MAGNETIC PROPERTIES MONTE CARLO SIMULATION OF $La_{1-x}Ca_xMnO_3$ FERROMAGNETIC-ANTIFERROMAGNETIC BILAYER USING A COMPOSED INTERFACE APPROXIMATION

David Angulo, Elisabeth Restrepo

Departamento de Física y Química, Universidad Nacional de Colombia Sede Manizales, Manizales, Colombia

Introduction

Colossal magnetoresistance (CMR), present in ferromagnetic manganites thin films has been widely used in magnetic field sensors and read heads for magnetic memories. Although many perovskites show this phenomenon, the $La_{1-x}Ca_xMnO_3$ (LCMO) manganite presents a stronger CMR effect [1].
Furthermore, thin bilayer systems of antiferromagnetic-ferromagnetic (AFM/FM) has been used as well, due the phenomenon present in such systems named Exchange Bias (EB), specially important for magnetic storage devices applications [2]. Exchange Bias arises from magnetic coupling at the bilayer interfaces; this effect is characterized by a shift of the magnetic hysteresis loop along the magnetic field axis. AFM/FM systems properties have been studied not only experimentally but also theoretically. However, few approximations to a non-abrupt interface have been made. E. Restrepo *et al.* analyzed the effect that roughness in the interface of an AFM/FM coupled bilayer has on EB [4]. Conclusions of that work are remarkable; topology and nature of the interface on a coupled AFM/FM bilayer are decisive characteristics that define EB behavior. Some theories stand that in the AFM/FM $La_{1/3}Ca_{2/3}MnO_3/La_{2/3}Ca_{1/3}MnO_3$ interface, a composed material as $La_{1/2}Ca_{1/2}MnO_3$ is created [6], thus this layer should be modeled as well. Since the $x=1/2$ LCMO can be formed in both phases, FM and AFM [7], the aim of this work is to find the effect that this interface produces in magnetic and electrical transport properties on a bilayer of AFM/FM LCMO through Monte Carlo simulation using Metropolis algorithm.

Model Detail

$La_{2/3}Ca_{1/3}MnO_3/La_{1/3}Ca_{2/3}MnO_3$ bilayer was built by using a composed interface. This interface was modeled as a $La_{1/2}Ca_{1/2}MnO_3$ that according to phase diagram, at x=1/2 the stoichiometry of the material allows a coexistence of FM and AFM phases. Two approximations were compared. Figure 1 shows the system construction.
The distribution of magnetic ions, depending on the stoichiometry was carried out according to the literature reports [2].
The Hamiltonian that describes the system is shown in equation 1.

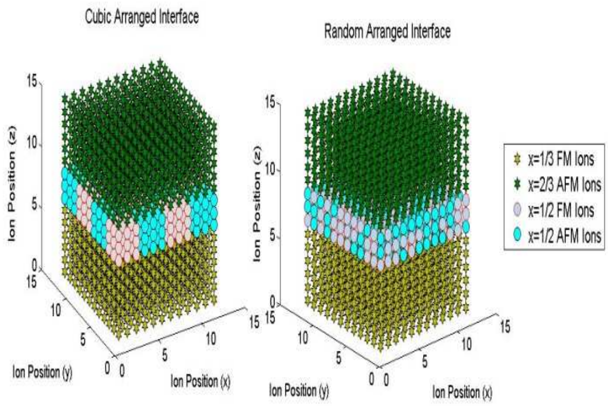

Fig. 1 Bilayer Construction: *First layer of FM $La_{2/3}Ca_{1/3}MnO_3$ phase, upper layer of AFM $La_{1/3}Ca_{2/3}MnO_3$ phase. Cubic Arranged (left) and Random Arranged (right) $La_{1/2}Ca_{1/2}MnO_3$ with FM and AFM phases put together.*

$$H=-J_{ex}\sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j - K_{an}\sum(\boldsymbol{S}_i \cdot \hat{a}_k)^2 - h\sum(\boldsymbol{S}_i \cdot \hat{a}_h) \quad (1)$$

First term represents the exchange coupling between first neighbors. The J_{ex} parameter sign determines the nature of the phase, either it is FM (positive) or AFM (negative). Contribution of magnetocrystalline anisotropy is represented in the second term, where K_{an} is the anisotropy constant and $\hat{a}_k$ is the unit vector in the direction of the easy axis, which in our case is the (1 0 0) direction. The last term, corresponding to the Zeeman effect, represents the contribution of an external constant magnetic field (h), in the direction of the unit vector $\hat{a}_h$. Magnetic ions Mn^{4+}, Mn^{3+eg} and $Mn^{3+eg'}$ on the i^{th} position are described by the classical Heisenberg Spin $\boldsymbol{S}_i$. The spin magnitudes depend on the electronic configurations of the corresponding ion.
For interfacial constants case, the model suggested by M. Kiwi was employed [8]. It consists on using two different exchange parameters alternated where $J_i \neq J_{i+1}$. The selected values are determined as multiples of exchange AF parameter ($\alpha \times J_{AF}$). This is due to interfacial interaction is normally AF type. In this work, values of α were *0.5* and *2* obtained by means of several simulations that allowed to fit experimental reports [9].
Monte Carlo method and metropolis algorithm were used in order to get the system to the ground state. Calculations were carried out during 1.5×10^4 steps per site, discarding the first 7.5×10^3 and averaging the remainder.

Results and Discussion

Magnetoresistance

Results of simulations carried out with proposed approximations are shown in figure 2.

