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Shell thickness and dynamic magnetic field effects on the critical phenomena of magnetic core-shell nanoparticles with spherical geometry

Yusuf Yüksel

Department of Physics, Dokuz Eylül University, Tr-35160 İzmir, Turkey

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ABSTRACT

By using Monte Carlo simulations for classical Heisenberg spins, we study the critical phenomena and ferrimagnetic properties of spherical nanoparticles with core-shell geometry. The particle core is composed of ferromagnetic spins, and it is coated by a ferromagnetic shell. Total size of the particle is fixed but the thickness of the shell is varied in such a way that the shell layer is grown at the expense of the core. Effects of the shell thickness, as well as dynamic magnetic field parameters such as oscillation period and field amplitude on the magnetization profiles, dynamic hysteresis loops and phase diagrams have been investigated for the present system. It has been found that as the shell thickness varies then the easy axis magnetization of the overall system may exhibit *Q*-, *P*-, *L*- and *N*- type behaviors based on the Neél terminology. We also found that three distinct anomalies originate in the thermal variation of specific heat with increasing field period. Dynamic hysteresis loops corresponding to off-axial magnetization components exhibit unconventional behavior such as double rings with symmetric shapes around the vertical axis over the $h(t) = 0$ line which may originate due to the stochastic resonance behavior of these components.

1. Introduction

In recent years, magnetic fine materials in forms of nanowire, nanotube and nanoparticle structures have gained a great deal of theoretical and experimental attention [1]. Compared to their bulk counterparts, these nanoscaled materials may exhibit very peculiar magnetic properties which can be controlled by adjusting their size and shape. With the recent developments in experimental preparation techniques, nanoparticles gained particular attention. In biomedical applications, they are used in drug delivery in cancer thermotherapy and magnetic hypertermia [2–6]. Furthermore, magnetic nanoparticles based on core-shell morphology are very promising than simple particles for different biomedical purposes due to several major reasons [7]. On the other hand, in terms of magnetic recording applications, in order to increase the areal density of a recording system, one must decrease the bit size, and must use smaller particles. However, below a critical size, as a result of decreased magnetic anisotropy energy, the system loses its stability against thermal fluctuations due to superparamagnetic effect which can be beaten by exchange bias (EB), a phenomenon peculiar to thin films and core-shell nanoparticles [8–12]. Although conventional EB systems are composed of a ferromagnetic (FM) core which is in contact with an antiferromagnetic (AFM) oxide [13–17], there are also systems with inverted structures showing EB phenomena [18,19].

Very recently, the influence of the roughened interfaces on the EB phenomena in FM core-AFM shell nanoparticles have been investigated by Evans et al. [20], and they established a connection between the degree of the interfacial roughness and the EB field. Apart from this, Dimitriadis et al. [21] found that in case of geometrically sharp interfaces, cubic particles exhibit a higher coercivity and lower EB field than spheres of the same size. Moreover, according to their results, as the interface roughness increases then the cubic and spherical particles exhibit similar behavior. These results show us that, geometric structure of the interface plays important role on the magnetic behavior of nano structures. Theoretically, Kaneyoshi's elegant formulations [22–28] based on mean field and effective field theories provided new insights on the magnetic properties and critical behavior of fine particles in nanowire and nanotube geometries. Since then, several theoretical attempts have been made for the investigation of nano-scale magnetism in systems with a wide variety of geometrical interfacial shapes including cubic [29–33] and spherical [34–39] particles, as well as nanoribbon [40], graphyne [41], hexagonal [42–44], and segmented nanowire [45] structures. In Refs. [26,28,33,34,38,43,44], the authors also studied the influence of quenched randomness due to diluted surfaces and interfaces, as well as random magnetic fields on the EB phenomenon and other several magnetic properties such as thermal dependence of ferrimagnetic and ferromagnetic properties.

