## Nanocomposites and nanomaterials

# Phase transitions in Ising-like spin-crossover model with nonlinear intersite interaction

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The spin-crossover compounds are the class of inorganic coordination molecular complexes of the chemical elements with $d^4$-$d^7$ electronic configuration of the outer orbital which form the ligand environment with transient metal ion centered in octahedral ligand field. These materials are characterized by two spin states: low-spin (LS) state with diamagnetic properties and high-spin (HS) state with paramagnetic behavior. The LS and HS spin configuration can be interconversed by the action of external controlling field. The transition is supported by drastic change of material's properties that are evidence of the occurrence of phase transition. Among the properties that undergo changes during spin transition the special interest represents the molecular volume changes that renormalize the intersite interaction in the spin lattice. The compressibility of the lattice provoked by the volume changes lead to appearance of additional internal pressure in the system [1].

The Hamiltonian of the system with pressure takes the form

(1)

where is pressure, is molecular volume change during transition between the spin states, is ligand field splitting energy, is the degeneracy ratio between HS and LS states. Since the pressure changes the molecular volume, the inter-molecular interaction is changed also. Therefore in Eq. (1) the intersite interaction may be replaced by its expansion in a series on volume changes with accounting the nonlinear terms

. (2)

From Monte Carlo simulations the temperature-induced spin transition curves for various values of volume increasing were obtained. By detailed analysis of critical temperatures during cooling and heating processes the state diagram has been built. On the diagram are shown the regions of second-order and first-order phase transition together with the region of two-step transition.

1. *Gudyma Iu.V., Ivashko V.V.* Spin-crossover molecular solids beyond rigid crystal approximation // Nanoscale Res. Let. – 2016. – **11**. – 196 (8pages).