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Transport properties of armchair graphene nanoribbons under uniaxial strain: A first principles study

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ABSTRACT

In this work, transport properties of armchair graphene nanoribbons (AGNRs) under uniaxial strain are considered using density functional theory. We found that carrier mobility of AGNRs depends strongly on uniaxial strain. The electron mobility of 5-AGNR is up to 38.5×10^4 $cm^2/V\,s$ at an elongation of 6%. However, the dependence of the effective mass of electrons and holes of AGNR on uniaxial strain can almost be described by the same function and their effective masses coincide at an elongation of 10%. The sensitivity to strain of the transport properties of AGNRs opens many ways for applications in nanoelectromechanical devices.

1. Introduction

Due to extraordinary mechanical, transport and electromechanical properties, low-dimensional carbon materials, such as carbon nanotubes (CNTs) and graphene nanoribbons (GNRs), have attracted many scientists both theoretical and experimental in recent years [1–4]. Both CNTs and GNRs are quasi one-dimensional systems, and can be a semiconductor or a metal depending on their topological structure [5,6]. However, GNRs have a planar structure leading to ease of designing nanonodevices where a GNR is one of device's components. Therefore studies of electronic and transport properties of GNRs play an important role in their applications to nanoelectronic devices.

Electronic and transport properties of GNRs have been studied by different methods [7–11]. Using first-principles calculations, one shows that we can control the band gap of armchair graphene nanoribbons (AGNRs) by strain [8]. Besides, the band gap modulation of strained AGNRs depends strongly on the quantum confinement at the edge of the nanoribbons [8]. Electronic properties of GNRs under strain have also been studied by many groups [12–14]. Structural and electronic properties of a system of GNRs encapsulated in carbon nanotubes have also been investigated using the dispersion-corrected density functional theory [15]. The effect of impurities and edge roughness scattering on the mobility of GNRs has been studied [16]. In addition, the dependence of electron transport [17] and time-dependent ballistic transport [18] of GNRs on ribbon width has been theoretically investigated. Molecular dynamics simulations have shown that the strain strength plays an important role in thermal transport and thermal rectification of AGNRs [19]. Via the Landauer formalism, Lehmann et al. [20] have confirmed that the transport properties of GNRs are very sensitive to uniaxial longitudinal strain and edge termination. They have also shown that the band gap of AGNRs can appear at the critical strain value and it also strongly depends on the concentration of defects in the case of non-ideal AGNRs [20]. In the small strain limit, they could change the electrical conductivity from an insulator to a conductor by using uniaxial strain [21]. In this case, the dependence of carrier effective masses on uniaxial strain is important to modulation of electrical conductivity of GNR.

In the present work, we theoretically study the transport properties of strained AGNRs by using first principles calculations. The effect of uniaxial strain on the electronic properties and carrier mobility of AGNRs is studied. We estimate the fluctuation of the carrier effective mass in nanoribbons under small uniaxial strain. The role of uniaxial strain in change of the electronic and transport properties of AGNRs is also discussed.

2. Model and computational details

In the present work, we study AGNRs under engineering uniaxial strain. All dangling bonds at the edges of the GNR will be assumed to be saturated by hydrogen atoms. The schematic of an AGNR under uniaxial strain is shown in Fig. 1. In this study, all

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calculations for AGNRs with various ribbon widths (via dimer lines N across the ribbon) were performed using density functional theory (DFT) with Quantum Espresso *ab initio* simulation package [22]. The ultrasoft pseudopotential with the general gradient approximation of the PBE exchange correlation functional was adopted. The cutoff energy of plane waves was 520 eV. Geometrically, we fully optimized the structure of AGNRs by using *ab initio* calculations with PBE density functional theory [23–25]. The structure of ribbons was relaxed until all atomic forces were less than 0.001 eV/Å, and the convergence criterion for the total energy at each self-consistent field iteration was 0.01 meV. Electronic properties of AGNRs are calculated using DFT-D2. For all calculations, we used large enough supercells, in which the distance between the adjacent sheets is at least 25 Å. Previously, we have successfully used this method for a similar system such as GRN or GNR placed on a semiconductor substrate [10,26–28].

At room temperature, the electron velocity υ is 10^5 m/s. The lattice constant of AGNRs is smaller than the wave-length of the electron ($\lambda \approx 7$ nm). Hence, we believe that the delocalized charge is scattered only by acoustic phonons and we use the deformation potential theory of Bardeen and Shockley [29] to describe this scattering process. In the framework of the effective mass approximation and electron-acoustic phonon scattering mechanism in a one–dimensional semiconducting system, via the average value of the momentum relaxation time τ, the mobility can be written as follows [30]

$$\mu = e\frac{\overline{\tau}}{|m^*|} = \frac{e\hbar^2 C}{(2\pi k_B T)^{1/2}|m^*|^{3/2}E_1^2}, \quad (1)$$

where E_1 is the deformation potential constant, e is the electron charge, $m^* = \hbar^2(\partial^2 E/\partial k^2)$ is the effective mass of the charge, C is the stretching modulus caused by the longitudinal acoustic phonon along the ribbon, k_B is Boltzmann's constant, and T=298 K is the temperature chosen in present calculations.

