Non-equilibrium Green function simulations of graphene, silicene, and germanene nanoribbon field-effect transistors

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Abstract. Ballistic performance of graphene, silicene, and germanene-nanoribbon field-effect transistors (FETs) with a gate-length of 10 nm has been numerically investigated. The graphene-nanoribbon FET is found to have the largest ON-current when one compare FETs with a nanoribbon channel having a nearly equal band-gap $E_g \approx 0.5$ eV. The graphene device exhibits the largest OFF-current due to the smallest effective-mass enhancing the source-drain direct tunneling.

Keywords: graphene, silicene, germanene, nanoribbon, FET, NEGF

1. Introduction

Graphene, a monolayer of carbon (C) atoms forming a dense honeycomb two-dimensional crystal structure [1], offers the prospect of creating future nanoelectronics devices. Other group IV elements, such as silicon (Si) and germanium (Ge), have stable honeycomb monolayers [2], namely silicene and germanene, and can be also applied to electronic devices [3,4]. We have assessed the performance potentials of graphene, silicene, and germanene-nanoribbon (GNR, SiNR, and GeNR) field-effect transistors (FETs) [5,6] employing the ballistic top-of-the-barrier (ToB) FET model [7]. The ToB FET model ignores the source-drain (S-D) tunneling, and can be applied only to long-channel FETs whose S-D tunneling is insignificant. In the present study, we have performed non-equilibrium Green function (NEGF) simulations of GNR, SiNR, and GeNR FETs to assess an impact of the S-D tunneling on the device performance.
2. Device model

We consider a nanoribbon FET structure whose schematic diagram is given in Fig. 1. The structure is similar as considered in Ref. [8]. The channel consists of a semiconducting armchair-edge nanoribbon (A-NR) of width $w$. The back-gate bias, $V_b$, controls the carrier density in the nanoribbon, and the top-gate bias, $V_g$, controls the channel potential modifying the drain current, $I_d$. The device parameters and the bias condition are summarized in Table 1.

![Schematic diagram of the nanoribbon FET structure](image)

Figure 1: Schematic side and top views of the nanoribbon FET structure together with the coordinate system used in the present study. The channel consists of a semiconducting armchair-edge nanoribbon.

| Parameter                  | Symbol | Value     |
|----------------------------|--------|-----------|
| Top-gate length            | $L_g$  | 10 nm     |
| Source-extension length    | $L_s$  | 20 nm     |
| Drain-extension length     | $L_d$  | 20 nm     |
| Device width               | $W_{dev}$ | 30 nm   |
| Top-oxide thickness        | $t_{ox}$ | 2 nm     |
| Back-oxide thickness       | $t_{box}$ | 20 nm   |
| Drain voltage              | $V_d$  | 0.05 V    |
| Top-gate voltage           | $V_g$  | $-0.5 \rightarrow +0.5$ V |
| Back-gate voltage          | $V_b$  | 2 V       |

Table 1: Device parameters and bias condition
3. Calculation method

We calculate the current-voltage characteristics using a non-equilibrium Green function (NEGF) method \([9–11]\) within the nearest-neighbor tight-binding approximation. The channel of the device consists of a semiconducting A-NR with the number of dimer lines of \(N\). The nanoribbon width, \(w\), is related to \(N\) by the relation \(w = \frac{1}{2}(N - 1)a_0\), where \(a_0\) is the lattice constant. The Hamiltonian describing an isolated A-NR channel can be defined by the matrix element between the \(i\)-th and the \(j\)-th atoms:

\[
H_{ij} = \begin{cases} 
V(x_i, y_i) & (i = j) \\
-\gamma & \text{(neighboring atoms } i, j) \\
0 & \text{(otherwise)} 
\end{cases} 
\]  

(1)

Here \((x_i, y_i)\) is the \(i\)-th atom position, \(V(x, y)\) the potential profile on the A-NR channel, and \(\gamma\) the transfer energy between neighboring atoms. In the present study, the values of \(\gamma\) for silicene and germanene are extracted from the Fermi velocities of the first-principles calculations (see Table 2). Figure 2(a) shows the energy gap, \(E_g\), in semiconducting A-NRs as a function of \(N\). For performance comparison of GNR, SiNR, and GeNR devices, we consider A-NRs with \(E_g \approx 0.5\,\text{eV}\); i.e. A-GNR with \(N = 18\), A-SiNR with \(N = 6\), and

| Graphene | Silicene | Germanene |
|----------|----------|-----------|
| Lattice constant (nm) | \(a_0\) | 0.246 | 0.386 | 0.405 |
| Transfer energy (eV) | \(\gamma\) | 2.79 | 1.13 | 1.02 |

Figure 2: (a) Energy gap in semiconducting armchair-edge nanoribbons (A-NRs) as a function of the number of dimer lines, \(N\), for even numbers of \(N\). Lines connecting marks are a guide to the eye only. (b) Band dispersion near the Dirac point for A-NRs with \(E_g \approx 0.5\,\text{eV}\): A-GNR with \(N = 18\) (left), A-SiNR with \(N = 6\) (center), and A-GeNR with \(N = 6\) (right).
A-GeNR with \( N = 6 \) (see the horizontal gray line in Fig. 2(a) and Fig. 2(b)).

