Extended Abstracts of the 2011 International Conference on Solid State Devices and Materials, Nagoya, 2011, pp1264-1265

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Theoretical Study of AC Response of Defective Carbon Nanotubes: Tube Diameter Dependence

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1. Introduction

Metallic carbon nanotubes (CNTs) are potential candidates for interconnects in next-generation nanoelectronic devices due to their large allowable current density and high electron mobility. Toward CNT nanoelectronics, a considerable amount of effort has been devoted to the investigation of the DC electronic response of CNTs thus far.

For controlling ultrafast electronic CNT-based devices, understanding of the AC transport properties is also a key in addition to the DC electronic transport properties. Thus far, several theoretical investigations on AC response of pristine metallic CNTs have been reported, and they indicate that the AC response strongly changes in sub-THz region [1,2]. Most recently, the effect of contact between metallic electrode and CNT on the AC response has also been analyzed, and the results predict that the properties of the AC response depend on the contact-coupling strength and are correlated with the DC one: as the DC conductance decreases, the low-frequency admittance changes from inductive response to capacitive one [3]. The correlation between the low-frequency admittance behavior and the DC conductance one is well-known in other systems [4,5].

Although important features as the above have been revealed, our understanding of the AC response of CNTs is not enough in the sense that to the best of our knowledge, the effects on atomistic defects and impurities have not been examined at all. Considering the fact that coherent DC conductance in CNTs is significantly influenced by atomistic defects and impurities [6], we can expect their strong influence on AC transport. Since defects and impurities are inevitably introduced in real electronic devices, the understanding of their influence on AC transport in CNTs is of great technological importance as well as scientific interests.

In this paper, we perform a theoretical analysis of AC transport in the low-frequency region in metallic single-walled carbon nanotubes (SWNTs) with a single atomic vacancy. In doing so, we focus on the inductive-capacitive transition of susceptance when the Fermi-level is changed, and discuss the tube diameter dependence of the transition.

2. Numerical simulation methods

We simulate the admittance in metallic SWNTs using the Keldysh nonequilibrium Green's function (NEGF) method [7,8] within the wide-band limit (WBL) approximation [8], combined with the nearest neighbor π-orbital tight-binding model [1-3]. In the NEGF formalism, the metallic SWNT is divided into three regions: scattering region, and semi-infinite left/right regions. In this study, a single atomic vacancy is introduced in the center of the scattering region with the length of 12.546 nm, which corresponds to 51 unit cells.

In low-frequency region, the admittance $Y(\omega)$ can be approximately expressed as $Y(\omega) = G_{DC} + iE\hbar\omega$, where G_{DC} is the DC conductance, E is the emittance [4,5], and ω is the angular frequency of AC bias voltage. According to the sign of emittance, the low-frequency response is called either inductive or capacitive: the positive (negative) emittance means that the current follows (leads) the voltage as is the response of an inductive (a capacitive) circuit. In this study, we examine the emittance behavior, focusing on the inductive-capacitive transition.

3. Results and discussions

First, we investigate the Fermi-level (ε_F) dependence of the DC conductance in armchair SWNTs with a single atomic vacancy (Fig. 1). Around $\varepsilon_F = 0$ eV, the DC conductance decreases due to the electron scattering by the defect level induced by the vacancy, in contrast to the case without introducing a vacancy (denoted by the short-dashed line in Fig. 1). The DC conductances of the SWNTs with a single atomic vacancy are the same at $\varepsilon_F = 0$ eV regardless of the tube diameter. On the other hand, the dip of the DC conductance becomes sharper as the diameter becomes larger. This is because the defect level in the SWNT with a larger diameter is much localized than that with a smaller diameter.

Next, we examine the Fermi-level dependence of the emittance behavior (Fig. 2). The capacitive response appears around $\varepsilon_F = 0$ eV, regardless of the diameter, in contrast to the response in a pristine metallic SWNTs, which is always inductive. This capacitive response can be ascribed to the electron scattering by the defect level. More interestingly, the inductive-capacitive transition occurs when ε_F is varied around the defect level. This transition occurs when the DC conductance averaged over transmission channels with the weight proportional to their density of state (aver-

aged DC conductance) becomes a half of the quantum conductance, as in the cases examined in Ref. [3]. This correspondence between the inductive-capacitive transition and the averaged DC conductance is related to the parity symmetry of the system [3-5]. Furthermore, it is noteworthy that the emittance at $\varepsilon_F = 0$ eV depends on the diameter although their DC conductance is the same regardless of the diameter. This contradicts with our naïve guess from the previous theoretical studies [3-5]. Considering the Kramers-Kronig relation between the real and imaginary parts of admittance, this behavior implies that the frequency dependent terms of conductance, which is ignored in the approximate expression written previously in this paper, have the diameter dependence. The physical origin of this behavior is speculated to be related to the degree of localization of the defect level.

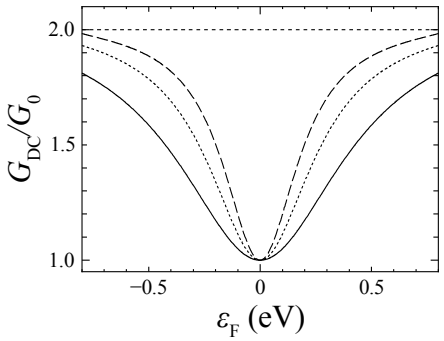

Fig. 1. Fermi-level dependence of the DC conductance of armchair SWNTs with a single atomic vacancy. Solid, dotted, and dashed lines show the DC conductance behaviors of (6,6), (8,8), and (10,10) SWNTs with a single atomic vacancy, respectively, and short-dashed line shows that of pristine armchair SWNTs. G_0 is the quantum conductance unit.

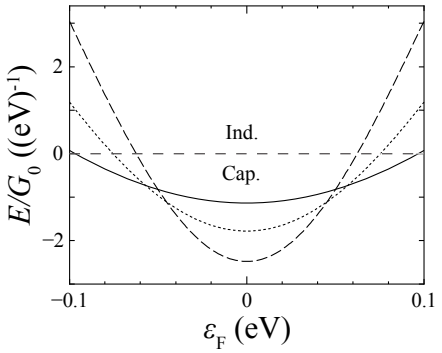

Fig. 2. Fermi-level dependence of the emittance in armchair SWNTs with a single atomic vacancy. Solid, dotted, and dashed lines show the emittance behaviors of (6,6), (8,8), and (10,10) SWNTs with a single atomic vacancy, respectively.

4. Conclusions

We studied the AC electronic response in metallic SWNTs with a single atomic vacancy, using the NEGF method within the WBL approximation combined with the nearest neighbor π-orbital tight-binding model. We found that the emittance shows the inductive-capacitive transition due to the electron scattering by the defect level. Moreover, we found that the emittances $\varepsilon_F = 0$ eV are different each other depending on the diameter, though their DC concuctances are the same. In the presentation, we will discuss the physical origins of these behaviors in detail.

Acknowledgements

We acknowledge partial financial support from Grant-in Aids for Scientific Research on Innovative Area "Materials Design through Computics: Complex Correlation and Non-Equilibrium Dynamics" and on Priority Areas "Carbon Nanotube Nano-Electronics" and "New Materials Science Using Regulated Nano Spaces Strategy in Ubiquitous Elements" and the Global COE Program "Global Center of Excellence for Mechanical System Innovation" from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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