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Electron doping effects on the electrical conductivity of zigzag carbon nanotubes and corresponding unzipped armchair graphene nanoribbons

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ABSTRACT

The Kubo formula is used to extract the electrical conductivity (EC) of different diameters of doped zigzag carbon nanotubes and their corresponding unzipped armchair graphene nanoribbons, as a function of temperature and chemical potential, within the tight-binding Hamiltonian model and Green's functions approach. The results reveal more sensitivity to temperature for semiconducting systems in addition to a decrease in EC of all systems with increasing cross-sections.

1. Introduction

Carbon nanotubes (CNTs) [1,2] and graphene nanoribbons (GNRs) [3] are two allotropes of the carbon crystals with quasi-one-dimensional (1D) honeycomb structure similar to graphene [4,5]. A single-walled CNT (SWCNT) is a cylindrically shaped GNR with a diameter that ranges from about 0.5 to 5 nm and lengths of the order of micrometers to centimeters. The structure of CNTs is specified by the chiral vector, $\boldsymbol{C}_h = n\boldsymbol{a}_1 + m\boldsymbol{a}_2 \equiv (n, m)$, where $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are primitive vectors of graphene and the integers n and m characterize the number of unit vectors along two directions in the lattice of graphene (Fig. 1). If $m = 0$, the CNTs are named zigzag CNTs (zCNTs) [6,7].

GNRs are narrow strips of graphene sheets while the armchair GNR (aGNR) has an armchair cross-section at the long edges. Width of the aGNRs can be identified by number of armchair lines, W, present in direction of their width and indicated by W-aGNR. Moreover, aGNRs show a departure from the electronic properties of graphene sheets, most notably the opening of a band gap due to the quantum confinement and edge effects [8]. Denoting Δ_W the energy gap of a W-aGNR around the Fermi level, they are orderly categorized as $\Delta_{3q} \geq \Delta_{3q+1} \geq \Delta_{3q+2} = 0$, which q is a positive integer number. Moreover, it has been verified experimentally and theoretically that GNRs are derived by unzipping the CNTs [9–13]. It has been proven that unzipping metallic zCNTs always results in narrow-gap semiconducting aGNRs, but for semiconducting zCNTs, it may lead to either a metallic or a narrower gap semiconducting aGNR [6,14].

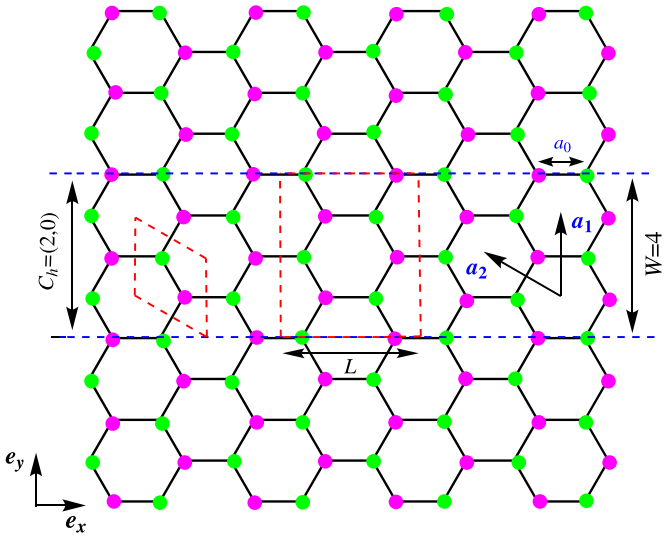

Fig. 1. Geometry of a graphene honeycomb lattice with the interatomic distance a_0 and primitive vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The longitudinal slice enclosed in dashed lines is an 4-aGNR with the primitive vector $\boldsymbol{L} = 3a_0\boldsymbol{e}_x$. The aGNR results in a zCNT if its long edges, two points of which are connected by the chiral vector $\boldsymbol{C}_h = (2, 0)$, fold in to coincide. The red dashed lines illustrate the boundaries of the BLUCs of graphene (left) and aGNR (right).

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CNTs and GNRs are carbon-based nanomaterials, and their electronic properties can be altered by either electron donors or electron acceptors [15–19]. For example, the effect of nitrogen (N) and boron (B) doping on the electronic and field emission properties for CNTs and GNRs has been reviewed by Yu and Zheng [15] where they have shown the doping of N atoms into the CNTs can improve the field emission properties of these carbon based materials, while the doping of B atoms has no positive effect on [15]. Electrical conductivity (EC) enhancement in SWCNTs bundles doped with bromine and potassium has been investigated by Lee et al. [16]. The structure and electronic properties of potassium-doped SWCNTs have been studied by conduction electron spin resonance, EC, and x-ray diffraction, using electrochemical methods by Claye et al. [17]. Also, effects of B and N doping on charge transport in GNRs have been investigated by Biel et al. [18] where they have concluded it is strongly dependent on the symmetry and width of the ribbon, as well as the position of the dopants. In addition, first principle calculations of the electronic properties of N-doped GNRs with zigzag edge have been presented by Yu et al. [19]. Some works have also investigated the thermal properties of CNTs and GNRs by different methods [20–23]. Likewise, have been reported many efforts concerning their mechanical [24,25] and optical properties [26–29].

