Electro-Thermal Simulation of Graphene Nanoribbon Interconnects

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***Abstract*—The electro-thermal simulation of graphene nanoribbon (GNR) interconnects is presented in this paper. The Boltzmann transport equation (BTE) is solved under the relaxation time approximation (RTA). The power density, which is obtained by the Boltzmann–Poisson approach, is used as the Joule-heating source in heat conduction equation to calculate the temperature profile along the GNR. The result is then sent back to the BTE for updating the distribution function. This process is iterated until self-consistency is achieved. Based on this method, the current-voltage characteristics of metallic GNRs with different lengths and bias conditions are investigated.**

Keywords—Boltzmann transport equation (BTE), graphene nanoribbon (GNR), heat conduction equation, relaxation time approximation (RTA).

I. INTRODUCTION

In the last decade, carbon nanomaterials, such as carbon nanotube (CNT) and graphene nanoribbon (GNR) have aroused a lot of research interest for the next generation of interconnect applications [1]. For example, based on the basic Boltzmann transport equation (BTE) and combined with the dispersion relation for graphene, the current density distribution across the GNR structure was investigated in [2]. Nevertheless, solving the BTE is a heavy computational burden when dealing with complicated microscopic scattering processes. Recently, an effective technique has been proposed to relief this burden by employing the relaxation time approximation (RTA) [3]. The RTA can not only capture essential features of quasi-ballistic transport in the decananometer scale, but also enable us to obtain the solution of BTE in an efficient way.

On the other side, some approaches based on the compact equivalent circuit models have also proposed for the analysis of electrical characteristics of GNR interconnects, where the effects of conduction channels as well as edge roughness were considered [4]. This kind of methods, however, were under the simplified mean free path (MFP) assumption, which would lead to inaccurate results under high bias condition.

In this paper, a novel approach for the electro-thermal simulation of GNR interconnects is presented. The scattering term in the BTE is dealt with the RTA, which enables direct and efficient solution of the BTE. The current-voltage characteristics of GNRs are obtained by solving the coupled BTE, Poisson equation and heat conduction equation in a self-consistent way, where the effect of self-heating is taken into consideration. Thus, the proposed method can provide more accurate prediction of the current-voltage characteristics of GNR interconnects.

II. BTE-BASED SIMULATION OF GNRS

The layout of a GNR interconnect with length L and width w is shown in Fig. 1. Pd or Au metal can afford near Ohmic contacts to the GNR at two terminals.

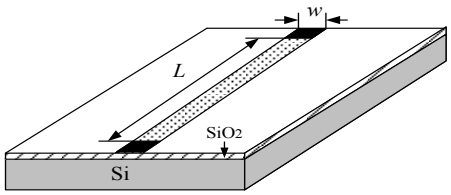

Fig. 1. The schematic of GNR interconnect located on the substrate.

Due to the confinement in the transverse direction of the GNR, we only consider the transport along the longitudinal direction. Ignoring the thickness of carbon atoms layer, the BTE of GNR can be written as:

$$\frac{\partial f}{\partial t}-\frac{e\xi(x)}{\hbar}\frac{\partial f}{\partial k}+v(k)\frac{\delta f}{\delta k}=J(F,f) \tag{1}$$

where e is the electron charge, $\xi(x)$ is the electric field strength, $v(k)$ is the electronic group velocity, f is the distribution function and $J(F,f)$ is the collision integral which can be treated by the RTA [3],

$$J(F,f)=\frac{F(k)-f(x,k,t)}{\tau} \tag{2}$$

where τ is relaxation time and $F(k)$ is Fermi equilibrium distribution function.

For the simulation of GNR interconnect, the relaxation time in (2) is given by $\tau = l_{eff}/v_f$, where v_f is the Fermi velocity, and l_{eff} is defined by

$$l_{eff}^{-1}=l_e^{-1}+\left(l_\Omega+l_{hp}\right)^{-1} \tag{3}$$

here, l_e is the elastic MFP caused by the line edge roughness and acoustic phonons, l_Ω is the distance that electron must accelerate in the electric field to reach a threshold energy, and l_{hp} stands for the high-energy phonon scattering MFP.

