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Magnetotransport properties simulation in FM/AF/FM Trilayer of $La_{1-x}Ca_xMnO_3$ Manganite

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Simulations of hysteretic and electrical transport properties such as resistivity and magnetoresistance in Ferromagnetic/Antiferromagnetic/Ferromagnetic (FM/AF/FM) trilayer systems of $La_{1-x}Ca_xMnO_3$ manganite are shown in this paper; for possible spin valves applications. Simulations were carried out by using the Monte Carlo method, Metropolis algorithm, and classical Heisenberg and Kronig-Penney models. FM layers were modeled as an x=1/3 manganite and AF layer as an x=2/3 one. Hysteresis loops showed exchange bias phenomenon in agreement as was expected. Resistivity values were obtained varying different parameters such as temperature, external magnetic field and FM and AF layers thickness, observing typical behavior. The FM layer presented a Metal-Insulator transition around the Curie temperature (T_C). On the other hand, the AF layer did not undergo any transition and curves showed a negative slope. Finally systems composed by FM and AF layers exhibited a behavior corresponding to a mixture of both phases.

Keywords: Monte Carlo simulation; manganites; exchange bias; magnetoresistance.

Este trabajo muestra simulaciones de propiedades histeréticas y de transporte eléctrico tales como resistividad y magnetoresistencia en sistemas de tricapas Ferromagneticas/Antiferromagneticas/Ferromagnéticas (FM/AF/FM) de manganitas de $La_{1-x}Ca_xMnO_3$, con posibles aplicaciones a válvulas de espín. Las simulaciones fueron llevadas a cabo usando el método de Monte Carlo, el algoritmo de Metrópolis y los modelos de Heisenberg Clásico y Kronig-Penney. Las capas FM fueron modeladas considerando $x = 1/3$, y la AF como $x = 2/3$. Los ciclos de histéresis mostraron fenómeno de Exchange Bias de acuerdo a lo esperado. Los valores de resistividad fueron obtenidos variando diferentes parámetros como temperatura, campo magnético externo y espesor de las capas FM y AF. Se observó un comportamiento típico en la resistividad, la capa FM presentó una transición Metal-Aislante alrededor de la temperatura de Curie (T_C). Por otro lado la capa AF no sufrió ninguna transición, y sus curvas mostraron una pendiente negativa. Finalmente se encontró que las propiedades de transporte eléctrico en de los sistemas compuestos por capas FM/AF/FM presentaron un comportamiento correspondiente a la combinación de las ambas fases.

Descriptores: Simulación Monte Carlo; manganitas; exchange bias; magnetoresistencia.

PACS: 75.70.-i; 75.50.Gg; 75.70.Cn; 75.47.Lx

1. Introduction

Spin valves are devices built with coupled systems of Magnetic/Insulator/Magnetic materials. Their applications in read heads, sensors and transistors are widely reported in literature [1-4]. Phase diagram of $La_{1-x}Ca_xMnO_3$ manganite (LCMO), allows the structure to have either Metal-Ferromagnetic nature (FM) or Insulator-Antiferromagnetic nature (AF) [5]. According to this, spin valves can be built by (LCMO) trilayers, taking advantage of their Giant Magnetoresistance effect (GMR) which consists on the high decrease of resistivity (20%-100%) in presence of a low magnetic field [5]. Another typical phenomenon in such systems is the so-called Exchange Bias (EB). This effect, characterized by a shift in the hysteresis loop is a feature of study in spin valves as well [6]. Explanation of this phenomenon is still an open research subject. Although many models have been proposed for describing it [7-10], the model developed by Lederman et. al. has shown interesting results from the simulation point of view [11].

Many materials have been used for developing spin valves, however few works have reported the possible use of LCMO heterostructures as candidates [12] because of their low critical temperature ($\sim$ 260K). Nevertheless reported simulations on multilayers of FM/AF LCMO show that these kind of systems are feasible structures for spintronics devices in the low temperatures domain [13-14].

The aim of this paper is to study electrical transport properties and hysteretic behavior by means of simulations of a LCMO thin trilayer system (FM/AF/FM), which are deciding characteristics for constructing spin valves devices.

