Journal of Magnetism and Magnetic Materials 441 (2017) 548–556

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Research articles

Nonmagnetic impurities and roughness effects on the finite temperature magnetic properties of core–shell spherical nanoparticles with antiferromagnetic interface coupling

Erol Vatansever *, Yusuf Yüksel

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

ARTICLE INFO

Article history:
Received 16 February 2017
Received in revised form 21 May 2017
Accepted 7 June 2017
Available online 10 June 2017

Keyword:
Core–shell nanoparticles, Roughness effects
Nonmagnetic impurities
Monte Carlo simulation

ABSTRACT

Being inspired by a recent study (Dimitriadis et al., 2015), we study the finite temperature magnetic properties of the spherical nanoparticles with antiferromagnetic interface coupling including quenched (i) surface and (ii) interface nonmagnetic impurities (static holes) as well as (iii) roughened interface effects. The particle core is composed of ferromagnetic spins, and it is surrounded by a ferromagnetic shell. By means of Monte Carlo simulation based on an improved Metropolis algorithm, we implement the nanoparticles using classical Heisenberg Hamiltonians. Particular attention has also been devoted to elucidate the effects of the particle size on the thermal and magnetic phase transition features of these systems. For nanoparticles with imperfect surface layers, it is found that bigger particles exhibit lower compensation point which decreases gradually with increasing amount of vacancies, and vanishes at a critical value. In view of nanoparticles with diluted interface, our Monte Carlo simulation results suggest that there exists a region in the disorder spectrum where compensation temperature linearly decreases with decreasing dilution parameter. For nanoparticles with roughened interface, it is observed that the degree of roughness does not play any significant role on the variation of both the compensation point and critical temperature. However, the low temperature saturation magnetizations of the core and shell interface regions sensitively depend on the roughness parameter.

1. Introduction

When the size of a magnetic system is reduced to a characteristic length, the system has a bigger surface to volume ratio giving rise to a great many outstanding thermal and magnetic properties compared to the conventional bulk systems [1]. Advanced functional magnetic nanostructures in different geometries, such as nanowires, nanotubes, nanospheres, nanocubes are center of interest because of their technological [2–4] and scientific importance as well as biomedical applications [5–7]. From the experimental point of view, many studies have been carried out to discuss and understand the origin of the fascinating physical properties observed in magnetic nanoparticles [7–11]. For example, recently the multi-functional core–shell nanowires have been synthesized by a facile low-cost fabrication process [7]. Based on this study, it has been shown that a multidomain state at remanence can be obtained, which is an attractive feature for the biomedical applications. In another interesting study, the authors show the presence of a robust antiferromagnetic coupling between core and shell in ferrimagnetic soft/hard and hard/soft core–shell nanoparticles based on Fe-oxides and Mn-oxides [10]. They have also used a computational model to support the physical facts observed in the experiment. Moreover, it is a fact that core–shell nanoparticle systems exhibit two important phenomena, namely exchange bias and magnetic proximity effects. These are completely due to the interface effects of the system. For detailed reviews on the exchange bias and magnetic proximity phenomena, the readers may follow the references [12–16].

Ferrimagnetic materials have a compensation temperature under certain conditions. At this special temperature region, the net magnetization of the sample vanishes below its critical temperature [17]. The phenomenon of ferrimagnetism in bulk material is associated with the counteraction of opposite magnetic moments with unequal magnitudes located on different sublattices in the same system. According to the Refs. [18,19], interestingly coercive field presents a behavior with a rapid increment at the compensation point. Existence of such a point has a technological importance [20,21], because at this point only a small magnetic field is required and enough to change the sign of the net

---

* Corresponding author.
E-mail address: erol.vatansever@deu.edu.tr (E. Vatansever).

http://dx.doi.org/10.1016/j.jmmm.2017.06.046
0304-8853/© 2017 Elsevier B.V. All rights reserved.

magnetization. However, the origin of the compensation point found in the nanostructures is quite different from those observed in the ferrimagnetic bulk materials. Magnetic nanoparticles can exhibit a compensation point due to the existence of an antiferromagnetic interface coupling at the ferromagnetic core and ferromagnetic shell interface even if the lattice sites in the core and shell parts of the system are occupied by identical atomic spin moments. Hence, investigation of ferrimagnetism in nanoparticle systems has opened a new and an intensive field in the research of the critical phenomena in magnetic nanoparticles. For example, the critical and compensation temperatures properties of cylindrical nanowire and nanotube systems have been performed by means of Effective-Field Theory with single-site correlations [22,23]. In these studies, the authors have also focused their attention on the effects of the surface and its dilution on the magnetic properties of the considered system, and it is reported that these systems display a compensation point for appropriate values of the system parameters. Very recently, thermal and magnetic phase transition features of a core–shell spherical nanoparticle with binary alloy shell have been studied by making use of Monte Carlo simulation based on single-spin flip Metropolis algorithm [24]. Here, the authors claim that the system may demonstrate one, two or even three compensation points depending on the selected Hamiltonian as well as on the concentration parameters. In addition to these, critical behaviors of core–shell nanoparticles with ferromagnetic materials but with antiferromagnetic interface exchange coupling are studied by means of a self-consistent local mean-field analysis [25]. It has been found that compensation temperature depends on all the material parameters, namely the core and shell radius, and the magnetic field.

