Pressure Influence on Transitions in Spin-Crossover Nanostructures

Gudyma Iu.V., Ivashko V.V.

Chernivtsi National University, Chernivtsi, Ukraine

A compressible model of spin-crossover nanostructure in framework of the Ising-like model with two order parameters and effect of elastic strain on interaction potential is presented [1]. By using this model can be effectively studied the influence of pressure on the spin transition. Magnetic ions occupy a simple regular cubic lattice with homogeneous and isotropic deformations. The Hamiltonian of the model is given by

$$H = -h\sum_i s_i - \sum_{\substack{i,j \\ i \neq j}} J_{ij} s_i s_j + \frac{1}{2} K\xi^2 - P\xi . \qquad (1)$$

Here $h = -(\Delta - k_B T \ln g)$ is generally the energy distance between the HS (High-Spin) and the LS (Low-Spin) states, where Δ is directly related to the strength of crystal field per site, $k_B T$ is the thermal energy, $g = g_H/g_L$ is the electro-vibrational degeneracy ratio between the HS and LS states. Variable s_i is a fictitious classical spin which has two eigenvalues ±1, corresponding to the LS and HS states respectively, J is the inter-ion interaction potential upon homogeneous elastic strain, K is the bulk modulus of the lattice (the elastic constant). Variable $\xi = (a - a_0)/a_0$ indicates the change of the relative inter-ion distance, where a_0 is the average distance between neighboring spins at an equilibrium temperature T_{eq} and an atmospheric pressure, a is the average distance between neighboring spins at a temperature T, P is the external uniform pressure.

On the basis of this model, the thermodynamic function (entropy) of the system was obtained:

$$S = k_B \ln[z(x)] + k_B(\ln g - x) < s > -(\partial K/\partial T)\xi^2 , \qquad (2)$$

where $z(x)=2\cosh(x)$, $x=(2zJ<s> + h)/k_B T$, $<s>=2n_H - 1$, $p=P/N$, $K=K/N$, n_H and ξ are two order parameters of the system, and N - number of molecules.

The entropy had shown us the existence of two basic types of transitions that occurs in a framework of our model: continuous high–spin ↔ low–spin transitions over a broad temperature range; discontinuous high–spin ↔ low–spin transitions associated with a first-order phase transition at a definite temperature.

Also we have obtained a phase diagram witch gives more complete description of diffusionless processes occurring in the spincrossover nanostructure [1]. The results obtained show that the increase of the strain component leads to the forthcoming first-order phase transition. The kind of phase transition, in general, depends on the magnitude of inter-ion interaction.

1. Gudyma Iu., Ivashko V., Linares J. Diffusionless phase transition with two order parameters in spin-crossover solids // *Journ. of Appl. Phys*, **116**(17), (2014), 173509.