Physics-Based Solution for Electrical Resistance of Graphene Under Self-Heating Effect

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***Abstract*—In this brief, we present a physics-based solution for the temperature-dependent electrical resistance of a suspended metallic single-layer graphene (SLG) sheet under Joule self-heating. The effect of in-plane and flexural phonons on the electron scattering rates for a doped SLG layer has been considered, which particularly demonstrates the variation of the electrical resistance with increasing temperature at different current levels using the solution of the self-heating equation. The present solution agrees well with the available experimental data done with back-gate electrostatic method over a wide range of temperatures.**

***Index Terms*—Graphene, phonons, self-heating effect.**

I. Introduction

In RECENT years, metallic graphene materials have demonstrated withstanding and possessing a reportedly very high breakdown current density and thermal conductivity (on the order of 10^8-10^9 A $\cdot$ cm^{-2} [1]–[3] and 600–7000 W $\cdot$ m^{-1} $\cdot$ K^{-1} [4], respectively, at 300 K), which makes them fit to emerge as potential candidates for next-generation interconnect materials in integrated circuits. However, applications near the limiting breakdown current have also resulted in Joule heating over the metallic single-layer graphene (SLG) surface [5]–[7], which initiates our motivation to study the temperature-dependent electrical resistance (R) through the solution of the Joule-heating equation containing a temperature-dependent thermal conductivity (κ).

Over the past few years, extensive experiments on electrical and thermal resistances in SLG have been reported. On one hand, R has been found to decrease with temperature (T) over all ranges [8], [9], where the testified lateral dimension was less than 10 nm which makes the SLG act as a semiconductor [10], while, for larger SLG sheet, R increases within the same range of T [11]–[13] exhibiting a metallic behavior. These studies are rather categorized through the interactions of in-plane and out-of-plane phonons with the electrons, respectively. Conflicts on the variation of R not only have arisen but also did its impact on defining κ. According to Balandin [3] and Nika *et al.* [13], it is the in-plane phonons which possess large mean free paths and thus are responsible for such a high κ. This follows from their *ab initio*-based full in-plane phonon dispersion relation which has been further evaluated through a number of simulative works using rigorous molecular dynamics approach, such as the use of the valence-force-field method for the determination of the exact phonon group velocities and Umklapp scattering selection rules [14]. It is also stated that the contribution to κ from the ZA phonon modes is small because of the large Gruneisen parameter and small group velocity. On the contrary, based on the numerical solution to the linearized phonon Boltzmann's transport equation and Lennard–Jones potential, Mariani and von Oppen [14] and, later, Lindsay *et al.* [15] predicted that about 60% of the Umklapp and normal processes involving ZA mode are forbidden, causing a decrease in the intrinsic relaxation rate which leads to a significant increase of κ in suspended SLG. In addition, the ZA phonon dispersion relation is treated as nonlinear or rather quadratic in nature that makes the thermal conductivity to follow a $T^{1.5}$ law variation below 300 K, also exhibited experimentally elsewhere [17], [18]. This formalism has further been used [19]–[21] and considered by others [22], [23] and suggested that the inclusion of ZA modes is inevitable in order to explain the κ of both suspended and supported SLGs where the ZA mode is usually damped due to leakage through the substrate.

In this brief, we thus present a physics-based model for the determination of R for a suspended metallic SLG sheet considering self-heating and the in-plane and out-of-plane phonon scattering contributions. We demonstrate that the effect of T distribution as a result of a temperature-dependent κ over the doped SLG layer due to the Joule heating has substantial control on R. The present contemporary model signifies the realization of $R(T)$ via the Joule-heating method, exhibiting an excellent match with the available experimental data over a wide range of temperatures done by using the gate electrostatic method [11].

