First-principles study on electron transport property through graphene strips

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Abstract

We perform first-principles calculations for the electron-transport properties of graphene strips suspended between semi-infinite electrodes. The transport properties of graphene strips depending on the type of defects and the transport direction are investigated. The π states of carbon atoms play a main role in the electron transport, while the σ states also contribute to the transport through a graphene strip with a vacancy. Additionally, the electron-transport paths in the armchair direction are much affected by the existence of doped impurity atoms compared with those in zigzag direction.

Introduction

The carbon-based materials, such as a carbon nanotube and fullerene, are promising for application to new electronic devices that will succeed conventional silicon-based devices, and the nanoelectronics with carbon-based materials is currently one of the rapidly-expanding fields in physics and chemistry. It is important to understand the structural and electronic properties of such materials. Graphene is also attracting interest. In this study, the first-principles electron-transport property calculations are carried out for defect-containing graphene suspended between semi-infinite electrodes and the effects of defects on electrons flowing through graphene are examined.

Computational Scheme

The computational scheme is based on the real-space finite-difference (RSFD) method[1] within the framework of the density functional theory. The norm-conserving pseudopotential method and the local spin density approximation are employed to represent the ionic Coulomb potential and the exchange-correlation interactions between electrons, respectively. The transport properties of graphene strips sandwiched

between semi-infinite Au jellium electrodes (Fig. 1) are calculated by the overbridging boundary-matching method. The grid spacing is set to be 0.38 a.u., and the distances between the graphene strip and electrodes are taken to be 3.1 (2.8) a.u. for armchair-(zigzag-)direction transport.

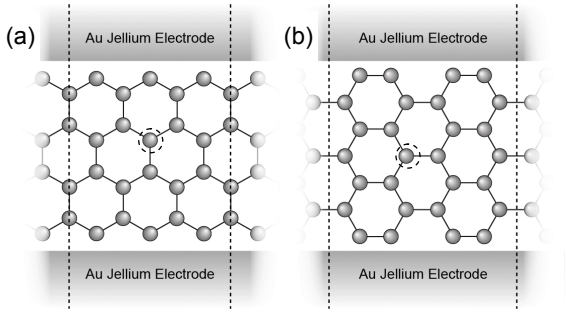

Fig. 1. Schematic view of computational models for (a) armchair-direction and (b) zigzag-direction transport. In calculations, a surrounded atom with dashed circle is replaced by a defect.

Results and Discussions

In this study, one carbon atom in the graphene strips is replaced by a vacancy or an impurity atom (boron or nitrogen), and the effects of defects on the transport properties are analyzed by comparing the results with those of the perfect model without defects. In the case of the graphene strips without defects, the conductivity is mainly contributed to by the π orbitals, and the σ orbitals play a secondary role. For the graphene strip with a vacancy, a spin polarization is manifested and σ-orbitals of carbon atoms around the vacancy play an important role in the electron transport, although the π-orbitals of carbon atoms mainly contribute to the transport in the other models.

In the impurity-doped graphene strips, the spatial flowing paths of conducting electrons in the zigzag direction are less sensitive to the existence of defects than those in the armchair direction. However, the conductances of the zigzag-direction model are much affected by impurities as well as those of the armchair-direction one. This is caused by the robust features of the conductivities against disorders in the graphene for zigzag-direction transport. Consequently, the effects of impurities on the electron conductivity and transport path are clearly observed in the flowing path for the armchair-direction transport. On the other hand, for the zigzag-direction transport, the transmission probability becomes higher (lower) owing to increasing (decreasing) of π electrons which contribute to the electron transport in the nitrogen- (boron-)doped graphene strip while the current flowing path is insensitive to the impurity atom.

References

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