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Local Spin Induced Magnetism In The Monolayer Nanographene

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Abstract. In this paper, we investigated local spin orientation (up or down) effects on magnetizations of the monolayer nanographene by using effective field theory developed by Kaneyoshi. It is found that the monolayer nanographene and its components have very small magnetization (mC1≈mC2≈mC3≈mMLNG≈2.31x10-18≈0) at T≈0.00 for the Jd1<0 (C1-spin up, C2-spin down and C3-spin up). On the other hand, for Jd2<0, Jd3<0, Jd4<0, and Jd5<0, the monolayer nanographene and its components (C1, C2 and C3 atoms) have very large local spin induced magnetization (mC1≈mC2≈mC3≈mMLNG≈1;1>>2.31x10-18) than those of the Jd1<0. These results clearly indicate that the local spin orientation in the monolayer nanographene has very strong effect on its magnetism.

Keywords: Nanographene, Monolayer nanographene, Spin, Spin orientation, Magnetism, Effective field theory.

Tek Tabakalı Nanografende Lokal Spin Etkili Manyetizma

Özet. Bu çalışmada, Kaneyoshi tarafından geliştirilen etkin alan teorisi kullanılarak, tek tabakalı nanografenin mıknatıslanmalarına lokal spin yönelimlerinin (yukarı ya da aşağı) etkileri incelendi. Tek tabakalı nanografenin ve bileşenlerinin Jd1<0 (C1-spin yukarı, C2-spin aşağı ve C3-spin yukarı) için T≈0.00'da çok küçük mıknatıslanmaya (mC1≈mC2≈mC3≈mMLNG≈2.31x10-18≈0) sahip olduğu bulundu. Diğer taraftan, Jd2<0, Jd3<0, Jd4<0 ve Jd5<0 için, tek tabakalı nanografen ve bileşenleri (C1, C2 ve C3 atomları), Jd1<0'dakinden çok büyük lokal spin etkili mıknatıslanmaya (mC1≈mC2≈mC3≈mMLNG≈;1>>2.31x10-18) sahiptirler. Bu sonuçlar açıkça, lokal spin yönelimlerinin, tek tabakalı nanografenin manyetizması üzerinde çok güçlü bir etkiye sahip olduğunu göstermektedir.

Anahtar Kelimeler: Nanografen, Tek tabakalınanografen, Spin, Spin yönelimi, Manyetizma, Etkinalanteorisi.

1. INTRODUCTION

Monolayer graphene discovered in 2004 by Novoselov et al.[1]. It is a new material that consists of Carbon atoms with honeycomb (hexagonal) lattice in one atom thickness. Because of its unique properties such as it consists of one layer, being strongest than steel, having high thermal and electrical conductivity, it is a promising material that can be used in areas such as; transistors, battery charges, energy storing devices, magnetic drug delivery systems, artificial magnetic systems, flat screens, coating material in automobiles and planes. Therefore, mono, two and multilayer graphene systems had come in to center of

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interest. Although it has a short history as 15 years, many works have been done on graphene and graphene based systems by using different experimental [2-22] and theoretical methods [23-29].

On the other hand, effective field theory developed by Kaneyoshi, which successfully identifies many magnetic nanosystems such as nanoparticles, thin films, nanowires and nanotubs [30-47] and enables the magnetic properties of these nanosystems to be successfully obtained, modeling nanosystems, it has emerged as a successful theoretical method which is used for defining and examining magnetic systems and applied continuously to different nanosystems. For example, using the effective field theory, the magnetic properties of the cubic nanowire [48], the hexagonal Ising nanowire [49], the mixed Ising nanoparticles [50], the spin-1 Ising nanotube [51], cylindrical transverse spin-1 Ising nanowire [52], cubic nanowire [53], a kinetic cylindrical Ising nanotube [54], honeycomb thin film [55], diluted transverse Ising nanowire [56], core/shell nanowire system [57], a mixed core/shell nanotube [58], core/shell spin-1 Ising nanowire [59] and cylindrical Ising nanowires [60-63] were investigated in detailed in literature.

Although the magnetic properties of many nanosystems were investigated using effective field theory, a small number of studies were reported on the magnetic properties of nanographene systems were investigated by using effective field theory in the literature [64-71]. However, local spin orientation effects on the magnetizations of the monolayer nanographene (MLNG) have not been studied yet for ϴCTA=1300. Therefore, in this paper, we investigate the local spin orientation (up or down) effects on magnetizations of the MLNG by using effective field theory developed by Kaneyoshi in detailed.