Exchange Bias and Magnetoresistance phenomena will be discussed as a function of applied magnetic field, temperature and layers thickness.

2. Model detail

FM/AF/FM trilayer systems were built by using LCMO manganites. FM and AF materials were modeled with $La_{2/3}Ca_{1/3}MnO_3$ and $La_{1/3}Ca_{2/3}MnO_3$ stoichiometries respectively. Figure 1 shows the system phases distribution. Lower and upper layers correspond to FM phase (x=1/3). On the other hand, intermediate layer corresponds to AF phase (x=2/3).

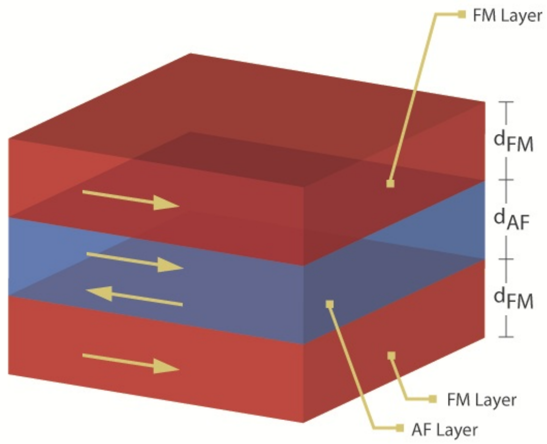

FIGURE 1. System construction. Lower and upper layer correspond to FM phase (x=1/3). Intermediate layer correspond to AF phase (x=2/3).

The system is described by the next Hamiltonian:

$$H = \pm J_{ex} \sum S_i \cdot S_j \pm K_{an} \sum (S_i \cdot a_k)^2 \pm h \sum S_i \cdot a_h \qquad (1)$$

The first term represents the exchange coupling between first neighbors. The J_{ex} parameter sign determines the phase nature, wether it is FM (positive) or AF (negative). The contribution of the Magnetocrystalline anisotropy is represented in the second term, where K_{an} is the anisotropy constant and is the unit vector in the direction of the easy axis, that 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. Magnetic ions Mn^{4+}, Mn^{3+eg} and $Mn^{3+eg'}$ (where superscripts *eg* and *eg'* stand for different Mn^{3+} ions with electrons in the higher levels of the $3d$-orbital) 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, being 2 for Mn^{4+} and 3/2 for Mn^{3+}. Values for each parameter are shown in table I.

Interface interactions were established according to the model proposed by M. Kiwi [11]. In this model, an additional anisotropy is added to the system produced by uncompensated moments at the interface. In order to introduce this anisotropy, two different exchange parameters (J_{in1} and J_{in2}) are proposed for the interface case. These parameters represent the exchange with the first sublattice and the second one at the interface. In this case we have J_{in1}=2×J_{AF} and J_{in2}=0.5×J_{AF}. Periodic boundary conditions were used for (100) and (010) directions and free conditions for lower and upper surface of FM layers. Relation ξ between AF and FM thickness was studied ($\xi = d_{AF}/d_F$). Metropolis algorithm was applied trough Monte Carlo method in order to take the system to the equilibrium. Calculations were carried out during 2×10^4 steps per site, discarding first 1×10^4 and averaging the remainder. In order to obtain EB, system was cooled from 260K to the desired values of temperature. The cooling process was carried out with a cooling field of 4kOe. Once the trilayer reached the desired temperature, hysteretic and magnetoresistivity curves were obtained by applying an external magnetic field.

TABLE I. Exchange interaction values and magnetocrystalline anisotropy. Values taken from [14]

Parameter	Interaction	$x = 1/3$	$x = 2/3$
J_{ex}	Mn^{4+}/Mn^{3+eg}	7.77	-15.54
	$Mn^{4+}/Mn^{3+eg'}$	3.65	-7.3
	$Mn^{3+eg}/Mn^{3+eg'}$	4.65	-9.3
	Mn^{4+}/Mn^{4+}	–	-8.6
K_{an}		1.25	6.24

