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## Remarkable features of magnetic properties in transverse Ising nanoislands



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#### ABSTRACT

The phase diagram and magnetizations in two transverse Ising nanoislands with the same structures which are consisted of the two layers are examined by using the effective-field theory with correlations. The effects of interlayer coupling and two transverse fields at the center and the perimeter atoms on them are examined. We find remarkable features in them which come from the frustration induced by the interlayer coupling and two transverse fields.

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#### 1. Introduction

Nowadays, magnetic nanomaterials, such as nanoparticles, nanoislands, nanofilms, nanowires, nanotubes and so on, have attracted considerable attention experimentally and theoretically, related with their technological and biomedical applications. The magnetic properties of nanomaterials are due to the distinct contributions of inside, perimeter and surface atoms. The remarkably different contributions of surface and perimeter spins govern the nanomagnetism of a material and points to the new way of finding important possible technological applications. From the academic point of view, the magnetism of a single-domain nanoparticle (or nanoisland) and a nanoscaled thin film can be addressed to the research. The thickness dependence of transition temperature, the temperature dependence of magnetization, the critical exponent  $\beta$  and the Neel hyperbola for paramagnetic susceptibility [1] in these materials have been obtained by the use of some elaborate experimental techniques [2–4], in addition to hysteresis loops which are important for the manufacture of magnetic recording media. From the experimental point of view, at the present time, it is almost impossible to study the morphology of the very same particle in conjunction of magnetism. The experimental topography of a nanoparticle displays a discontinuous (or island-like) architecture composed of well-separated and nonuniform particles with an average island diameter [5,6]. As far as we know, the contribution to the magnetic properties from such islands has not been taken into account theoretically.

In a series of recent works [7-12], we have examined the phase diagrams and the magnetizations of nanoscaled Ising (or transverse

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http://dx.doi.org/10.1016/j.jmmm.2014.08.062 0304-8853/© 2014 Elsevier B.V. All rights reserved. Ising) thin films consisting of a few magnetic layers by the use of the effective-field theory with correlations (EFT) [13,14]. The EFT corresponds to the Zernike approximation (ZA) [15] and it is believed to give more exact results than those of the mean field approximation. In them, when the value of r ( $r=J_r/J$ ) is taken as a very small or a very large value, some interesting phenomena have been found in the magnetic properties of the systems with thickness L (from L=2to L=10), such as the appearance of a broad maximum in the variation of transition temperature  $(T_c)$  as a function of r for the site dilution, while such a phenomenon has not been obtained for the bond dilution. Here, J<sub>r</sub> is the interlayer coupling between the surface and the next inner layer, when the value of the inner layer coupling is fixed at J. In particular, a new type of frustration has been obtained in the systems [10–12], when a uniform transverse field is applied and a large value of r is selected. Furthermore, such a frustration has been also found in the transverse Ising nanoisland consisting of two layers with eighteen atoms in total [16].

The aim of this work is, within the theoretical framework of the EFT, to investigate the effects of interlayer coupling and two transverse fields ( $\Omega_S$  and  $\Omega$ ) on the magnetic properties (phase diagram, magnetizations) in two nanoscaled transverse Ising islands with the same structural aspect as that in Ref. [16], since the effects of a uniformly applied transverse field ( $\Omega_S = \Omega$ ) have been examined in Ref. [16]. Here,  $\Omega_S$  is the transverse field at the perimeter spin and  $\Omega$  is the transverse field at the central (inside) spin.

#### 2. Model and formulation

We consider the 3D nanoisland (or nanoparticle), as depicted in Fig. 1, in which they are consisted of the surface shell and the core. The core (white circles) is surrounded by the surface shell (black

y<sub>s</sub>



Fig. 1. Schematic representation of two transverse Ising nanoislands. In Fig. (A), the above and below layers are consisted of 9 spin-1/2 atoms, where 8 black circles and 1 white circle represent the same magnetic atoms. In Fig. (B), the above and below layers are consisted of 5 spin-1/2 atoms, where 4 black circles and 1 white circle represent the same magnetic atoms. The lines connecting the black and white circles in each figure represent the three nearest-neighbor exchange interactions  $(J_{S_r} | and J_r)$ .

circles). Each site on the figure is occupied by a Ising spin. Each spin is connected to the nearest neighbor spins with an exchange interaction. The surface spins are coupled to the center spin with an exchange interaction J. The atoms on the surface shell are connected by the exchange interaction J<sub>s</sub>. Each spin on the upper layer is connected to the corresponding spin on the lower layer with an exchange interaction J<sub>r</sub>. The choice corresponds to the experimental facts [5,17], as discussed in [16]. In this work, let us formulate the system depicted as Fig. 1(B), since the phase diagram and the magnetizations of the system shown in Fig. 1 (A) has been formulated in [16] and the numerical results of them have been examined for the case of  $\Omega_{S} = \Omega$ .

