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Investigation of phase diagrams for cylindrical Ising nanotube using cellular automata

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ABSTRACT

Recent developments in the field of applied nanoscience and nanotechnology have heightened the need for categorizing various characteristics of nanostructures. In this regard, this paper establishes a novel method to investigate magnetic properties (phase diagram and spontaneous magnetization) of a cylindrical Ising nanotube. Using a two-layer Ising model and the core-shell concept, the interactions within nanotube has been modelled. In the model, both ferromagnetic and antiferromagnetic cases have been considered. Furthermore, the effect of nanotube's length on the critical temperature is investigated. The model has been simulated using cellular automata approach and phase diagrams were constructed for different values of inter- and intra-layer couplings. For the antiferromagnetic case, the possibility of existence of compensation point is observed.

1. Introduction

In recent years, a growing body of research in nanoscience is devoted to magnetic nanoparticles and their applications. Due to surface effects [1], magnetic properties of nano-scaled particles are far different from the bulk material, and are highly dependent on size and dimensionality of the material [2,3]. Magnetic nanoparticles also have multiple applications in biomedicine [4], drug delivery [5], Magnetic Resonance Imaging (MRI) [6], permanent magnets [6], long-lasting memories [7] and recording media [6]. Among all possible nanostructures, carbon nanotube exhibits interesting mechanical and thermal behaviour as well as electrical behaviour, which turns it into a possible replacement for silicon in future electronic devices [8].

Cylindrical Ising nanotube can be modelled using a core-shell structure, as adopted for various nanoparticles, e.g. in [9–19]. The core-shell model has been theoretically successful in explaining magnetic behaviour of nanoparticles [20]. This structure also has some advantages, as the carbon shell protects magnetic core from oxidation and corrosion and increases its lifetime [21] and also make the nanoparticle more compatible with biological systems [6]. The mathematical model of a nanoparticle could be solved using Mean Field Theory (MFT) [22] and Effective Field Theory (EFT) [15–18]. Results obtained by MFT are well known to be unreliable because it neglects non-trivial thermal fluctuations [23]. Although EFT was proposed to increase the accuracy of MFT [24], the results obtained by EFT lack in quantitative exactness [25]. Furthermore, these methods are usually time consuming and mathematically complex in some cases [25]. Recently, numerical methods using computer simulation have received attention for investigating Ising model. Monte Carlo (MC) simulation using the Metropolis algorithm was firstly introduced in [26] and adopted in several researches [8–13,27] to extract critical properties for nanomagnets. Another simulation-based numerical method is Cellular Automata (CA), firstly introduced in [28], which preserves dynamical information of the system. Q2R and Creutz algorithms for CA have been presented in [29] for studying statistical mechanics problems. Q2R automaton is fast, reversible and deterministic but it turns out that probabilistic algorithms, such as Glauber [30], are more realistic [25]. In several researches, CA has been successful in explaining nanomagnetic behaviours. For example, in [25] two-layer Ising and Potts models were considered and phase transition diagrams were investigated. The anisotropic two-layer Ising and Potts models are also studied in [31] and critical point and shift exponents are computed using CA method. A Creutz automaton is applied to a 4-dimensional Ising model by Aktekin in [32] and critical characteristics as well as size-dependent properties were studied. Ahmadi

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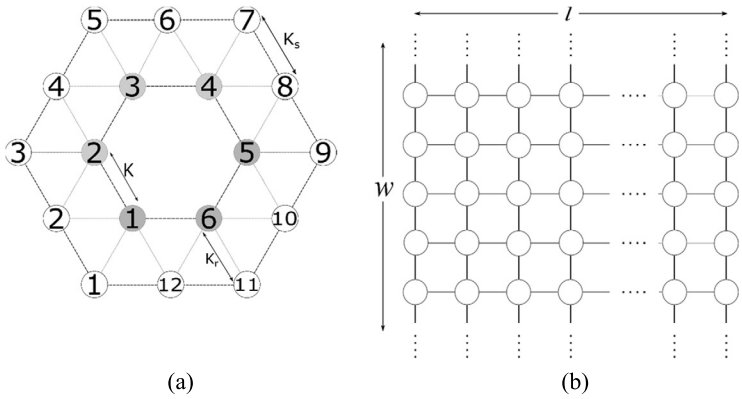

Fig. 1. Schematic representation of nanotube from, a. cross-section view, b. side-on view.

and Ghaemi in [33] has studied critical properties of an anisotropic two-layer Ising model on Kagome lattice using a CA approach with the Glauber algorithm. Recently, CA is applied on a honeycomb lattice to investigate phase diagrams of nano-films and nanotubes [34]. The CA method is further applicable to nanoscience problems, not yet widespread in this field.