As a ferrimagnetic property, compensation temperature T_{comp}

E-mail address: yusuf.yuksel@deu.edu.tr.

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plays an important role on the magnetic recording technology. Origin and existence conditions of T_{comp} in nano systems is a widespread motivation of vast majority of recent papers. In these works, the model is based on a FM core in contact with a FM shell. Core and shell layers are assumed to be interacting via an AFM interface coupling. According to Refs. [29,32,36,42], cubic and spherical particles may exhibit a T_{comp} within a certain range of shell exchange coupling strength J_S. However, variation of T_{comp} with interfacial exchange coupling strength $|J_{IF}|$ is not so clear. Namely, by comparing the models considered in Refs. [29,30], one obtains qualitatively different results for cubic particles depending on the spin variable occupying the particle core, although the shell layer is occupied by the same spin variable. Results regarding the dependence of T_{comp} on the shell thickness are also noteworthy to discuss. For a spherical particle, both the transition temperature T_C and compensation temperature T_{comp} decrease with increasing shell thickness, and they saturate at finite values corresponding to their bulk counterparts [36]. However, we have an opposite scenario for a cubic particle with the same spin components [32]. Whether this interesting result is a consequence of different particle geometries or due to the interface roughness, etc. has not been discussed by the authors. Apart from these, there are also some important works which have reported important and noteworthy results. For instance, according to Refs. [36,42], spherical and hexagonal particles may exhibit two compensation points for large interface exchange coupling. For a spherical nanoparticle with ferrimagnetic binary alloy shell, one, two and even three compensation points can be found for appropriate choice of system parameters [37]. Moreover, in the presence of time dependent magnetic fields, it has been noted in Ref. [39] that T_{comp} decreases with increasing field amplitude, but in the basis of this claim, the authors considered only a small portion of the phase space in their work. On the other hand, as another adjustable control parameter, oscillation period of the external field may also play an important role on the critical behavior and ferrimagnetic properties of core-shell nanoparticles. Nevertheless, to the best of our knowledge, a detailed examination of these issues does not exist in the literature, and in this regard, the problem still needs particular treatment. In this context, our aim in the present work is to clarify the dynamic aspects of ferrimagnetic properties of core-shell nanoparticles in the presence of time dependent magnetic fields. To this end, the outline of the work can be summarized as follows: In Section 2, we introduce our model, and give simulation details considered throughout the paper. Section 3 is devoted to our results and related discussions. Finally, Section 4 contains our conclusions.

2. Model and formulation

As our model, we consider a spherical particle which has been depicted schematically in Fig. 1 with a FM core which is surrounded by a FM shell. At the core-shell interface (which is composed of the outermost core and the innermost shell layers) we define an AFM exchange coupling. The interface region consists of two successive mono-layers. The total radius of the particle and the thickness of the shell are denoted by R and R_S, respectively. A classical Heisenberg spin resides at each lattice site of a simple cubic structure, and the nearest neighbor sites are separated from each other by unitary lattice spacing.

The system can be defined according to the following Hamiltonian

$$\mathcal{H} = -J_C\sum_{\langle ij\rangle}\mathbf{S}_i.\,\mathbf{S}_j - J_S\sum_{\langle kl\rangle}\mathbf{S}_k.\,\mathbf{S}_l - J_{IF}\sum_{\langle jk\rangle}\mathbf{S}_j.\,\mathbf{S}_k - K_C\sum_i (S_i^z)^2 - K_S\sum_k (S_k^z)^2 - \mathbf{h}(t).\sum_{i'}\mathbf{S}_{i'}, \quad (1)$$

where $\mathbf{S}_i$ represents a classical Heisenberg spin vector with unit magnitude, and the former three sums are taken over the nearest-neighbor sites whereas remaining terms are taken over all the lattice sites. In practice, spin structure of interface in such systems is experimentally inaccessible, and it is quite a challenge to determine

