Nanocomposites and nanomaterials

Ising-like model of compressible spin crossover molecular solids

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The molecular complexes of transition metals with the electronic configuration $d4-d7$ can have both high spin (HS) and low spin (LS) central ions and are called spin crossover solids. The compressible model of spin-crossover compounds we consider in simplest way. The deformations are homogeneous and isotropic. Magnetic ions occupied a cubic regular lattice. In mean-field approach the Gibbs free energy per spin is given by:

$$g = zJ < s >^2 + K\xi^2 - p\xi - \ln[z(x)]\,, \qquad (1)$$

where z is the number of nearest neighbors of magnetic ion, J is the interaction integral upon homogeneous deformations, $< s >= 2n_H - 1,$ K is the bulk modulus of the lattice, p is the pressure, $z(x) = 2\cosh(x),$ $x = (2zJ < s > +h)/k_B T,$ $h = -(\Delta - k_B T \ln g)$ is the uniform "magnetic field", Δ is directly related to the crystal field on site, T is the temperature. Values n_H and ξ are two coupled order parameters. If we take into account the explicit dependence of Gibbs free energy on the temperature (1), we obtain the entropy for this system:

$$S = k_B(\ln[z(x)] + (\ln g - x) < s >), \qquad (2)$$

where $\ln g$ is the electrovibrational degeneracy ratio between the HS and LS states in our model. The obtained numerical results enable us to construct the energy diagram, which in turn confirm the presence of first and second order phase transitions in such compounds. The dependence of the critical temperature and the coefficients of Landau expansion of the Gibbs free energy on the external pressure are derived.

The possibility to address spin states (high-spin state and low-spin state in considering model) through external stimuli opens the perspectives to construct new kinds of switches and magnetic storage [1,2].

1. *P. Gütlich and H. Goodwin, eds., Spin Crossover in Transition Metal Compounds I-III, Top. Curr. Chem. No. 233-235 (Springer-Verlag, Berlin/Heidelberg, 2004).*
2. *M. A. Halcrow, ed., Spin-Crossover Materials: Properties and Applications (Wiley, Chichester 2013).*