Deterministic Boltzmann Equation Solver for Graphene Sheets Including Self-Heating Effects

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Abstract: A deterministic Boltzmann equation solver for graphene sheets is developed. The self-heating effect is included. The Boltzmann transport equation is expanded with the Fourier harmonics. The remote phonon scattering as well as the intrinsic phonon scatterings are considered. The angle-dependent term of the remote phonon scattering is accurately implemented. Impact of the maximum order of the Fourier harmonics expansion on the simulation results is demonstrated. Negative differential mobility is clearly observed in the simulation with the self-heating effect.

Introduction: The quasi-ballistic transport simulation of the monolayer graphene sheet has gained much research interest [1]-[10]. The mobility calculation with the relaxation time approximation can be performed easily in the low-field regime. However, when the high-field transport is of concern, the full solution of the Boltzmann transport equation should be obtained. For this purpose, the Monte Carlo method has been widely adopted [3] [5]-[7] [9] [10]. As an alternative choice to the Monte Carlo, the deterministic Boltzmann solver can be found [11].

In this work, we present the simulation results for the monolayer graphene sheet, obtained by our in-house graphene simulator, which is a deterministic Boltzmann equation solver based on the Fourier harmonics expansion.

Simulation framework: We have implemented an in-house Boltzmann equation solver based on the Fourier harmonics expansion [11]. Throughout this work, the H-transformation is applied to get the stabilized scheme. In order to employ the H-transformation in the graphene sheet simulation, the special boundary condition is imposed as shown in Fig. 1.

The remote phonon scattering as well as the intrinsic phonon scatterings are considered. Note that the remote phonon scattering is anisotropic. Without relying on the analytical approximation, the scattering rate (including the Thomas-Fermi screening) is expanded with the Fourier harmonics numerically. The impurity scattering is neglected.

When the self-heating effect is taken into account, an outer loop for the graphene temperature is solved [12]. For a 300 nm-thick SiO_2 substrate, the lumped thermal resistance of 2.8×10^{-7} m^2 K W^{-1} is used [13].

Isothermal result: In order to verify the correctness of our implementation, the simulation results are compared with those obtained by Monte Carlo simulations [7] [14]. Since these Monte Carlo simulations are isothermal, the self-heating effect is also neglected in our simulation. Fig. 2 shows the low-field mobility as a function of the electron density. Two cases – suspended graphene and graphene on SiO_2 substrate – are considered. In the case of the suspended graphene, only the intrinsic phonon scatterings in the graphene are considered. Fig. 3 shows the drift velocity of the suspended graphene as a function of the applied electric field. When the maximum order of the Fourier harmonics expansion (mmax) is 1, the drift velocity is overestimated. However, with the mmax of 3 or 5, excellent agreement is obtained. Similar result for the graphene on the SiO_2 substrate is shown in Fig. 4. The electron distribution is shown in Fig. 5. The centroid of the distribution is shifted by ~0.3 nm^{-1} in this case.

Electron velocity at a high electric field (20 kV cm^{-1}) is shown in Fig. 6. Impact of the deformation potential of the acoustic phonon scattering is estimated. For the nominal value (6.8 eV in [14]), the high-field velocity shows a moderate decrease. This trend was previously reported in [7]. When a higher value for the deformation potential (25 eV in [12]) is adopted, although the absolute value is reduced, the reduction ratio does not change significantly.

Self-heating result: With the self-heating effect the high-field behavior of the drift velocity changes considerably, as shown in Fig. 7. Compared to the isothermal simulation results in Fig. 4, the negative differential mobility becomes more prominent in the simulation with the self-heating effect.

Fig. 8 shows the graphene temperature as a function of the electric field. As the electric field becomes larger, the graphene temperature is elevated. In this example, the temperature can be as large as 700 K at an electric field of 20 kV cm^{-1}. A simple estimation from the isothermal simulation result fails for high electric fields.

Conclusion: The deterministic Boltzmann equation solver for the graphene sheet has been developed. The self-heating effect has been included by solving the thermal resistance equation. Excellent agreement with previous Monte Carlo results has been obtained. It has been shown that the high-field saturation behavior is affected by the self-heating effect considerably.

Reference:

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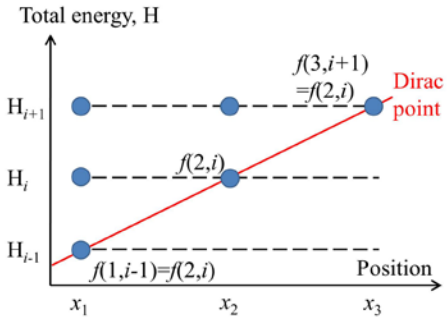

Fig. 1. Discretization scheme adopted in this work. For boundary points in the real space, the distribution at the center point is referred with shifting the energy index.

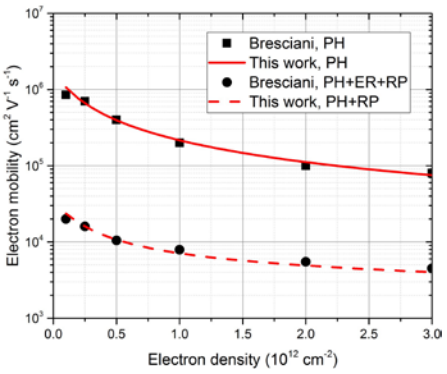

Fig. 2. Electron mobility as a function of the electron density. Scattering parameters are adjusted to [7].

