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Monte Carlo study of magnetization plateaus in a zigzag graphene nanoribbon structure

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ABSTRACT

The Monte Carlo simulation has been applied to discuss the step effect on a zigzag graphene nanoribbon structure in a longitudinal magnetic field. The effects of the singe-ion anisotropies, longitudinal magnetic fields and temperature on the magnetization plateaus have been investigated in detail. Our results show that the number of magnetization plateaus for the system dissatisfy $2S+1$ criterion at low temperatures, originating from not only the competition between the anisotropy and the external magnetic field, but also the contributions of edge effects. It has been found that the single-ion anisotropy plays a significant role in modulating the spin configurations of the zigzag graphene nanoribbon structure. In addition, the effects of single-ion anisotropies and external magnetic fields on the magnetization, the susceptibility, the internal energy and the blocking temperature have been examined.

1. Introduction

Over two decades, there are increasingly dramatic breakthroughs in the progress of materials with excellent nanostructures, such as nanoparticles [1–3], nanowires [4,5], nanotubes [6], nanoislands [7], nanodisks [8], nanographene [9,10]. Particularly, nanographene has speedily developed into one focus of nanomaterials since the two-dimensional graphene with a honeycomb structure was succesfully prepared. As a new derivative, graphene may be derived from a macromolecule produced by chemical reactions [11,12]. It is considered as an effective approach to adjust the gap energy and dominate magnetic properties for the graphene [13]. Graphene has been devoted to more explorations since the first appearance in 2004 [14,15]. Because graphene is a zero gap semiconductor, it offers a challenge how to open and regulate the band gap, which makes it possible for the graphene material to apply in high tech-electronic devices. A few of techniques are employed with diverse processes to overcome this limitation. Of which one way is the quantum confinement of electrons by forming graphene nanoribbons (GNRs) [16,17]. Either it can explain magnetism or modify the electronic structure for the non-magnetic materials.

By means of the epitaxial graphene pattern or cutting the exfoliated graphene sheet along one straight line, it is feasible to fabricate graphene nanoribbons with two typical types of edges: armchair and zigzag edges [18]. Considerable theoretical investigations have revealed that the electrical and magnetic properties of GNRs can be modulated by the edge structures and the ribbon width [19]. Naturally, armchair graphene nanoribbons (AGNRs) are not beneficial for magnetic ordering in theory [20], whereas zigzag graphene nanoribbons (ZGNRs) can display relatively more plentiful information about interesting magnetic structure and magnetic behaviors such as peculiar transport properties and magnetism [21]. Owing to the electron spin polarization behaviors spontaneously at zigzag edge states, ZGNRs are discovered to be magnetic semiconductor, in which the C atoms at each edge couple ferromagentically to each other and antiferromagnetically to those of the opposite edge [22]. As a typical feature of AFM ground state in ZGNRs, half metallicity is especially significant for special spintronic devices [23]. In order to stabilize the half metallicity in ZGNRs, the energy difference between ferromagnetic and antiferromagnetic (FM-AFM) ground states may be very small (several meV per unit cell), and it is likely for FM-AFM energy to take on the metal state at finite temperature. In view of this, a great number of theoretical explorations are concerned with the effects of adsorptions with magnetic transition metal (TM) atoms [24], the

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replacement of edge C atoms by nonmagnetic atoms such as N [20], H [25] and B [26], heteroatoms-doping [27], carrier density [28], edge state [29], topological defect vacancies [30], as well as external electrical and magnetic field [31] to achieve the reasonable prediction and explanation for magnetic mechanism in ZGNRs.

Another interesting theoretical study has illustrated that the sufficiently strong magnetic field can drive the spin-polarized edge states in ZGNRs from antiferromagnetic to ferromagnetic coupling, leading to a phase transition from the ground state to the magnetized state. Conversely, the increase of the temperature enables the spins to become disordered and unpolarized state, magnetic anisotropy effect can be used to keep the spin ordering [32]. As a result, by aid of the external conditions, ZGNRs in finite temperature can exhibit the ground state, spin disordered or magnetized state. Therefore, controlling multiple spin configuration states of ZGNRs under different physical parameters may be of important theoretical and practical significance in designing spin transistors and spin logic devices [33]. As is well-known, the Ising model as one of the basic models of statistical physics has been successfully extended to describe various magnetic nanosystems and plays a significant role in understanding magnetic phase transitions and electric polarization behaviors of spin systems. Theoretically, by building various Ising models, the effects of various physical parameters such as the crystal-field, the exchange coupling, the temperature and the longitudinal magnetic field upon magnetic performances of graphene nanoribbons have been deeply examined. L. B. Drissi et al. have studied magnetic behaviors of a mixed-spin (1/2, 1) nanoribbon with the core-shell structure under the effect of an antiferromagnetic interface coupling by the Monte Carlo (MC) simulation [34]. They have found a number of distinctive behaviors, for example, single and triple hysteresis loops as well as compensation temperatures. The influence of the locations and the number of spin-3/2 substituted magnetic atoms upon magnetic phase transitions of the doped mono-, bi- and tri-graphene nanoribbons with different configurations have been analyzed in great details [35]. Related results have indicated that the critical temperature T_c relies on the number of dopants, while in view of configurations with fixed magnetic impurities, it could be found that T_c has the stronger sensitivity to edges. In addition, by using the mean field theory and the MC simulation, the temperature dependences of magnetizations and susceptibilities have been thoroughly explored for the pure graphene nanoribbons [36]. Particularly, the low/strong external magnetic fields and ribbon widths on critical temperatures, transition temperatures and hysteresis loops have been also investigated. These results have further proved the important functions of the temperature, the anisotropy and the longitudinal magnetic field to graphene nanoribbon systems.

