Simulation of Semiconductor Processes and Devices 2016
Edited by E. Bär, J. Lorenz, and P. Pichler

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

Sung-Min Hong and Suhyeong Cha
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology
Gwangju, Republic of Korea
Email: smhong@gist.ac.kr

***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.**

***Keywords*—Graphene; Boltzmann transport equation; Remote phonon scattering; Self-heating effect**

I. 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]. Especially, when the graphene sheet is placed on top of a substrate layer, dominant impact of the remote phonon scattering on the electron transport has been extensively investigated.

As much as the solution technique for the Boltzmann transport equation is involved, the Monte Carlo method is not the only available method. As an alternative choice to the Monte Carlo, the deterministic Boltzmann solver can be found [11]. The Pauli principle can be naturally incorporated in the deterministic approach, because the distribution function is determined at every discretized point [12].

In this work, we present 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. In order to gain better understanding on the velocity saturation, the lattice temperature is considered as an unknown variable. In [13], the same problem was addressed with a hydrodynamic model.

The structure of this extended abstract is as follows: In Section II, the simulation framework is briefly introduced. The isothermal results are shown in Section III. The self-heating simulation results are shown in Section IV. Finally, the conclusion is made in Section V.

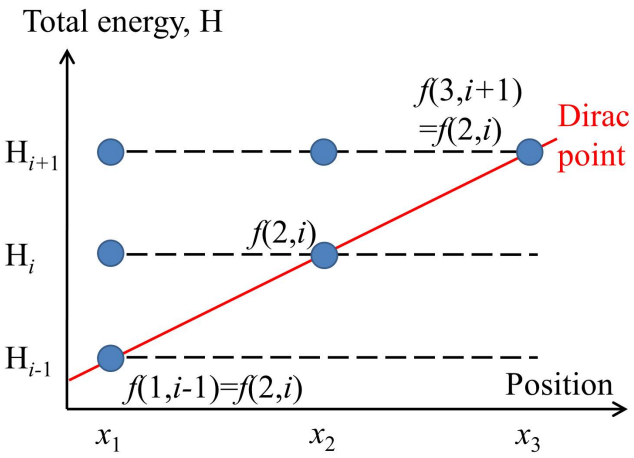

Fig. 1. Discretization scheme adopted in this work. For boundary points in the real space, the distribution at the center point is referred. The product of the electric field and the node spacing in the real space is chosen to be identical to the energy spacing (written in eV).

II. Simulation Framework

Since the graphene has a two-dimensional momentum space, the angle dependency of transport parameters (such as the density-of-states, the scattering rate, and the distribution function) should be resolved with a set of basis functions. We have implemented an in-house Boltzmann equation solver based on the Fourier harmonics expansion [11]. Throughout this work, the H-transformation [11] [14] is applied to get the stabilized scheme. Adoption of the H-transformation makes the future extension to the nanoscale device simulation easier.

In order to employ the H-transformation in the graphene sheet simulation, the special discretization scheme is employed, as shown in Fig. 1. Three points (x_1, x_2, and x_3 in the figure) are assigned in the real space. For the center point (x_2), the Boltzmann transport equation is written in a conventional way. For boundary points in the real space (x_1 and x_3), the distribution at the center point is referred. In the case depicted in Fig. 1, the boundary conditions are given by

$$f(1, i-1) = f(2, i) = f(3, i+1), \tag{1}$$

978-1-5090-0818-6/16/$31.00

where $f(i_x, i_H)$ is the distribution function defined at the (i_x,i_H) point. By considering the three-point device with appropriate boundary conditions, it is possible to simulate the graphene sheet without significant modification of the device simulation code.

The linear dispersion relation of the graphene sheet is assumed without any correction. For an electron whose momentum is given by $\mathbf{k}$,

$$\varepsilon_k = \hbar v_F k, \tag{2}$$

where ε_k is the kinetic energy of an electron and $k = |\mathbf{k}|$. A small spacing of 5 meV is used in the simulation. The Fermi velocity (v_F) of 10^6 m sec^{-1} is used. Since the Fermi energy level is assumed to be located well above the Dirac point, only the electron transport is taken into account.