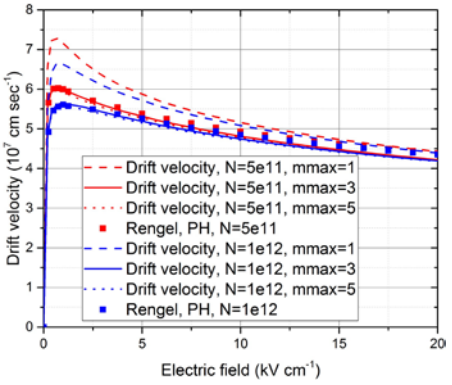

Fig. 3. Drift velocity as a function of the applied electric field for electron density of 10^{12} cm^{-2}. The suspended graphene is assumed.

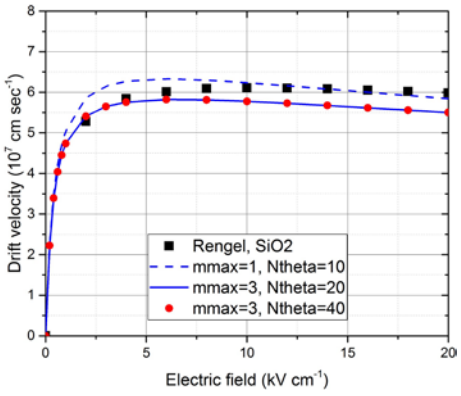

Fig. 4. Drift velocity as a function of the applied electric field for electron density of 10^{12} cm^{-2}. The monolayer graphene on the SiO_2 substrate is assumed.

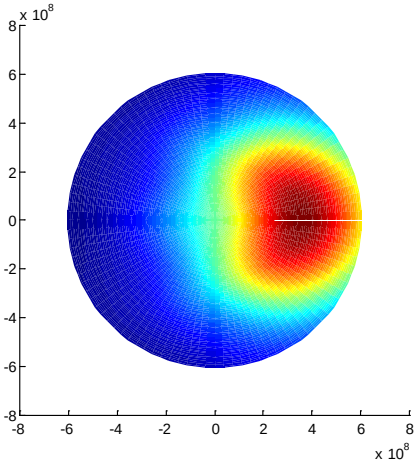

Fig. 5: k-space distribution function (shown only up to 0.4 eV for clarity) at an electric field of 20 kV cm^{-1}. The electron sheet density is 10^{12} cm^{-2}. (mmax=5)

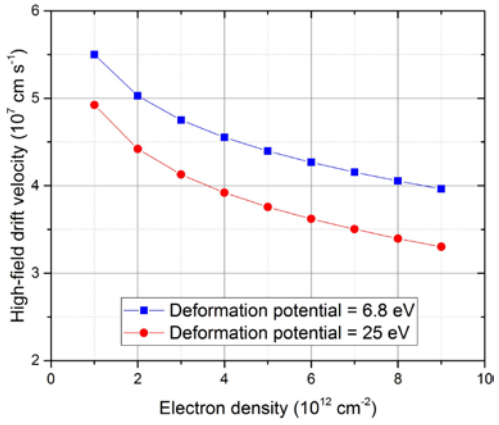

Fig. 6. Velocity at an electric field of 20 kV cm^{-1}. Two different values of the deformation potential (6.8 eV and 25 eV) of the acoustic phonon scattering are considered.

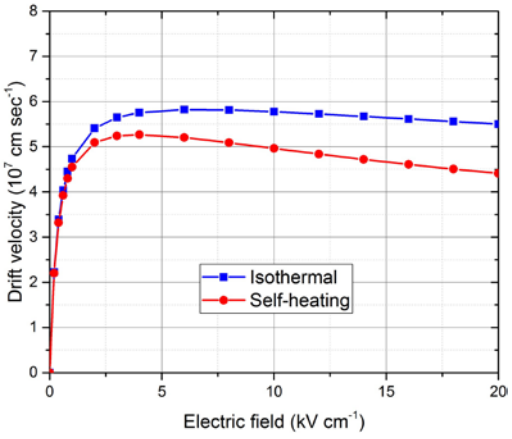

Fig. 7. Impact of the self-heating on the drift velocity. The monolayer graphene on the SiO_2 substrate is assumed.

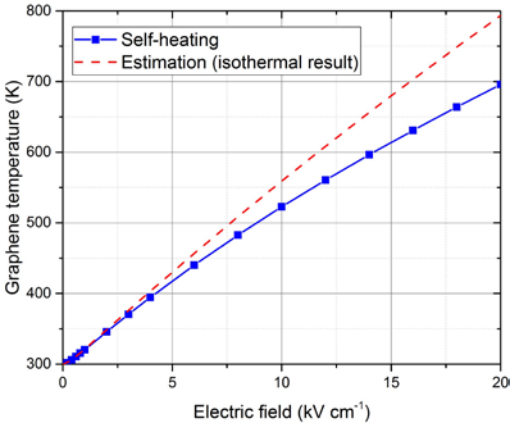

Fig. 8 Graphene temperature as a function of the electric field. Estimation from the isothermal simulation result is also shown.