This paper is organized as follows. Section 2 describes the theoretical methods. Section 3 introduces the theoretical results and discussion. Section 4 is reserved for the conclusions.

2. THEORETICAL METHOD

The aim of this paper to investigate the local spin orientation (up or down) effects on magnetizations of the monolayer nanographene (MLNG) by using effective field theory developed by Kaneyoshi [72]. To obtain the the local spin orientation (LSO), we the exchange interactions between C1, C2 and C3 atoms of the MLNG. Namely, when $J_{d1}<0$, the spin direction of the C1 and C2, C2 and C3 is opposite, when $J_{d2}<0$ and $J_{d3}<0$, the spin direction of the C1 and C3 is opposite, when $J_{d4}<0$, the spin direction of the C1 and C2 is opposite, and when $J_{d5}<0$, the spin direction of the C2 and C2 is opposite. However, when all $J>0$ [73], all of the the spin of the MLNG are up (see Fig.2(f)).

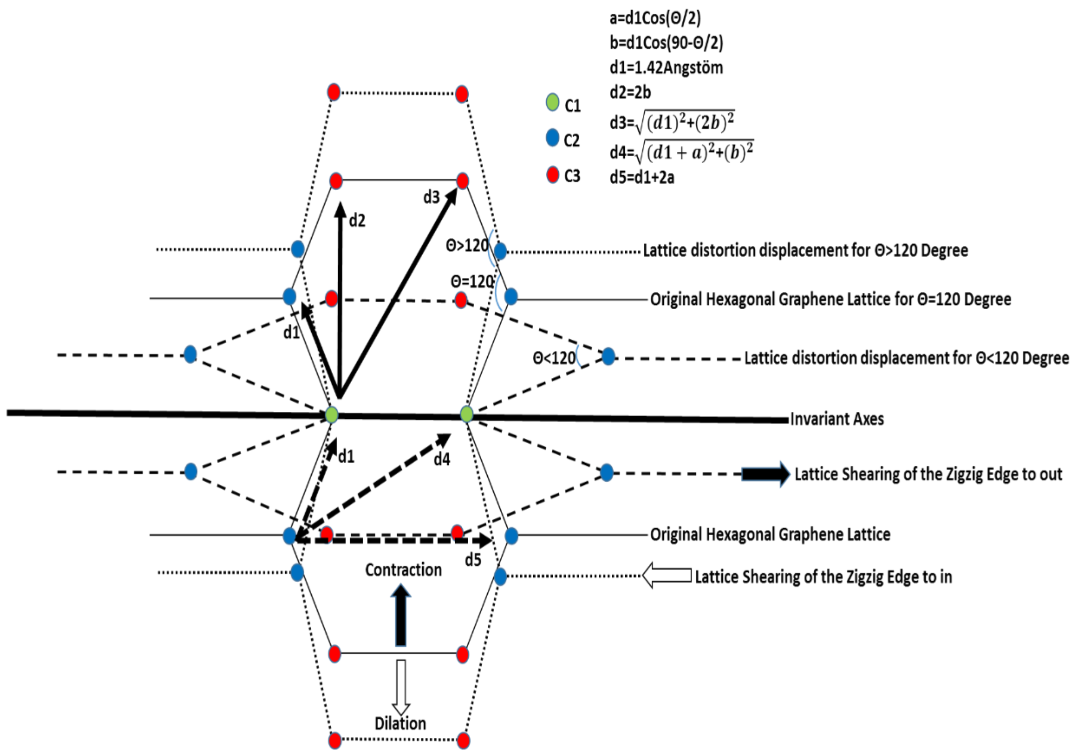

Figure 1. (Color online) Schematic representation the MLNG [73].

In our previous work [73], we investigated the effects of the twinning angle on the magnetizations of the MLNG. Since the MLNG system is same, we shall follow the same model and the same equations of the effective field theory of the MLNG given in our previous work [73] in detailed. Therefore, the Hamiltonian and the magnetizations of the MLNG and its components C1, C2 and C3 are given by [73],