The intrinsic phonon scatterings, such as intravalley acoustic phonons, optical phonons, and intervalley acoustic phonons, are considered. Their model parameters are taken from [15] and [16], unless stated otherwise. In addition to the intrinsic phonon scatterings, the remote phonon scattering are considered. Note that the remote phonon scattering is anisotropic. Its transition rate from $\mathbf{k}$ to $\mathbf{k}'$, $S(\mathbf{k}'|\mathbf{k})$, is given by

$$S(\mathbf{k}'|\mathbf{k}) = A_{\pm}\frac{\exp(-2qd)}{2(\epsilon(q))^2 q}(1+\cos\theta)\delta(\varepsilon_{k'} - \varepsilon_k \pm \hbar\omega), \tag{3}$$

where $A_{\pm}$ is a proportional coefficient, $q = |\mathbf{k}' - \mathbf{k}|$ is the momentum transfer, d is the distance between the graphene layer and the substrate, $\epsilon(q)$ is the dielectric function, θ is the angle difference, $\hbar\omega$ is the phonon energy, and $\delta(\cdot)$ is the Dirac delta function. The upper sign is for the phonon absorption, while the lower one is for the phonon emission.

The angle dependency of $S(\mathbf{k}'|\mathbf{k})$ cannot be expanded with the Fourier harmonics easily in an analytic form. Therefore, without relying on the analytical approximation, the transition rate (including the Thomas-Fermi screening) is expanded with the Fourier harmonics numerically. For this purpose, the angle variable is discretized with a predefined value of Ntheta. The impurity scattering is neglected.

III. Isothermal Results

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. Scattering parameters are adjusted to [7]. 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. In this case, the remote phonon scattering is suppressed. 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 with the Monte Carlo results is obtained.

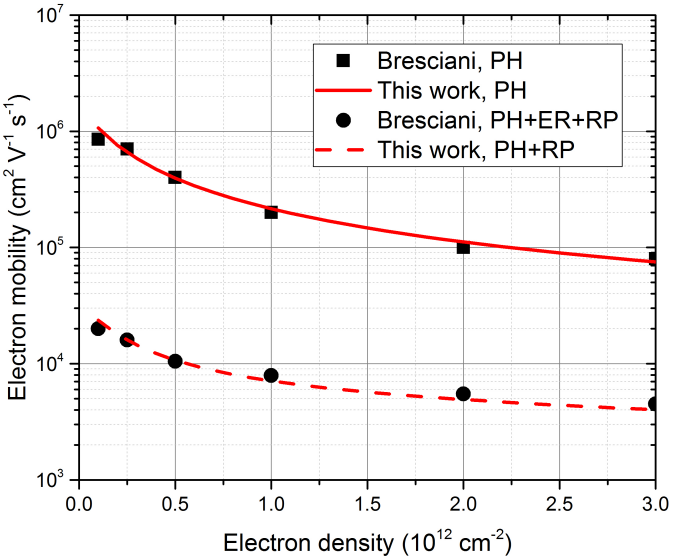

Fig. 2. Electron mobility as a function of the electron density. Scattering parameters are adjusted to [7]. (Isothermal)

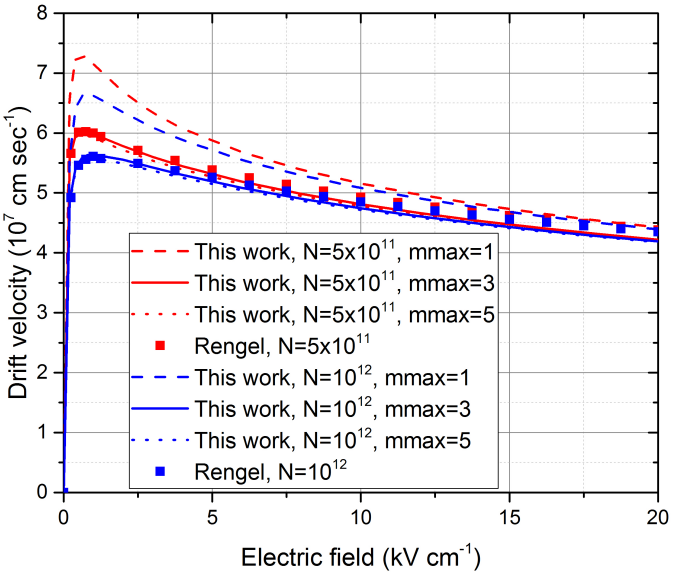

Fig. 3. Drift velocity as a function of the applied electric field for electron densities of 5×10^{11} cm^{-2} and 10^{12} cm^{-2}. The suspended graphene is assumed. (Isothermal)

Similar result for the graphene on the SiO2 substrate is shown in Fig. 4. Moreover, the impact of Ntheta is rather small for the simulated values (10, 20, and 40). Of course, for the nanoscale devices, the impact of mmax and Ntheta should be carefully investigated.

