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Magnetic and thermodynamics properties graphene monolayer with defects

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HIGHLIGHTS

- Ising model of a graphene monolayer with defects is suggested.
- Magnetic and thermodynamics properties of the system have been studied.
- A broad maximum of the magnetization has been found.
- Unusual behavior of the specific heat has been explained.

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ABSTRACT

Magnetic and thermodynamics properties of a graphene monolayer with defects are studied within the effective-field theory with correlations. The magnetization, the internal energy, and the specific heat as functions of temperature for different anisotropy and the defect concentration are calculated. Plateaus behaviors of the magnetization have been found. The reason that a broad maximum presents on the magnetization curve in some parameter range have been explained. Similar result has been also found experimentally in graphene. The results show the magnetic properties can be adjusted by controlling the defect concentration.

1. Introduction

As one of the most promising materials, graphene has attracted much interest in exploring its unique physical and chemical properties [1–7]. Now it is widely applied in semiconductor [8,9], biomedicine detection [10,11], super-capacitor [12], electromagnetic interference shielding [13], sensors [14,15]. The ideal graphene shows diamagnetism, but the graphene with carbon atom defects may display magnetism. More and more researchers focus on such novel metal-free magnetic materials in experimentally. Ji et al. have proposed an optical system that for the first time provided a practicable method for exploring the quantum magnetic correlation of polarized photons [16]. Wang et al. have reported the graphene-based materials display ferromagnetic properties at room temperature [17]. From the experimental results they believe that ferromagnetism comes from the defects on graphene. Scanning tunneling microscopy reported that a sharp electronic resonance was at the Fermi energy around [18]. Each vacancy formed to local magnetic moments. The results showed the possibility of magnetic states of graphene by randomly deleting individual C atoms. Khurana et al. have also noted ferromagnetism behavior in the graphene

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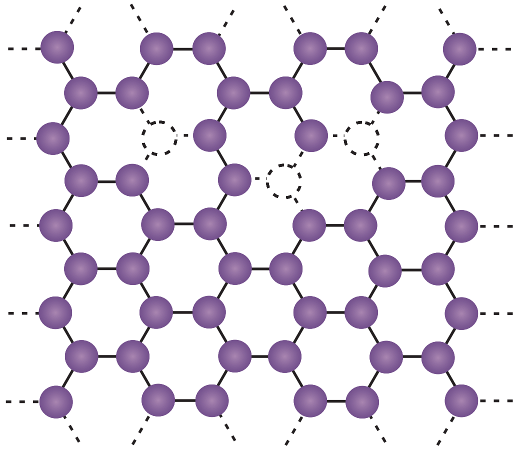

Fig. 1. Schematic representation of a graphene monolayer with defects. The hollow balls are randomly defects.

with the defects [19]. The carbon atomic defects play important role in controlling the magnetism in graphene. A single layer of graphene with defects has been prepared by chemical vapor deposition [20]. The size and density of defects in graphene samples were caused by ion irradiation. This ion implantation technique can be used to control the defects in graphene. Recent experimental evidence has shown magnetic behavior of graphene with defects [21]. The localized state of the atomic defects splits to induce magnetic properties. Miao et al. have prepared graphene with a high temperature synthesis method and then controlled the defect concentration with heat treatment [22]. To control defects concentration makes magnetism manageable in graphene. Based on first-principles the magnetic properties of graphene with defects have been studied [23]. It is found the itinerant magnetism mainly comes from defect-induced extended states. The values of magnetic moments are sensitive to the defect concentration. The exchange coupling between the magnetizations is ferromagnetic or antiferromagnetic, depends on whether the defects match to the same or different sublattices. The role of defects on the magnetic properties of carbon materials has also been studied [24]. The magnetization for graphitic structures decreases more rapidly with increase of vacancy density. The nitrogen at a vacancy has been found to produce larger macroscopic magnetic signals compared to a single carbon vacancy. It is possible for tuning the magnetic properties of carbon material by making atomic defects. Valencia et al. have proposed ab initio theory to study magnetic properties of graphene with defects [25]. They predict an integer magnetization for a graphene with a single vacancy. Single vacancy with periodic array provided scatter spin exchange because of the specific symmetry of the graphene. The magnetic properties of carbon-based, honeycomb and graphene have been widely studied by Monte Carlo simulation [26–36]. In added two-dimension such as MoS2 monolayer with defects also appears magnetic properties [37]. We shall study the effects of defect on magnetic and thermodynamics properties of a graphene monolayer with defects within the effective-field theory with correlations. These results will be helpful to better understand the mechanism of magnetic properties of graphene with defects.

Theoretical and experimental progresses suggest the magnetic properties of graphene can be controlled by defect concentration. It stimulates our study of the effects of defect concentration on magnetic properties of a graphene. We consider a graphene with defects plotted in Fig. 1. The hollow balls are randomly single defects. Recently, based on molecular orbital calculation and first-principles to find the high spin-5/2 state matching to the lowest energy is more stable for graphene [38]. It has up and up spin pairs with stronger ferromagnetic exchange coupling. Thus, Ising model with spin-5/2 is proposed to describe a graphene with defects. We have studied magnetic properties of nano-graphene bilayer and sandwich-like structure by using the effective-field theory with correlations (EFT) in our previous work [39,40]. This method (EFT) has been successfully applied to solve various spin Ising problems. The aim of this paper is to apply the EFT onto the magnetic behavior of the graphene monolayer with defects. To find out how the anisotropy and the defect concentration affect the magnetic and thermodynamics properties of a graphene.

The paper is arranged as follows. In Section 2, a graphene monolayer with defects is proposed to describe by Ising model. In Section 3, the magnetic and thermodynamics properties of a graphene monolayer with defects are studied. Finally, the summary is given in Section.

2. Calculation methods

In this section we present the effective-field theory with correlations and differential operator technique [41–44] for a graphene monolayer with defects in Fig. 1 to gain expressions the magnetization and the internal energy. Ising model is a spin model in statistical physics, which can be used to describe a graphene monolayer with defects. The Hamiltonian for this