Core-shell approach to magnetite nanoparticles

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Abstract. The influence of the magnetite cluster size on various magnetic properties (magnetic moment, Curie temperature, blocking temperature etc.) is experimentally investigated. A phenomenological theory analogous to the Weitzsäcker approach in the nuclear physics is developed, metrological parameters for the cluster size being discussed. The Monte Carlo simulations for the classical Heisenberg model with different bulk and surface magnetic moments are performed.

Nanoscale magnetic materials are of interest for applications in ferrofluids, high-density magnetic storage, high-frequency electronics, high-performance permanent magnets, magnetic refrigerants. Magnetism of nanoparticles is the area of intensive development that touches many fields including material science, condensed matter physics, biology, medicine, biotechnology, planetary science etc. In particular, iron oxide colloids have a low toxicity and show good biocompatibility, which makes them applicable in various areas of medicine, e.g., drug delivery systems and hyperthermia treatment of cancer. In particular, iron oxide colloids have a low toxicity and show good biocompatibility, which makes them applicable in various areas of medicine, e.g., drug delivery systems and hyperthermia treatment of cancer. For the use in magnetic separation, MR tomography, magnetic hyperthermia and other applications, methods of metrological control of magnetic nanoparticles are being developed.

We performed experiments on the influence of the cluster size on various magnetic properties (magnetic moment, Curie temperature, blocking temperature etc.) for magnetite 4–22 nm nanoparticles synthesized by co-precipitation. Both clean (uncovered) and covered clusters were investigated. Temperature and magnetic field dependences of magnetic moment were measured, and ESR spectra for nanoparticles were obtained at temperatures 4.2–380 K.

The experimental data were interpreted on the basis of core-shell model. A phenomenological theory analogous to the Weitzsäcker approach in the nuclear physics was developed, metrological parameters to determine the cluster size being discussed. The corresponding microscopical Ising and classical Heisenberg models with modified surface moments are analyzed in the mean-field approximation.

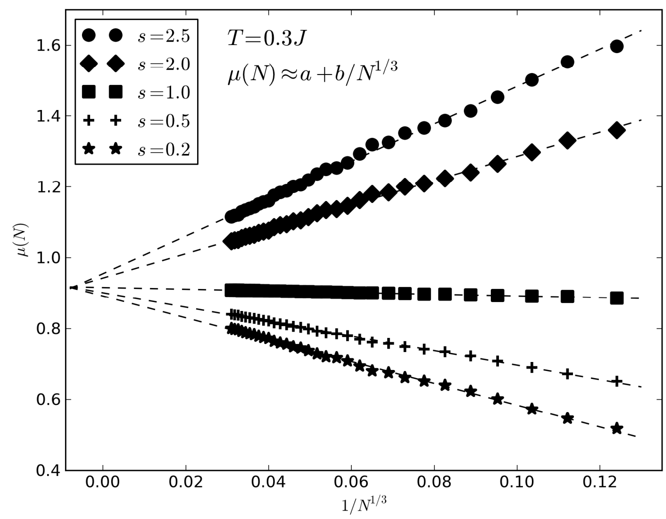

Fig. 1 Dependence of the nanoparticle magnetic moment on $1/N^{1/3}$ for temperature $T = 0.3\,J$, J being the exchange parameter

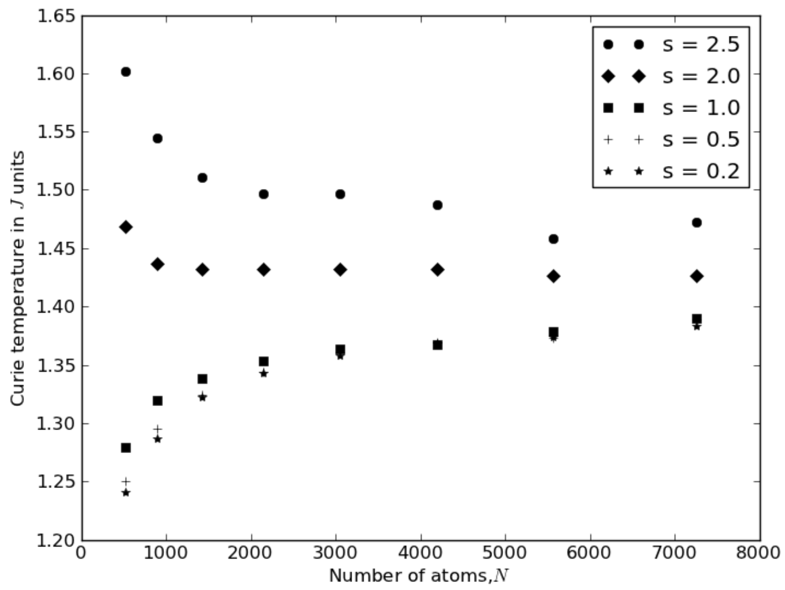

Fig. 2 Dependence of the nanoparticle Curie temperature on the number of atoms for different *s* values

To obtain more reliable conclusions and estimations, Monte Carlo simulations for the classical Heisenberg model with different bulk and surface magnetic moments were carried out. The corresponding results on the dependences of the nanoparticle magnetic moment and Curie temperature on the number of atoms *N* are presented in Figs.1-3 for the spherical particle with different surface magnetic moments (*s* is the ratio of surface and bulk moments). The calculated dependences turn out to agree qualitatively with the predictions of the Weitzsäcker model.

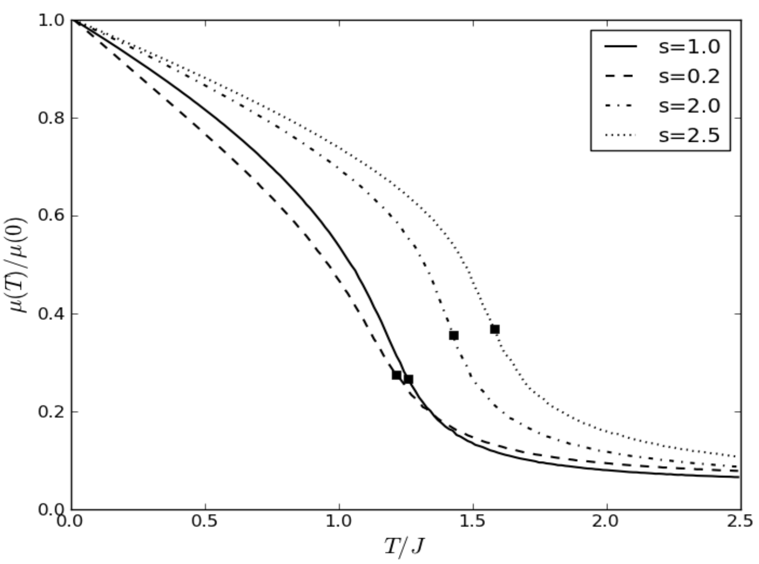

Fig. 3. Typical temperature dependences of magnetic moment of nanoparticles containing *N*=515 atoms with different surface moments (*s* values)

The combination of informative methods of magnetic diagnostics with phenomenological and microscopical models model for nanoparticles allows us to obtain the dependence of specific magnetic moment of nanoparticles on the number of its constituent magnetic formula units, as well as highlight the contributions from bulk and surface sites to magnetzation.