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The phase diagrams with influence of biquadratic exchange coupling on martensitic–austenitic transformations for core–surface nanoparticles

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ABSTRACT

Recently, origin of the martensite–austenite transitions in core–surface type magnetic nanoparticles has been investigated theoretically and it has been indicated that repulsive biquadratic exchange coupling ($K<0.0$) causes the coexisting martensite and austenite phases. In the present paper, the phase diagrams of homogeneous and composite nanoparticles in the $k_BT/J_0-D/J_0$ plane are studied for the presence and absence of attractive biquadratic exchange interaction in addition to repulsive biquadratic exchange interaction. Significant changes in the phase diagram points are discussed in the presence of martensitic and austenitic transformations. Four regions in the phase diagrams are found as second-order, martensitic–austenitic, T_{Cid} and first-order phase transition regimes.

1. Introduction

This paper constitutes the continuation of the theoretical treatment of core–surface (CS) type magnetic nanoparticles (NPs) presented recently in our published papers [1,2], hereafter denoted as Paper I and Paper II in the following. Papers I and II describe the martensitic and austenitic transformations (MT–AT) occurred in hexagonal and cubic NPs, respectively. The theoretical approach used was based on the Blume–Emery–Griffiths (BEG) model [3]. Its Hamiltonian contains bilinear (J) and biquadratic (K) exchange couplings as well as single-ion anisotropy (D) term in the presence of an external magnetic field (h). The main aim in these papers was to investigate the hysteretic splitting and magnetization (m) vs. induced temperature (k_BT/J_0) (k_B Boltzmann constant, T temperature and $J_0=J$) for the homogeneous (HM) and composite (CM) NPs by using the pair approximation (PA) technique introduced by Kikuchi for the bulk materials [4]. In the previous works [1,2], the MT–AT was strongly influenced by non-zero K which gives rise to the coexisting martensite (M) and austenite (A) states. The M–A phase co-existence in CS smart NPs systems is an interesting feature which is seen between the first- and second-order phase transition lines in the phase transformations for the negative K values. Also, nonzero D values caused splitting in hysteresis loops.

Apart from above results, recent calculations based on effective field theory with correlations [5–7] and simulations results using the Monte-Carlo technique [8,9] yielded a variety of phase diagrams without MT–AT for some nanosystems, such as core/shell nanowires [10]. There are also theoretical models that predict the crossover in phase diagrams from bulk iron (Fe)–nickel (Ni) alloys to NPs with martensitic transitions [11]. In spite of these studies, not all aspects of the phase transitions and the shell (R) evolution of Curie temperatures have been obtained for the CS-NPs using spin-1 BEG Hamiltonian. Especially, the phase diagrams of hexagonal NPs with M–A and first-/second-order phase regions have not yet been reported. A detailed investigation of biquadratic (K) effect on the structural and magnetic properties for these NPs reveals various regions in phase diagrams.

In this paper, the phase diagrams which occur in the hexagonal lattices of HM- and CM-CS-type NPs are studied intensively both in the presence and absence of attractive biquadratic interaction ($K\geq 0.0$) in addition to repulsive biquadratic interaction ($K<0.0$) [12]. The model and methodology used in the present investigation is the same one used for earlier study [1]; therefore, the details for the theoretical model can be seen from this reference. Magnetization calculations are carried out for only noninteracting NPs on hexagonal lattice which has the shells related to the radius (R) of the particles [13]. Indeed, features in the $k_BT/J_0-D/J_0$ plane associated with various structural (M–A) and magnetic (first-/second-order) phases have been observed in detail.