Recently, many researchers have investigated different mixed-spin Ising systems under the external magnetic field for many years [37–39]. They have demonstrated the special significance of the external magnetic field on the magnetic properties for nanosystems. At low temperatures or ground state, magnetic Ising nanomaterials may display spin ladders, exchange biases, magnetization plateaus as well as other outstanding performances. The eligible condition $s\text{-}m =$ integer for existing magnetization plateaus have early come into the view of theoretical studies [40]. Since the first report of the magnetization plateau for one nearest-neighbour Ising model, more and more devotions have been immersed in studying magnetization plateaus of mixed-spin magnetic systems [41]. Based on the effective-field theory (EFT), Jiang et al. have examined the influences of different crystal-field anisotropies on magnetization plateaus for one ferrimagnetic nanoparticle [42]. Of investigations it has found the dissatisfaction of the $2S + 1$ criterion for the magnetization plateaus under the effect of larger crystal-field anisotropies. It is colorful to investigate magnetization plateaus on $\pm J$ Ising square lattices and triangular lattices by the MC simulation [43,44]. At low temperatures, irregular behaviors from the single-ion anisotropy have been also found in the hysteresis loops. X.Y. Chen et al. have studied magnetization plateau phenomena for the positive anisotropy under the influence of the longitudinal magnetic field in an antiferromagnetic mixed-spin (1, 3/2) Ising system with the classical MC simulation [45]. By using both the molecular-field theory and density-matrixre normalization group calculations, magnetic characteristic behaviors have been explored with the homogenous crystal-field anisotropy for one ferrimagnetic mixed-spin (1, 3/2) Ising chain [46]. It turned out that the anisotropy plays a vital part in the occurrence of magnetization plateaus. Besides, with increasing the longitudinal magnetic field from 0 to its saturation value h_s, it is not difficult to discover $2S + 1$ magnetization plateaus in low-dimensional magnetic materials with the magnetic field h [40,45,47]. As far as ferromagnetic and antiferromagnetic mixed-spin systems are concerned, they have strong dependences on crystal-field anisotropies, temperatures and the magnetic dipolar interactions [48,49]. It could be observed the magnetization plateaus within the anisotropy at the magnetization process in a spin-3/2 chain system [50]. With respect to experimental observations, magnetization plateau phenomena have also emerged in diverse systems, such as $NbFeTe_2$ [51], $Fe_xMg_{1\text{-}x}Cl_{12}$ [52], $La_{0.67\text{-}x}A_xCa_{0.33}MnO_3$ [53], novel organic tetraradical crystal BIP-TENO [54] as well as the quasione-dimensional Ni-compounds [55,56] and the quasitwo-dimensional compound $SrCu_2(BO_3)_2$ [57].

Interestingly, recent theoretical studies have also been focused on the graphene nanostructure by the establishment of different mixed-spin Ising models. Using the EFT, E. Kantar have investigated the magnetic hysteresis, compensation behaviors and phase diagrams of the bilayer honeycomb lattices (BHL) system with AB stacking geometry by building spin-1/2 Ising model [58]. Especially the dynamic phase transitions, the dynamic hysteresis curves and compensation types of the BHL structure in the oscillating magnetic field have been studied in details [59,60]. R. Masrour et al. have applied the MC simulation to explore the effect of magnetic atom doping of graphene strucrure by a spin-2 Ising model [61]. Described by a mixed-spin (3, 7/2) Ising model, the magnetic properties of a bi-layer decorated graphene structure has been examined within the MC simulation [62]. In our previous work, we have applied the MC simulation and mixed-spin Ising models to study magnetic and thermodynamic properties of different low-dimensional nanomaterials, such as the nanographene bilayer [63], the nanowire [64] and the magnetic films [65]. Especially, the step effects on molecular-based magnets under the influences of single-ion anisotropies, exchange couplings and temperatures [66]. Whether magnetization plateaus exist or not in such a ZGNRs system? Do they satisfy the $2S + 1$ criterion? In remarkable, less attention has been paid to the connection of appearing magnetization plateaus with the variation of spin configurations for diverse single-ion anisotropies and longitudinal magnetic fields in a ZGNRs structure. Recently, the magnetization plateaus of the sandwich-like nanographene have been discussed with the EFT [67]. In addition, AGNRs can be also express metallic and semiconductor properties depending on the ribbon width under certain conditions, but different from that of AGNRs, ZGNRs system is always semiconductor and can exhibit more fascinating edge effect since localized edge states, edge magnetism and susceptibility can develop them into special magnetic materials without d or f electrons [34,35,68], which may be favor for ample potential applications in spintronic devices. However, less literature has been reported on multiple spin states related to magnetization evolution in an external magnetic field for the relevant investigations of