Orissa Journal of Physics
ISSN 0974-8202

Vol. 24, No.1
February 2017
pp. 101-105

Theoretical Model study of the Effect of different Substrates on Electron Specific Heat in Graphene in Paramagnetic Limit

R PANDA[1], S SAHU[1] and G C ROUT[2,*]

[1]School of Applied Sciences (Physics), KIIT University, Bhubaneswar, Pin-751024
[2]Condensed Matter Physics Group ,Physics Enclave, Plot No.- 664/4825, Lane -[4]A,Shree Vihar, C. S. Pur, PO- Patia, Bhubaneswar- 751031, Odisha, India

* E-mail-gcr@iopb.res.in

Received: 22.11.2016 ; *Revised : 11.12.2016* ; *Accepted : 8.1.2017*

Abstract. We address here a tight binding model calculation taking into account of the substrate effect, electron correlations and different band fillings in monolayer graphene. The model Hamiltonian is solved by Zubarev's Green's function technique. Hence sublattice electron densities are calculated self-sufficiently taking 120×120 grid points of the electron momentum. The effect of substrate induced gap on temperature dependent electron specific heat is investigated.

Keywords: Graphene, Electron specific heat, Paramagnetism

PACS No: 75.75.+a , 75.50. Xx

1. Introduction

The last few years were marked with the exploration of new allotropic modifications of carbon and related nanostructures. Graphene is a two-dimensional (2D) material with over 100-fold anisotropy of heat flow between the in-plane and out-of-plane directions. High in-plane thermal conductivity is due to covalent sp^2 bonding between carbon atoms, whereas out-of-plane heat flow is limited by weak van der Waals coupling. Most thermal properties of graphene are derived from those of graphite and bear the imprint of the highly anisotropic nature of this crystal [1]. For instance, the in-plane covalent sp^2 bonds between adjacent carbon atoms are among the strongest in nature (slightly stronger than the sp^3 bonds in diamond), with a bonding energy of approximately 5.9 eV[2]. To increase the dissipation power, the necessity of removal of heat in electronic industry cannot be avoided. For next generation integrated circuits and

electronics, the rigorous search for materials that conduct heat well, has become essential. Graphene's high thermal conductivity is a challenge to understand, as because the theoretical model of two dimensional and nano scale physics are limited. The thermal energy stored inside the body is determined by the specific heat, and also this determines how quickly the body cools or heats. Earlier Sahu et al. have reported the microscopic theoretical studies on non-magnetic and magnetic properties of graphene-on-substrate[3,4,5]. More recently, we have considered a tight binding model calculation taking substrate effect, electron-electron interaction effect and have reported the important role played by the band filling on charge gap in paramagnetic limit in graphene [6]. Again we have also studied the evolution of charge gap in paramagnetic state of graphene-on-substrate in which the Coulomb interaction introduces a charge gap in graphene at Dirac point [7]. In continuation of this work, we present in this work we present this communication the role played by different substrates on the electron specific heat of monolayer graphene.

2 Tight-Binding Model Hamiltonian

The Hamiltonian consisting of the hopping of π-electrons up to first-nearest-neighbor is written as

$$H_1 = \sum_{k,\sigma} (\varepsilon_a \, a^{\dagger}_{k,\sigma} \, a_{k,\sigma} + \varepsilon_b \, b^{\dagger}_{k,\sigma} \, b_{k,\sigma}) + \sum_{k,\sigma} \left(\varepsilon_{1k} a^{\dagger}_{k,\sigma} \, b_{k,\sigma} + \varepsilon^{*}_{1k} b^{\dagger}_{k,\sigma} \, a_{k,\sigma}\right) \quad (1)$$

where $a^{\dagger}_{k\sigma}$ $(a_{k\sigma})$ is the creation (annihilation) electron operator for A-site and $b^{\dagger}_{k\sigma}$ $(b_{k\sigma})$ is the creation (annihilation) electron operator on sublattices B. Here ε_a and ε_b are the site energies at A and B sublattices respectively, while $\varepsilon_{1k} = -t_1\gamma_1(k)$ is the nearest neighbor electron hopping energy with hopping integral $t_1 \approx 2.78$ eV. In case of a graphene-on-substrate system, the electron interaction with the static potential induced by the substrate comes into play. As a result, a modulated potential, where A site have energy +Δ and B sites with energy –Δ , leads to the breaking of the symmetry between A and B sites and gives rise to a gap. Such a symmetry breaking Hamiltonian is written as

$$\mathrm{H_{sub}} = \Delta \sum_{\mathrm{i},\sigma} \mathrm{a^{\dagger}_{i,\sigma}} \, \mathrm{a_{i,\sigma}} - \Delta \sum_{\mathrm{j},\sigma} \mathrm{b^{\dagger}_{j,\sigma}} \, \mathrm{b_{j,\sigma}} \quad (2)$$

