Journal of Engineering Science and Technology
Vol. 12, No. 6 (2017) 1677 - 1684

MATHEMATICAL FORMULATION OF SURFACE CONDUCTIVITY FOR GRAPHENE MATERIAL

BALA R., MARWAHA A., MARWAHA S.*

Sant Longowal Institute of Engineering & Technology, Longowal
(Deemed University) Dist. Sangrur, Punjab, India
*Corresponding Author: marwaha_sanjay@yahoo.co.in

Abstract

The graphene material is currently being used in the design of nano components and devices for wireless applications in terahertz (THz) regime as it possesses a number of desirable electromagnetic and mechanical properties that assist in providing flexible and reconfigurable structures. The material tunable conductivity accounts for the superior electromagnetic properties. Very little efforts however are being done to provide simplified solution of the graphene surface conductivity to be utilized for design of nano devices. Hence the authors have presented the simplified analytical solution for graphene surface conductivity expressed in terms of the chemical potential.

Keywords: Graphene, Surface conductivity, Nano devices, Terahertz regime.

1. Introduction

Graphene's high electrical conductivity and high optical precision make it a candidate for transparent conducting electrodes, required for various high-speed electronics and high frequency applications due to its very high mobility and graphene's saturation velocity [1]. In particular, graphene's mechanical strength and flexibility are beneficial compared to indium tin oxide, which is brittle [2]. Single sheet of graphene is hard to make on a suitable substrate. So according to the radio wave absorption, stacked graphene layer on a silicon dioxide substrate increases the absorption of radio waves by 1.68% fractional bandwidth, extendable from microwave to THz frequencies, while remaining translucent to visible light. Scientific research in the wireless communications field is growing fast. The major challenges in wireless communications are ultra-high spectrum efficiency need for wide bandwidth, number of functions between the nano devices at a time with less interference. High data rates are required to carry multimedia communications at low power consumption.

Nomenclatures

f	Frequency, Hz
$f_d(\varepsilon)$	Fermi-dirac distribution function
k_B	Boltzmann constant , eV
n_s	Charge carrier density. Cm^{-3}
q_e	Electron charge, C
T	Temperature , kelvin
V_{DC}	External bias voltage, V
V_f	Fermi velocity, m/s
Z_s	Surface impedance , Ω

Greek Symbols

Γ	Electron scattering rate , eV
μ_c	Chemical potential , eV
$\hbar$	Reduced Planck constant , eVs
ε	Energy , joules
σ	Conductivity , Siemens
τ	Relaxation time , s
ω	Angular frequency of the photon , rad/s

Abbreviations

DC	Direct Current
ILATE	Inverse Trigonometric, Logarithmic, Algebraic, Trigonometric and Exponential
MATLAB	Matrix Laboratory
SPP	Surface Plasmon Polaritons
THz	Tera Hertz

To meet these challenges efficient communication system should be designed. So the current research is going towards designing nano devices at terahertz regime. The frequencies higher than microwaves offer many advantages including wider communication bandwidths, improved spatial directivity and resolution with system compactness. Currently researchers have realized that the unique features of graphene material makes it a very promising candidate to wireless communications among nano devices. The potential of graphene for use in photonic applications was evidenced by recent demonstrations of amplitude modulators, attenuators, satellite telemetry, Photomixers for continuous-wave terahertz emission, Faraday and Kerr polarisation rotators, and non-reciprocal isolators. Additionally, the optical down-conversion of ultra short laser pulses by means of photoconductor materials has confirmed a sustained increase in performance in the last decades [3-4]. A lot of microwave and terahertz applications have also been suggested, such as antennas and interconnect [5-6]. For all the applications the major thrust is to mathematically model graphene-based plasmonic nano-components and devices which can operate efficiently at micrometer radio wavelengths.

Plasmonic propagation can be supported by graphene at THz, leading to extremely interesting properties for practical nano devices. The wavelength of surface plasmon polaritons for a given frequency is several hundred times smaller than the wavelength of freely propagating electromagnetic waves of the same frequency [7]. For using graphene as nano components major challenge is to mathematically model the new complex graphene material that would exhibit improved high frequency properties. The specific material properties that need improvement are lower losses, better impedance matching, high radiation efficiency and modified electromagnetic absorption characteristics compatible with nano devices on the basis of electromagnetic properties. There has however been relatively little effort in improving the materials technology in nano devices and simplifying mathematically the tunable graphene surface conductivity [8]. In this paper an attempt has been made to accurately model graphene based material with tunable conductivity for nano devices in the THz regime.