3. Results

Trilayer resistivity for three different values of ξ is shown in Fig. 2. A phase transition is present in all systems around 260K, which corresponds to Curie Temperature T_C for the FM phase and the Neel Temperature T_N for AF one. It shall be noticed that a small shifting on phase transition is observed when ξ varies as is reported [14,15]. At higher temperatures, paramagnetic regime is established and the slope of the graphic is negative which is the typical behavior of insulating phases. There also exists a low temperature region where the slope of the resistivity is negative, once the temperature reaches certain value T_B called blocking temperature, the slope becomes positive until phase transition is reached. This temperature is attributed to a blocking phenomenon that has been widely reported in literature [16,17]. T_B decreases as a function of AF thickness. This result is supported by several works [18]. Smaller values of ξ present a lower resistivity as external magnetic field is applied as it would be expected, since its behavior approaches to the Metallic-FM bulk. Configurations with larger values of ξ show insulator-like tendency with larger regions of negative slope before T_B, at ξ=1 blocking temperature approaches to transition.

Magnetoresistance ratio was calculated for each studied systems (Fig. 3). As the AF layer becomes thicker, the torque produced by AF layer spins on the interface is bigger, preventing the arrangement of FM layer spins. It shall be noticed that the larger values of ξ, the smaller values of MR are observed. This effect is presented because AF insulating phase has a much stronger contribution to the total resistivity of the system in that case.

When ξ=1, the shape of MR curve is different from configurations of lower AF thickness. Reference line at y=0 was drawn for analysis purposes. Figure 3 shows that at low values of ξ, MR ratio is always negative (resistivity decreases

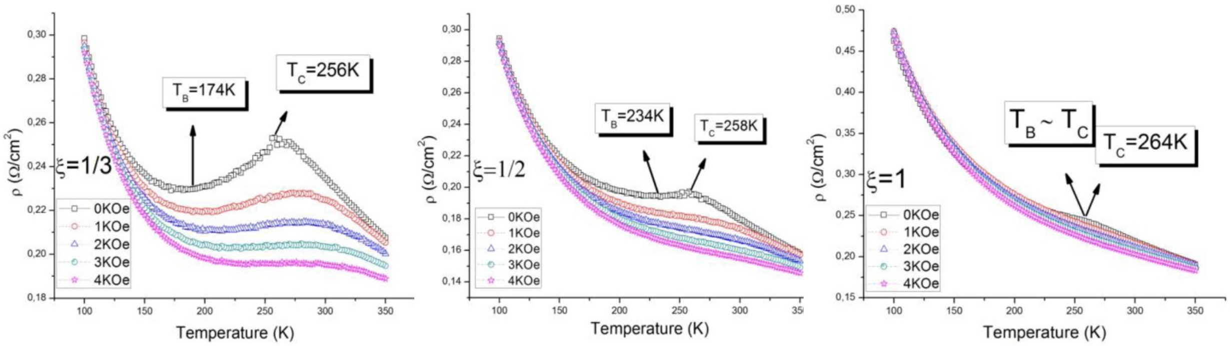

FIGURE 2. Resistivity values as a function of the temperature for several values of magnetic field (0kOe-4kOe) and three values of ξ. Transition temperature (TC) and blocking temperature (TB) are shown at Zero Field. Different values of external magnetic field change these parameters. When ξ =1 blocking temperature is overlapped with TC.