The Hamiltonian describing the Coulomb interaction with an effective repulsive Coulomb energy U is written as

$$H_U = U \sum_i \left[n_{i\uparrow}^a \, n_{i\downarrow}^a + n_{i\uparrow}^b \, n_{i\downarrow}^b \right] \quad (3)$$

For weak coupling, the Hamiltonian can be decoupled by Hartree–Fock mean-field decoupling scheme, i.e. $U n_{i\uparrow}^{\alpha} \, n_{i\downarrow}^{\alpha} \approx U \langle n_{i\uparrow}^{\alpha} \rangle \, n_{i\downarrow}^{\alpha} + U \langle n_{i\downarrow}^{\alpha} \rangle \, n_{i\uparrow}^{\alpha} - U \langle n_{i\uparrow}^{\alpha} \rangle \langle n_{i\downarrow}^{\alpha} \rangle$ where $\alpha \equiv a, b$ corresponding to A and B site interactions. The total Hamiltonian is given by $H = H_1 + H_{sub} + H_U$.

3. Calculation of entropy and electron specific heat

The Green's functions for A and B site electron operator can be defined as,

$$G_1(k,\omega) = \ll a_{k,\sigma}; a_{k,\sigma}^{\dagger} \gg_{\omega} \; ; \; G_2(k,\omega) = \ll b_{k,\sigma}; b_{k,\sigma}^{\dagger} \gg_{\omega} \quad (4)$$

By using Zubarev's Green's function technique , the final expressions of the above Green's functions are

$$G_1(k,\omega) = \frac{1}{2\pi} \frac{(\omega - \epsilon_{b,k})}{|D_\sigma(\omega)|}; \; G_2(k,\omega) = \frac{1}{2\pi} \frac{(\omega - \epsilon_{a,k})}{|D_\sigma(\omega)|} \quad (5)$$

For $|D_\sigma(\omega) = 0|$, we get two quasi-particle bands namely $\omega_{1k,\sigma}$ for valence band and $\omega_{2k,\sigma}$ for conduction band which are given by

$$\omega_{1k\sigma} = \frac{(\varepsilon_{a,k} + \varepsilon_{b,k}) + \sqrt{(\varepsilon_{a,k} - \varepsilon_{b,k})^2 + 4|\varepsilon_1(k)|^2}}{2} \quad (7)$$

$$\omega_{2k\sigma} = \frac{(\varepsilon_{a,k} + \varepsilon_{b,k}) - \sqrt{(\varepsilon_{a,k} - \varepsilon_{b,k})^2 + 4|\varepsilon_1(k)|^2}}{2} \quad (8)$$

where, $\varepsilon_{a,k} = \varepsilon_a + \Delta + U\langle n^a \rangle$ and $\varepsilon_{b,k} = \varepsilon_b - \Delta + U\langle n^b \rangle$.

In order to study the effect of substrate induced gap, on the thermal properties of graphene, we write free energy for graphene in terms of the quasi-particle energies $\omega_{\alpha,k,\sigma}$ $(\alpha = 1,2)$ as

$$F = -k_B T \sum_{\alpha,k,\sigma} [\ln\{1 + e^{-\beta(\omega_{\alpha,k,\sigma})}\}] \quad (9)$$

where k_B is the Boltzmann constant and $\beta = \frac{1}{k_B T}$. The entropy of the system is defined for $S = -\frac{1}{N}\left(\frac{\partial F}{\partial T}\right)_{V,\mu}$. Further the temperature dependence specific heat is calculated numerically from entropy (S) and is given below

$$\bar{C}_V = \frac{C_V}{k_B} = \left(T \frac{\partial s}{\partial T}\right)_{V,\mu} \quad (10)$$

The physical quantities are made dimensionless by NN hopping integral $t_1 = 2.78eV$. The parameters are: the Coulomb energy $= \frac{U}{t_1}$, substrate induced gap $d_1 = \frac{\Delta}{t_1}$ and temperature $t = \frac{k_B T}{t_1}$.

