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Effects of Edge Termination on Conductance in Zigzag Graphene Interconnects

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Abstract

To examine the effects of edge defects and edge atom termination on the electrical properties of graphene nanoribbon (GNR) interconnects, we studied ab-initio calculations of zigzag-edged GNRs (ZGNRs) with artificial edge defects. Edge termination with hydrogen and fluorine atoms was considered in this work. In the transmission spectrum calculated for ideal (defect-free) ZGNRs, a peak at Fermi energy, which derived from curved flat bands around Fermi energy, appeared regardless of hydrogen or fluorine atom termination. In the case of edge-defected ZGNRs, edge-termination with a fluorine atom can considerably suppress the decrease in the transmission spectrum caused by artificial edge defects, while hydrogen termination is not effective for preserving the transmission spectrum of the edge state channels. From the results of theoretical calculations, we propose some design strategies of the GNR interconnects in terms of the robustness of current conduction paths.

1. Introduction

Graphene nanoribbons (GNRs) have attracted much attention as a promising material to replace Cu in the next generation of Si LSIs because of their high electron mobility and high electro-migration tolerance. Intercalation or doping technologies for graphene that lower electrical conductivity have been reported by several groups [1, 2]. However, with the minimum feature size of LSI interconnects becoming smaller, manufacturing variants, such as edge roughness, cannot be avoided as long as lithography and dry etching processes are utilized. In addition, intercalants of GNRs can easily escape from the GNR interlayers when the width of the nanoribbons becomes narrower. Several theoretical calculations have predicted that the electrical properties of GNRs are strongly affected by edge roughness [3, 4]. Moreover, the effects of edge atom termination on electrical properties ZGNRs were calculated in several studies [5, 6]. Even so, there are few studies on the electronic structures of GNRs having edge roughness with edge atom termination. In this work, we studied the electronic structures and transmission properties of zigzag-type-edge GNRs (ZGNRs) with artificial edge defects and different edge-terminating atoms by using ab-initio calculations with the non-equilibrium Green's function.

2. Method and Models of Calculation

To calculate the electronic structures, we used the density functional scheme for the local density approximation as exchange-correlation functions. Atomistix Toolkit (ATK-DFT) software [7] based on the non-equilibrium Green function (NEGF) was used for calculating the transmission spectra of GNR. Figure 1 shows the spatial model of our calculations. A mono-layer ZGNR, which is 5-nm long and 1.8-nm wide, is sandwiched with graphene electrodes between which fixed voltages are applied. The edges were assumed to be terminated with hydrogen and fluorine atoms. We provided a small edge defect to ZGNRs, as shown in Fig. 1.

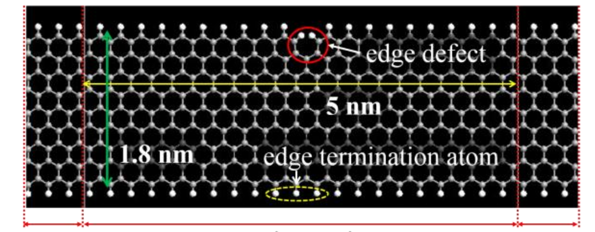

Fig. 1. Schematic model of spatially-optimized ZGNR used for theoretical calculation in this study.

To estimate electrical transport properties, we calculated transmission spectra (T(E)) at each electron energy (E) because linearity between conductance (G(E)) and T(E) is assured as given by Eq. (1),

$$\mathrm{G(E)} = \frac{e^2}{\mathrm{h}} T(E) \qquad (1)$$

T(E) is provided by the summation of transmission coefficients for respective conductance channels from the left to the right electrode at each energy level.