2. Simplified Formulation of Graphene Surface Conductivity

From the previous literature it is known that the electromagnetic fields for metallic conducting devices are governed by classical Maxwell's equations, the graphene is however represented by a conductivity surface arising from a semi-classical intraband mode and quantum-dynamical interband mode [8]. The Kubo's formula has therefore been used to calculate the graphene surface conductivity as a function of frequency. The surface conductivity of an infinite graphene film consists of two parts: first term is intraband and second term interband contributions in Eq. (1), correspond to the intraband electron-phonon scattering process and interband electron transition respectively. In the infrared and visible range (short wavelength), the graphene optical conductivity is determined by interband transitions whereas, for terahertz range (long wavelengths) is dominated by intraband transitions. This simple conductivity model has been used here which ignores the magnetic field hall conductivity as graphene is assumed to be only electrically biased [9-11].

$$\sigma(i\omega, \mu_c, \Gamma, T) = -j\frac{q_e^2(\omega+2j\Gamma)}{\Pi\hbar^2}\left[\frac{q_e^2}{(\omega+2j\Gamma)^2}\int_0^\infty \varepsilon\left(\frac{\partial f_d(\varepsilon)}{\partial\varepsilon}-\frac{\partial f_d(-\varepsilon)}{\partial\varepsilon}\right)d\varepsilon-\int_0^\infty\frac{f_d(-\varepsilon)-f_d(\varepsilon)}{(\omega+2j\Gamma)^2-\left(\frac{4E}{h}\right)^2}d\varepsilon\right] \quad (1)$$

Here ω is angular frequency of the photon, Γ is electron scattering rate expressed in terms of relaxation time as $\tau=\frac{1}{2\Gamma}$, ħ is the reduced Planck constant or Dirac constant, i.e., $\hbar = \frac{h}{2\Pi}$, where h is Planck constant, T is room temperature, the Fermi-dirac distribution function $f_d(\varepsilon)=\left(1+e^{\frac{\varepsilon+|\mu_c|}{k_BT}}\right)^{-1}$ and k_B is the Boltzmann constant. It is noted that for highly doped or gated graphene $\frac{\mu_c}{k_BT} < 1$, so the carrier density and chemical potential can be expressed as $n_s = \frac{\mu_c^2}{\Pi\hbar^2V_f^2}$ and $\mu_c \approx \sqrt{\Pi\hbar^2v_f^2n_s}$ respectively. For present analysis when $\frac{\mu_c}{k_BT} > 1$,therefore the

chemical potential of graphene is determined in terms of carrier density from the expression given by

$$n_s = \frac{2}{\Pi\hbar^2 V_f^2}\int_0^\infty \varepsilon\left[f_d(\varepsilon-\mu_c)-f_d(\varepsilon+\mu_c)\right]\partial\varepsilon \tag{2}$$

For the present case we consider positive values of chemical potential i.e. $\mu_c > 0$. Now Eq. (2) is solved using substitutions $A = \int_0^\infty \varepsilon\left[f_d(\varepsilon-\mu_c)\right]\partial\varepsilon$ and $B = \int_0^\infty \varepsilon\left[f_d(\varepsilon+\mu_c)\right]\partial\varepsilon$.

The first Fermi-dirac distribution term can be expressed as

$$f_d(\varepsilon-\mu_c) = \frac{1}{\left(1+e^{\frac{\varepsilon-2\mu_c}{k_BT}}\right)} \tag{3}$$

Therefore

$$A=\int_0^\infty \frac{\varepsilon}{\left(1+e^{\frac{\varepsilon-2\mu_c}{k_BT}}\right)}\partial\varepsilon \tag{4}$$

Using the approximation $1+e^{\frac{\varepsilon-2\mu_c}{k_BT}} \approx e^{\frac{\varepsilon-2\mu_c}{k_BT}}$ Eq. (4) reduces to

$$A = \int_0^\infty \varepsilon\left(e^{\frac{2\mu_c-\varepsilon}{k_BT}}\right)\partial\varepsilon = e^{\frac{2\mu_c}{k_BT}}\left[\int_0^\infty \varepsilon\left(e^{\frac{-\varepsilon}{k_BT}}\right)\partial\varepsilon\right] \tag{4a}$$