4. Results and Discussion

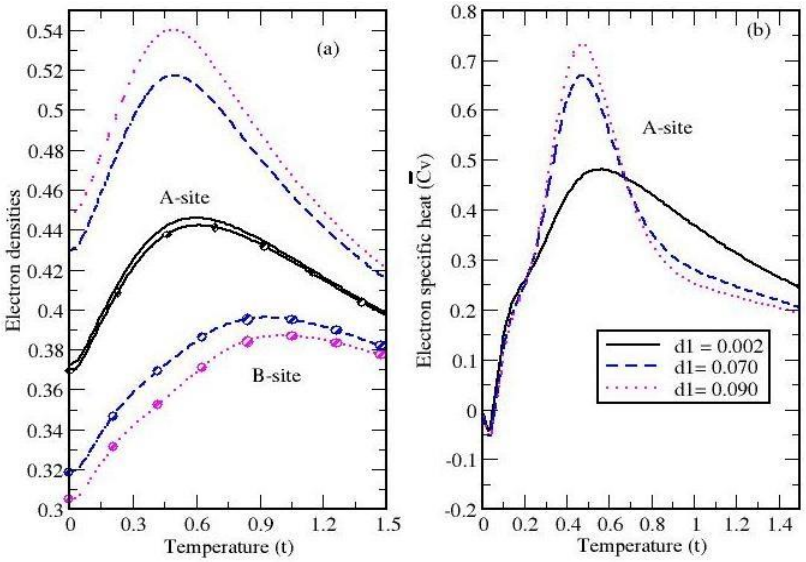

Fig 1(a). The plot of electron densities vs. temperature (t) of both sites for different substrate induced gap $d_1 = 0.002, 0.070, 0.090$ (for continuous line, dashed line, dotted line at A site and same lines with circles for B-site),at electron density $n = 1$. Figure1 (b) shows the plot of electron specific heat vs. temperature (t) for different values of substrate induced gap $d_1 = 0.002, 0.070, 0.090$ and at electron density $n = 1$.

The electron densities at A and B-sublattices of the honeycomb lattice of graphene is calculated from the correlation functions derived from the corresponding electron Green's functions given in equations (4) and (5). They shown in the Figure 1(a) for different values of substrate induced gap. Since the electron densities in two sublattices are different, a charge gap develops in graphene due Coulomb interaction. Figure 1(a) shows that the electron density at A-sublattice is higher than that of B-sublattice. Further the temperature dependent electron density at A-site exhibits a sharp peak associated with charge gap at temperature ≈ 0.5 , while the electron density at B-sublattice exhibits a flat peak associated with charge gap at temperature $t \approx 0.6$ to 0.9 . In addition to this, the electron densities display flat dips associated with substrate induced gap at very low temperatures. It is to note here that the peak in electron densities shifts to

higher temperatures with increase of substrate induced gap ($d_1 = 0.0002$ to 0.090).

The electron specific heat is calculated from electron free energy given in equation 9 by using the formula given in equation 10. The electron specific heat is computed numerically for different substrate induced gaps ($d_1 = 0.0002, 0.070, 0.090$) as shown in figure 1(b). The specific heat exhibits a sharp dip associated with the substrate induced gap at very low temperatures($t_s \approx 0.02$) and a sharp peak at higher temperatures $t_c \approx 0.5$ associated with charge gap. The specific heat decreases very sharply at higher temperatures. Further the specific heat is suppressed with increase of substrate induced gap throughout the temperature range. The suppression of specific heat is more near the charge gap temperature (t_c).

5. Conclusions

We have considered a tight binding model study taking into account of substrate effect, band filling and electron-electron interaction in paramagnetic limit. The electron densities and temperature dependent specific heat are computed numerically. The temperature dependent electron densities and specific heat exhibit dips and peaks associated with substrate effect and charge gap effect respectively. The specific heat is suppressed with increase of substrate induced gap. We present here the preliminary work and the detailed study of the thermal properties like entropy, specific heat and the specific heat coefficient will be reported elsewhere for different values of substrate induced gap, band filling and Coulomb correlation energy [7].

References

[1] H.O. Pierson, Handbook of Carbon, Graphite, Diamond and Fullerenes: Properties, Processing and Applications (Noyes Publications, Park Ridge, NJ, 1993).

[2] MC Schabel, JL Martins, *Phys. Rev*. **B 46**, 7185 (1992)

[3] S Sahu, GC Rout, *Physica* B **461**, 49-56 (2015)

[4] S Sahu, GC Rout, *J. Magn. Magn. Mater*. **407**, 396-405 (2016)

[5] S Sahu, SKS Parashar, GC Rout, *AIP Conf. Proc*., **1724**,020111 (2016)

[6] R Panda, S Sahu, GC Rout, *AIP Conf. Proc*. (2017) [In press]

[7] R Panda, S Sahu, GC Rout, *OJP*. (2017) [Communicated]