3. Result and Discussion

Figure 2 presents the electron energy dependence of the transmission spectrum for ideal (edge-defect-free) ZGNRs with hydrogen and fluorine termination. The coordinate origin of the horizontal axis in Fig. 2 corresponds to the Fermi level of ZGNRs with respective terminating atoms. Several staircase features in the transmission spectrum appear for the ideal ZGNR and indicate an increase in the number of electron conduction channels at the quantized sub-band energy levels. In Fig. 2, the transmission spectrum

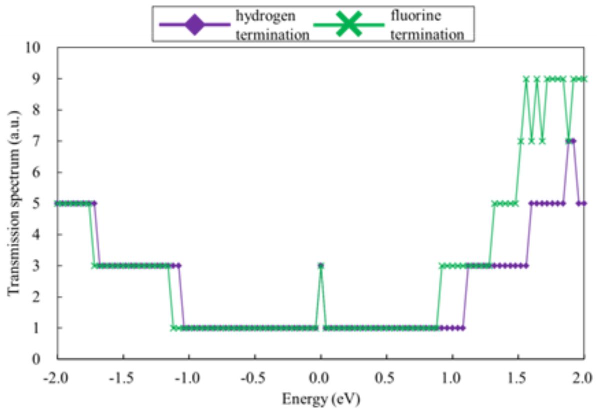

Fig. 2. Electron energy dependence of transmission spectra for ideal (edge-defect-free) ZGNRs with hydrogen and fluorine termination.

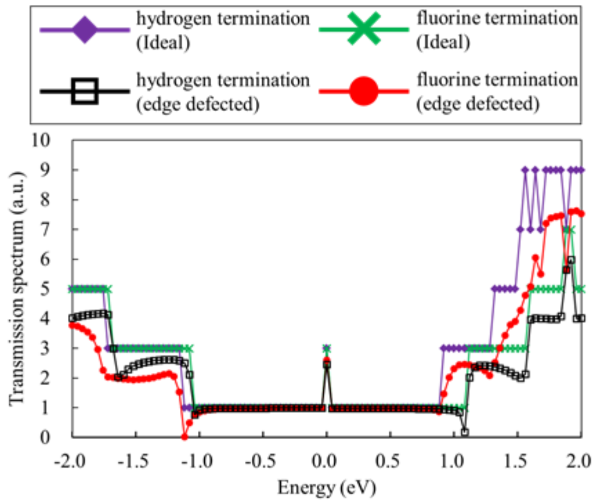

Fig. 3. Electron energy dependence of transmission spectra for ideal (edge-defect-free) and edge-defected ZGNRs with hydrogen and fluorine termination.

presents a peak value of 3 at Fermi level regardless of hydrogen or fluorine atom termination, indicating the existence of three different channels. The peaks at Fermi energy derive from curved flat bands around Fermi energy [6]. These calculation results suggest that the fluorine-terminated ZGNR has edge state conduction channels as well as the hydrogen-terminated one.

Figure 3 shows transmission spectra of edge-defected ZGNRs, whose edges are terminated with hydrogen and fluorine atoms. For comparison, the transmission spectra for edge-defect-free ZGNRs (shown in Fig. 2) were displayed again in Fig. 3. (Here we call hydrogen- and fluorine-terminated ZGNR as H-ZGNR and F-ZGNR, respectively.) The transmission spectrum of H-ZGNR decreased from 3 to 2.46 with the existence of the small edge defect, since conduction channels in edge states can easily be disconnected by edge defects with the width of a single six-membered ring as represented in Fig. 1.

On the other hand, the transmission spectrum of F-ZGNR slightly decreased from 3 to 2.6 when the similar edge defect was introduced. At Fermi energy, a ZNGR has three conduction channels and the impacts of edge effects were different between individual channels. Comparing transmission coefficients of F-ZGNR (t_F) and H-ZGNR (t_H) in the most affected channel, the value of t_F was 1.6 times larger than that of t_H. According to these calculation results, edge termination with fluorine atoms is more effective for maintaining the electron transport properties in edge-defected ZGNRs than hydrogen termination.

4. Conclusions

The effects of edge atom termination on conductance decrease in edge-defected ZGNRs were theoretically examined. According to our calculation results, the transmission spectrum in Fermi energy has a peak value due to curved flat band appearing at around Fermi energy, regardless of hydrogen and fluorine termination in edge-defect-free ZGNR. In addition, decrease in the transmission spectrum for edge-defected ZGNRs can be alleviated by edge termination with fluorine atoms. From above-mentioned results, fluorine termination can be one of the promising methods for developing nanoscale interconnects based on edge-defected ZGNRs

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