Progress on quantum transport simulation using empirical pseudopotentials

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I. I NTRODUCTION

After performing one-dimensional simulation of electron transport in narrow quantum wires without gate control in Ref [1], [2] using the open boundary-conditions full-band plane-wave transport formalism derived in Ref [3], we now extend the work to simulate three-dimensionally field-effect transistors (FETs) with a gate bias applied and obtain their transport characteristics. We optimize multiple procedures for solving the quantum transport equation (QTE), such as using a selected eigenvalue solver, the fast Fourier transform (FFT), block assignment of matrices, a sparse matrix solver, and parallel computing techniques. With an expanded computing capability, we are able to simulate the transistors in the sub-1 nm technology node as suggested by the ITRS [4], which features ∼5 nm physical gate length, ∼2 nm body thickness, ∼0.4 nm effective oxide thickness (EOT), ∼0.6 V power supply voltage, and a multi-gate structure. Here we simulate an armchair graphene nanoribbon (aGNR) FET using a gate-all-around architecture and obtain its transport properties. We will discuss the numerics concerning the matrix size of the transport equation, memory consumption, and simulation time.

II. T HEORY

As shown in Ref. [2], the Schrödinger equation describing the electronic band structure in one-dimensional (1D) nanosstructures in the (x-z) plane, surrounded by a large vacuum padding in the (x-y) plane to decouple the structures, using the empirical pseudopotential method is

$$\sum_{G'} \left( \frac{\hbar^2}{2m} |k + G'\rangle \delta_{G'G} + V_{lat}(G'G) \right) u^G_{k'} = E_k u^G_k,$$  \hspace{1cm} (1)

where \( k = (0, 0, k_z) \) is the wavevector along the axial z-direction. This constitutes an eigenvalue problem of rank given by the number of reciprocal-space vectors \( N_G \) within the energy-cutoff sphere of radius \( E_{cut} \). The QTE describing the 1D electron transport along the z direction is a linear system of the form

$$\begin{pmatrix} -\Delta H & \Sigma_L & \Sigma_R \end{pmatrix} \begin{pmatrix} \Sigma_R \end{pmatrix} \phi = [\text{RHS}]_{\Sigma_L}^{[\text{inj}]} + [\text{RHS}]_{\Sigma_R}^{[\text{inj}]},$$  \hspace{1cm} (2)

where \( \Sigma_L, \Sigma_R, \Sigma_D \) are the self-energies of the contacts, \( \phi \) is the envelope wavefunction, and \([\text{RHS}]_{\Sigma_L}^{[\text{inj}]} \) and \([\text{RHS}]_{\Sigma_R}^{[\text{inj}] \Sigma_D} \) are the terms representing the amplitudes of the waves injected from the contacts (self-energies). Using finite difference (FD) and discretizing a device into \( N_z \) slices along the transport direction with a step-size \( \Delta \), the Hamiltonian \( H \) takes a block tridiagonal form

$$H = \begin{bmatrix} T^- & D^{-1} & T^+ & 0 & 0 & \cdots \nolimits & \cdots \\ 0 & T^- & D^0 & T^+ & 0 & \cdots \\ 0 & 0 & T^- & D^1 & T^+ & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$  \hspace{1cm} (3)

where the operator \( D^i \) is a dense matrix of rank \( N_G \) that includes the lattice and external potential (gate and source/drain bias) in the i-th slice, and the Hermitian operators \( T^+ \) and \( T^- \) are diagonal matrices also of rank \( N_G \). Therefore, the rank of \( H \) is \( N_G \times N_z \). The self-energy matrix \( \Sigma_L \) is added to \( D^1 \) and \( \Sigma_R \) is added to \( D^N \). Solving Eq. (2) and Poisson’s equation self-consistently for different drain-source bias and gate bias, the current-voltage characteristics of the device can be obtained. Since we have not yet implemented in our computer program the capability to account for bound and quasi-bound states, we are unable to perform full self-consistent calculations. Therefore, for now we solve Eq. (2) with an external potential obtained from a self-consistent calculation within a simple semiclassical drift-diffusion approximation. This is performed by solving the two-dimensional Schrödinger equation in all slices, calculating the charge density using local quasi-Fermi level, and then solving Poisson’s equation to update the potential. An approximate device current is calculated from the obtained envelope wavefunctions \( \phi \).