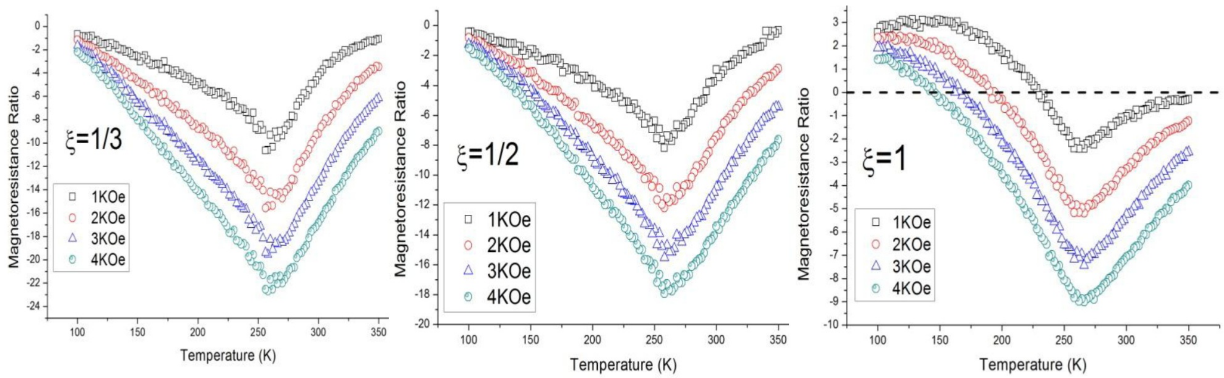

FIGURE 3. %MR as function of Temperature. ξ =1/3 and 1/2 have a regular behavior of magnetoresistance. Applied magnetic field always produces a decrease in the resistivity for all ranges of temperature. On the other hand, ξ =1 has the special feature that low temperatures increases resistivity and high temperatures present regular MR effect.

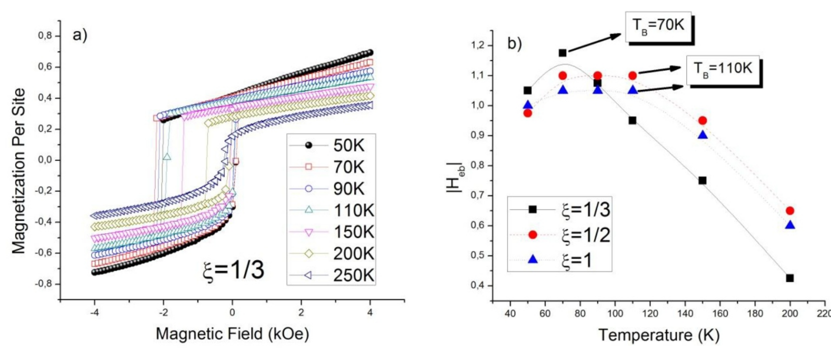

FIGURE 4. a) Hysteresis Loops for different values of Temperatures. Exchange Bias phenomenon is exhibited. b) Variation of the Exchange Field as a function of temperature. In ξ =1/3. A lower blocking temperature is exhibited around 70K and when ξ grows enough, a higher blocking temperature is established around 110K.

with regard to zero field system) which is the regular GMR behavior. However, when AF layer becomes thicker (ξ=1) a small resistivity increase (1%-4%) is observed when magnetic field is applied for low temperature ranges; as the temperature becomes higher regular Magnetoresistance effect is recovered. This particular phenomenon is produced by competition between torque exerted by AF layer, magnetic force and temperature influence on spin arrangement. At low temperatures, spins remain frozen [19], and magnetic force is overcome by the thick AF layer torque [16] observing positive MR ($\rho_H > \rho_0$). As temperature grows, spins gain mobility so that magnetic force can overcome AF torque recovering regular MR behavior ($\rho_0 > \rho_H$).

It can be concluded that at thinner AF layer compared with the FM one, a higher GMR effect is exhibited.

Hysteresis Loops were obtained for all trilayers systems. The specific case of ξ=1/3 is shown in Fig. 4, a shift in the direction of the applied field axis is observed which is the characteristic of EB. Both, Exchange Field (H_{eb}) and Coercive field (H_c) have a tendency to decrease as the temperature grows and approaches to T_C (where they become 0). Similar curve shapes arise from different values of ξ. Variation of the exchange field for each one of them is shown in Fig. 4 as well. This figure shows again a blocking phenomenon where a strong decreasing tendency in $|H_{eb}|$ is observed when T_B is reached. This result is similar to those reported by [20] and [21].

4. Conclusions

Magnetic trilayers systems of FM/AF/FM were studied regarding different relations of AF and FM thickness d_{AF}/d_{FM}. Resistivity for each one of the systems present a blocking temperature lower than transition temperature and strongly dependent on values of ξ and h. Magnetoresistance phenomenon for low values of ξ show similar behaviors with MR ratios between 10% and 25%, however an abnormality in the shape of MR ratio is observed for $\xi=1$ in the low temperature region. Exchange Field also shows a blocking temperature where $|H_{eb}|$ suddenly decreases. Despite the fact that values of T_B for resistivity and hysteresis loops are not equal they are attributed to the same blocking phenomenon which has shown a nonlinear dependence on conditions of the system.

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