Full-band and atomistic study of electron-phonon interaction in graphene nanoribbons

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Abstract. Transmission function through metallic armchair-edge graphene nanoribbons is calculated within non-equilibrium Green’s function method including full-band electron–optical-phonon interaction. Structures appear in transmission function, which are originated in both zone-center and zone-edge optical-phonon scattering.

1. Introduction
Recently, Novoselov et al. successfully fabricated field-effect transistors (FETs) of graphene [1]. Graphene sheets have also been patterned into narrow nanoribbons to produce graphene nanoribbons (GNRs) with a width of several tens of nanometers down to a few nanometers. One can control the band-structure of GNRs by changing their width and orientation relative to the graphene crystal structure. Graphene-based FETs are now considered to be one of most promising device structures for future integrated circuits. For improvements in the transport properties of GNRs, it is essential to identify the major sources of carrier scattering. Since graphene-based FETs operate at room temperature, electron-phonon interaction is considered to play an important role as a dominant scatterer. In the present work, we have numerically studied effects of electron–optical-phonon interaction in metallic armchair-edge GNRs (A-GNRs). We have calculated transmission function through A-GNRs using the method developed by Frederiksen et al. [2] based on non-equilibrium Green’s function (NEGF) [3–5]. The electron and phonon dispersion curves are obtained within tight-binding approximation, and optical-phonon scattering are taken into account within full-band and atomistic NEGF formalism.

2. Calculation method
2.1. Electronic states
We use a tight-binding model to describe the electronic states of GNRs. The wave function is written as

\[ \Psi(r) = \sum_{R_n} \Psi(R_n) \phi(r - R_n), \]

where \( \phi(r) \) is the wave function of the \( p_z \) orbital of a carbon atom located at the origin and \( R_n \) represents the position of a carbon atom. The Hamiltonian is written as

\[ H = \sum_{nm} E_{nm} |\phi_{nm}\rangle \langle \phi_{nm}| + \sum_{nm\neq n'm'} \gamma_{nm,n'm'} |\phi_{nm}\rangle \langle \phi_{n'm'}|, \]

where \( E_{nm} \) is the energy of the electron in the \( nm \) band, \( \gamma_{nm,n'm'} \) is the coupling constant between the \( nm \) and \( n'm' \) bands, and \( |\phi_{nm}\rangle \) and \( |\phi_{n'm'}\rangle \) are the wave functions of the electrons in the \( nm \) and \( n'm' \) bands, respectively.

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where $E_{nm}$ is the on-site energy, $\gamma_{nm,n'm'}$ is the transfer integral between orbitals, $n$ is a unit cell number, and $m$ is a site number in a unit cell (see inset of Fig. 1). We consider nearest-neighbor interaction with the transfer integral of $-\gamma_0$ and the case without potential ($E_{nm} = 0$). Although the case with a non-zero potential would be important, we only consider the zero potential case in the present study for investigating fundamental properties of GNRs with phonon scattering.

2.2. Optical-phonon modes

We describe the optical-mode lattice vibration by considering two types of restoring forces between carbon atoms [6]. One is restoring force for the bond lengths and the other is that for the bond angles. In the present study, we ignore edge effects on phonon modes and assume bulk phonons for simplicity.

2.3. Electron-phonon interaction

We include the full-band electron-phonon interaction in NEGF formalism by using the method developed by Frederiksen et al. [2]. The transfer integral between an atom labeled $i$ and an atom labeled $j$ depends on the change of the lattice displacement as

$$
\gamma_{ij}(|d_i + u_i(R_i) - u_j(R_j)|) = \gamma_0 + \frac{1}{b} \frac{d\gamma_0}{db} d_i \cdot |u_i(R_i) - u_j(R_j)|, 
$$

where $u(r)$ is the lattice displacement, $d_i = R_i - R_j$ are the vectors connecting nearest neighbor carbon atoms ($l = 1, 2, 3$) [7], and $b$ is the bond length without the lattice displacement [8–10].

By solving the dynamical equation of the two restoring forces between carbon atoms, we obtain the normal mode vector $e_\mu$ (normalized $e_\mu \cdot e_\mu = 1$) and the eigen-frequency $\omega_\mu(q)$. Here $\mu$ is the mode number and $q$ is the phonon wavevector. The quantized expression for $u_i$ is then written as

$$
u_i(R) = \sum_\mu \sum_q (e_{\mu i}) e^{i\vec{q} \cdot \vec{R}} \sqrt{\frac{\hbar}{2MN\omega_{\mu}(q)}} (b^\dagger_{\mu,-q} + b_{\mu,q}),
$$

$$
u_j(R - d_i) = \sum_\mu \sum_q (e_{\mu j}) e^{i\vec{q} \cdot \vec{R}} \sqrt{\frac{\hbar}{2MN\omega_{\mu}(q)}} (b^\dagger_{\mu,-q} + b_{\mu,q}),
$$

