Superlattices and Microstructures 113 (2018) 524–533

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Magnetic compensation and critical properties of a mixed spin-(2, 3/2) Heisenberg single-walled nanotube superlattice

Bin-Zhou Mi [a,*], Cui-Ju Feng [a], Jian-Guo Luo [b,**], De-Zhi Hu [b]

[a] College of Science, North China Institute of Science and Technology, Beijing 101601, China
[b] School of Mechanical & Electrical Engineering, North China Institute of Science and Technology, Beijing 101601, China

ARTICLE INFO

Article history:
Received 20 September 2017
Received in revised form 20 November 2017
Accepted 20 November 2017
Available online 20 November 2017

Keywords:
Magnetic nanotubes
Mixed spins
Easy-axis single-ion anisotropy
Magnetic compensation and critical properties
Quantum effects

ABSTRACT

In recent years, some theoretical interests have been focused on the binary alloy nanotubes and nanowires with mixed spins. Compared with ferrimagnetic nanowires, few studies have been done on ferrimagnetic nanotubes. In this paper, the magnetic properties of a mixed spin-(2, 3/2) Heisenberg single-walled nanotube superlattice are calculated by use of the double-time Green's function method within the random phase approximation and the Anderson and Callen's decoupling. Magnetic compensation and critical properties are obtained for a wide range of parameters in the Hamiltonian, and magnetic phase diagrams are plotted in the related planes. For Heisenberg single-walled nanotube superlattice model with Néel-type magnetic structure, anisotropy must be taken into account, and the easy-axis single-ion anisotropy is considered in this paper. The next nearest neighbor exchange interactions J_{bb} and/or single-ion anisotropy strength D_b of the smaller spin sublattice were necessary in order to obtain a compensation point. The influence of the wall diameter number of the tubes, m, an important parameter of the system, on the compensation behavior is considered. Calculation shows that as J_{bb} and D_b are fixed, only when m is beyond a certain minimum value, m^{min}, can compensation temperature T_{com} appears, where the next nearest neighbor exchange interactions J_{aa} and single-ion anisotropy strength D_a of the larger spin sublattice are absent. The compensation temperature and critical temperature increase with m rising, which indicates that the longitudinal correlation effect is enhanced and the fluctuation effect is weakened with the increase of m.

1. Introduction

In recent years, magnetic nanostructured materials, i.e., nanotubes and nanowires, have attracted great interest in experimental [1–6] and theoretical [6–16] studies due to their promising applications, such as ultrahigh-density magnetic storage devices, biomagnetic sensors, nanomedicine, molecular devices, catalysts, and nanoelectronic devices, etc. Experimentally, binary alloy magnetic nanotube and nanowire arrays, such as FeCo nanotubes [17], FeNi nanotubes [18,19] and nanowires [19,20], CoNi nanotubes [21], CoPt nanotubes and nanowires [22], have been fabricated by various experimental techniques. Seen from the perspective of the theory, the magnetic properties of nanotubes and nanowires can be described by

* Corresponding author.
** Corresponding author.
E-mail addresses: mbzfjerry2010@ncist.edu.cn (B.-Z. Mi), luojg_1598@126.com (J.-G. Luo).

https://doi.org/10.1016/j.spmi.2017.11.037
0749-6036/

the well-known Ising model and Heisenberg model using various theoretical techniques and numerical methods, such as micromagnetic simulation [6,7], Monte Carlo simulations [8–10], effective-field theory [11–13], First-principles calculations [14,15], and double-time Green's function method [16]. Geometrically, nanotubes are described by their external and internal radii, R and r, respectively, and longitudinal length L. Here we define the ratio $\beta_0 \equiv r/R$, so that $\beta_0 = 0$ represents a nanowire and β_0 close to 1 corresponds to a nanotube with very thin walls. In this paper, we consider the single-walled nanotube lattice model, i.e. $L \rightarrow \infty$, and $\beta_0 = 1$ [23–25].