III. S IMULATIONS AND RESULTS

An atomistic model of an aGNR with six dimer lines along the width direction \( x \) is shown in Fig. 1a and a device model of 6-aGNRFET is shown in Fig. 1b. The channel has \( p^+ \) doping and the source and drain contact have \( n^+ \) doping. The discretization is shown in Fig. 1c and 1d. The band structure of the 6-aGNR is calculated by solving Eq. (1) and shown in Fig. 2. The self-consistent external potential and charge distribution within the aforementioned semiclassical drift-diffusion simplification are shown in Fig. 3 and their distribution after non-equilibrium quantum transport simulation are shown in Fig. 4. The I-V characteristics are shown in Fig. 5. Some information about the numerical details of the calculations is shown in Table. I.
Fig. 1: Device model of 6-aGNRFET with an overall length $L=30a_3=12.78$ nm, a physical channel length $L_g=5.12$ nm, a body width $W=0.62$ nm, and an EOT=0.62 nm. Electron transport is along the $z$ direction. The device is discretized along $z$ into $N_z=121$ slices with $\Delta z=a_3/4=0.11$ nm and discretized in the cross-sectional ($x$-$y$) plane using a finite element mesh. Notice that this particular triangular mesh is used to calculate the bands in the interesting energy range, and FFT calculations.

Fig. 2: The electronic dispersion of the first six low-energy conduction bands (CBs) is shown in (a). Within 100 meV from the bottom of the CB, only one conducting channel is observed. The electron probability distribution $|\psi(r_j)|^2$ is shown in (b). This is obtained by averaging the square of the cross-sectional wavefunction over one unit cell along $z$. A selected eigenvalue solver from IBM ESSL package is used to calculate the bands in the interesting energy range, and FFT is used to calculate $|\psi(r_j)|^2$ from Eq. (1).

Fig. 3: Approximate potential and charge distribution, averaged along $y$, in the ($x$-$z$) plane after self-consistent calculation with the semiclassical assumption for a 6-aGRNFET with a drain-source bias $V_{DS}=0.4$ V and a gate bias $V_{GS}=0.2$ V.

Fig. 4: Potential and charge distribution, averaged along $y$, in the ($x$-$z$) plane from Eq. (2) for a 6-aGRNFET. Quasi-bound states can be observed in the region close to the drain contact. Note that variation of the electron density corresponds to the location of individual atoms.

Fig. 5: Current-voltage characteristics of a 6-aGRNFET.

**TABLE I: Rank of the matrices, simulation time, and memory consumption when simulating a 6-aGRNFET**

<table>
<thead>
<tr>
<th>$N_G$</th>
<th>$t_s$ (s, Eq. (1))</th>
<th>$t_h$ (h)</th>
<th>LDM</th>
<th>$t_h$ (h)</th>
<th>Memory (GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>701</td>
<td>10</td>
<td>2.5&lt;sup&gt;a&lt;/sup&gt;</td>
<td>84821</td>
<td>0.2&lt;sup&gt;b&lt;/sup&gt;</td>
<td>5.0&lt;sup&gt;c&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup> Simulation time required to obtain the starting potential self-consistently for each applied bias.
<sup>b</sup> Simulation time required to solve Eq. (2) for a single injection energy. E. MPI is used to solve Eq. (2) in parallel for all the injection energies.
<sup>c</sup> Peak memory required to solve Eq. (2). A sparse matrix solver UMFPACK is used to save memory.

**REFERENCES**