Hamiltonian;

$$\begin{aligned} H = &-J_{\mathrm{d1}}\sum_{\langle \mathrm{C1,C1}\rangle} S^z_{\mathrm{C1}}S^z_{\mathrm{C1}} - J_{\mathrm{d1}}\sum_{\langle \mathrm{C1,C2}\rangle} S^z_{\mathrm{C1}}S^z_{\mathrm{C2}} - J_{\mathrm{d1}}\sum_{\langle \mathrm{C2,C3}\rangle} S^z_{\mathrm{C2}}S^z_{\mathrm{C3}} - J_{\mathrm{d1}}\sum_{\langle \mathrm{C3,C3}\rangle} S^z_{\mathrm{C3}}S^z_{\mathrm{C3}} \\ &-J_{\mathrm{d2}}\sum_{\langle \mathrm{C1,C3}\rangle} S^z_{\mathrm{C1}}S^z_{\mathrm{C3}} - J_{\mathrm{d2}}\sum_{\langle \mathrm{C2,C2}\rangle} S^z_{\mathrm{C2}}S^z_{\mathrm{C2}} - J_{\mathrm{d3}}\sum_{\langle \mathrm{C1,C3}\rangle} S^z_{\mathrm{C1}}S^z_{\mathrm{C3}} - J_{\mathrm{d4}}\sum_{\langle \mathrm{C1,C2}\rangle} S^z_{\mathrm{C1}}S^z_{\mathrm{C2}} \\ &-J_{\mathrm{d5}}\sum_{\langle \mathrm{C2,C2}\rangle} S^z_{\mathrm{C2}}S^z_{\mathrm{C2}} - h\left(\sum_{\mathrm{C1}} S^z_{\mathrm{C1}} + \sum_{\mathrm{C2}} S^z_{\mathrm{C2}} + \sum_{\mathrm{C3}} S^z_{\mathrm{C3}}\right) \end{aligned} \quad (1)$$

M**agnetizations;**

$$\begin{aligned} m_{\mathrm{C1}} = &[\cosh(J_{\mathrm{d1}}\nabla)+\mathrm{m}_{\mathrm{C1}}\sinh(J_{\mathrm{d1}}\nabla)]^1[\cosh(J_{\mathrm{d1}}\nabla)+\mathrm{m}_{\mathrm{C2}}\sinh(J_{\mathrm{d1}}\nabla)]^2[\cosh(J_{\mathrm{d4}}\nabla)+\mathrm{m}_{\mathrm{C2}}\sinh(J_{\mathrm{d4}}\nabla)]^2 \\ &[\cosh(J_{\mathrm{d2}}\nabla)+\mathrm{m}_{\mathrm{C3}}\sinh(J_{\mathrm{d2}}\nabla)]^2[\cosh(J_{\mathrm{d3}}\nabla)+\mathrm{m}_{\mathrm{C3}}\sinh(J_{\mathrm{d3}}\nabla)]^2 F_{\mathrm{s}\text{-}1/2}(x)\big|_{\mathrm{x}=0}, \\ m_{\mathrm{C2}} = &[\cosh(J_{\mathrm{d1}}\nabla)+\mathrm{m}_{\mathrm{C1}}\sinh(J_{\mathrm{d1}}\nabla)]^1[\cosh(J_{\mathrm{d4}}\nabla)+\mathrm{m}_{\mathrm{C1}}\sinh(J_{\mathrm{d4}}\nabla)]^1[\cosh(J_{\mathrm{d2}}\nabla)+\mathrm{m}_{\mathrm{C2}}\sinh(J_{\mathrm{d2}}\nabla)]^1 \\ &[\cosh(J_{\mathrm{d5}}\nabla)+\mathrm{m}_{\mathrm{C2}}\sinh(J_{\mathrm{d5}}\nabla)]^1[\cosh(J_{\mathrm{d1}}\nabla)+\mathrm{m}_{\mathrm{C3}}\sinh(J_{\mathrm{d1}}\nabla)]^1 \\ &[\cosh(J_{\mathrm{d4}}\nabla)+\mathrm{m}_{\mathrm{C3}}\sinh(J_{\mathrm{d4}}\nabla)]^1 F_{\mathrm{s}\text{-}1/2}(x)\big|_{\mathrm{x}=0}, \\ m_{\mathrm{C3}} = &[\cosh(J_{\mathrm{d2}}\nabla)+\mathrm{m}_{\mathrm{C1}}\sinh(J_{\mathrm{d2}}\nabla)]^1[\cosh(J_{\mathrm{d3}}\nabla)+\mathrm{m}_{\mathrm{C1}}\sinh(J_{\mathrm{d3}}\nabla)]^1[\cosh(J_{\mathrm{d1}}\nabla)+\mathrm{m}_{\mathrm{C2}}\sinh(J_{\mathrm{d1}}\nabla)]^1 \\ &[\cosh(J_{\mathrm{d4}}\nabla)+\mathrm{m}_{\mathrm{C2}}\sinh(J_{\mathrm{d4}}\nabla)]^1[\cosh(J_{\mathrm{d1}}\nabla)+\mathrm{m}_{\mathrm{C3}}\sinh(J_{\mathrm{d1}}\nabla)]^1 F_{\mathrm{s}\text{-}1/2}(x)\big|_{\mathrm{x}=0}, \end{aligned} \quad (2)$$

