11th International Conference on Advanced Materials
ICAM 2009
Rio de Janeiro Brazil
September 20 - 25

Critical Behavior of $La_{2/3}Ca_{1/3}MnO_3$ Magnetic Thin Films: Monte Carlo Simulation

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Abstract – Within the framework of a three-dimensional Heisenberg model with nearest magnetic neighbor interactions, and using a Monte Carlo–Metropolis algorithm for equilibrium and energy minimization, the canonical ensemble averages for magnetization, magnetic susceptibility and specific heat of stoichiometric manganite $La_{(1-x)}Ca_xMnO_3$ were computed. In the model, atoms are distributed on a perovskite simple cubic type structure for which interactions arising from ferromagnetic Mn^{3+}- Mn^{3+} (*eg- eg'*), Mn^{3+}- Mn^{4+} (*eg-d*^{3}) y Mn^{3+}-Mn^{4+} (*eg'-d*^{3}) . On the basis of finite-size scaling theory, our best estimates of critical exponents for the correlation length, specific heat, magnetization and susceptibility are: ν =0.40, α =0.21, β=0.17 and γ =0.75 respectively.

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The ferromagnetic transition in doped manganese has had revived interest since the discovery of colossal magnetorresistence phenomena [1,2]. Recent refinement of the experimental techniques and the improvement of the sample quality make it possible to discuss critical phenomena of this transition in detail [3]. However, the investigations, the estimates of the exponents are scattered and have not covered yet. For this reason it is necessary to shed light on this problem for the theoretical viewpoint. One theoretical work is presented by N. Furukawa and Y. Motome [3] investigated the critical phenomena of double-exchange models for manganites by using finite size scaling analysis on unbiased numerical results. Those results were in agreement with those obtained by Heisenberg models. Regarding to $La_{1-x}Ca_xMnO_3$, one of the most used Ca concentration is x=0.333, due to its special magnetic and transport properties [4]. It makes important to study not only experimentally but also theoretically its critical behavior. In this work, the critical exponents ν , β, γ and α of $La_{2/3}Ca_{1/3}MnO_3$ low T_c were obtained assuming that the magnetic transition is the second order. The simulation is carried out by using Monte Carlo-Metropolis algorithm and Heisenberg model.

The structure and valence of manganites has been investigated by E. O. Wollan and W. E. Koehler [5]. In this model, magnetic ions Mn^{3+} and Mn^{4+} ions are represented by Heisenberg spins type spin, while oxygen, lanthanum and calcium ions are considered as non-magnetic. The critical exponents were obtaining from the magnetization (m), energy, magnetic susceptibility (χ), specific heat (C) and four order cumulante (U_4) results as a temperature function for values different of size system L. In the figure 1 is showed the procedure employ to find the critical exponent ν with the average of maximum slopes for Ln m, m and U_4. Also, the transition temperature, was established with T(χmax) and T(Cmax) from ν value (figure 2). The other exponents were determined based in the relations: $M \alpha L^{-\beta/\nu}$, $C \alpha L^{\gamma/\nu}$, $C \alpha L^{\alpha/\nu}$. The results obtained for critical exponents were ν =0.40, α =0.21, β=0.17 and γ =0.75, and a critical temperature of 259 K similar to its reported in the literature. It was concluded that employed Monte Carlo method a critical behavior results of $La_{2/3}Ca_{1/3}MnO_3$ fulfilled with the Rushbrooke equality.

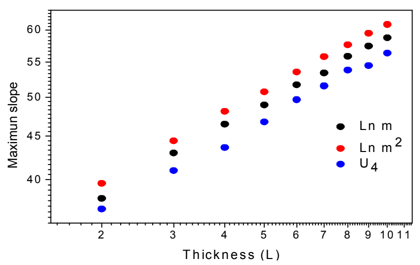

Figure 1: Maximum slope as function of thickness (L) for Ln m, m^2 and U_4 to find ν exponent.

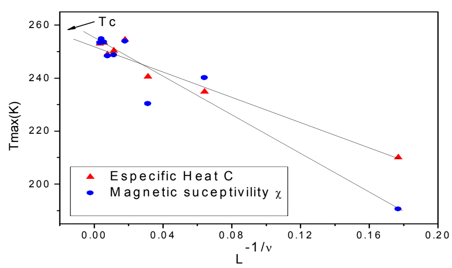

Figure 2: T(cmax) y T(Cmax) to obtain Tc

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