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2. Results and discussion

Fig. 1 shows magnetization (m) as a function of temperature (k_BT/J_0) for hexagonal lattices of CM-NPs in various D values ranging from -0.16 to -0.11 marked on the respective curves when $R=8$, $K=-0.5$, $h=0.0$. The representation view of the hexagonal nanoparticle (NP) is given in the inset of Fig. 1a. Similar data were also reported in Paper I and is reproduced here for review of results with $K<0.0$. At $D=-0.11$, on increasing the temperature, a broad second-order transition from ferromagnetic (FM) to paramagnetic (PM) phase has been observed while a first-order transition takes place when $D=-0.16$. In Fig. 1a, the temperatures T_{C2} and T_{C1} demonstrate the Curie temperatures for these transitions. The M and A phase coexistence region occurs for $D=-0.14$ and -0.118 values. On increasing and decreasing the temperature, the M and A phase transitions have been obtained by using the maximum and minimum values of D for the particle. The characteristic temperatures for the onset and finish of martensite (M_S, M_{S1}, M_F, M_{F1}) and austenite transitions (A_S, A_{S1}, A_F, and A_{F1}) are marked on the $D=-0.118$ and -0.14 curves of Fig. 1b. The magnetization is sharply increasing from A_S to A_F while it is decreasing from A_{F1} to A_{S1} with increasing temperature. The phase between A_{F1} and A_{S1} is called weakly austenitic phase. The similar behavior of magnetization with decreasing temperature displays weakly and strongly martensitic states between M_{F1}–M_{S1} and M_F–M_S, respectively. The thermal transition between M_F–M_S and A_F–A_S with M_{F1}–M_{S1} and A_{F1}–A_{S1} is accompanied by a hysteresis called thermal hysteresis loop [14,15]. It displays the thermal response of magnetic properties emerging at nanoscale. The loops for $D=-0.14$ are smaller than that of $D=-0.118$.

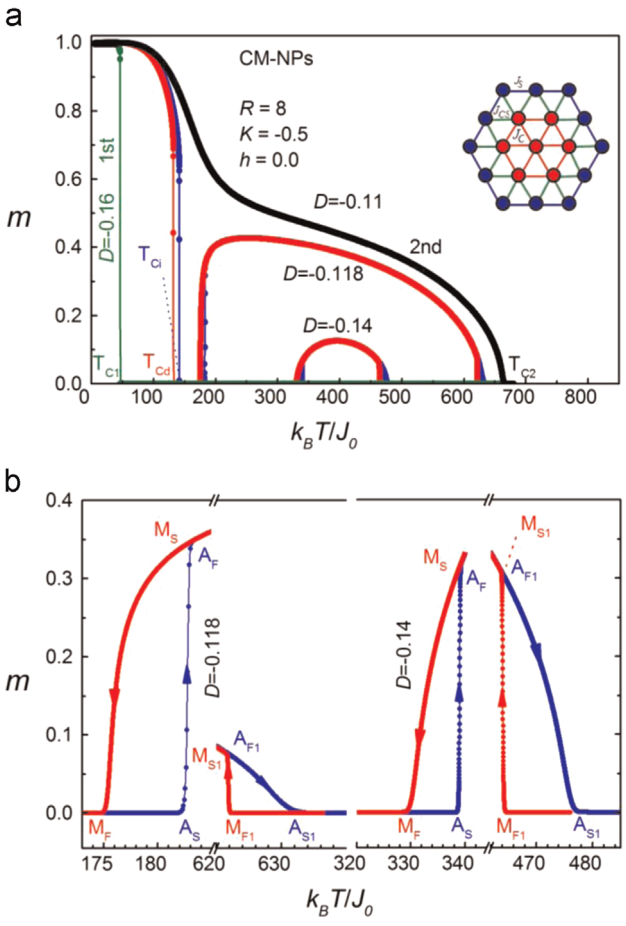

Fig. 1. (a) Temperature (k_BT/J_0) variation of magnetization (m) for several values of D. (b) Thermal hysteresis loops for $D=-0.118$ and -0.14. $R=8$, $K=-0.5$ and $h=0.0$.

