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A quadrangular transverse Ising nanowire with an antiferromagnetic spin configuration

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HIGHLIGHTS

- Phase diagrams and magnetizations are discussed by the use of the EFT.
- The effects of an antiferromagnetic spin configuration on them are examined.
- Some novel types are reported for the thermal variations of magnetizations.
- The reentrant phenomena with a compensation point and so on are found.

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ABSTRACT

The phase diagrams and the temperature dependences of magnetizations in a transverse Ising nanowire with an antiferromagnetic spin configuration are investigated by the use of the effective-field theory with correlations (EFT) and the core–shell concept. Many characteristic and unexpected behaviors are found for them, especially for thermal variation of total magnetization m_T. The reentrant phenomenon induced by a transverse field in the core, the appearance of a compensation point, the non-monotonic variation with a compensation point, the reentrant phenomena with a compensation point and the existence of both a broad maximum and a compensation point have been found in the thermal variations of m_T.

1. Introduction

In recent years, the transverse Ising model (TIM) and its variants have been applied to the examinations of various nanoscaled ferroelectric (or ferromagnetic) systems, such as thin films, nanoparticles, nanowires and nanotubes. The reason is based on their physical properties and their possible applications in different areas. The ferroelectric (or ferromagnetic) properties of these systems clearly become different from bulk counterparts, when the physical size of such a system is reduced to a characteristic length, such as a few atomic length. In particular, surface effects give the distinct contributions to these physical properties, since a large fraction of the atoms in them exist at the surface. Experimentally, magnetic nanowires, such as Fe and Ni single crystal nanowires [1,2], have been fabricated. They have unique magnetic properties clearly different from their bulk, because of the above-mentioned reasons, and exhibit ferromagnetic behaviors. In recent theoretical works, we have found the unconventional surface effects in the TIM nanosystems, namely the reentrant phenomenon induced by a transverse field in the core, while the transverse field at the surface shell is zero [3,4], and the unique thermal variations of magnetizations due to the antiferromagnetic spin configuration at the surface shell [5]. In bulk insulating magnetic materials, the spin configuration of them are normally antiferromagnetic. Nowadays, it is not difficult experimentally to fabricate insulating nanowires [6,7]. As far as we know, however, any insulating magnetic nanowire with an antiferromagnetic spin configuration has not been reported experimentally and theoretically. The main physical reason may come from the fact that it is not known what magnetic properties may be obtained from the investigation of such a system.

Now, we can find a lot of theoretical works on the various types of magnetic nanowires. In these works, the spin configurations in the core and shell are normally ferromagnetic or ferrimagneic, except the work [5,8,9]. These systems have been studied by using a variety of theoretical techniques, mainly the mean-field theory

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(MFA), the effective-field theory with correlations (EFT) and the Monte Carlo simulation (MC) (For the references, see the recent works [10–13]). The recent works for nanosystems [14,15] prove that the results obtained from the EFT have the same topology as those obtained from the MC, while the results obtained from the MC are smaller than those of the EFT. The EFT corresponds to the Zernike approximation [16] and it is believed to give more exact results than those of the MFA, since it includes automatically some correlations between a central spin and the near neighbor spins. However, the theoretical investigations of TIM nanowires with ferromagnetic spin configurations at the surface and in the core are not so much discussed. They have mainly been examined by the EFT and the MFA [4,5,17,18]. In particular, the possibilities of reentrant phenomena in such a TIM nanoswire which are free from disorder-induced frustration have been discussed by the use of the EFT. Traditionally, the reentrant phenomena have been found in a variety of disordered magnetic systems experimentally and theoretically [19,20], especially spin glass systems in which the effects of frustration due to the change of sign in exchange interactions play important ingredient. A ferromagnet in a random field also exhibits the reentrant phenomena [21], which is equivalent to the Ising antiferromagnet with randomly quenched exchange interactions in a uniform field.

The aim of this work is, within the theoretical framework of the EFT, to investigate the phase diagrams and the temperature dependences of magnetizations in the quadrangular TIM naonowire with an antiferromagnetic spin configuration. In Section 2, the models and formulations for the system are given. In Section 3, the phase diagrams are examined. The thermal variations of magnetizations are examined in Section 4. The possibilities of reentrant phenomena which are free from disorder-induced frustration, as discussed in [4,5], are discussed for the present system. For the present system, we have found a number of unexpected and novel kinds of thermal variations of magnetization.