II. Model Development, Results, and Discussions

We start with the calculation of the Fermi-level 2-D electron density of states (DOS) as

$$D(E_F) = \frac{g_s g_v}{(2\pi)^2} \frac{\partial A_s}{\partial E_F} \tag{1}$$

where g_s and g_v which are equal to two are the electron spin and valley degeneracies, $A_s = \pi(k_x^2 + k_y^2) = \pi k_s^2$, and $E = \hbar \upsilon_F k_s$ is the SLG electron band structure near the K-point symmetry. Using these, the Fermi-level DOS can be written as $D(E_F) = 2E_F/\pi\hbar^2\upsilon_F^2$, where υ_F is the Fermi velocity $\sim 10^6$ m $\cdot$ s^{-1} and $\hbar$ is the reduced Planck's constant. Under the application of a static longitudinal bias qV_D, the 2-D carrier density can

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then be written from the Fermi-level shifting of $E_F = qV_d + \hbar v_F\sqrt{\pi n_{2\text{-D}}}$, where $n_{2\text{-D}}$ is the electron concentration in the SLG sheet. The use of these definitions in the expression of linearized Boltzmann resistance $R = (2/q^2 v_F^2 D(E_F))(1/\tau)$ leads to

$$R(T) = \frac{\pi\hbar^2}{q^2 E_F}\frac{1}{\tau} \tag{2}$$

in which $1/\tau$ is the resultant scattering rate due to in-plane and flexural phonons and is given by Matthiessen's rule as $1/\tau = (1/\tau_{\text{in-plane}}) + (1/\tau_{\text{flexural}})$, where [18]

$$\frac{1}{\tau_{\text{in-plane}}} \approx \left[\frac{g^2}{2v_L^2} + \frac{\hbar^2 v_F^2\beta^2}{4a^2}\left(\frac{1}{v_L^2}+\frac{1}{v_T^2}\right)\right]\frac{E_F}{2\rho\hbar^3 v_F^2}k_B T \tag{3}$$

$$\frac{1}{\tau_{\text{flexural}}} \approx \left(\frac{g^2}{2} + \frac{\hbar^2 v_F^2\beta^2}{4a^2}\right)\frac{(k_B T)^2}{64\pi\hbar\varsigma^2 E_F}\ln\left(\frac{k_B T}{\hbar\omega_c}\right). \tag{4}$$

Here, k_B is the Boltzmann's constant, $g \approx 3$ eV is the screened deformation potential constant, $\beta \approx 2-3$, $\varsigma = 1$ eV is the bending rigidity, $a = 1.4$ Å is the distance between the nearest carbon atoms, $\rho = 7.6\times10^{-7}$ kg/m^2 is the mass density, and $v_L = 2.1\times10^4$ m/s and $v_T = 1.4\times10^4$ m/s are the longitudinal and transverse sound velocities, respectively [18]. In deriving (3) and (4), it has been assumed that the Bloch–Gruneisen temperature ($T_{\text{BG}} = 57$ K, 38 K, and 0.1 K) is far less than the room temperature for longitudinal, transverse, and flexural phonons at $n_{2\text{-D}} = 10^{12}$ cm^{-2}, respectively, and the domination of the absorption or emission of two phonons for $T \gg T_{\text{BG}}$.

Thus, in order to find $R(T)$ due to the self-heating from a constant current i_D, we rewrite the Fermi level E_F using (2) and the allied definition as

$$E_F^3 - AE_F^2 - B = 0 \tag{5}$$

where $A = (i_D\pi\hbar^2/q)C + \hbar v_F\sqrt{\pi n_{2\text{-D}}}$ and $B = (i_D\pi\hbar^2/q)D$, where, from (3) and (4), one can write $1/\tau_{\text{in-plane}} = CE_F$ and $1/\tau_{\text{flexural}} = D/E_F$. The solution to (5) is the lowest real positive value given by $E_F = (S+U) + (A/3)$, in which $S = \sqrt[3]{Q}$, $Q = -(G/2) + \sqrt{H}$, $H = (G^2/4) + f^3/27$, $G = -((2A^3+27B)/27)$, $f = -A^2/3$, $U = \sqrt[3]{T_1}$, and $T_1 = -(G/2) - \sqrt{H}$. With this solution of E_F, the profile of $R(T)$ from (2) in the suspended metallic SLG can be evaluated through the solution of the Joule self-heating equation