where $N$ is the number of unit cells, $M$ is the mass of a carbon atom, and $b^\dagger_{\mu,q}$ and $b_{\mu,q}$ are the creation and destruction operators, respectively. Inserting Eqs. (4) and (5) into Eq. (3), we obtain

$$
\gamma_{i,j} = \gamma_0 + \sum_\mu \sum_q (M_{\mu,q})_{i,j} (b^\dagger_{\mu,-q} + b_{\mu,q}),
$$

where $M_{\mu,q}$ is the electron–optical-phonon coupling defined as

$$
(M_{\mu,q})_{ij} = \frac{1}{b} \frac{d\gamma_0}{db} d_i \cdot (e_{\mu i} - e_{\mu j}) e^{i\vec{q} \cdot \vec{R}} \sqrt{\frac{\hbar}{2MN\omega_{\mu}(q)}}.
$$

2.4. NEGF formalism

The electron-phonon interaction is included into NEGF formalism through electronic self-energies caused by the optical-phonon scattering $\Sigma_{ph}^\tau(\varepsilon)$ as (we follow the notation as in Ref. [2])

$$
\Sigma_{ph}^\tau(\varepsilon) = \sum_\mu \sum_q \int_{-\infty}^{\infty} \frac{d\varepsilon'}{2\pi} M_{\mu q}^\dagger \left\{ \frac{4}{\hbar \omega_{\mu}(q)} \text{Tr}[G^{<}(\varepsilon')M_{\mu q}] 
+ D^\mu_{\mu}(\varepsilon, \varepsilon') G^{<}(\varepsilon') M_{\mu q} + D^\mu_{\mu}(\varepsilon - \varepsilon') G^r(\varepsilon') M_{\mu q} \right\}.
$$
\[
\Sigma_{\text{ph}}^{\mu}(\varepsilon) = \sum_{\mu} \sum_{q} \int_{-\infty}^{\infty} \frac{d\varepsilon'}{2\pi} M_{\mu,q} D_{\mu}^{\mu,\Sigma}(q, \varepsilon - \varepsilon') G_{\mu}(\varepsilon') M_{\mu,q},
\]

where \( G^{\mu} \) are the lesser and greater electron Green function and \( D_{\mu}^{\mu,\Sigma} \) are the noninteracting phonon Green functions. The retarded electron Green function is given by

\[
G'(\varepsilon) = ((\varepsilon + i0)I - H - \Sigma^r_{\mu}(\varepsilon) - \Sigma^r_{\mu}(\varepsilon) - \Sigma_{\text{ph}}^{\mu}(\varepsilon))^{-1},
\]

where \( \Sigma^r_{\mu,R} \) are the contact self-energies. We calculated the retarded Green function \( G' \) self-consistently using Eqs. (8) and (10). Transmission function is then obtained by

\[
T(\varepsilon) = \text{Tr} \left[ \Sigma^<_{\mu} G^{>}(\varepsilon) - \Sigma^<_{\mu} G^{<}(\varepsilon) \right].
\]

3. Result and Discussion

Figure 1 shows the band-structure of an A-GNR with a width of \( W = (7/2)a \) (\( a \) is the lattice constant). We set the transfer integral to \( \gamma_0 = 3.03 \text{ eV} \). Figure 2 shows optical-phonon scattering rate at an edge atom (marked in the inset of Fig. 1) as a function of electron energy. We set the phonon occupation factor to zero and consider the emission process only. We find high scattering rate at an edge atom (marked in the inset of Fig. 1).

Figure 3 shows the transmission function through A-GNRs with a width of \( W = (7/2)a \) for \( L = (5\sqrt{3}/6)a, (11\sqrt{3}/6)a, \) and \( (17\sqrt{3}/6)a \). In Fig. 3, we also plot the transmission function without electron-phonon interaction for comparison. The electron-phonon interaction has strong impact on the transmission for electron energies near the band center (\( \varepsilon \approx 3 \text{ eV} \)), while weak impact near the band edges (\( \varepsilon \approx 0 \text{ eV} \) and \( 9 \text{ eV} \)). We find several structures appearing on the transmission function, which can be attributed to not only zone-center phonons (\( \hbar \omega = 196 \text{ meV} \)) but also zone-edge phonons (\( \hbar \omega = 162 \text{ meV} \)) (see Fig. 4). When electron kinetic energy
becomes higher than optical phonon energy, phonon emission occurs with the probability being proportional to the final density-of-states. This results in the structures on the transmission function.

4. Summary
We have calculated transmission function through metallic A-GNRs within NEGF method including full-band electron–optical-phonon interaction. We find structures appearing in transmission function, which are originated in both the zone-center and zone-edge optical-phonon scattering. We also find that the electron-phonon interaction has strong impact on the transmission for electron energies near the band center, while weak impact near the band edges.

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