2. Models and formulations

We consider the transverse Ising nanowire with a tetragonal structure in which each layer (or section) is parallel to the (001) surfaces, as depicted in Fig. 1. The each site (white and black circles) on the figure is occupied by a Ising spin. A spin in each layer is coupled to the two spins on the next layers with an exchange interaction J_R ($J_R \geq 0.0$). On the surface, there exists the negative exchange interaction ($-J_S$ and $J_S > 0.0$). The four atoms at the surface (or white circles) in each layer are coupled to the center (or core) atom (or black circle) with the negative exchange interaction ($-J$ and $J > 0.0$). Accordingly, the black and white circles in the figure represent the up- and down- spin directions, when the transverse fields (Ω_S and Ω) at the surface- and core-atoms are taken as zero (or $\Omega_S=\Omega=0.0$). When $\Omega_S=\Omega=0.0$, the spin configuration of the system is an uncompensated collinear antiferromagnetet. One should notice that the quadrangular prism is necessary for the nanowire to get a stable antiferromagnetic spin configuration. Furthermore, when $\Omega_S \neq 0.0$ and $\Omega \neq 0.0$, one should notice that the spin configuration of the system is a canted (or noncollinear) antiferromagnetet.

The Hamiltonian of the present system is given by

$$H = J_S \sum_{(ij)} \sigma_i^z \sigma_j^z + J \sum_{(mn)} \sigma_i^z \sigma_m^z - J_R \sum_{(il)} \sigma_i^z \sigma_l^z - \Omega_S \sum_{(i)} \sigma_i^x - \Omega \sum_{(m)} \sigma_m^x, \tag{1}$$

where $\sigma_i^\alpha (\alpha = z,\ x)$ is the Pauli spin operator with $\sigma_i^z = \pm 1$. The surface exchange interaction J_S is often defined as

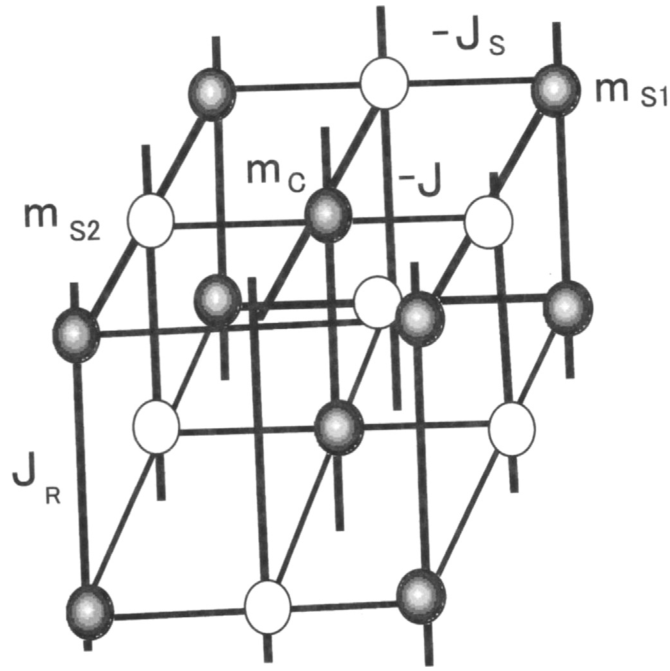

Fig. 1. Schematic representations of a quadrangular nanowire. The black and white circles represent magnetic atoms. The black and white circles represent the up- and down spin directions. The lines connecting the white and black circles represent the nearest-neighbor exchange interactions ($-J_S$, J_R and $-J$).

$$J_S = J(1 + \Delta_S) \tag{2}$$

in order to clarify the effects of surface on the physical properties in the system. In this work, we only examine the two longitudinal magnetizations ($m_{S1} = <\sigma_i^z>$ and $m_{S2} = <\sigma_i^z>$) on the surface shell and one longitudinal magnetization ($m_c = <\sigma_m^z>$) on the core in the z direction, since, in order to obtain the phase diagrams of the present system, only the longitudinal magnetizations are necessary. In fact, the transverse magnetizations of the TIM systems show some finite values in the whole region of temperature and do not exhibit normally any characteristic phenomenon, when the transverse fields take some finite values (see the recent work [5] on the TIM nanowire with an antiferromagnetic spin configuration at the surface). Let us at first define the total magnetization m_T per site in the nanowire as follows:

$$m_T = (1/9)[8m_S + m_C], \tag{3}$$

with

$$m_S = (1/2)[m_{S1} + m_{S2}], \tag{4}$$

where m_S is the averaged magnetization per site at the surface shell.

Within the framework of the EFT [22,23], the magnetizations of Eqs. (3) and (4) in the nanowire can be given by

$$m_{S1} = \left[\cosh(B) + m_{S1}\sinh(B)\right]^2 \left[\cos h(A) - m_{S2}\sinh(A)\right]^2 F_S(x)|_{x=0} \tag{5}$$

$$m_{S2} = \left[\cosh(B) + m_{S2}\sinh(B)\right]^2 \left[\cosh(A) - m_{S1}\sinh(A)\right]^2 \left[\cosh(C) - m_C\sinh(C)\right] F_S(x)|_{x=0} \tag{6}$$

$$m_C = \left[\cosh(C) - m_{S2}\sinh(C)\right]^4 \left[\cosh(B) + m_C\sinh(B)\right]^2 F(x)|_{x=0}, \tag{7}$$

where A, B and C are defined by $A = J_S D$, $B = J_R D$ and $C = J D$. $D = \partial/$