A finite-length isolated A-NR channel is attached to the source and the drain electrodes. These electrodes can be accounted for by the self-energies \( \Sigma_s(E) \) and \( \Sigma_d(E) \) in the NEGF method. The self-energies are calculated using the method of Ref. 12. In the ballistic limit, the drain current, \( I_d \), can be written as

\[
I_d = \frac{2e}{h} \int T(E) [f_s(E) - f_0(E)] dE,
\]

where \( f_s(E) \) (\( f_0(E) \)) is the electron distribution function in the source (drain) electrode, and \( T(E) \) is the transmission function given by

\[
T(E) = \text{trace}[\Gamma_s(E)G(E)\Gamma_d(E)G^\dagger(E)]
\]

with \( G(E) = [E - H - \Sigma_s(E) - \Sigma_d(E)]^{-1} \), \( \Gamma_{\alpha}(E) = i[\Sigma_s(E) - \Sigma_d(E)] \) \( (\alpha = s, d) \). We adopt the recursive Green function algorithm for calculating the Green function \( G(E) \) [13].

The three-dimensional potential profile is self-consistently determined with the NEGF transport equation. Poisson equation is solved with the Neumann boundary condition on the surfaces except on the gate electrodes where the Dirichlet boundary condition is applied. Since the nanoribbon width considered in the present study is very narrow, we neglect the \( y \)-dependence of the potential profile in the channel region.

4. Results and discussion

Figure 3 shows the calculated electron density spectra and the \( V_g \)-dependence of the one-dimensional electron density, \( n_{1D} \), at \( T = 300 \text{ K} \). As can be seen in Fig. 3(a), electrons

![Figure 3](image-url)

Figure 3: (a) Electron density spectra (palette color mapped image) and the band-edges (solid lines) for A-GNR \( (N = 18) \) FET. (b) One-dimensional electron density at the source edge (solid lines), at the drain edge (dashed lines), and at the bottleneck point (dotted lines). Red for A-GNR \( (N = 18) \), green for A-SiNR \( (N = 6) \), and blue for A-GeNR \( (N = 6) \).
mainly occupy the lowest subband due to a large subband separation. We see in Fig. 3(b) that \(n_{1D}\) are almost equal among A-GNR, A-SiNR, and A-GeNR FETs. We also see in Fig. 3(b) that \(n_{1D}\) at the source- and the drain-edges are weakly affected by \(V_g\) and that \(n_{1D}\) at the drain-edge is slightly smaller than that at the source-edge. These features can be attributed to the device structure in which the carrier density is controlled mainly by the back-gate bias (see Fig. 1).

Figure 4 shows (a) the transfer characteristics and (b) the transconductance at \(T = 300\) K. We find that the A-GNR FET exhibits the largest ON-current, \(I_{ON}\), and the largest maximum transconductance. This can be attributed to the fact that the A-GNR has the smallest effective-mass (see Fig. 2(b)). Note that the one-dimensional electron densities are almost equal among A-GNR, A-SiNR, and A-GeNR FETs (see Fig. 3(b)) and the difference in \(I_{ON}\) is mainly determined by the difference in the electron velocity. The small difference between \(I_{ON}\) of A-SiNR FET and that of A-GeNR FET can be attributed to the threshold-voltage difference due to the small \(E_g\) difference (see Fig. 2(b)). We see in Fig. 4(a) that the OFF-current, \(I_{OFF}\), of the A-GNR FET is significantly larger than that of the A-SiNR and that of A-GeNR FET. This is due to the large tunneling current in the A-GNR FET as shown in Fig. 5, where we can clearly see that the tunneling component dominates in the A-GNR FET. Note that the fact that the smaller effective-mass leads to the large S-D tunneling and its impact on the device performance have been extensively discussed in a context of the conventional semiconductor FET scaling [14].

5. Conclusion

We investigated ballistic performance of A-GNR, A-SiNR, and A-GeNR FETs with a gate-length of 10 nm. We find that the A-GNR FET has the largest ON-current when we compare...
Figure 5: Conduction-band edge profile (solid lines) and the current density spectra $J(E)$ (dotted lines) for (a) A-GNR, (b) A-SiNR, and (c) A-GeNR FETs. The tunneling component appearing in $J(E)$ at $E \approx 0$ eV dominates in A-GNR FET.

FETs with a nanoribbon channel having a nearly equal band-gap $E_g \approx 0.5$ eV. The A-GNR FET exhibits the largest OFF-current due to the smallest effective-mass enhancing the source-drain direct tunneling.

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