For further simplification, substitute $\frac{1}{k_BT} = \alpha$, $\alpha\varepsilon$=y then $\alpha\partial\varepsilon=\partial$y in Eq. (4a),

$$A = e^{\frac{2\mu_c}{k_BT}}\left[\int_0^\infty \varepsilon\left(e^{-\alpha\varepsilon}\right)\partial\varepsilon\right] = e^{\frac{2\mu_c}{k_BT}}\left[\int_0^\infty \frac{y}{\alpha}\left(e^{-y}\right)\frac{\partial y}{\alpha}\right] = e^{\frac{2\mu_c}{k_BT}}\frac{1}{\alpha^2}\left[\int_0^\infty y\left(e^{-y}\right)\partial y\right] \tag{4b}$$

Solving this equation by using application of integration methods based on ILATE rule the simplified expression is obtained as

$$A = e^{\frac{2\mu_c}{k_BT}}(k_BT)^2 \tag{4c}$$

Similarly, the second term of carrier density expression given by $B = \int_0^\infty \varepsilon\left[f_d(\varepsilon+\mu_c)\right]\partial\varepsilon$ is solved correspondingly to obtain the solution as

$$B = (k_BT)^2 \tag{5}$$

Hence using the values of *A* and *B* in Eq. (2), the carrier density is obtained as

$$n_s = \frac{2}{\Pi\hbar^2 V_f^2}(k_BT)^2\left(e^{\frac{2\mu_c}{k_BT}}-1\right) \tag{6}$$

where V_f is the Fermi velocity (~ 3×10^6 m/s in graphene), ε is the energy and μ_c is graphene chemical potential. The parameter of great interest for evaluating the performance of the graphene based nano devices is the chemical potential of

graphene, i.e., the level in the distribution of electrons energies at which a quantum state is equally likely to be occupied or empty. The chemical potential μ_c can be accurately extracted by numerically solving Eq. (6).

3. Results and Discussion

The graphene SPP can therfore be tuned by material doping which is further controlled by the external bias,V_{DC}. Hence the graphene conductivity σ or corresponding surface impedance $Z_s=1/\sigma$ can be dynamically controlled by V_{DC}. This property can be used to create tunable nano devices with dynamic control. At the THz frequency region , the application of an external DC bias allows to increase chemical potential, thus reducing losses and increases the inductive behaviour of the graphene sheet.

The first term of conductivity represented by Eq. (1) corresponds to intraband transition in which the real part contributes to energy absorption or dissipation due to the intraband electrons and after utilizing the solution explained above, can now be expressed as

$$\sigma(\text{int}raband) = j\frac{q_e^2 k_B T}{\Pi\hbar^2\left(\omega + j\tau^{-1}\right)}\left(\frac{\mu_c}{k_B T} + 2\ln\left(e^{\frac{-\mu_c}{k_B T}} + 1\right)\right) \tag{7}$$

In the recent years many researchers are using the Kubo's expression to find out tunability of graphene material but to the best of our knowledge very little consideration has been given to provide the accurate solution of the expression to analyze the effect of chemical potential on conductivity in simplified form [11-12]. Therefore the authors have suggested here an accurate mathematical modeling of graphene surface conductivity in a simple manner. The first attempt was performed using the Mathematica software, which however could not provide the converged solution. Thereafter MATLAB code was generated for the expression considering $\mu_c \neq 0$, and using the values of different parameters as q_e=1.6×10^{-19}C with Coulomb charge (C)= 6.25×10^{19} electrons, k_BT= 0.0256eV where k_B is Boltzmann constant, $\hbar$ = 6.582×10^{-16} eVs, Γ =0.11eV, ω=2πf where f is frequency.