The Hamiltonian of the system is given by

$$H = -J_{S} \sum_{\substack{\sigma_{i} \\ (ij)}} \sigma_{j}^{Z} - J \sum_{\substack{\sigma_{m} \\ (mn)}} \sigma_{m}^{Z} - J_{r} \sum_{\substack{\sigma_{m} \\ (im)}} \sigma_{m}^{Z} - \Omega_{S} \sum_{\substack{\sigma_{m} \\ (m)}} \sigma_{m}^{X},$$
(1)

where  $\sigma_i^{\alpha} (\alpha = z, x)$  is the Pauli spin operator with  $\sigma_i^2 = \pm 1$ .  $\Omega_s$  and  $\Omega$  represent the transverse fields at the surface shell and in the core, respectively, since the transverse fields may be different at the surface and in the core. The first (ij) and second (mn) terms in the Hamiltonian (1) represent the contributions from the surface shell and the core, respectively. The third term shows the contribution from the interlayer interaction.

The surface exchange interaction J<sub>S</sub> is often defined as

$$\mathbf{J}_{\mathrm{S}} = \mathbf{J} \left( 1 + \Delta_{\mathrm{S}} \right), \tag{2}$$

in order to clarify the effect of surface shell on physical properties in the system. In particular, when the value of  $I_s$  is given by  $I_s=0.0$ (or  $\Delta_{\rm S} = -1.0$ ) in (3), the system shown as Fig. 1(B) represents the system as shown in Fig. 2, in which the atoms at the corner of each square (half black and half white circle) represent the nonmagnetic atoms. The system represents one of the transverse Ising islands with the same structural aspect as that in Fig. 1(A).

Within the framework of the EFT [13,14], we can obtain the longitudinal magnetizations  $m_s$  ( $m_s = \langle \sigma_i^Z \rangle$ ) at the surface shell and the longitudinal magnetization  $m_c$  (  $m_c = \langle \sigma_m^Z \rangle$  ) in the center for the system shown in Fig. 1(B), as coupled equations:

$$m_{S} = \left[\cosh(A) + m_{S} \sinh(A)\right]^{2} \left[\cosh(C) + m_{C} \sinh(C)\right]$$
$$\left[\cosh(B) + m_{S} \sinh(B)\right] f_{S}(x)|_{x = 0}$$
(3)

 $m_{\rm C} = \left[\cosh{(\rm C)} + m_{\rm S}\sinh{(\rm C)}\right]^4 \left[\cosh{(\rm B)} + m_{\rm C}\sinh{(\rm B)}\right]f(x)|_{x=0}$  (4)

where A, B and C are defined by  $A=J_S$  D,  $B=J_r$  D and C=J D. D=d/dx is the differential operator. Here, the functions  $f_{S}(x)$  and f (x) are defined by

$$f_{S}(x) = (x/y_{S}) \tanh (\beta y_{S})$$
and
$$f(x) = (x/y) \tanh (\beta y)$$
(5)
with

$$y_{\rm S} = (X^2 + \Omega_{\rm S}^{-1})^{1/2}$$
  
and

$$y = (x^2 + \Omega^2)^{1/2},$$
 (6)

where  $\beta = 1 / k_{\rm B}T$  and T is a temperature.

Furthermore, the transverse magnetizations  $m_S^X = < \sigma_i^X >$  and  $m_{\text{C}}^{\text{X}} = <\sigma_{m}^{\text{X}}>\,$  are also given by the same equations as those of Eqs. (3,4), only replacing the functions  $f_S(x)$  and f(x) in Eqs. (3,4) by the new functions  $h_s(x)$  and h(x), respectively. The new functions  $h_s(x)$  and h(x) are defined by

$$h_{S}(x) = (\Omega_{S}/y_{S}) \tanh (\beta y_{S})$$
  
and  
$$h(x) = (\Omega/y) \tanh (\beta y)$$
(7)



Fig. 2. Schematic representation of a transverse Ising nanoisland. The above and below layers are consisted of 9 spin-1/2 atoms, where 8 black circles and 1 white circle represent the same magnetic atoms and the half black and half white atoms represent a nonmagnetic atom. The lines connecting the black and white circles represent the two nearest-neighbor exchange interactions (J and J<sub>r</sub>).

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