Phase Transitions in the Core / Shell Model of Magnetic Nanoparticles

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The present work proposes to study the phase transitions to a specific model of magnetic nanoparticle (MNP) formed by a ferromagnetic core, covered with a material that has differentiated magnetic properties from the center. This construction is called "Magnetic Nanoparticle Core / Shell Model". For this purpose, the structure was computationally simulated in two and three dimensions using the Ising model.

First, with the purpose of simulating ripples observed experimentally in the hysteresis curve of a MNP core/shell of cobalt ferrite and covered by maghemite with a diameter of 3 nanometers, was projected a fictitious magnetic nanoparticle made up of four sub-structures with different magnetic moments, one core plus three layers. Thus, it was observed that there was a marked damping behavior of the magnetization in function of the temperature and magnetic field externally applied. This smoothing generated, at low temperatures, corrugations in the hysteresis curve similar to the observations found experimentally. Therefore, these disorders can be interpreted as a variation of the magnetization of the layered material.

In a second analysis, the curve adjustment was performed for the magnetization of the MNPs, being accomplished for the alignment of the spins core (transition 1) and shell (transition 2) at different temperatures and considering the definition of critical exponentes according to the classical theories of phase transitions and critical phenomena, concluding that:

1. The first transition in two-dimensional networks: performance features according to the expected theory simulations in two dimensions, but the values of the critical exponents differ subtly from the theory based on the Ising model, making the phase transition more damped;

2. A second transition in two-dimensional networks: behaves according to the defining equation of the critical exponents only in temperatures very close to the transition and their values tend to smoother the magnetization curve;

3. The first transition in three-dimensional network: Presented critical exponent well defined and close to the already consolidated theory;

4. The second transition in three-dimensional network: It presented critical exponent with considerable variation according to the simulated parameters, however, maintains the behavior characteristic based on a power function.

The Monte de Carlo method was chosen as a way of sampling the system configurations and all the simulations were elaborated in programming language "C".