The electron distribution is shown in Fig. 5. The electric field strength is 20 kV cm^{-1}. 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

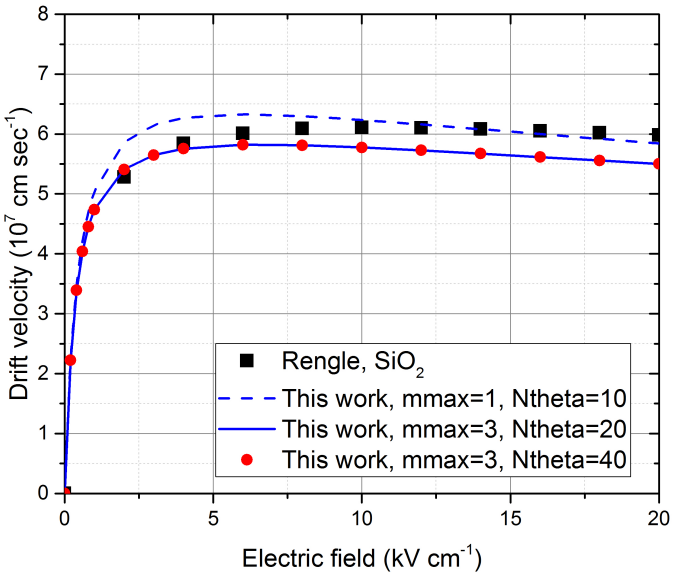

Fig. 4. Drift velocity as a function of the applied electric field for electron density of 10^{12} cm^{-2}. The monolayer graphene on the SiO_2 substrate is assumed. (Isothermal)

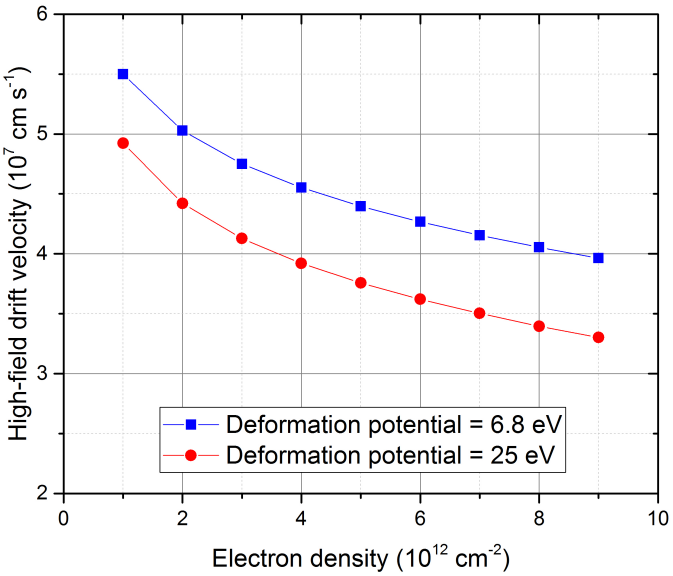

Fig. 6. Velocity at an electric field of 20 kV cm^{-1}. Two different values of the deformation potential (6.8 eV and 25 eV) of the acoustic phonon scattering are considered.

