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Dynamic phase transitions in $La_{2/3}Ca_{1/3}MnO_3$ manganites: A Monte Carlo simulation study

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ABSTRACT

This work presents a study of dynamic phase transitions in samples of perovskite type manganites of $La_{2/3}Ca_{1/3}MnO_3$, when they were submitted to the influence of an external magnetic field that includes both a time dependent and a time independent magnetic fields. This study was carried out based on Monte Carlo simulations and using the Metropolis algorithm and the mixed spin Ising model. Exchange parameters are proposed to simulate this material. These exchange parameters were obtained in order to reproduce the critical temperature for $La_{2/3}Ca_{1/3}MnO_3$. Results showed that it exists a competition between different factors that generate order or disorder in the magnetic behavior of that material. It was observed that, as the time independent field increases, the critical temperature increases. Moreover, simulations showed that as the amplitude or the period of the time dependent magnetic field increases, the critical temperature decreases. This behavior allows to assert that an time dependent magnetic field induced disorder while a time independent field induces order.

1. Introduction

In the last years, several works have been focused on studying materials with potential magnetic properties. For instance, perovskite type manganites exhibit remarkable magnetic transition phenomena, allowing their application in the development of storage information and logical devices [1,2]. When these materials are exposed to an external magnetic field, which includes terms both time independent and time dependent, it is possible that the system does not respond in a simultaneous way, because the magnetic field contributes or does not contribute to the ordering of magnetic moments. This causes a dynamic phase transition in the system [3–5]. Vatansever and Polat [6] have considered an analysis of a ferromagnetic material, in a generic way, under the influence of a time independent field, named bias field, and other time dependent, named oscillating field. They argued that the amplitude and period of the field affect the dynamic critical nature of the system. Robb et al. [7] described the dynamic phase transition phenomena in a bidimensional Ising model, employing Monte Carlo method. In another study, these authors studied dynamic phase transitions in magnetic multilayers [8]. Idigoras et al. [9] suggested that bias field is the conjugate field to dynamic order parameter. Gallardo et al. [10], using Monte Carlo simulations and kinetic Ising model, studied the evolution of a magnetic system under the simultaneous influence of time dependent and independent magnetic fields. Yüksel [11] investigated the magnetization dynamics in terms of magnetic hysteresis loops as a function of bias field and the period and the amplitude of the oscillatory field, in an uniaxial ferromagnetic nanowire. These calculations are qualitatively in agreement with the recent experimental results obtained for uniaxial cobalt films, in which, it was concluded that the bias field is the conjugate field of the dynamic order parameter. Even though there are several theoretical studies about the influence of time dependent magnetic field on magnetic properties of nanostructures, most of these works are applied to generic models, without considering real materials as mixed valence manganites, where there are several interactions between nearest neighbors. Furthermore, the physics behind these phenomena requires a deeper analysis.

Some of the aforementioned works have employed the Ising model. The Ising model is a good test case for Monte Carlo simulations in statistical physics, since it is quite nontrivial, but the solution of the Ising model by simulation is quite straightforward, avoiding high computational costs and allowing to have a good inside of the system behavior. The Ising model simulation illustrates the microscopic view in greater detail and, although the manganite studied in this work is highly symmetric and isotropic, the Ising model allows to reach a suitable understand of its magnetocaloric behavior, avoiding the high computational costs that

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the Heisenberg or other models imply. On the other hand, Monte Carlo method has been so useful to study the magnetic behavior of nano-structured system due to its straightforward implementation and versatility. Moreover, by means of Monte Carlo simulations, it is possible to study magnetic phase diagrams of complex systems as well as complex phenomena such as exchange bias and compensation behavior [12–14].

According to the recent publication performed by Patricia Riego et al. [15], systems that are in non-equilibrium can undergo qualitative and modifications in their dynamic behavior, depending on external critical parameters, entailing dynamic phase transitions. This behavior is of great importance in superconductivity, charge-density waves, chemical systems, magnetic materials, among others. Studying these dynamic phase transitions, for instance in the case of manganites, it is possible to obtain relevant information regarding to the system dynamics, being interesting for many scientific fields. Furthermore, the simulation of these phenomena gives the possibility to have a better understanding and description of the thermal equilibrium. Manganites, like $La_{1-x}Ca_xMnO_3$, exhibit many interesting properties like a rich magnetic phase diagram for different concentration values. Moreover, this kind of manganites could present spinodal nano-decomposition of La and Ca [16–21]. However, to study this phenomenon is required sophisticated simulations which include first-principles calculations [17].

In this work, we study the behavior of perovskite type manganites, $La_{2/3}Ca_{1/3}MnO_3$, in presence of both a bias and a time oscillating magnetic fields, by means of Monte Carlo simulations. We have employed the mixed spin Ising Model in order to describe the ferromagnetic material behavior [22,23]. For evaluating the influence of bias and time oscillating magnetic, we have varied the bias field and the period and amplitude of the time dependent magnetic field, while the other variables remain constant. Notwithstanding the time in the simulations is measured in Monte Carlo steps, the scaling properties, as singularities in time, and the magnetic behavior should be unchanged for the different algorithms [24].

