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Monte Carlo study of magnetic properties and critical behavior of Sr_2CrMoO_6

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ABSTRACT

We performed the Monte Carlo simulation (MCs) in order to study the magnetic properties and the critical behavior of Sr_2CrMoO_6. Within this magnetic oxide, the Cr^{3+} and Mo^{5+} ions form two interpenetrating ferromagnetic sublattices with opposite spins directions (Cr^{3+}up and Mo^{5+}down). The exchange interaction between these sublattices is assumed to be ferrimagnetic. The effects of the system parameters on critical temperatures and as a result on the phase diagrams are shown by using reduced values of parameters. The phase transitions and the magnetic stability are investigated in the framework of Ising model. For specific values of the system parameters, the existence of a compensation point is shown. Furthermore, to investigate the critical behavior, the critical exponents are calculated, they indicate that the compound belongs to a three dimensional Ising universality class. The reduced transition temperature is also found.

1. Introduction

Sr_2CrMoO_6 compound belongs to double-perovskite oxide family which has as reference chemical formula A_2MNO_6 (A can be an alkaline-earth such as barium, calcium or strontium or a lanthanide, M and N are respectively a magnetic and non-magnetic transition metal and O is the oxygen) [1–5]. Since several years, Sr_2CrMoO_6 double-perovskite oxide is subjected to interesting studies due to its multiple properties making it potential candidate for various spintronics applications [6,7]. Properties such as colossal magnetoresistance [8], half-metallicity [9], semiconductor behavior [10] and magnetodielectricity [11] were detected in Sr_2CrMoO_6. Its magnetic properties are particularly interesting for the fact that Sr_2CrMoO_6 double-perovskite compound has a high magnetic ordering temperature [12,13], which is crucial for the fabrication of magnetic devices operating at room temperature. Furthermore, Sr_2CrMoO_6 presents the particularity to be used for anode of solid oxide fuel cell (SOFC) with hydrocarbon fuels [14].

In this picture, we are especially interested by the Sr_2CrMoO_6 magnetic properties. In previous works, its magnetic properties have been studied in experiment for high Curie temperatures [5,6,9,15]. It was shown that Mo^{5+} magnetic moments order antiparallely with Cr^{3+} moments by a superexchange interaction, inducing to a ferrimagnetic ordering at 450 K [16]. Due to the similar ionic sizes [17] of Cr^{3+} (0.615 A°) and Mo^{5+} (0.61 A°) ions, A low magnetic moment (2.0 μB per formula unit) has been found. It was also shown that Cr^{3+} ($3d^3$, $S = 3/2$) and Mo^{5+} ($4d^1$, $\sigma = ½$) ions are believed to be ferrimagnetically coupled within a cubic lattice with Fm3m space group [9]. This structure is subdivided into two interpenetrating ferromagnetic sublattices, respectively, of Cr^{3+} and Mo^{5+} ions. According to X-ray absorption spectroscopy, in undoped Sr_2CrMoO_6 magnetic oxide, Cr^{3+} can be only in 3+ state ($3d^3$), sparing any valence compensation with Mo^{5+} ($4d^1$) [8,15]. Ferrimagnetic phase resulting from antiferromagnetic coupling between spins $\sigma = ½$ and $S = 3/2$ has suggested some studies [18–21] about mixed Ising systems in the presence of a crystal-field. These studies reported the influence of the ferrimagnetic coupling and of the crystal-field on the magnetic behavior and also found Compensation behaviors in these systems. On the other hand, other works about magnetic properties of perovskites such as Sr_2CrReO_6 [22] or $LaMnO_3$ [23] motivated our investigations.

The aim of this work is to propose a theoretical model which takes into account the crystal-field and the exchange interactions

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between σ–*S*, σ–σ and *S*–*S* spins in order to describe the region, in the parameters spaces, in which the ferrimagnetic state, experimentally observed, is stable. In addition this study exhibits a rich variety of phase diagrams, including the compensation phenomenon. This work also aims to find the universality class of the Sr_2CrMoO_6 compound by calculating the critical exponents in the framework of the defined ferrimagnetic state. Thus, using the Monte Carlo simulation in the framework of the proposed model, we report the magnetic properties and the critical behavior of ordered Sr_2CrMoO_6 and present phase diagrams of its intrinsic physical quantities.

Thus, in Section 2, we present the Hamiltonian model used. We devote the Section 3 to make a MC simulation analysis for an essential clearness in the discussion. In Section 4, we report and discuss our results. Naturally, the Section 5 is reserved for conclusion.

2. Hamiltonian model

The purpose of this paper is to bring out the effects of the exchange interactions and of the crystal-field on phase diagrams of the ferrimagnetic Sr_2CrMoO_6 while pointing out some phenomena such as the phase transitions, the stability regions and the compensation between spins σ and *S*. The lattice size effect on the magnetization and the magnetic susceptibility are also shown. We will also calculate the different critical exponents related to the size effect and the reduced transition temperature.