Based on the band structure at equilibrium, we can fit two curves for the bottom of the conduction band and the top of the valence band near the $k = 2\pi/3$ point, whence we got the effective masses m_e and m_h for electron and hole, respectively. It is well-known that carriers without a very sharp density of state near the edges of frontier bands could contribute to the real conduction process in an energy range wider than the thermal energy k_BT. In this work, the thermal energy of $10k_BT$ [31] is used to obtain the carrier effective mass and then the carrier mobility.

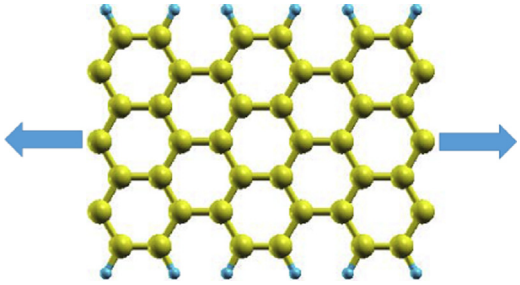

Fig. 1. (Color online) Schematic of an AGNR under uniaxial strain. Yellow and blue balls stand for carbon and hydrogen atoms, respectively.

3. Results and discussion

In the present study, we consider only 5-, 6-, and 7-AGNRs, which represent the three categories of $(3n-1)$-, $3n$-, and $(3n+1)$-AGNRs. We first consider the electronic structure of AGNRs after relaxation at zero strain. At the equilibrium state, AGNRs are semiconductors with direct energy gap. Our previous work shows that the electronic band gaps at zero strain for 5-, 6-, and 7-AGNRs are 0.5691, 0.9833, and 1.6889 eV, respectively [10]. We all know that carbon nanomaterials are very sensitive to defects and mechanical strain. The electronic properties of AGNRs are strongly dependent on uniaxial strain. Our calculations show that the total energy is minimum at the equilibrium state for all AGNRs. The dependence of the total energy of AGNRs on uniaxial strain can be described as a parabola. Besides, the shift of the conduction/valence band of AGNRs depends linearly on uniaxial

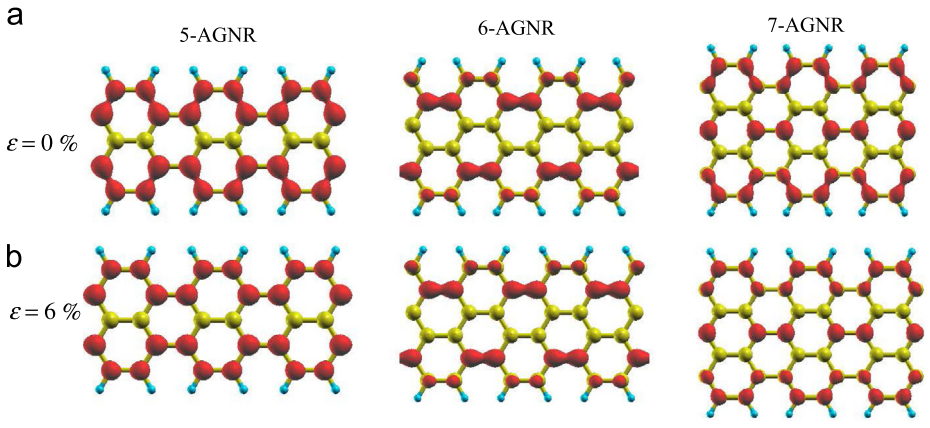

Fig. 2. (Color online) Charge density of the conduction band of AGNRs at the Γ point.

Table 1
The stretching modulus $C(10^{10}$ eV/cm), valence band deformation potential constant E_{1v}, conduction band deformation potential constant E_{1c} (eV), hole effective mass $|m_h^*|$, electron effective mass $|m_e^*|$ (m_0), relaxation time for hole τ_h and electron τ_e (ps), hole mobility μ_h, and electron mobility $\mu_e(10^4$ cm^2/V.s) of AGNRs.

	C	E_{1v}	E_{1c}	m_h^*	m_e^*	τ_h	τ_e	μ_h	μ_e
5-AGNR	40.45	9.48	2.78	0.104	0.100	0.63	7.44	1.06	13.11
6-AGNR	44.75	4.30	10.20	0.223	0.230	2.31	0.40	1.82	0.31
7-AGNR	48.90	5.11	12.45	0.170	0.230	2.04	0.32	2.11	0.28