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Phase diagram of the double perovskite Sr_2CrReO_6: Effective-field theory

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ABSTRACT

The double perovskite Sr_2CrReO_6 has very important characteristics for spintronic applications. It is a ferrimagnetic material distinguished by its high Curie temperature $T_c \approx 635$ K. We made this statistical study to further reveal the different ways in which this compound can behave with respect to interaction couplings and crystal fields prevailing in the system. We used as approximation an effective field theory (EFT) without correlation in the context of the Ising model. Thus we report different phase diagrams, firstly in relation to the exchange couplings present in the model adopted, and secondly in relation to the crystal fields of Cr and Re. We compare the results found by this method with those found by other statistical methods. Several phase transitions are detected and reentrant phenomenon was observed.

1. Introduction

Magnetoresistive semi-metals are a class of materials that begins to have a great interest in the development of practical applications. Discovery of giant magnetoresistance in metallic multilayers Fe/Cr [1] helped launch many studies under the veil of a new science. This is spintronics or spin electronics science that focuses on the spin of the electron rather than its charge. The low-field magnetoresistance (LFMR) was the origin of the construction of magnetic sensors (position sensors and potentiometers without contacts) based $La_{2/3}Sr_{1/3}MnO_3$ [2]. A major constraint experienced by this type of $La_{1-x}Sr_xMnO_3$ materials is the rapid diminishing of their magnetoresistance with temperature. This Magnetoresistance becomes zero at their Curie temperature not exceeding 360 K. The double perovskites are generally materials having a higher T_c. This property has attracted much interest in this type of materials.

One area of research in this type of material is directed in favor of storing information via the giant magnetoresistance heads. Another area is directed to the realization of non-volatile RAM comprising two half-metal layers separated by an insulating tunnel barrier. These RAM have the advantage of non-volatile information against SRAM and DRAM "classic" (the information remains in memory even without power supply) which leads to a very low energy consumption.

Ordered double perovskites with the formula $A_2BB'O_6$ (with A an alkaline earth, B a magnetic transition metal ion and B'' a non-magnetic ion) take great interest in the scientific research thanks to their magnetic properties. For example, the magnetoresistance observed in the compound Sr_2FeMoO_6 at large room-temperature [3], then double perovskites that show very high Curie temperature compared to simple perovskites, namely Sr_2CrReO_6 with ($T_c \approx 635$ K) [4,5] and Sr_2CrOsO_6 with ($T_c \approx 725$ K) [6,7]. Remains to mention that, the magnetic coupling in these materials is associated with a substantially charge carriers semi-metal character at the Fermi level [8,9]. For these reasons, these materials are becoming more powerful candidates for spintronic applications [10,11].

The important progress that knew the manufacturing technology of thin films allows producing prototypes which are increasingly pure. Recently our compound was synthesized with the least possible defects [12]. Especially the defects of anti-site less than 20% which stands as the major defect that affects the properties of such materials. The same group of researchers reports that the compound synthesized by pulsed laser deposition on (001)-oriented substrates presents high saturation magnetization of 0.8 and high coercivity of 1.1 T, as well as a strong magnetic anisotropy [12]. These properties are very similar to those found by theoretical studies of pure crystalline compound [13,14]. Thus a detailed study of this compound in its pure crystalline state is important to analyze its magnetic behavior towards different

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interaction couplings and crystal fields that govern it. We choose in this study a powerful analysis tool that has proven efficiency in statistical physics. This tool is effective field theory (EFT) which is more accurate than the standard mean-field theory [15]. More precisely we use the approximation based on the effective field theory with the use of the differential operator as a mathematical tool [16], then insert it into the identity of Callen [17].

This letter is organized as follows: In Section 2 we develop the EFT by the use of the differential operator technique in the frame work of adopted Ising model. Section 3 is reserved for the obtained phase diagrams. A conclusion is reported in Section 4.

2. Model and formulation

Based on the crystalline structure of an ideal double perovskite [3] the two atoms which contribute to the magnetization Cr/Re are located in two nested Face Centered Cubic (FCC) lattices (in fact, the cell is not a perfect FCC, but centered quadratic which allows to take into account the slight distortion). We take it as a FCC to simplify the model this leads to withdraw from this structure following parameters: $J_1(J_1<0)$ is the interaction coupling between Cr and Re ions. $J_2(J_2>0)$ is the interaction constant between Cr atoms. $J_3(J_3>0)$ is the interaction constant between Re atoms (Fig. 1). Δ_{Cr} and Δ_{Re} are the crystal fields of the two sub-lattices Chromium and Rhenium, respectively [14].