$$\sigma(\text{int}raband) = \frac{3.009\times10^{10}}{6.28f + 0.22j}\left(\frac{\mu_c}{k_B T} + 2\ln\left(e^{\frac{-\mu_c}{k_B T}} + 1\right)\right) \tag{7a}$$

$$\sigma_{int ra(realpart)} = \frac{0.66198\times10^{10}}{39.44f^2 + 0.0484}\left(\frac{\mu_c}{0.0256}\right) + \frac{0.66198\times10^{10}}{39.44f^2 + 0.0484}\left(2\ln\left(e^{\frac{-\mu_c}{0.0256}} + 1\right)\right) \tag{7b}$$

$$\sigma_{\text{int}ra(\text{i}mg.part)} = j\frac{18.896f\times10^{10}}{39.44f^2 + 0.0484}\left(\frac{\mu_c}{0.0256}\right) + \frac{18.896f\times10^{10}}{39.44f^2 + 0.0484}\left(2\ln\left(e^{\frac{-\mu_c}{0.0256}} + 1\right)\right) \tag{7c}$$

Figures 1 and 2 respectively show the real and imaginary part of intraband conductivity at terahertz frequencies regime obtained from their corresponding equations.

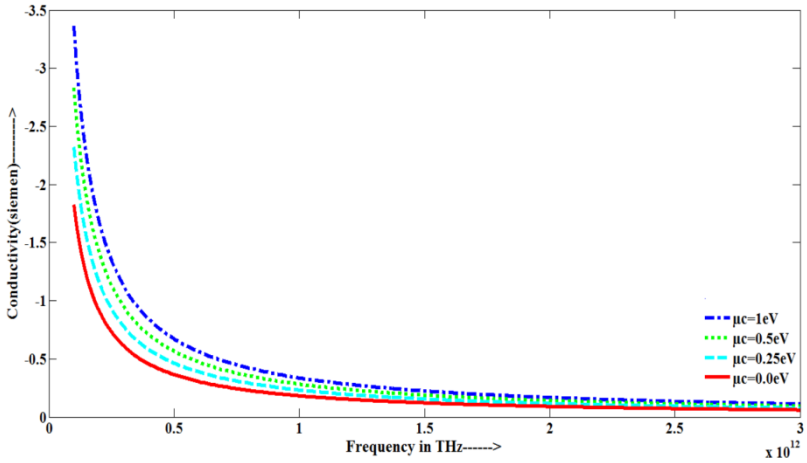

Fig. 1. Real part of the intraband conductivity at room temperature (T = 300° K) for different values of chemical potential

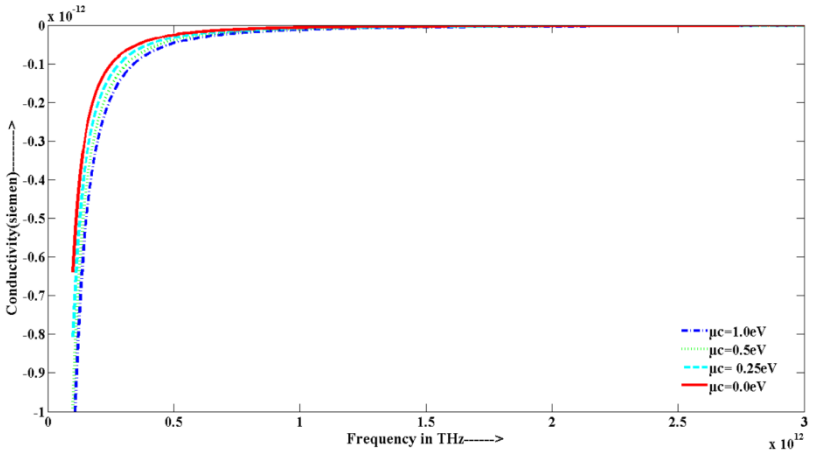

Fig. 2. Imaginary part of the intraband conductivity at room temperature (T = 300° K) for different values of chemical potential.

Further Eq. (7) can be simplified for $\mu_c = 0$,

$$\sigma(\text{int}raband) = \frac{q_e^2 k_B T}{\Pi\hbar^2}(2\ln 2)\left(\frac{j}{(\omega + j\tau^{-1})}\right) = j\frac{262.06 f \times 10^{10}}{39.44 f^2 + 0.0484} \tag{8}$$

So, for this case, it can be observed that we obtain the simplified intraband term of the graphene conductivity which is similar to the available Drude-like form [13] i.e.

$$\sigma\text{int}ra(simplified) = j\frac{q_e^2 \mu_c}{\Pi\hbar^2(\omega + j\tau^{-1})} \tag{9}$$

The high frequency conductivity can be well described by Drude model and it has been observed that the free carrier absorption is directly related to high frequency conductivity of electrons in graphene. Therefore as the frequency increases the lower frequency free carrier absorption under intraband absorption transition also increases. Such intraband transitions are responsible for conductivity behaviour of graphene in THz regime as validated by the spectroscopy measurements performed by Wang [14-15].