In the Hamiltonian, J_i (i = d1, d2, d3, d4 and d5) is the exchange interaction between two nearest and next neighbor Carbon atoms. The values of the J_i are obtained by using the relationship $J_i = k_i/nd_i$; where, k_i (i = 1, 2, 3, 4 and 5) is a constant that defines the type of magnetization and nd_i (i = 1, 2, 3, 4 and 5) is the normalized lattice distance such as, $nd_1 = d_1/1Å = 1.42Å/1Å = 1.42$. $S^z = \pm 1$ is the Pauli spin operator. h is the external magnetic field. In the magnetizations, $\nabla = \partial / \partial x$ is the differential operator and the function of $F_{S\text{-}1/2}(x)$ is defined by as follows for the spin-1/2 Ising particles [73].

$$F_{s\text{-}1/2}(x) = \tanh[\beta(x+H)] \tag{3}$$

where $\beta = 1/k_B T_A$, k_B is the Boltzmann's constant, T_A is the absolute temperature. We used the reduced temperature, $T = k_B T_A/J$, and the reduced applied field, i.e. $H = h/J$ in all calculations. The total magnetization of the MLNG is given by [73],

$$MT_{MLNG} = \frac{1}{10}[2\, m_{C1} + 4\, m_{C2} + 4\, m_{C3}]. \tag{4}$$

3. THEORETICAL RESULTS

We obtained the temperature and local spin orientation dependence of the magnetization of the monolayer nanographene (MLNG) for the critical twinning angle ($\Theta_{CTA}=130^0$) of zigzag edge in Figs.2(a)-(f). In Fig.2(a), magnetizations of the MLNG (MTMLNG) and its component (mC1, mC2 and mC3) are obtained for Jd1<0 (in other word, C1-spin up, C2-spin down and C3-spin up). As we clearly see that antiferromagnetic orientations of the spin of the nearest neighbor atoms (Jd1<0) cause almostly zero magnetization (mC1≈mC2≈mC3≈mMLNG≈2.31x10-18≈0) at T≈0.00 (this means that TC≈0.00). On the other hand, antiferromagnetic orientations of the spin of the next-nearest (Jd2<0 and Jd4<0) and third-nearest (Jd3<0 and Jd5<0) neighbor atoms cause a very highest magnetization behaviors than those of the nearest neighbor atoms (Jd1<0) ($m_{C1} \approx m_{C2} \approx m_{C3} \approx m_{MLNG} \approx 1 >> m_{C1} \approx m_{C2} \approx m_{C3} \approx m_{MLNG} \approx 2.31 \mathrm{x} 10^{-18} \approx 0$) at T≈0.00 in Figs.2(b), (c), (d), (e) and for all J>0 in Fig.2(f) for which the local spin induced Curie temperature are obtained as TC=1.57, 2.15, 1.04, 2.47 and 2.738 (after Ref. [73]), respectively. By using these results, we suggest that it is possible to obtain magnetism with the changing of the local spin direction of the MLNG and other magnetic systems. We call such magnetism as local spin induced magnetism (LSIM) and local spin induced Curie temperature ($LSIT_C$).