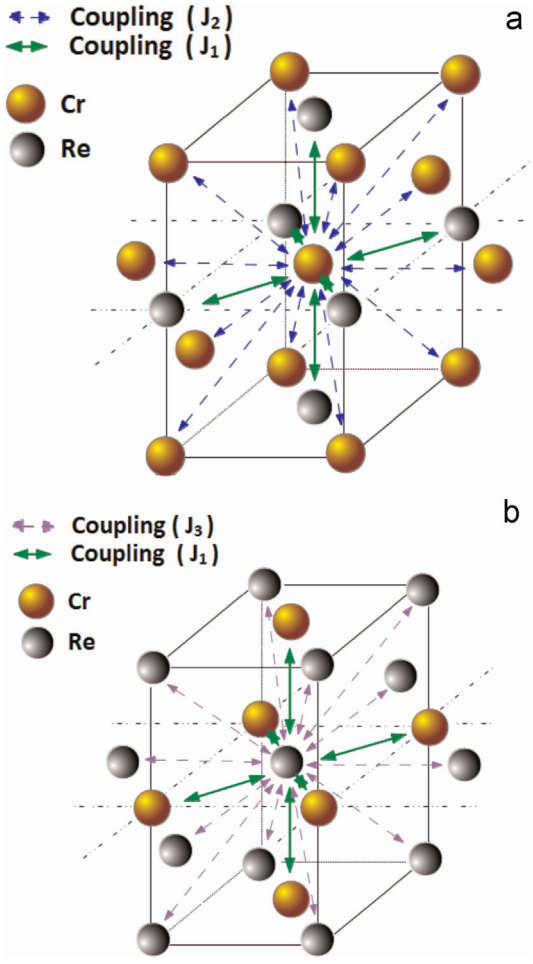

Fig. 1. 3D-illustration of the coupling interactions taken into account for this model. (a) First finite cluster centered on a chromium atom. (b) Second finite cluster centered on a rhenium atom.

Thus, the Hamiltonian of the Ising model for this system can be given by

$$H = -J_1\sum_{(i,j)} S_i\sigma_j - J_2\sum_{(i,j)} S_iS_j - J_3\sum_{(i,j)}\sigma_i\sigma_j - \Delta_{Cr}\sum_i (S_i)^2 - \Delta_{Re}\sum_i (\sigma_i)^2 \quad (1)$$

where (i,j) denotes the nearest neighbor spins at i and j sites. $S_i = \pm 3/2, \pm 1/2$ and $\sigma_i = \pm 1, 0$ are the respective spins of Cr and Re.

We focus our analysis on the ferrimagnetic phase reported in the ground state phase diagram [14] because several studies have predicted this phase at ground state [4,18,19]. This phase described J_1 negative, J_2 positive and J_3 positive. We also discover the behavior of the system when J_2 and J_3 become negative.

The originality of our development comes from the fact that we took into account the interactions of the first nearest neighbors which are 6 in number, and second nearest neighbors which are 12 in number (Fig. 1).

Thus we distinguish two Hamiltonian equations corresponding to two finite clusters

– A first cluster centered on S_0 (Fig. 1(a))

$$H' = -J_1S_0\left(\sum_{i=1}^{6}\sigma_i\right) - J_2S_0\left(\sum_{i=1}^{12}S_i\right) - \Delta_{Cr}(S_0)^2 \quad (2)$$

– The second centered on σ_0 (Fig. 1(b))

$$H'' = -J_1\sigma_0\left(\sum_{i=1}^{6}S_i\right) - J_3\sigma_0\left(\sum_{i=1}^{12}\sigma_i\right) - \Delta_{Re}(\sigma_0)^2 \quad (3)$$

We start by finding the identity of Callen [17] of our spin system. The use of the differential operator technique [16] allows finding the mean-values of $\langle S_i\rangle$ and $\langle\sigma_i\rangle$ exactly in the forms

$$\langle S_i\rangle = \left\langle e^{(3D_x+D_y)E_i'}\right\rangle f(x,y)_{x=y=0} \quad (4)$$

with

$$E_i' = \frac{1}{2}K_1\sum_{i=1}^{6}\sigma_i + \frac{1}{2}K_2\sum_{i=1}^{12}S_i \quad (5)$$

and

$$\langle\sigma_i\rangle = \left\langle e^{D_xE_i''}\right\rangle g(x)_{x=0} \quad (6)$$

with

$$E_i'' = K_1\sum_{i=1}^{6}S_i + K_3\sum_{i=1}^{12}\sigma_i \quad (7)$$

where the functions $f(x,y)$ and $g(x)$ are defined by

$$f(x,y) = \frac{(3/2)e^{d_1}sh(x) + (1/2)sh(y)}{e^{d_1}ch(x) + ch(y)} \quad (8)$$

$$g(x) = \frac{e^{d_2}sh(x)}{e^{d_2}ch(x)+1} \quad (9)$$

$K_1 = J_1/T$, $K_2 = J_2/T$, $K_3 = J_3/T$ are temperature reduced couplings; $D_x = \partial/\partial x$, $D_y = \partial/\partial y$ are differential operators; $d_1 = \Delta_{Cr}/T$, $d_2 = \Delta_{Re}/T$ are temperature reduced crystal fields.Quadratic terms are given by