Geometry influence on the hysteresis loops behaviour in $La_{2/3}Ca_{1/3}MnO_3$ nanoparticles: Monte Carlo simulation on a Heisenberg-like model

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1. Introduction

Theoretical investigation with Monte Carlo simulations predicts that spin-switching hysteresis of diferent materials complexes appears even in nanoparticles, but the hysteresis width does not depend only on the interaction strength between molecules but also strongly on the shape and size of the nanoparticles. [1].

2. The model

The manganite $La_{2/3}Ca_{1/3}MnO_3$ is a ferromagnetic compound below 260 K. It is characterized for having three types of ions as Mn^{4+} $(S = 3/2)$, which is bonded with $Ca2+$ ions, Mn^{3+eg} and $Mn^{3+eg'}$ $(S = 2)$ that are related to La^{3+}. Magnetic ions are represented by classical Heisenberg spins. The Hamiltonian used in this work is [2]:

$$H = \sum_{i \neq j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j - K_B \sum_i \mathbf{s}_i \cdot \hat{a} - K_S \sum_k \mathbf{s}_{k\hat{n}} - h \sum_i \mathbf{s}_i \cdot \hat{h}$$

The first sum runs over nearest magnetic neighbors with a coordination number of six. The second term gives the core cubic magnetocrystalline anisotropy, the unit vector $\hat{a}$ indicates the easy axis direction. The third term accounts for single ion site surface anisotropy. The fourth term shows the influence of external magnetic field. The simulations were carried out for nanoparticles with shapes presented in fig.1.

3. Results

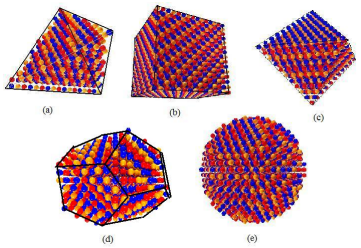

Fig.1: Nanoparticle shapes (a)Tetrahedron (b)Cube (c) Octahedron (d) Dodecahedron (e) Sphere

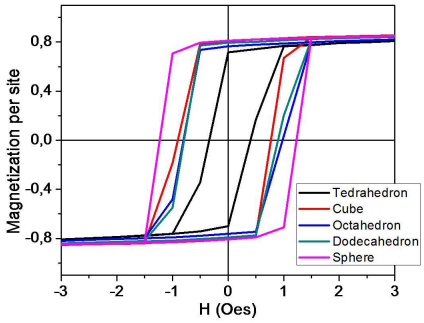

Fig. 2: Hysteresis loops for nanoparticles with different shapes.

Fig. 1 presents the diferent shapes of nanoparticles employed in the simulations. Fig. 2 shows the hysteresis loops for the nanoparticles. Greater coercive field H_c was observed in the sphere curve. It is possible due to it shape contains higher quantity of ions.

4. Conclusions

Simulation of hysteresis loops for nanoparticles with different shapes was carried out observing changes in the coercive field, depending on the geometry and the number of ions.

5. Submission

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