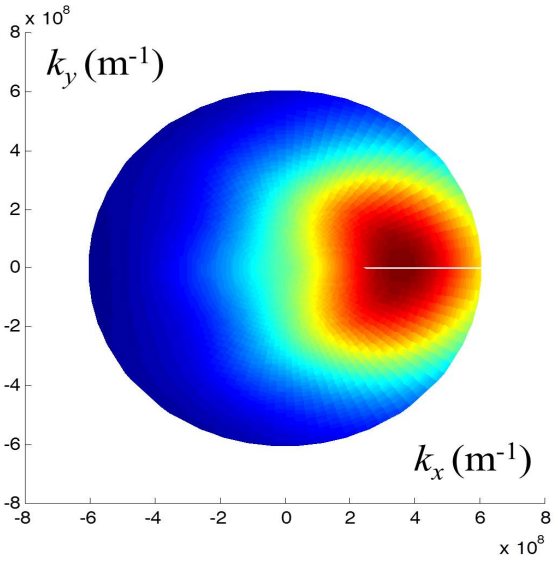

Fig. 5. Electron distribution function in the momentum space at an electric field of 20 kV cm^{-1}. For clarity, it is shown only up to 0.4 eV. The SiO_2 substrate is considered. The electron sheet density is 10^{12} cm^{-2}.

acoustic phonon scattering is estimated. For the nominal value (6.8 eV in [16]), 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 [13]) is adopted, although the absolute value is reduced, the reduction ratio does not change significantly.

IV. Self-Heating Results

When the self-heating effect is taken into account, an outer loop for the graphene temperature is solved [13]. For a background temperature of T_0, the graphene temperature $T_{graphene}$ is obtained by

$$T_{graphene} = T_0 + R_{thermal} P, \tag{4}$$

where $R_{thermal}$ is the lumped thermal resistance and P is the dissipated power per unit area. For a 300 nm-thick SiO_2 substrate, the lumped thermal resistance of 2.8×10^{-7} m^2 K W^{-1} is used [17].

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 non-self-consistent estimation for the graphene temperature, which is based on the isothermal simulation result, fails for high electric fields. It demonstrates the necessity of the self-consistent solution.

V. Conclusion

The deterministic Boltzmann equations 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 saturaton behavior is affected by the self-heating effect considerably.

Acknowledgment

This work was supported by the EDISON Program (Grant No. 2012M3C1A6035304) and the Pioneer Research Center

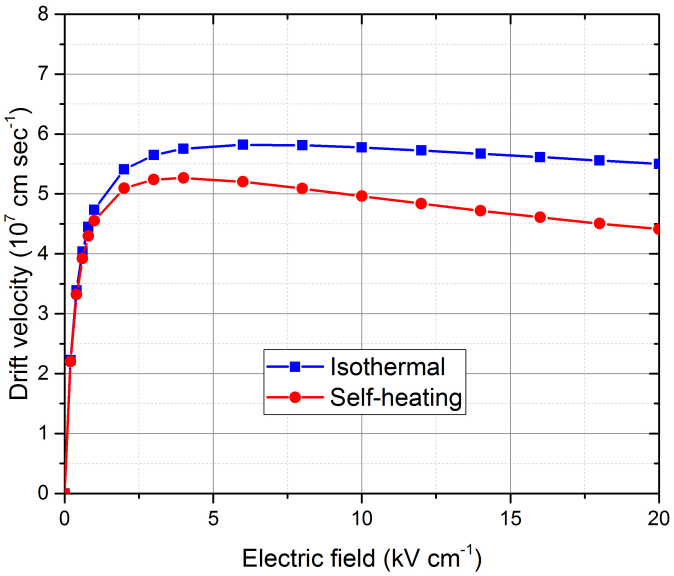

Fig. 7. Impact of the self-heating on the drift velocity. The monolayer graphene on the SiO_2 substrate is assumed.

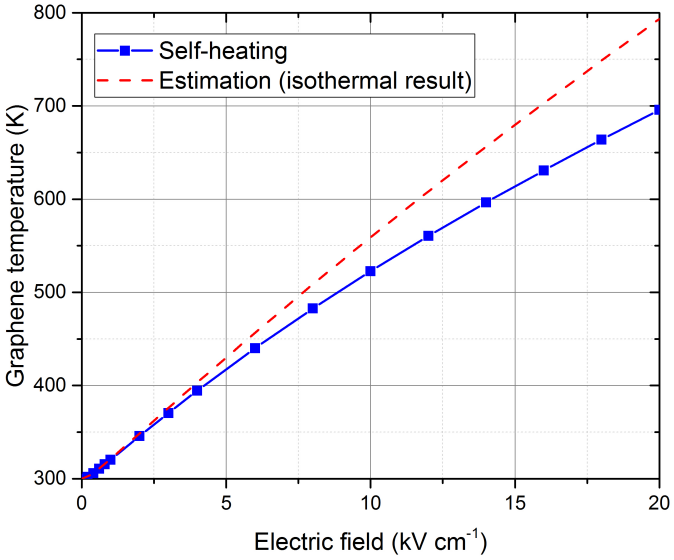

Fig. 8. Graphene temperature as a function of the electric field.