Although the mechanism and physics underlying of the critical behavior of the magnetic nanoparticles may be treated and understood with idealized interfaces and surfaces of the nanoparticle, real magnetic nanoparticles have some small defects. From this point of view, experimental systems showing exchange bias may contain statistical distributions due to the presence of randomly located defects in the system [26,27]. Recently, Ho and coworkers have attempted to address the magnetic properties of a fer romagnetic/antiferromagnetic core–shell nanospherical particle including the vacancies at the antiferromagnetic interface, based on Monte-Carlo simulation method [28]. It is found that the frustrated spins at the ferromagnetic interface is another pinning-source generating exchange bias phenomenon, in addition to the antiferromagnetic shell spins. Furthermore, the influences of nonmagnetic defects on the exchange bias of core–shell nanoparticles have been analyzed by benefiting from Monte Carlo simulation, and it is shown that exchange bias can be tuned by defects in different positions [29]. Apart from these, Evans et al. [26] presented exchange-bias calculations for FM core/AFM shell nanoparticles with roughened interfaces. They showed that the magnitude of exchange bias is strongly correlated with the degree of roughness. Moreover, in a very recent paper, Dimitriadis et al. [30] simulated cubic and spherical particles showing exchange bias phenomenon. According to their results, in terms of exchange bias characters, the distinction between cubic and spherical particles is lost for moderate roughness.

Based on the previously published studies, it is possible to mention that thermal and magnetic properties of the core–shell nanoparticles containing the surface and interface defects and also roughened interfaces are complicated and interesting compared to the clean nanoparticle systems. It is certain that the studies taking these effects into account play a crucial role in having a better insight of the physics behind real magnetic nanoparticle systems. However, much less attention has been given to determine the influences of the disorder and roughness on the critical behavior of the core–shell nanoparticles, and there are still many unresolved issues. Motivated by these facts, we intend to search answers for the following questions:

- What are the effects of the nonmagnetic impurities at the surface and interface of a core–shell type spherical nanoparticle on the critical and compensation behavior? Is it possible to control the magnetic behavior of the core–shell nanoparticles by means of concentration of the vacancies?
- What kind of physical relationships may emerge between the physical properties of the system and the interface roughness?

The main motivation of the paper is to make an attempt to determine the physical facts underlying these questions. Furthermore, particular attention has been dedicated to elucidate the effects of the system size on the critical behavior of the system. We believe that the findings obtained in this work would be beneficial for the future theoretical and experimental research in magnetic nanoparticles including disorder effects.

The outline of the remainder parts of the paper is as follows: In Section 2, we present the model and simulation details. The results and discussion are given in Section 3, and finally Section 4 includes our conclusions.

2. Model and simulation details

We consider a spherical nanoparticle which has been schematically depicted 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 monolayers. 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

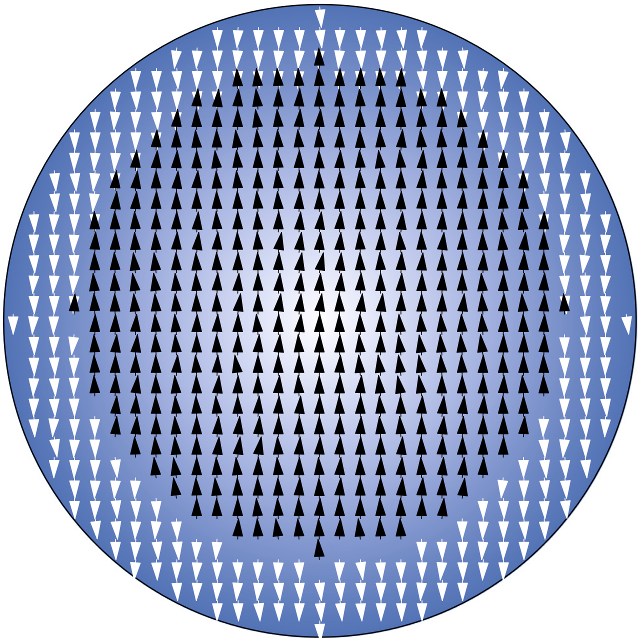

Fig. 1. Schematic representation of an ideally purified spherical nanoparticle composed of classical Heisenberg spins. FM core of radius R_c is coated by an FM shell of thickness R_S. Total radius of the particle is denoted by $R = R_c + R_S$. At the interface, the outermost core and the innermost shell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