In this theoretical study, the EC of doped zCNTs with different diameters and their corresponding unzipped aGNRs of different widths are investigated by TB Hamiltonian model and Green's functions approach. Using band representation of the Green's functions, EC of the systems is calculated by Kubo formula [30–35]. Introduced in section II are the mentioned model and method as well as the temperature-dependent EC. The two last sections include the results, discussion and conclusion.

2. Hamiltonian model and Green's function method

The band representation TB Hamiltonian model in the second quantization form for π-electrons of a quasi-1D lattice reads as follows [36,37]:

$$\widehat{\mathcal{H}} = \sum_{s=\pm}\sum_{b=1}^{N_b}\sum_{k\in \mathrm{FBZ}}^{N_c} (\xi_s^{(b)}(k) - \mu)\hat{c}_{s,k}^{(b)\dagger}\hat{c}_{s,k}^{(b)}, \tag{1}$$

in which s = + (-) symbolizes the conduction (valence) band, b serves as the sub-band index, N_b indicates the number of the sub-bands, $k \equiv k_x$ shows a 1D wave vector in the first Brillouin zone (FBZ), N_c is the total number of the Bravais lattice unit cells (BLUCs) and μ is the chemical potential energy. $\hat{c}_{s,k}^{(b)\dagger}$ ($\hat{c}_{s,k}^{(b)}$) stand for the creation (annihilation) operators of the π-electrons with the corresponding quantum numbers, and $\xi_s^{(b)}(k)$ are the eigenvalues of the Hamiltonian. The π bands of the both systems in nearest-neighbor (nn) approximation are available by following expressions:

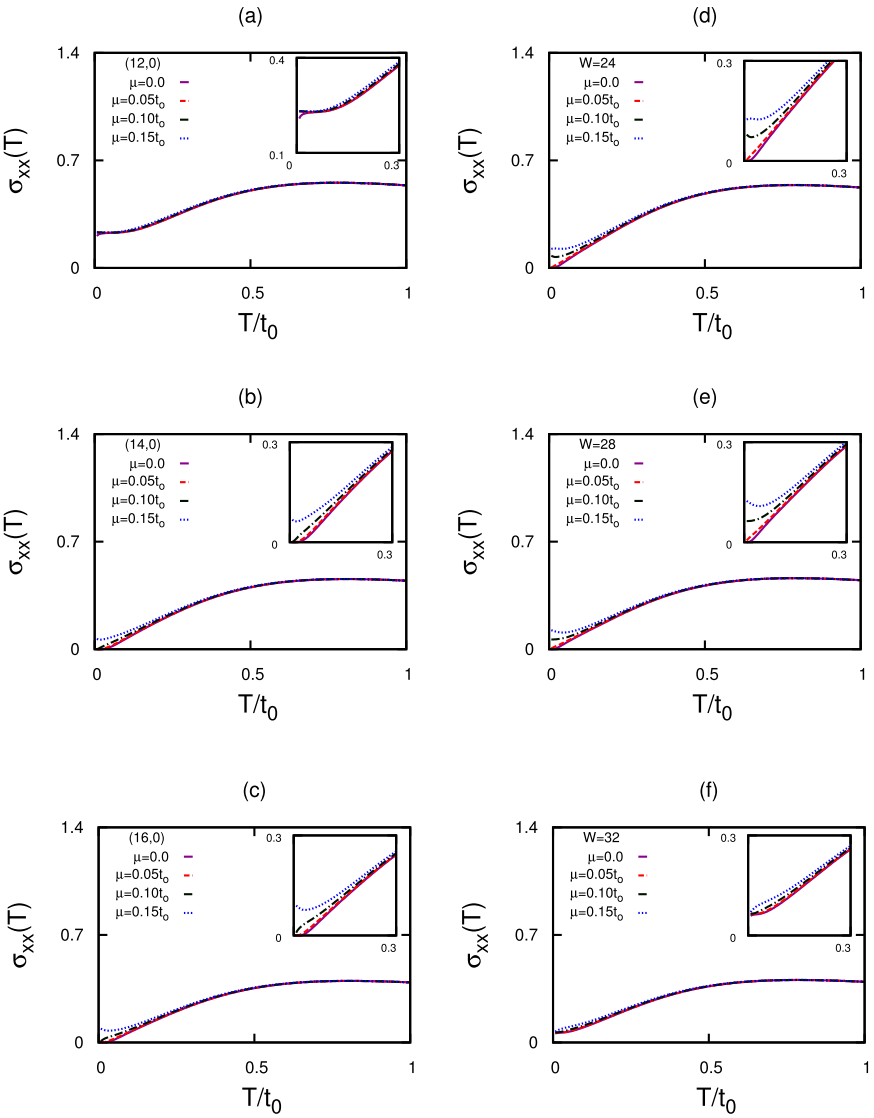

Fig. 2. The EC curves for $\mu = 0.0$ (solid violet lines), $\mu = 0.05t_0$ (dashed red lines), $\mu = 0.1t_0$ (dashed-dotted black lines) and $\mu = 0.15t_0$ (dotted blue lines) of the (12, 0), (14, 0) and (16, 0) zCNTs in panels (a–c) respectively (left), along with corresponding 24-, 28- and 32-aGNRs in panels (d–f) (right).