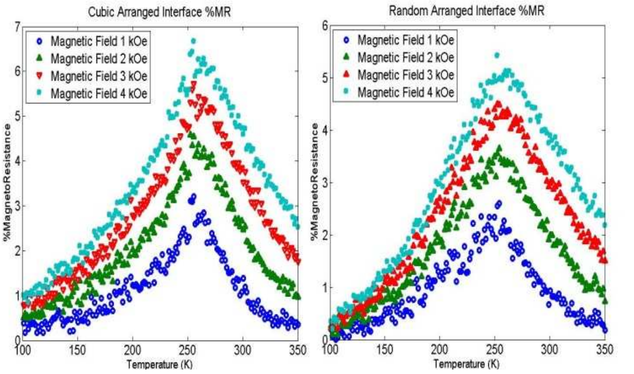

Fig. 2 *Magnetoresistance vs Temperature: MR effect in Cubic Arranged Interface (CAI) (left) and Random Arranged Interface (RAI) (right)*

In this figure, both models show the expected temperature transition around *260K*. It corresponds to a metallic-insulator transition. The shape of the curves is similar to reported in literature for these materials. However, CAI presents a little higher MR values compared with RAI. Moreover transition in RAI is smoother than the former. Explanation to this phenomenon lies in the fact that a random arrange of $x=1/2$ ions is a less abrupt approximation to interface interactions.

Hysteresis Loops

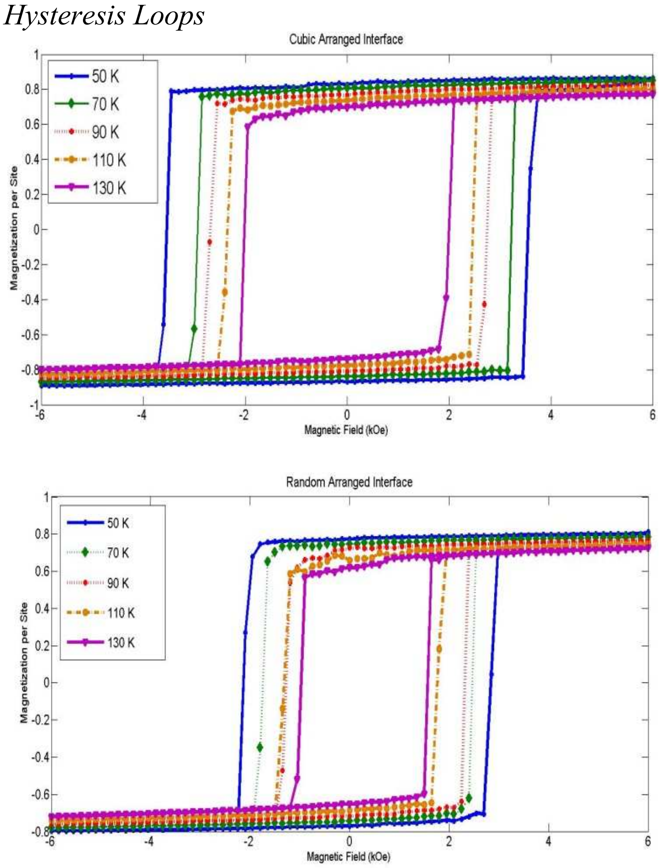

Fig 3. *Hysteresis Loops at different cooling temperatures for CAI (up) and RAI (down)*

Several calculations about hysteretic behavior were made. Figure 3 shows the interface effect on the magnetic properties of the system.-

Several temperatures, below and above the block temperature (around *77 K*) were chosen for the simulation. A weak influence on the EB is exhibited for both arrangements. This result is supported by reports which stand that imperfections on AFM/FM interface bilayers could not favor apparition of EB. Moreover, it seems that Coercive Force is enhanced by CAI as the temperature decreases. This effect is also observed in a lower scale for RAI.

Conclusions

The influence of Cubic Arranged and Random Arranged approximations to non-abrupt interface in FM/AFM LCMO on the magnetic and electrical transport properties was analysed. Magnetoresistance curves showed typical behavior with a metallic-insulator transition close to the Curie temperature as is reported in the literature [6].

Exchange Bias and Coercive Force were studied for different cooling temperature. It seems that the non-abrupt interface does not affect strongly the EB phenomenon.

References

1. Y. Tokura, Y. Tomioka, J. Magn. Magn. Mater. 200 (1999) 1.
2. E. Dagotto, T. Hotta, A. Moreo, Physics Reports 344 (2001) 1-153
3. W. Kuch, L. I. Chelaru, F. Offi, J. Wang, M. Kotsugi, and J. Kirschner, Nat. Mater. 5, 128 (2006); M. Blamire and B. Hickey, ibid. 5, 87 (2006).
4. E. Restrepo, G. Orozco, J. Urrea, J. F., J. C. Vargas, J. C. Riaño, J. Restrepo, J. Matter. Sci. *In Press*
5. J. Spray, U. Nowak, J. Phys. D: Appl. Phys. 39 (2006) 4536-4539
6. E. Dagotto, T. Hotta, and A. Moreo, Phys. Rep. 344, 1 (2001).
7. P. Radaelli, Phys. Rev. B 55 (1999) 3015.
8. D. Lederman, R. Ramírez and M. Kiwi., Phys. Rev. B 70,184422 (2004).
9. J.C Riaño-Rojas, R. Restrepo-Parra, G. Orozco-Hernandez, J. Restrepo, J.F Jurado and C. Vargas-Hernandez, IEEE. Tarns. Magn. 45 (2009) 5196-5199.