$$A_c\nabla(\kappa\nabla T) - p = 0 \tag{6}$$

where $A_c = \delta W$ is the SLG cross-sectional area with δ and W being the interplanar thickness and the width, respectively, $p = i_D^2 R(T)/L$, L is the sheet length, and contacts are assumed to be ideal. The Dirichlet boundary conditions are that the SLG ends have been kept at temperatures of 10 K and 450 K, respectively. Furthermore, in this case, we assume that κ of the SLG sheet is isotropic (where, roughly, in the sub-0.1-μm SLG film geometry, it exhibits anisotropy [24]), which transforms (6) to a 1-D problem. The realization of the quadratic wave vector phonon-dependent κ ($\omega_q = \alpha q^2$, where $\alpha \approx 4.6\times10^{-7}$ m$^2\cdot$s^{-1} denotes the ZA phonon diffusion constant) constitutes the scattering contributions from edge roughness ($1/\tau_E = (\sqrt{\pi}/2F\sqrt{LW})(\partial\omega_q/\partial q)$) and Umklapp ($1/\tau_U = (32/27)|\gamma_{\text{ZA}}|^4(k_B T/M(\partial\omega_q/\partial q)^2))^2\omega_B$), in which F is the geometric factor, M is the mass of the carbon atom, ω_B is the ZA phonon branch frequency, and $|\gamma_{\text{ZA}}|$ is the Gruneisen parameter for the ZA mode.[1] The use of these two scattering rates defines $\kappa^{-1} = \kappa_{\text{low}}^{-1} + \kappa_{\text{high}}^{-1}$, where $\kappa_{\text{low}} = 4.58(Fk_B/2\delta)(LW/\alpha)^{1/2}(k_B T/\pi\hbar)^{3/2}$ and $\kappa_{\text{high}} = (27/16\pi\delta)(k_B/\hbar)^3(M\alpha/|\gamma_{\text{ZA}}|^2)^2(\theta^4/\hbar\omega_B)(1/T^2)$, in which $\theta = 1000$ K, the SLG Debye temperature. This particularly exhibits that κ for suspended metallic SLG follows a T^{-2} law due to the second-order three-phonon Umklapp process. Using this aforementioned temperature-dependent κ in the 1-D Joule self-heating equation leads to the temperature distribution over the SLG layer for a given value of current. Thus, for a known value of the temperature profile, the temperature-dependent electrical resistance can finally be estimated using (2). We now compare our theoretical model with that of the back-gate electrostatic method done by Bolotin *et al.* [11] as shown in Fig. 1. The application of the back-gate voltage changes the Fermi level of the graphene which, under the known value of the gate capacitance, allows estimating E_F and, thus, $R(T)$ by varying the system-in-cryostat temperature. However, for an interconnect (although suspended), where the two ends can be at two different temperatures, our Joule-heating formalism also converges to the same nature of the resistance variation with temperature. The advantage of our present analysis lies in the fact that one has the ability to control over the current and the end point temperatures which are extremely necessary conditions for interconnect architecture. This is shown in Fig. 2, where the variation of R as a function of temperature for a doped SLG ($n_{2\text{-D}} = 10^{12}$ cm^{-2}) at various current levels has been plotted. The SLG dimensions are taken as $L = 1$ μm and $W = 1.5$ μm. It can be seen from Fig. 2 that, under the Joule-heating effect, the resistance exhibits a linear T dependence at lower temperatures while following a quadratic T^2 law at higher temperatures. This is due to the crossover of the in-plane phonon scattering at lower temperatures to the out-of-plane flexural phonon. The reason for such a dependence of the resistance is the dominant flexural phonon modes at higher temperature which exhibits a quadratic dispersion relation. Furthermore, we see that, as the current levels are increased, the resistance decreases. This, at first, seems to be contradictory since a rise in current should also rise T over the surface, as a result of which $R(T)$ increases. However, in this case, due to the linear energy–wave vector relationship of the electrons, the