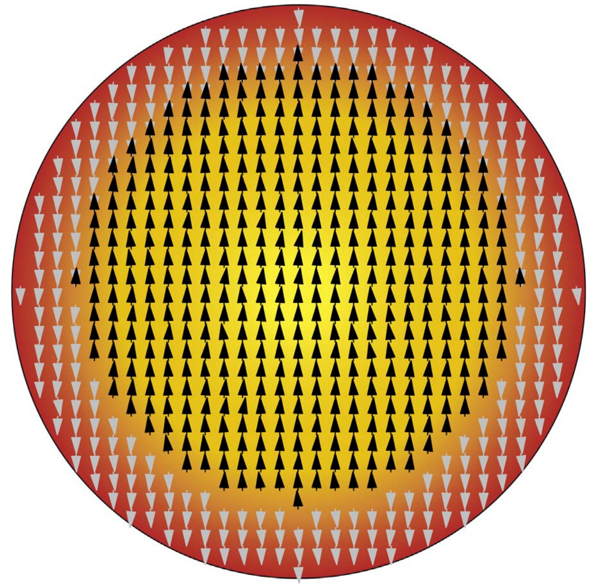

Fig. 1. Schematic representation of spherical nanoparticle model: FM core of radius R_c is coated by an FM shell of thickness R_S. Total radius of the particle is denoted by $R = R_c + R_S$. At the interface, the outermost core and the innermost shell layers interact with an AFM exchange coupling.

the magnetic nature near interface. Therefore, in order to theoretically investigate the ferrimagnetic properties of the system, we consider the following Hamiltonian parameters: Spin-spin interactions between core and shell spins are taken as ferromagnetic ($J_{C,S} > 0$) whereas interactions at the core-shell interface are of antiferromagnetic type ($J_{IF} < 0$). Due to the reduced coordination number at the surface, FM exchange interactions between shell spins are usually smaller than those between core spins. Hence, we select $-J_{IF} = J_S = 0.5J_C$. Easy axis magnetization of the particle is assumed to be along the z direction by assigning nonzero values for the z components of the uniaxial anisotropy constants K_C and K_S for the particle core and shell, respectively. In order to emphasize the surface effects, we set $K_C = 0.1J_C = 0.1K_S$ [46]. The last term in Eq. (1) is the contribution of the Zeeman energy to the total internal energy of the system and $\mathbf{h}(t)$ is a time dependent magnetic field. For simplicity, we consider only the longitudinal part of the external field which is given as $\mathbf{h}(t) = h_0\sin(\omega t)\hat{z}$ where h_0 and ω are the amplitude and angular frequency of the periodically oscillating longitudinal magnetic field, respectively.

Total radius R has been kept fixed as R=25.0 throughout the simulations, corresponding to a particle with $N_T = 65267$ spins, however the shell thickness has been varied at the expense of the core which mimics the case of the production process for the surface chemically modified nanoparticles [47]. For the structural parameters of the simulated particle samples with different shell thickness, see Table 1. Our simulations are based on an improved Metropolis algorithm for classical Heisenberg spins [48–50], and we apply free boundary conditions in all directions.

Following physical quantities have been calculated in the simulation process:

- Time series of the instantaneous magnetization components

$$M_{core}^{\alpha}(t) = \frac{1}{N_C}\sum_{i=1}^{N_C} S_i^{\alpha},\ M_{shell}^{\alpha}(t) = \frac{1}{N_S}\sum_{i=1}^{N_S} S_i^{\alpha},\ M_{int}^{\alpha}(t) = \frac{1}{N_{int}}\sum_{i=1}^{N_{int}} S_i^{\alpha},\ M_{total}^{\alpha}(t) = \frac{1}{N_T}\sum_{i=1}^{N_T} S_i^{\alpha} \quad \text{with } \alpha = x, y, z. \quad (2)$$

- Period averages of the instantaneous magnetizations (i.e. dynamic order parameters for $h_0 \neq 0$)