Program (Grant No. 20120009603) through the National Research Foundation of Korea funded by the Ministry of Science, ICT & Future Planning.

References

[1] E. H. Hwang and S. Das Sarma, "Acoustic phonon scattering limited carrier mobility in two-dimensional extrinsic graphene," Physical Review B, vol. 77, p. 115449, 2008.

[2] S. Fratini and F. Guinea, "Substrate-limited electron dynamics in graphene," Physical Review B, vol. 77, p. 195415, 2008.

[3] J. Chauhan and J. Guo, "High-field transport and velocity saturation in graphene," Applied Physics Letters, vol. 95, p. 023120, 2009.

[4] A. Konar, T. Fang, and D. Jena, "Effect of high- gate dielectrics on charge transport in graphene-based field effect transistors," Physical Review B, vol. 82, p. 115452, 2010.

[5] X. Li, E. A. Barry, J. M. Zavada, M. Buongiorno Nardelli, and K. W. Kim, "Surface polar phonon dominated electron transport in graphene," Applied Physics Letters, vol. 97, p. 232105, 2010.

[6] M. Bresciani, P. Palestri, D. Esseni, B. Szafranek, and D. Neumaier, "Interpretation of graphene mobility data by means of a semiclassical Monte Carlo transport mode," Solid-State Electronics, vol. 89, pp. 161-166, 2013.

[7] M. Bresciani, A. Paussa, P. Palestri, D. Esseni, and L. Selmi, "Low-field mobility and high-field drift velocity in graphene nanoribbons and graphene bilayers," International Electron Device Meeting, pp. 724-727, 2010.

[8] Z.-Y. Ong and M. V. Fischetti, "Theory of remote phonon scattering in top-gated single-layer graphene," Physical Review B, vol. 88, p. 045405, 2013.

[9] H. Hirai, H. Tsuchiya, Y. Kamakura, and N. Mori, "Electron mobility calculation for graphene on substrates," Journal of Applied Physics, vol. 116, p. 083703, 2014.

[10] R. Rengel, E. Pascual, and M. J. Martín, "Influence of the substrate on the diffusion coefficient and the momentum relaxation in graphene: The role of surface polar phonons," Applied Physics Letters, vol. 104, p. 233107, 2014.

[11] S.-M. Hong, A.-T. Pham, and C. Jungemann, Deterministic Solvers for the Boltzmann Transport Equations, Springer-Verlag, 2011.

[12] S.-M. Hong and C. Jungemann, "Inclusion of the Pauli principle in a deterministic Boltzmann equation solver based on a spherical harmonics expansion," Journal of Computational Electronics, vol. 9, pp. 153-159, 2010.

[13] A. Y. Serov, Z.-Y. Ong, M. V. Fischetti, and E. Pop, "Theoretical analysis of high-field transport in graphene on a substrae." Journal of Applied Physics, vol. 116, p. 034507, 2014.

[14] A. Gnudi, D. Ventura, G. Baccarani, F. Odeh, "Two-dimensional MOS-FET simulation by means of a multidimensional spherical harmonics expansion of the Boltzmann transport equation," Solid-State Electronics, vo. 36, p. 575-581, 1993.

[15] K. M. Borysenko, J. T. Mullen, E. A. Barry, S. Paul, Y. G. Semenov, J. M. Zavada, M. Buongiorno Nardelli, and K. W. Kim, "First-principles analysis of electron-phonon interactions in graphene," Physical Review B, vol. 81, p. 121412, 2010.

[16] R. Rengel, C. Couso, and M. J. Martín, "A Monte Carlo study of electron transport in suspended monolayer graphene," Spanish Conference on Electron Devices, pp. 175-178, 2013.

[17] V. E. Dorgan, M.-H. Bae, and E. Pop, "Mobility and saturation velocity in graphene on SiO_2," Applied Physics Letters, vol. 97, p. 082112, 2010.