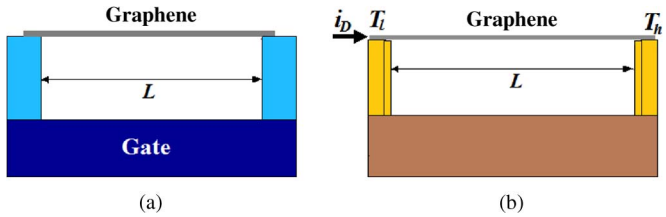

Fig. 1. (a) Schematic of suspended SLG adapted from [11] using a back-gate electrostatic method and (b) our Joule-heating model of suspended SLG whose ends are at two different temperatures with a constant current i_D.

[1]The expressions of κ for various cases are derived from [25]

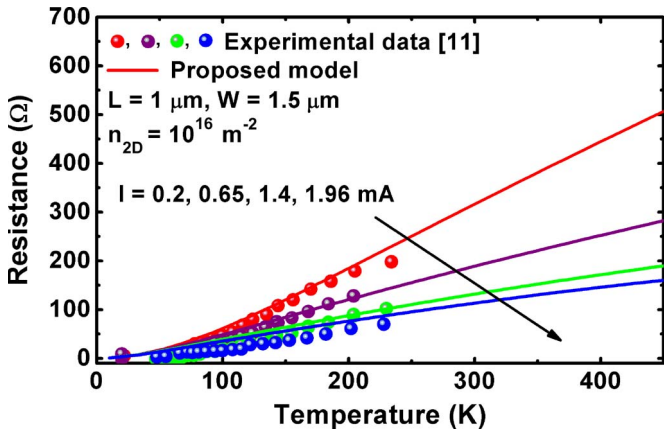

Fig. 2. Electrical resistance as a function of temperature for doped SLG at various current levels. The solid curves correspond to the proposed model, and the symbols are the experimental data from [11].

resistance is an inverse function of the Fermi energy. Thus, as the current increases for a fixed value of the temperature, the Fermi level increases, which eventually decreases $R(T)$. It can be seen that our theoretical solution is in excellent agreement with the available experimental data over a wide range of temperatures [11]. At this point, it should be noted that we did not consider the effect of isotope scattering. However, the thermal conductivity model in such case can be done by adding the term $1/\tau_i = (1/4)S_0\Gamma_m(q\omega_q^2/(\partial\omega_q/\partial q))$ [13] to the total phonon scattering rate, where S_0 is the cross-sectional area per one atom where $r_0 = 0.14$ nm is the carbon–carbon distance with Γ_m as the strength of the impurity scattering whose determination is an extremely challenging work. However, the order of Γ_m can be estimated from the knowledge of experimental data and is generally found to be in the range of 10^{-6}–10^{-3} for low level to high level of isotope addition for most materials. Using these, our model finds an excellent match when Γ_m is considered to be within 10^{-7}–10^{-6}, which is essentially as good as pure SLG. In addition, we have considered a more general model of edge roughness scattering [26] which provides the fundamental insight to phonon-assisted thermal conductivity in any material. The boundary scatterings are the Casimir limit of the edge roughness scattering. Hence, we see that, for a suspended metallic SLG under Joule-heating effect and for further embedded SLG interconnects, the results of our model can be used as to predict the electrical resistance from a thorough knowledge of the surface temperature distribution.

III. Conclusion

In this brief, a novel approach has been conveyed to estimate the SLG sheet $R(T)$. Using the solution of the Joule self-heating equation at different current levels and formulating a temperature-dependent thermal conductivity, we estimate the suspended metallic SLG $R(T)$. Our present theoretical model can be put as an alternative way to measure $R(T)$ via the known values of currents and end point temperatures which also agrees well with the available back-gate electrostatic experimental data [11] over a wide range of temperatures.

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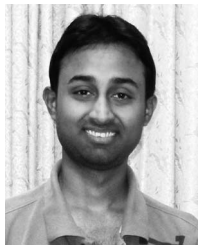

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