4. Conclusions

In this research paper, simplified mathematical formulation for graphene material conductivity has been presented. The Kubo's formula for graphene conductivity has been utilized and analytically simplified. Further MATLAB code is generated to plot the intraband term of surface conductivity as a function of frequency. The vision of a monolayer of carbon atom as graphene is hence examined as a new platform for one-atom-thick nano devices for high data rates in wireless application.

References

1. Wang, H.; Nezich, D.; Kong, J.; and Palacios, T. (2009). Graphene frequency multipliers. IEEE Electron Device Letters, 30(5), 547-549.
2. Meyer, J.C.; Geim, A.K. ; Katsnelson, M.I. ; Novoselov, K.S. ; Booth, T.J.; and Roth, S. (2007). The structure of suspended graphene sheets. *Nature*, 446(7131), 60-63.
3. Auston, D.H.; Cheung, K.P.; and Smith, P.R. (1984). Picosecond photo conducting hertzian dipoles. *Applied Physics Letters*, 45(3), 284-286.
4. Berry, C.W.; Wang, N.; Hashemi, M.R.; Unlu, M.; and Jarrahi M. (2013). Significant performance enhancement in photoconductive terahertz optoelectronics by incorporating plasmonic contact electrodes. *Nature Communications*, 4(1622), (arXiv:1209.1680v1)
5. Hanson, G.W. (2005). Fundamental transmitting properties of carbon nanotube antennas. *IEEE Transactions on Antennas and Propagation*, 53(11), 3426-3435.
6. Hagmann, M.J. (2005). Isolated carbon nanotubes as high-impedance transmission lines for microwave through terahertz frequencies. *IEEE Transactions Nanotechnology*, 4(2), 289-296.
7. Lin, Y.-M.; Jenkins, K.A.; Valdes-Garcia, A.; Small, J.P.; Farmer, D.B.; and Avouris, P. (2009). Operation of graphene transistors at gigahertz frequencies. *Nano Letters*, 9(1), 422-426.
8. Llatser, I.; Kremers, C.; Cabellos-Aparicio, A.; Jornet, J.M..; Alarcon E.; and Chigrin D.N. (2012). Graphene - based nano-patch antenna for terahertz radiation. *Photonics and Nanostructures-Fundamentals and Applications*, 10(4), 353-358.
9. Titz, D.; Bisognin, A.; Ferrero, F.; Luxey, C.; Jacquemod, G.; Laporte, C.; Ezzeddine, H.; Valente, M.; and Brachat, B. (2012). 60 GHz patch antenna using IPD technology. *Loughborough Antennas and Propagation Conference* (*LAPC*), Loughborough, UK.

10. Batovski, D.A. (2012). Graphene and communications technology. *Assumption University Journal of Technology*, 16(2), 105-114.
11. Gomez-Diaz J.S.; and Perruisseau Carrier, J. (2012). Microwave to THz properties of graphene and potential antenna applications. *International symposium on antennas and propagation*, Nagoya, Japan.
12. Skulason, H.S.; Nguyen, H.V.; Guermoune, A.; Sridharan, V.; Siaj, M.; Caloz, C.; and Szkopek T. (2011). 110 GHz measurement of large-area graphene integrated in low-loss microwave structures. *Applied Physics Letters*, 99(153504).
13. Horng, J.; Chi-Fan C.; Geng, B.; Girit, C.; Zhang, Y.; Hao, Z.; Bechtel, Hans A.; Martin, Michael C.; Zettl, A.; Crommie, Michael F.; Ron Shen, Y.; and Wang F. (2011). Drude conductivity of Dirac fermions in graphene. *Physical Review* B83(165113).
14. Bechtel, H.A.; Chen, C.; Crommie, M.F.; Geng, B.; Girit, C.; Horng, J.; Hao, Z.; Martin, M.; Shen, Y.R.; Wang, F.; Zhang, Y.; and Zettl, A. (2011). Intraband optical transitions in graphene. *CLEO*: 2011 - *Laser Science to Photonic Applications*, 1-2.
15. Kashuba, A.B. (2008). Conductivity of defectless graphene. *Physical Review* B78(085415).