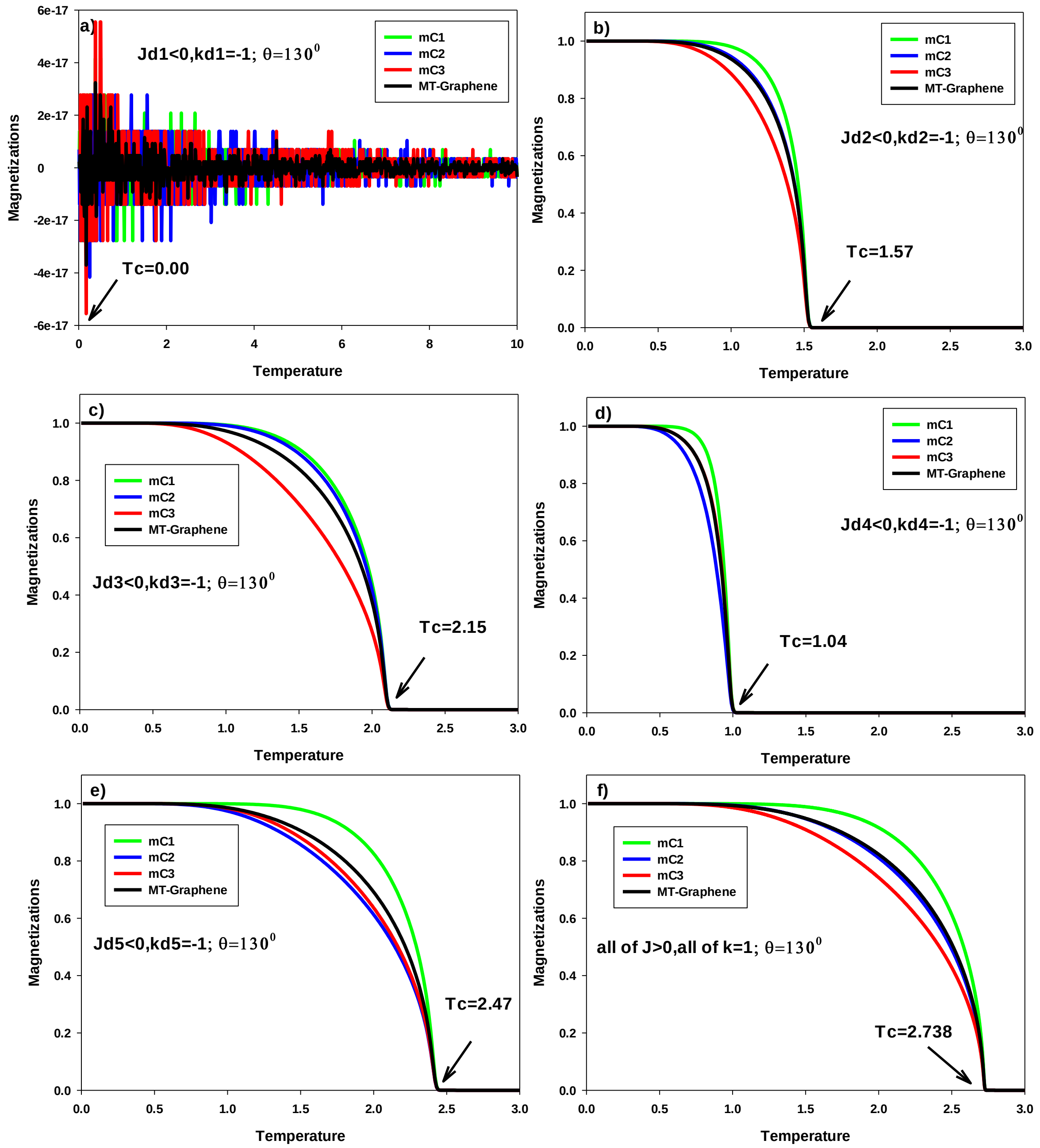

Figure 2. (Color online) Local spin induced magnetism (LSIM) and local spin induced Curie temperature (LSIT$_C$) in the MLNG.

4. CONCLUSIONS

Local spin orientation (up or down) effects on magnetizations of the monolayer nanographene (MLNG) by using effective field theory developed by Kaneyoshi. It is found that;

1. MLNG and its components have a very small magnetism $m_{C1} \approx m_{C2} \approx m_{C3} \approx m_{MLNG} \approx 2.31x10^{-18} \approx 0$ at T≈0.00 for Jd1<0.

2. MLNG and its components have very large magnetism $m_{C1} \approx m_{C2} \approx m_{C3} \approx m_{MLNG} \approx 1$ at T≈0.00 for $J_{d2}<0$, $J_{d3}<0$, $J_{d4}<0$, $J_{d5}<0$ and all J>0.

3. Curie temperature of the MLNG and its components is differ for each $J_{d1}<0$, $J_{d2}<0$, $J_{d3}<0$, $J_{d4}<0$, $J_{d5}<0$ and all $J>0$.

4. We call such magnetism as local spin induced magnetism (LSIM) and local spin induced Curie temperature ($LSIT_C$)

5. We hope that our results open a door to understanding of the magnetism in MLNG and other magnetic systems.

Acknowledgments

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