Nanocomposites and nanomaterials

Compressible behavior of spin-crossover nanomaterials and spin-crossover transition

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A compressible model of spin-crossover nanostructure in the 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. The Hamiltonian of the model is given by

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

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 with 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 homogeneous and isotropic change of the relative inter-ion distance, where a_0 is the average distance between neighboring spins at an equilibrium temperature 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. The entropy had shown the existence of two basic types of transitions that occurs in the framework of our model: continuous HS ↔ LS transitions over a broad temperature range; discontinuous HS ↔ LS transitions associated with a first-order phase transition at a definite temperature. Also we have obtained a phase diagram that gives complete description of diffusionless processes occurring in the spin-crossover nanostructure [1]. The results obtained show that the increase of the strain leads to the first-order phase transition. The kind of phase transition 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 // J. Appl. Phys.-2014.-**116**. N 17. -173509.