In this article, we have adopted a CA approach to simulate a two-layer Ising nanotube and to plot phase diagrams for ferromagnetic as well as antiferromagnetic cases. The CA model is implemented using C-language programming, accompanied with Dislin software and compiled on Linux OS. Using the results of simulation, phase diagrams, i.e. curves showing variations in the reduced critical temperature with respect to changes in surface and intra-layer couplings, are plotted. Also, investigation of spontaneous magnetization (in this article called "magnetization" for convenience) versus reduced temperature diagrams, shows that possibly a compensation point exists for the antiferromagnetic nanotube. The novel contribution of this paper is introduction of a mathematical relation between nanotube's length and its reduced critical temperature. No similar relation was proposed in the related literature reviewed thus far.

The rest of the paper is organized as follows: in Section 2 Ising and CA models of nanotube are constructed. Section 3 is devoted to presenting the simulation results and discussion. Finally, the main conclusions of the paper are stated in Section 4.

2. Mathematical model

To model a nanotube, firstly a proper configuration of Ising model parameters is selected, afterwards this model is defined as a CA model, adjusting the model in a way that could be used for a computer simulation. Through this article, we assume zero external magnetic field. We considered a core-shell structure for the nanotube. This approach has been used in a number of recent studies on nanosystems, e.g. [9,11,17]. In Fig. 1 the cross-section and side-on view of a nanotube is illustrated. The length of nanotube is denoted by l and its width is labelled w. Lines drawn between two nearby sites represent mutual interaction. This structure is conveniently represented by two square lattices, one to represent the surface and the other to represent the core, with w equal to 12 and 6 sites respectively. Spins within the core are denoted by $\sigma_{i,j}$ and those within the surface are indicated by $s_{i,j}$ where $i = 1, 2, \ldots, w$ and $j = 1, 2, \ldots, l$. Spin variables, $s_{i,j}$ and $\sigma_{i,j}$, can take values of $+1$ or -1 and are dimensionless. We adopt a probabilistic transition rule with Glauber algorithm as presented in [30] and the checkerboard approach to update each spin variable. In each time step, the probability, $p^+_{i,j}$, that spin state of each site in the lattice is up $(+1)$, is defined as

$$p^+_{i,j} = \frac{e^{-\beta E^+_{i,j}}}{e^{-\beta E^+_{i,j}} + e^{-\beta E^-_{i,j}}} \tag{1}$$

where $\beta = \frac{1}{k_B T}$ and k_B is the Boltzmann constant. The configuration energy for each spin at the surface is given by

$$\beta E^{\pm}_{i,j} = \pm\left\{-K_s(s_{i-1,j} + s_{i+1,j} + s_{i,j+1} + s_{i,j-1}) - K_r\sigma_{(i+1)/2,j}\right\} \tag{2}$$

for odd values of i and

$$\beta E^{\pm}_{i,j} = \pm\left\{-K_s(s_{i-1,j} + s_{i+1,j} + s_{i,j+1} + s_{i,j-1}) - K_r(\sigma_{i/2,j} + \sigma_{(i/2)+1,j})\right\} \tag{3}$$

for even values of i. The configuration energy for each spin within the core is given by

$$\beta E^{\pm}_{i,j} = \pm\left\{-K(\sigma_{i-1,j} + \sigma_{i+1,j} + \sigma_{i,j+1} + \sigma_{i,j-1}) - K_r(s_{2i-2,j} + s_{2i-1,j} + s_{2i,j})\right\} \tag{4}$$

Here $K_s = \frac{J_s}{k_B T}$ and $K = \frac{J}{k_B T}$ are dimensionless parameters which stand for exchange interaction between neighbouring spins within surface and within core, respectively. Exchange interaction between a spin on the surface and one in the core is also denoted by $K_r = \frac{J_r}{k_B T}$. Values assigned to K_s and K_r can be either positive or negative which corresponds to ferromagnetic and antiferromagnetic cases, respectively. The probability of down (-1) spin state at each site in the lattice is $1 - p^+_{i,j}$.

In the above equations, $s_{0,j} = s_{12,j}$, $s_{13,j} = s_{1,j}$, $\sigma_{0,j} = \sigma_{6,j}$, $\sigma_{7,j} = \sigma_{1,j}$ and $s_{i,0} = s_{i,l+1} = \sigma_{i,0} = \sigma_{i,l+1} = 0$. The average magnetization per site, which is dimensionless, is defined as

$$\langle m \rangle = \frac{\langle \sum_{i,j} \sigma_{i,j} + \sum_{i,j} s_{i,j} \rangle}{l(6+12)} \tag{5}$$

Furthermore, parameters r and Δ_s are defined as follows:

$$K_r = rK \tag{6}$$

$$K_s = K(1 + \Delta_s) \tag{7}$$

3. Results and discussion

3.1. Phase diagrams

For obtaining the critical point $(K_c = J/k_B T_c)$ several different methods exist. In this study we assume $l = 50$ sites for the nanotube, r varies from -1 to $+1$ in 0.25 steps, and Δ_s varies from -3 to $+1$. Therefore, both ferromagnetic and antiferromagnetic cases are considered. For each value of r and Δ_s, simulation is started

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