Kinetic Transport Model with Carrier-Carrier Scattering for Graphene Terahertz/Photonic Device Simulation

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INTRODUCTION

Device applications of graphene utilizing its unique electronic/optical properties have been investigated extensively. We have studied terahertz (THz) lasers and active plasmonic devices [1] based on interband population inversion in graphene, as well as photonic double-mixers [2] for optical-electrical signal conversion utilizing its very high mobility. The carrier-carrier (CC) scattering is one of the most important scattering mechanisms in graphene that influence on operation principles of those devices. For the THz lasers and active plasmonic devices, the fast quasi-equilibration of carriers by the CC scattering hinders population inversion in the THz region with optical pumping [3]. In photonic detectors and mixers, the photogenerated current is in general not conserved because the individual CC scattering conserves the total momentum but not the total velocity due to the linear dispersion [4]. Numerical simulation taking into account the CC scattering as well as other scattering mechanisms is inevitable to reveal its role on operation principles and performances of those graphene-based devices.

In this paper, we develop a kinetic transport model with the CC scattering based on a deterministic solution approach for the semi-classical Boltzmann equation and on the direct evaluation of the CC collision integral. Using the model, we conduct a transient simulation of photogenerated carriers and show that the current density is increased during the quasi-equilibration of initially non-equilibrium carrier distributions.

MODEL AND NUMERICAL METHODS

For a first step towards the development of a device simulation model with the CC scattering, we start from a spatially homogeneous case without any other scattering mechanisms (its extension to the inhomogeneous case and inclusion of other scattering mechanisms are straightforward, although the former is computationally more expensive). Our model is based on semi-classical Boltzmann equations for electrons and holes:

$$\frac{\partial f_{c\boldsymbol{p}}}{\partial t} = \sum_{c'=e,h} J_{cc'}, \tag{1}$$

where $f_{c\boldsymbol{p}}$ is the distribution function for carrier type c (e and h for electrons and holes, respectively). Here, $J_{cc'}$ is the collision integral for c-c' scattering:

$$\begin{aligned} J_{cc'}(\boldsymbol{p}) = \frac{4}{(2\pi\hbar)^4} \int d^2\boldsymbol{p}_1 \int d^2\boldsymbol{p}' W_{cc'}(\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}',\boldsymbol{p}'_1) \\ \times \left[f_{c\boldsymbol{p}'} f_{c'\boldsymbol{p}'_1} (1-f_{c\boldsymbol{p}})(1-f_{c'\boldsymbol{p}_1}) \right. \\ \left. - f_{c\boldsymbol{p}} f_{c'\boldsymbol{p}_1} (1-f_{c\boldsymbol{p}'})(1-f_{c'\boldsymbol{p}'_1}) \right] \end{aligned} \tag{2}$$

with $\boldsymbol{p}'_1 = \boldsymbol{p} + \boldsymbol{p}_1 - \boldsymbol{p}'$ and $W_{cc'}$ being the Coulomb scattering probability. $W_{cc'}$ contains a delta function representing the energy conservation, $\delta(p + p_1 - p' - p'_1)$, so that Eq. (2) reduces to a triple integral. For simplicity, we consider the Thomas-Fermi screening for the Coulomb scattering. The momentum space is descritized by grids in the p- and θ-directions with grid points $N_p = 192$ and $N_\theta = 80$, and Eq. (1) is solved numerically first by evaluating $J_{cc'}$ at each point (p_i, θ_j) in parallel and then by applying the third-order TVD Runge-Kutta scheme [5] for the time-step update.

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For a transient simulation of photocarriers generated by an optical pulse, we consider initial distribution functions of intrinsic graphene with photoexcited electrons and holes, $f_{c\boldsymbol{p}}|_{t=0} = [1 + \exp(v_F p/k_B T)]^{-1} + f_{ph} g(\theta) \exp[-(v_F p - \hbar\Omega/2)^2/(\hbar\Delta\Omega)^2]$, where $\hbar\Omega$ and $\hbar\Delta\Omega$ are the photon energy of the pulse and its spectral width, f_{ph} is a parameter characterizing the pulse intensity, and $g(\theta)$ represents the angular distribution of photogenerated carriers with θ being the angle between $\boldsymbol{p}$ and x-direction. Here, we artificially set an angularly asymmetric distribution $g = \exp(-\theta^2)$ which produces a nonzero initial photocurrent in the x-direction, in order to demonstrate the deviation of the current density from its initial value in time. This corresponds roughly to the situation where photogenerated electrons and holes are spatially separated by strong electric field in graphene right after the pulse excitation. In this situation, we can assume $J_{eh} \simeq 0$ and $f_e = f_h$ at any time.

RESULTS

We conducted a simulation described above with the following parameters: $f_{ph} = 0.1$, $\hbar\Omega = 0.8$ eV, $\Delta\hbar\Omega = 0.02$ eV, the initial temperature $T = 300$ K, and the dielectric constant $\epsilon = 4$. Figure 1 shows the electron distribution function as a function of the electron energy $\varepsilon = v_f p$ and the angle θ at different times. It is seen in Fig. 1 that the initial distribution with photongenerated electrons near $\varepsilon = \hbar\Omega/2$ is equilibrated in the p-direction very fast within the time scale of 100 fs, resulting in a very broad (hot) distribution in the p-direction. On the other hand, the quasi-equilibration in the θ-direction is much slower than that in the p-direction. This originates from the small-angle nature of the Coulomb scattering.

Figure 2 shows the x-component of the current density as a function of time, calculated from the distribution function. It is clearly seen that with the parameters used the current density increases about 44% after the pulse photoexcitation. We emphasize that accuracies of all the conservative quantities (concentration, energy density, x- and y-components of momentum density) were within 1.5%, so that the deviation of the current density is not due to numerical error. This increase can be utilized for optimizing the output current in photonic detectors and mixers. The result obtained demonstrates the importance of the CC scattering on graphene-based photonic devices and the necessity of further development of the device simulation model.

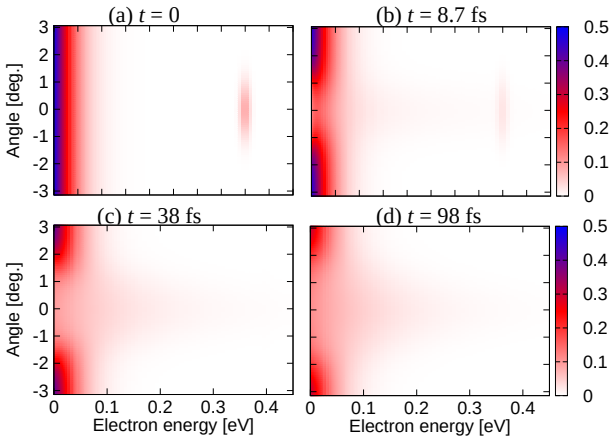

Fig. 1. Electron distribution function at (a) $t = 0$, (b) 8.7 fs, (c) 38 fs, and (d) 98 fs.

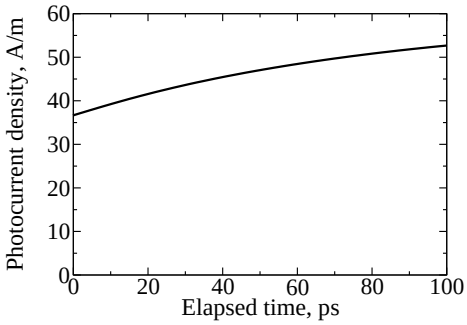

Fig. 2. Photocurrent density as a function of time.

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