Starting with an initial distribution function, we can get charge profile along the interconnect by [5]

$$\rho(x,t) = -2e\int f(x,k,t)\,dk \tag{4}$$

Then the charge density serves as an input to Poisson equation to derive the potential,

$$\nabla^2 V(x) = \frac{d^2V(x)}{dx^2} = -\frac{\rho(x)}{\varepsilon} \tag{5}$$

After that, the electric field ξ obtained by the derivative of the potential is coupled back into (1) to update the distribution function. This process is iterated until steady state is reached, and the steady-state current is given by,

$$I(x,t) = 2e\int v(k) f(x,k,t)\,dk \tag{6}$$

In the calculation process, we take the upwinding-difference method and central-difference method to deal with BTE and Poisson equation, respectively. Due to the limitation of space, they are not described here.

In order to investigate the electrical property of GNR interconnect over a wide range of temperatures and bias voltages, the self-heating effect should be included. The heat conduction equation is described by:

$$\frac{d}{dx}\left[A\kappa(T)\frac{dT(x)}{dx}\right] - g\left(T(x)-T_0\right) - I\frac{dV}{dx} = 0 \tag{7}$$

where T_0 is the temperature of substrate, A is the cross-sectional area, $\kappa(T)$ is GNR thermal conductivity (its value is assumed as a constant 2500 W/mK for simplicity in this paper), g is the net heat loss to the substrate per unit length.

Using the popular finite-difference method, the heat conduction equation can be solved with the boundary conditions. Then, the temperature profile is sent back to the BTE of (1) for updating the distribution function. This process is iterated until self-consistency is achieved.

III. Results and Discussions

As described in the previous sections, the power density obtained by the Boltzmann–Poisson approach is used as the Joule-heating source to calculate the temperature profile along the GNR. Fig.2 shows the steady temperature distribution of the GNR interconnect with the length of 500nm under different bias conditions. At low-bias voltage (0.5V), the maximum temperature rise in the middle of the line is less than 20K. As the applied voltage increases, the temperature along the GNR rises up gradually. In order to illustrate the self-heating effect, the performance of GNR interconnects with or without thermal coupling are compared in Fig. 3. It is shown that the results of the isothermal model (without coupling) underestimate the current. It is because that as the temperature increases, more electrons are involved into conduction and thus increasing the current. Therefore, the self-heating effect should be considered for accurate simulation of the GNR interconnects.

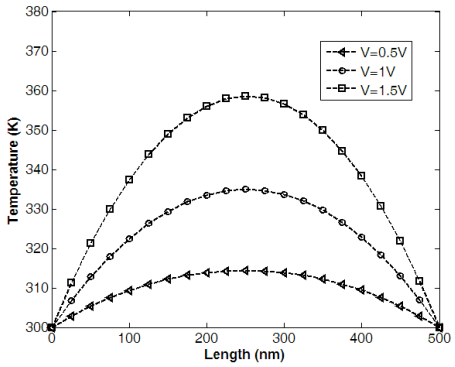

Fig. 2. Temperature distribution of GNR interconnect under different bias.

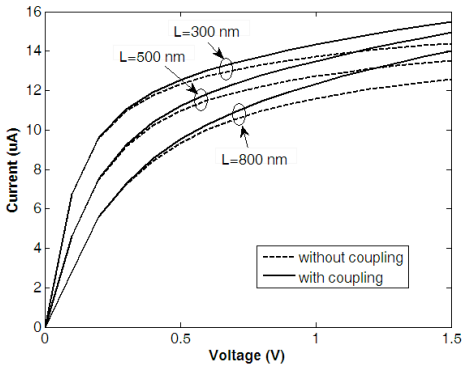

Fig. 3. Electro-thermal simulation results of GNR for different lengths.

IV. Conclusion

In this paper, the coupled BTE, Poisson equation, and heat conduction equation are solved self-consistently to investigate the current-voltage characteristics of GNR interconnects. Considering the high-energy phonons effect, the RTA is modified to deal with the scattering term in the BTE. The self-heating effect is also taken into account. The electro-thermal simulation of GNR interconnects with different lengths and bias conditions are illustrated by the numerical example.

Acknowledgment

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