Tolerance factor calculations report that ordered Sr_2CrMoO_6 crystallizes in a cubic structure within Fm3m space group [9]. Its crystalline magnetic lattice is subdivided by two ferromagnetic face-centered cubic sublattices, respectively, of the Mo^{5+} ($4d^1$, σ = ½) and Cr^{3+} ($3d^3$, *S* = 3/2) ions which alternate on sites.

The spins σ order antiparallely with the spins *S* by a superexchange interaction, inducing to a ferrimagnetic ordering between sublattices. For a lattice containing *N* particles, the Ising Hamiltonian of the system is defined as:

$$H = -J \sum_{<i,j>}^{\frac{N}{2}} S_i\sigma_j - J_{Mo} \sum_{<i,j>}^{\frac{N}{2}} \sigma_i\sigma_j - J_{Cr} \sum_{<i,j>}^{\frac{N}{2}} S_iS_j - \Delta \sum_{i}^{\frac{N}{2}} (S_i)^2. \quad (1)$$

where *J*, J_{Mo} and J_{Cr} are exchange interactions between nearest-neighbor pairs, respectively, of spins σ–*S*, σ–σ and *S*–*S*. Δ is the crystal-field parameter applied to spins S_i. Each spin-σ (*S*) is surrounded by 6 spins-*S* (σ) as first nearest-neighbors and 12 spins-*S* (σ) as second nearest-neighbors.

At zero temperature (T = 0), the system exhibits the four following initial configurations: F_e(½,3/2), F_e(½, ½), F_i(−½, 3/2) and A_f(−½, ½). However, for $J < 0$, only the antiferromagnetic *Af* and the ferrimagnetic F_i phases have a minimal ground-state energy. According to Equation (1), their corresponding ground-state energies are expressed as:

$$E_{Fi} = -\frac{9}{4} - \frac{3}{4}\frac{J_{Mo}}{J} - \frac{27}{4}\frac{J_{Cr}}{J} - \frac{9}{8}\frac{\Delta}{J}$$
$$E_{Af} = -\frac{3}{4} - \frac{3}{4}\frac{J_{Mo}}{J} - \frac{3}{4}\frac{J_{Cr}}{J} - \frac{1}{8}\frac{\Delta}{J} \quad (2)$$

With $J_{Mo} > 0$ and $J_{Cr} > 0$. Δ/J, J_{Mo}/J and J_{Cr}/J are, respectively, the reduced crystal-field applied to spins S_i and the reduced exchange interactions within sublattices of Mo^{5+} and Cr^{3+} ions. Thus, the equation $\Delta/J = -6J_{Cr}/J - 3/2$ denotes the coexistence function of *Af* and F_i phases, where the energies difference $(E_{Af} - E_{Fi}) = 0$. In all the following, we consider $J < 0$ and we express values of J_{Mo} J_{Cr} and Δ per unit of *J*, the exchange interaction between sublattices. MC simulation is used in order to investigate magnetic properties, size effects and the critical behavior.

3. Monte Carlo analysis

In order to compute the total magnetization, the magnetic susceptibility, the free energy and the specific heat, we used the Metropolis algorithm. We considered a cubic lattice of size L with periodic boundary conditions.

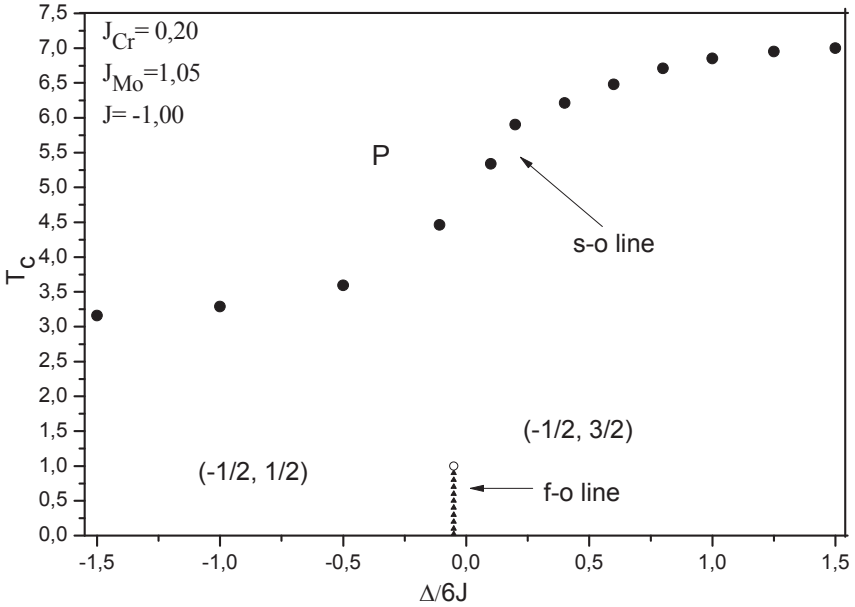

Fig. 1. The reduced critical temperatures as function of the reduced crystal-field parameter $\Delta/6J$ for $J = -1.00$, $J_{Mo}/J = -1.05$ and $J_{Cr}/J = -0.20$ and for the lattice size L = 16. The dashed line terminated by the tiny circle (end-point) is the first-order transition line (f-o line) plotted for low temperatures.