Effect of σ-band for Conduction of Metal/Graphene/Metal Junctions

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INTRODUCTION

Graphene, which is composed of a two-dimensional honeycomb lattice of carbon atoms, has a characteristic electronic structure near the Fermi level: its conduction and valence bands meet at only two states called Dirac points in the Brillouin zone and its energy momentum dispersion is linear near the Dirac points, that is, graphene is a gapless semiconductor in which electrons behave as massless electrons. The characteristics of electronic transport of such massless electrons have been intensively studied in graphene of infinite size as well as in finite-size nano-ribbons. The graphene has a zigzag edge and an arm-chair edge. The magnetization appears at the zigzag edge in the spin polarized graphene. The σ-band is neglected in the several theoretical studies for graphene because the σ-band is formed far the Fermi level. We show that the σ-band influence on the conduction in the graphene junctions.

MODEL and METHOD

Figure 1 shows the calculated structure of metal/graphene/metal lateral junctions with arm-chair edge contacts are shown in Figure 1. The zigzag edge of GNR is hydrogenated. The edge state of graphene disappears by hydrogenating. The width of GNR is 8 chains. The arm-chair edge of GNR is contacted the metal edge. We have used a sp^3 tight-binding model. The nearest-neighbor sp^3 model: s, p_x, p_y, and p_z orbital, or a p_z model: p_z orbital is used for the GNR. The metal lead is 2D semi-infinite square lattice with s-orbital. For the band parameters of the tight-binding model, we use are taken from Harrison's textbook. The conductance is calculated by using a recursive Green's function method and the Kubo formula [1].

RESULTS

The dispersions of 8 chains GNR with the sp^3 model are shown in figure 2. Fig. 2(a) and (b) show the non-spin-polarized GNR and the spin-polarized GNR, respectively. Fermi level is 0 eV. The almost sub-bands are consisted of the π-band of p_z orbital. We find the σ-band of s, p_x, p_y orbitals around 4.5 eV and –4.5 eV. In the spin-polarized GNR, a band gap of 0.84 eV opens (Fig. 1(b)). The band gap decrease with increasing the width of GNR. We use the spin-polarized GNR for the conduction calculation. Figure 3 and 4 show the calculated results of the conductance per spin around the conduction band bottom in the junction with the 50 and 500 lengths GNR, respectively. The light gray bold curve shows the conductance with sp^3 orbitals and a black thin curve shows the conductance with only p_z orbital for the graphene. When the graphene length is 50 chains, the conductance with sp^3 model is smaller than p_z model and the effective band gap is large. When the graphene length is 500 chains, the magnitude of effective band gap is nearly equal. However, the peak and dip of the magnitude of quantized conductance are different. In the sp^3 model, the s, p_x and p_y orbital of the graphene hybridize the p_z orbital of graphene via the metal lead. As a result, the calculated results of the conductance in the metal and graphene junctions differ between the sp^3 model and the p_z model.

REFERENCES

[1] S. Honda, A. Yamamura, T. Hiraiwa, R. Sato, J. Inoue, and H. Itoh, Phys. Rev. B **82**, 033402 (2010).

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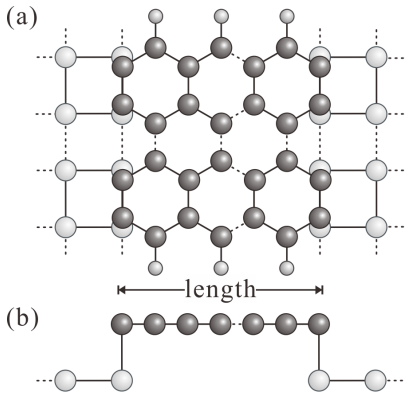

Fig. 1. (a) Top view and (b) side view of structure of metal/ graphene/ metal junction. The graphene hydrogenate. The black and gray and small gray spheres are carbon atoms and s-orb metals and hydrogen atoms, respectively. In this figure, the width and length of graphene are 4 chains and 3.5 chains, respectively.

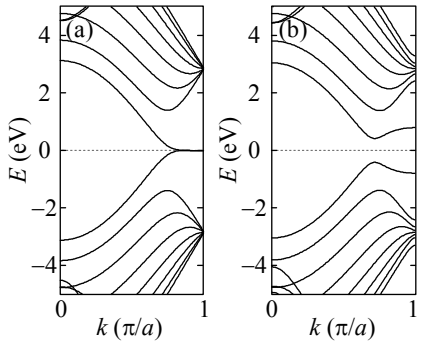

Fig. 2. The dispersion relations of (a) non-spin polarized and (b) spin polarized graphene nanoribbon. The width of graphene is 8 chains.

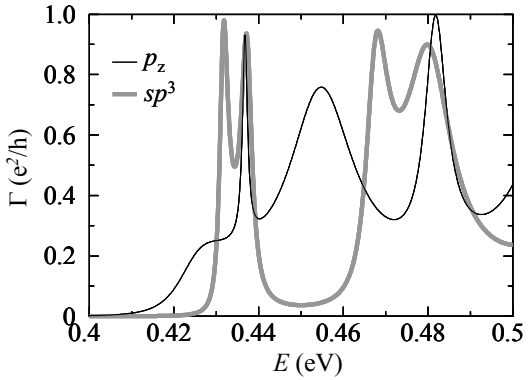

Fig. 3. Conductance of metal / graphene/ metal junction. The width and length of graphene nano ribbon are 8 chains and 50 chains, respectively.

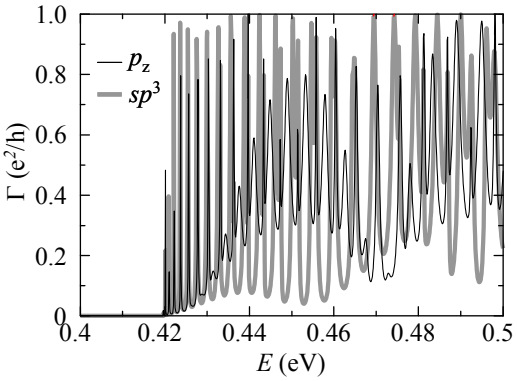

Fig. 4. Conductance of metal / graphene/ metal junction. The width and length of graphene nano ribbon are 8 chains and 500 chains, respectively.