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Influence of radial and tangential anisotropy components in single wall magnetic nanotubes. A Monte Carlo approach

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HIGHLIGHTS

- Magnetic behaviour of nanotubes with square cell has been studied by the Monte Carlo Method.
- Competition between exchange interaction and radial and tangential anisotropy is analysed.
- Ferromagnetic, radial or tangential and paramagnetic phases depend on anisotropy constant and temperatures values.

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ABSTRACT

Magnetic behaviour of nanotubes with square cell has been studied by the Monte Carlo Method, under the Metropolis algorithm and Heisenberg model. The Hamiltonian used includes nearest neighbour exchange interaction and radial and tangential direction for uniaxial anisotropy. Periodic boundary conditions were implemented at the sample's edges. Simulations were carried out varying the nanotube's diameter by changing the number of magnetic moments per ring and anisotropy values. Two transition temperatures were identified corresponding to states where moments were aligned as either ferromagnetic type or anisotropy direction. At low temperatures and low anisotropy values, the system exhibited a ferromagnetic alignment; as the anisotropy was increased, and continued in the low temperature range, spins were aligned in the anisotropy (radial or tangential) direction. As the temperature was increased, spins were reoriented in the ferromagnetic direction, generating a radial (tangential) anisotropy to ferromagnetic transition temperature. When the temperature continued increasing, the system transited toward the paramagnetic phase, appearing a ferromagnetic to paramagnetic transition phase temperature. In several cases studied here, between these two transition temperatures (anisotropy to ferromagnetic and ferromagnetic to paramagnetic transition phases), the magnetization of the system exhibited instabilities. These instabilities are caused because of the influence of the anisotropy values and the diameter of the nanotubes on the magnetic domains formation. As a consequence, there exist anisotropy values and diameters where metastable states were formed.

1. Introduction

Magnetic nanostructures have attracted the interest of scientific researches because of their technological applications [1,2]. For instance, the control of magnetic domains would allow the implementation of novel technologies in data storages,

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sensors, drug-delivery carriers, biomedical diagnosis agents and other possible applications. Magnetic nanotubes have been currently studied for that purpose, being a new challenge, especially because of their topological shape [3]. The shape is an important characteristic in nanotubes and other structures since their magnetic properties are quite different from those of the bulk and greatly affected by the nanostructure sizes [4]. Furthermore, the magnetization's easy axis is usually the same one of magnetic moments, as in the case of thin films. Nevertheless, in the case of nanotubes, the anisotropy direction mainly depends on the lattice structure and shape, being possible to observe radial and tangential components of the generated magnetocrystalline anisotropy. For instance, from the cubic crystalline structure [5], surface anisotropy is guided by structures of carbon nanotubes [6]. Competitions between radial, tangential, longitudinal and shape anisotropies could generate new and intriguing properties [3]. For instance, C.D. Salazar et al. [7] carried out a study of the anisotropy direction's influence on certain magnetic properties of square and hexagonal nanotubes. Nevertheless, a better analysis is required. Other authors reported studies of the anisotropy influence on different nanostructures as nanoparticles [8]. The nanotube shape influences the correlation between magnetic moments, specifically when the diameter presents a critical value with respect to the nanotube thickness and length [9]. In these cases, the correlation depends on the competition between exchange interaction (which attempts to orient in a parallel way the magnetic moments) and the radial or tangential influence generated by anisotropy. Due to this competition, magnetic domains should appear at a relatively short distance, at a certain number of atoms per ring and at a small temperature range, where anisotropy breaks the parallel alignment [5]. In the literature, works presenting simulations of magnetic nanotubes using the Monte Carlo method can be found. For instance, Masrour et al. [10] reported simulation of nanotubes with two spin configurations; in the Hamiltonian, they included exchange parameter, Zeeman effect and crystal field. Here, a competition between exchange interaction and crystal field, producing order and disorder, respectively, can be observed, according to these results, the total magnetization. In our work, we also are interested in presenting the competition between exchange parameter and the anisotropy influences. Although, in the literature, there are some reports regarding the anisotropy influence on nanostructures, it is required to perform more studies and to derive better analyses, especially in the case of nanotubes.

This work reports the results of tangential and radial anisotropy components in single wall nanotubes with square lattice structures and periodic boundary conditions. Transition temperatures are presented as a function of magnetic ions per ring, varying the anisotropy constant values with respect to the exchange parameters. The study focuses on the variations around the transition temperatures due to the generation of domains and other possible states favoured by the anisotropy direction.

2. Model description

Square single wall magnetic nanotubes were generated keeping the distance between magnetic ions equal to 1. A scheme of the sample is presented in Fig. 1(a). The classical Heisenberg model was considered with nearest neighbour interactions and one term for anisotropy. The corresponding Hamiltonian reads as follows:

$$\mathcal{H} = -\sum_{i,j} J_{exc} \vec{S}_i \cdot \vec{S}_j - \sum_i K_{an} \left(\vec{S}_i \cdot \hat{n}_i \right)^2 . \tag{1}$$

The first term corresponds to the exchange energy, where J_{exc} is the exchange parameter, which takes the value of 10 meV per pair interaction. $\left|\vec{S}_i\right| = \left|\vec{S}_j\right| = 1$, where j refers to the nearest neighbour atoms. The second term refers to uniaxial magneto-crystalline anisotropy, with K_{an}, where K_{an}/J_{exc} takes values between 0 and 1 and $\hat{n}$ provides the easy axis direction that can be radial or tangential as is observed in Fig. 1(b) and (c). Our research is focused on studying the competition between the anisotropy (radial or tangential) and the exchange parameter. Under this objective, it is required to use values that reflect similar energetic contributions to the system. These values may allow the competition not only at low but also at high temperatures; in our case, we chose values that produce critical temperatures at around 100 K. This value has evidenced high stability during the observable calculations using the Monte Carlo method and the classical Heisenberg model. Moreover, current researches are focused in obtaining high range anisotropies that allow the spins orientation to remain in the easy axis direction [11]. On the other hand, the number of ions included is $m \times L$, where m is the number of ion per ring and L is the nanotube length that was fixed in 50 ions. Simulations were based on Monte Carlo random states and the code is developed under FORTRAN 95 software. Energetic stability was implemented under Metropolis algorithm with the Boltzmann statistical distribution. Periodic boundary conditions at the ends of nanotube have been employed. The number of Monte Carlo steps (MCS) was 20×10^3 where 10×10^3 MCs were discarded for calculating the average of observables. The observables obtained were energy, magnetization, susceptibility and specific heat. Tangential anisotropy was also evaluated from the vorticity parameter. This parameter was obtained per ring from the sum of angles between radial vector and magnetic moment at each lattice point. According to the rotation direction per ring, vorticity was summed and separated in positive and negative values, and subsequently normalized.

3. Results and discussion

Figs. 2–4 present magnetic moments for some possible states that can occur in a nanotube of 18 ions per ring. All figures show the spin representations at two temperatures, (a) and (b) for 10 K, while (c) and (d) for higher temperatures; in

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