordon, *Phys. Rev. B* **78**, (2008) 121402.
- [8] T. Mueller, F. Xia, M. Freitag, J. Tsang, and Ph. Avouris, *Phys. Rev. B* **79**, (2009) 245430.
- [9] P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, (1964) B864.
- [10] W. Kohn and L.J. Sham, *Phys. Rev.* **140**, (1965) A1133.
- [11] D.M. Ceperley and B.J. Alder, *Phys. Rev. Lett.* **45**, (1980) 566.
- [12] J.P. Perdew and A. Zunger, *Phys. Rev. B* **23**, (1981) 5048.
- [13] D. Vanderbilt, *Phys. Rev. B* **41**, (1990) 7892.
- [14] M. Tsukada, Computer program package TAPP, University of Tokyo, Tokyo, Japan, 1983-2010.
- [15] J. Yamauchi, M. Tsukada, S. Watanabe, and O. Sugino, *Phys. Rev. B*, **54**, (1996) 5586.