More recently, it is worth noting that some theoretical interest has been focused on the binary alloy ferrimagnetic nanomaterials with mixed spins [26–31]. Unlike antiferromagnetic material, ferrimagnetic material has a measurable net magnetization at low temperatures, although the magnetization will vanish above a critical temperature T_C. The magnetizations in different sublattices have, in general, different temperature dependences. Therefore, they may cancel each other at some lower temperature, T_{com}, known as the compensation temperature. Such compensation behaviors have been observed in a number of real materials, which have many technological applications especially for thermo-magnetic and magneto-optical recordings, since at this compensation temperature the material undergoes a dramatic increase in its coercivity, such that only a small driving field can change the sign of the resultant magnetization. Therefore, it is important and meaningful to study the magnetic compensation properties of ferrimagnetic nanomaterials with mixed spins [26–31]. Particular theoretical attentions have been focused on the magnetic compensation and critical behaviors of the ferrimagnetic Ising nanowires [32–40] and Ising nanotubes [41,42] with mixed spins (1/2, 1) [32–35], mixed spins (1, 3/2) [36,41,42], mixed spins (1/2, 3/2) [37,38], and mixed spins (1, 2) [39,40]. For example, the magnetic properties and phase diagrams of ferrimagnetic mixed spin-1/2 and spin-1 cylindrical Ising nanowire are studied [32] by using the Monte Carlo Simulation and the effective field theory, and the effects of exchange interaction (J_S, J, and J_1) and anisotropy field (D) on the magnetic compensation properties and the critical properties are mainly considered. Calculations demonstrate that the system exhibits rich critical behaviors, which includes the first and second order phase transitions. The calculation also shows that the system can exhibit a magnetic compensation point depending on the values of J_S/J, J_1/J and D/J. Also the effects of the exchange coupling, the crystal field and the external longitudinal magnetic field on the magnetic and thermodynamic properties of the ferrimagnetic mixed spins-(1, 3/2) Ising nanowire with hexagonal core-shell structure are investigated [36] by using the Monte Carlo simulation techniques. The results show that the nanowire can demonstrate the compensation behavior, which depends on the critical exchange couplings J_{intk} and J_{sk} for the system. In addition, the compensation behavior of the mixed spin-1/2 and spin-3/2 hexagonal-type Ising nanowire system is examined [37] by using the effective field theory with correlations, and the N-, Q-, P-, R-, and S- type compensation behaviors are obtained relying on the values of Hamiltonian parameters. Similar characteristic phenomena have also been studied in the mixed spin-1 and spin-2 hexagonal Ising nanowire system [40]. Compared with ferrimagnetic nanowires, few studies have been done on ferrimagnetic nanotubes. In particular, the magnetic properties and thermodynamics of a double-wall cubic metal nanotube with mixed spins-(1, 3/2) are investigated [41,42] by the effective-field theory with correlations and the Monte Carlo simulation, respectively. Interestingly, it is found that [41] there are two or three magnetic compensation points for the magnetization curve of the double-wall cubic metal nanotube in some specific parameters. Although magnetic compensation and critical properties of ferrimagnetic Ising nanotubes were studied as described above, the research of magnetic compensation properties of ferrimagnetic Heisenberg nanotubes have still not been involved. The conditions of magnetic compensation point appears, especially the effects of the wall diameter of nanotubes on the magnetic compensation behaviors are deserved to be further studied.

Motivated by the above considerations, the magnetic compensation and critical properties of a mixed spin-(2, 3/2) Heisenberg single-walled nanotube superlattice are investigated by employing the double-time Green's functions (DTGFs) method. This paper mainly considers the effect of the easy-axis single-ion anisotropy and the next nearest neighbor interaction of the smaller spin sublattice, and the number of atoms in the cross section of nanotubes on the magnetic compensation and critical behaviors. The rest of this paper is organized as follows. We first put down the Hamiltonian of Heisenberg mixed spin-(2, 3/2) ferrimagnetic single-walled nanotube superlattice, and briefly outline the formulas derived by the DTGFs method. Then the numerical results and discussions are carried out in detail. At last the conclusions of this paper are summarized.

2. Model and formulas

First a two-dimensional (2D) square lattice with the nearest neighbor distance being a_0 is considered. One unit cell is depicted in Fig. 1, and a spin situated in each lattice site. Then the plane is rolled up along the diagonal direction of a cell to form a nanotube. This kind of rolling is just what was named as zigzag type tube [24,25]. In the present paper, we consider a Heisenberg ferrimagnetic single-walled nanotube superlattice of zigzag type, which is composed of two sublattices: a with spin $S_a = 2$ and b with spin $S_b = 3/2$, and the lattice constant is $b_0 = \sqrt{2}a_0$. The spins were assumed to interact via a Heisenberg exchange coupling limited to nearest neighbor (nn) and next nearest neighbor (nnn) sites. Moreover, easy-axis single-ion anisotropy was assumed to favor the nanotube axis. According to the Mermin–Wagner theorem [43], the isotropic Heisenberg model (without anisotropies and magnetic field) in less than three dimensions does not exhibit spontaneous magnetization (collective order) at finite temperatures. However, the spontaneous magnetization can occur when easy-axis single-ion anisotropy is introduced no matter how small it is [25,44,45]. In addition, single-ion anisotropy is quite common in real nanotube materials.