The paper is organized as follows: in section 2, we expose our model and Monte Carlo simulation procedure. In section 3, we presented the results and discussion. Finally, we included our conclusions in section 4.

2. Modeling and methods

In the manganite studied, the magnetic sites are organized in a perovskite structure (a simple cubic lattice) with a coordination number of six, as it was proposed by Hotta and Dagotto [25]. The sample is formed by a three-dimensional cube of size $L = 21$ m.u.c. (magnetic unit cells), with periodic boundary conditions, for a total of $N = 9261$ magnetic ions. The system presents a stoichiometry of $La_{2/3}Ca_{1/3}MnO_3$ where lanthanum (La) is a rare earth and calcium (Ca) is a divalent metal. The magnetic interactions are only considered between three types of ions: $Mn^{3+}_{eg'}$, Mn^{3+}_{eg} and Mn^{4+}, which may form the following bonds $Mn^{3+}_{eg'}$–O–Mn^{3+}_{eg}, $Mn^{3+}_{eg'}$–O–Mn^{4+} and Mn^{3+}_{eg}–O–Mn^{4+}. For a schematic representation see [26]. The ions were described with the mixed spin Ising model and the magnetic behavior of the system was modeled with a Hamiltonian including terms for nearest neighbors exchange interactions and Zeeman effect, and can be written as

$$\mathcal{H} = -J_{S-s}\sum_{\langle i,j\rangle} S_i s_j - J_{S-\sigma}\sum_{\langle i,j\rangle} S_i\sigma_j - J_{s-\sigma}\sum_{\langle i,j\rangle} s_i\sigma_j - H(t)\left(\sum_i S_i + \sum_j s_i + \sum_k \sigma_k\right) \quad (1)$$

where S, s and σ represent the spin values for $Mn^{3+}_{eg'}$, Mn^{3+}_{eg} and Mn^{4+}, respectively. The spin values were taken as $S = \pm 2, \pm 1, 0$, $s = \pm 2, \pm 1, 0$ and $\sigma = \pm 3/2, \pm 1/2$ for $Mn^{3+}_{eg'}$, Mn^{3+}_{eg} and Mn^{4+}, respectively. J_{S-s}, $J_{S-\sigma}$ and $J_{s-\sigma}$ represent the exchange constant between nearest neighbors for the bonds $Mn^{3+}_{eg'}$–O–Mn^{3+}_{eg}, $Mn^{3+}_{eg'}$–O–Mn^{4+} and Mn^{3+}_{eg}–O–Mn^{4+}, respectively. $H(t)$ is the magnetic field, which is composed by a bias field (h_{bias}) and a time oscillating magnetic field, and is written as

$$H(t) = H_{bias} + H_{osc}\sin(2\pi t/\tau) \quad (2)$$

where H_{bias} is the bias field value, H_{osc} and τ are the amplitude and period, respectively, of the time oscillating magnetic field and t is the time measured in Monte Carlo Steps per spin (MCS). The exchange parameters were computed carry out several simulations in order to reproduce the critical temperature for this material ($T_c \approx 270$ K). Hence, we have established $J_{S-s} = 1.66$ meV, $J_{S-\sigma} = 0.48$ meV and $J_{s-\sigma} = 2.77$ meV. Other way to compute the exchange parameter values is by means of first-principles calculations, where several quantum phenomena are taken into account [27,28]. However, this simulations are beyond the scope of this study.

To carry out the simulations, we start with a random state system from high temperature to low temperature. In order to compute the magnetic properties, the Metropolis Monte Carlo algorithm was employed. In each spin-flip attempt, a random site was selected and its spin value was tried to change, which was accepted or rejected according to the Metropolis algorithm. The numerical data were generated over 10 independent sample realizations by running the simulations for 2.5×10^4 MCS, which 1.0×10^4 were discarded for relaxation.

We have evaluated the normalized total magnetization as

$$m(t) = \frac{1}{M_s}\sum_i^N S_i(t) \quad (3)$$

where M_s is the saturation value of the magnetization.

The dynamic order parameter is defined as the average of $m(t)$ over a given field cycle i [7]:

$$Q_i = \frac{1}{\tau}\int_{(i-1)\tau}^{i\tau} m(t)\,dt \quad (4)$$

Therefore, we can compute the average dynamic order parameter as

$$\langle Q\rangle = \frac{1}{n}\sum_{i=1}^{n}|Q_i| \quad (5)$$

where n is the amount of field cycles, computed as $(2.5\times10^4 - 1.0\times10^4)/\tau$.

In order to estimate the critical temperature (T_c), we also have calculated the magnetic susceptibility, defined as

$$\chi = \frac{\langle Q\rangle^2 - \langle Q^2\rangle}{T} \quad (6)$$

T_c was computed as the temperature at which χ exhibits a global maximum.

3. Results and discussion

Fig. 1a shows the temperature dependence of the order parameter $\langle Q\rangle$ for $H_{bias} = 0.5$ meV, $\tau = 100$ MCS and values of $H_{osc} = 0.0$, 0.5, 1.0 and 1.5 meV. It is possible to visualize that, as H_{osc} increases, T_c tends to decrease. This behavior is due to