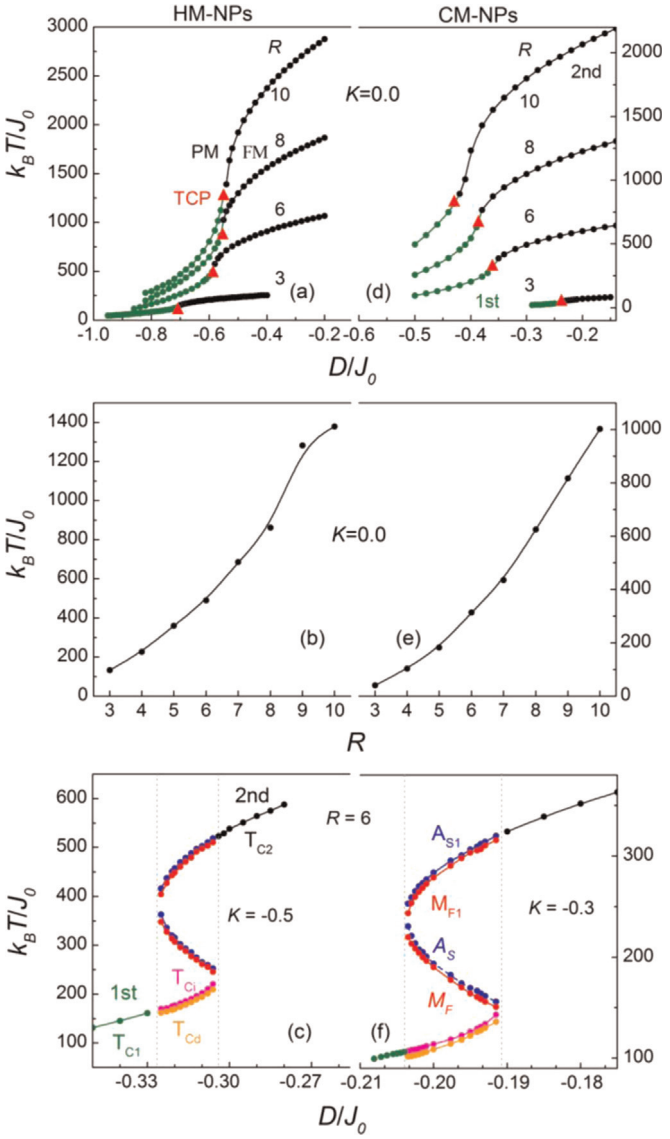

Fig. 2. The phase transformations of HM- (a) and (c) and CM- (d) and (f) NPs in the k_BT/J_0–D/J_0 plane for $R=3$, 6, 8 and 10 shells when $K=0.0$ and $R=6$ shells when $K<0.0$. The shell (R) evolution of k_BT/J_0 for HM- (b) and CM- (e) NPs for $K=0.0$, $h=0.0$.

To obtain more information about the behavior of phase transformations in the hexagonal HM- and CM-NPs, the phase transitions in the k_BT/J_0–D/J_0 plane and the shell evolution of k_BT/J_0 have been first illustrated in Fig. 2. Fig. 2a and d shows the phase transitions for some selected radius values ($R=3$, 6, 8, 10) in the k_BT/J_0–D/J_0 plane using $K=0.0$ value. In these figures, the green and black curves denote first- and second-order phase transition lines which separate the FM and PM phase regions. They join at a point called tricritical point (TCP) market by a red point. In the absence of biquadratic interaction ($K=0.0$), the first-order transition line (1st, green full circle) increases exponentially but the second-order phase transition line (2nd, black full circle) changes logarithmically as D/J_0 is increasing, illustrated for HM- and CM-NPs in Fig. 2a and d, respectively. In the HM-case, the TCP slowly shifts to right with increasing particle radius (Fig. 2a). However, this shift is reversed, i.e. to the left, when the particle is CM-type (Fig. 2d). Particle radius (R) evolution of k_BT/J_0 for HM- and CM-NPs is given in Fig. 2b and e for $K=h=0.0$. The Curie temperature