рамках современных представлений о МКЭ, а полученные новые экспериментальные данные могут быть использованы для практического применения.

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MONTE CARLO STUDY OF MAGNETIC NANOPARTICLES ADSORBED ON HALLOYSITE $Al_2Si_2O_5(OH)_4$ NANOTUBES

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Halloysite is natural biocompatible clay compound with multi-walled tubular form. It is wide spread and available at low price, which makes it attractive for both industry and research. This material found its application in medicine as container for drugs delivery. Load capability of halloysite nanotubes also allow to carry other functional compounds including catalysts and flame retardant agents [1]. Experiments show that the surface of halloysite is well suited for nanoparticles stabilization [2], which can be used for synthesis of nanotubes demonstrating magnetic properties.

This work is devoted to numerical study of magnetic nanoparticles (Fe, Co, Ni), adsorbed on halloysite surface. Existing experimental data for Ni nanoparticles is presented by hysteresis loops [2]. The classic inequilibrium Monte Carlo approach with solid angle restriction has been used for magnetization processes modeling. Hamiltonian of the system includes dipole-dipole interaction and field terms. The model also takes into account normally distributed sizes of nanoparticles and random orientation of their easy axes. The geometry of adsorbing surface is accounted in anisotropic dipole-dipole interaction:

$$J_{ij}^{\alpha\beta} = \frac{J_0}{R_{ij}^3}\left(\delta_{\alpha\beta} - \frac{3R_{ij}^{\alpha}R_{ij}^{\beta}}{R_{ij}^2}\right),$$

here R_{ij} and R_{ij}^{α} denote length and α-component (α = x,y,z) of the vector, pointing from i-th to j-th particle, respectively; $\delta_{\alpha\beta}$ is Kronecker symbol and $J_0 = \langle\mu\rangle^2$, where $\mu_i \sim V_i$ is magnetic moment of nanoparticle which is proportional to the particle volume.

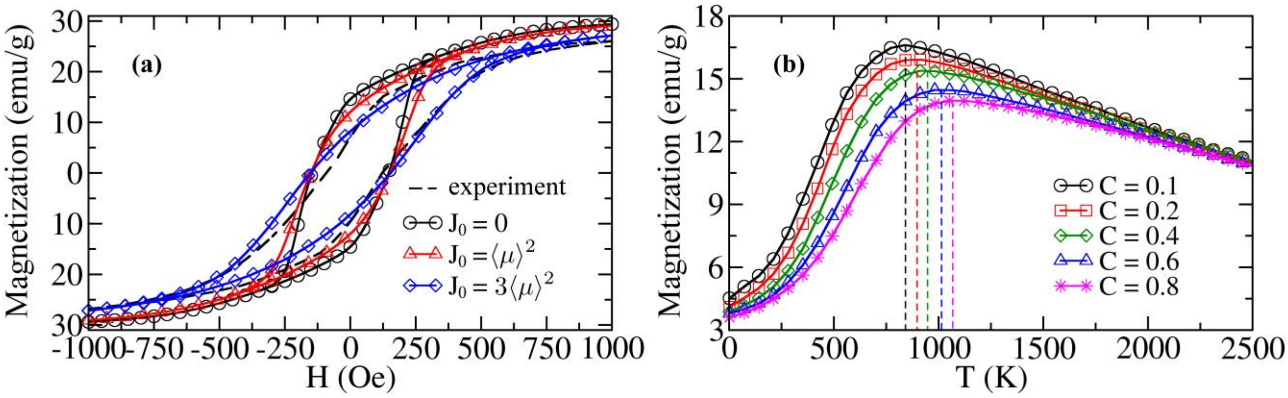

Fig. 1. Magnetic properties of Ni nanoparticles adsorbed on halloysite. (a) Hysteresis loops calculated for different values of J_0 and (b) ZFC-curves for different surface coverage.

Calculated hysteresis loops and ZFC (Zero Field Cooled) curves presented on Fig.1 are in good agreement with experimental data for Ni nanoparticles. It is clear, that the peak of ZFC curves moves to the region of high temperatures with increase of nanoparticles concentration, which can be interpreted as signature of superspin glass freezing. Using this approach, we also calculated hysteresis loops for Fe and Co nanoparticles and investigated influence of surface geometry on magnetic properties of the system.

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