Computational Condensed Matter xxx (2017) 1–5

Contents lists available at ScienceDirect

Computational Condensed Matter

journal homepage: http://ees.elsevier.com/cocom/default.asp

Low field magnetocaloric effect in the double perovskite Sr_2CrMoO_6: Monte Carlo simulation

O. El rhazouani*, A. Slassi

LMPHE, Department of Physics, Faculté des Sciences, Université Mohammed V, Rabat, Morocco

ARTICLE INFO

Article history:
Received 1 March 2017
Received in revised form
13 May 2017
Accepted 14 May 2017
Available online xxx

Keywords:
Double perovskite
Monte Carlo simulation
Magnetocaloric effect
Relative cooling power

ABSTRACT

Magnetocaloric effect (MCE) in double perovskite (DP) Sr_2CrMoO_6 has been investigated for low magnetic field change by using a Monte Carlo Simulation (MCS) in the framework of Ising model. Total magnetization and thermal derivative of the magnetization have been investigated. Magnetic entropy change has shown a significant extension around the transition temperature which is primordial for magnetic refrigeration. At transition temperature (T_C) equal to 458K, the maximum of magnetic entropy change, the adiabatic temperature change and the Relative Cooling Power (RCP) have shown an increase from 1.427 to 2.582$J\cdot Kg^{-1}K^{-1}$, from 5.43 to 8.71K, and from 18.33 to 28.62$J\cdot kg^{-1}$, respectively, for magnetic field changes 100Oe and 700Oe, which is large for low magnetic field compared to other magnetocaloric materials. The Large MCE at low-field makes Sr_2CrMoO_6 a very promising candidate for magnetic refrigeration above room temperature.

Contents

1. Introduction

Magnetic refrigeration is a cooling technology based on the use of a magnetic material in which a changing magnetic field can induce a Magnetocaloric effect (MCE) [1]. MCE is a physical concept that measures the capacity of a magnetic material to change its thermal behavior under application or removal of an external magnetic field. Classical refrigeration systems are mainly based on a compression/expansion vapor cycle [2], which is harmful to the environment and requires a large amount of energy. On the other hand, MCE refrigeration technology appears to be more beneficial, in term of environmental protection and energy costs reduction.

Designing efficient magnetic refrigerators working on a broader thermal range depends basically on the use of refrigerants that show a large magnetic entropy change ($|\Delta S_M|$). In this respect, a great theoretical and experimental deal effort has been made to search for magnetic materials that obey the large ΔS_M criterion. After the discovery of a large MCE in gadolinium element "Gd" [3], the latter has been considered for a long time to be the most suitable refrigerant for magnetic refrigeration in room temperature. However, problems encountered with Gd are its high cost and its transition temperature (T_C) cannot be

* Corresponding author.
E-mail address: doc.omarel@gmail.com (O. El rhazouani).

http://dx.doi.org/10.1016/j.cocom.2017.05.002
2352-2143/

adjusted readily [4].

In recent years, significant progress has been made in searching alternative materials, especially compounds without rare-earth elements and showing a large MCE near room temperatures. Magnetic perovskite oxides, compared to rare-earth metals, exalt promising and exciting properties going from smaller magnetic hysteresis to higher chemical stability and higher electrical resistivity, which makes them more suitable candidates for magnetic refrigeration at high thermal conditions, especially near room temperatures. Double Perovskite (DP) materials belong to the class of perovskite oxides that show the higher Curie temperatures measured until now in magnetic oxides. Recently, these materials have attracted a considerable amount of investigation due to the colossal magnetoresistance [5–10] and large MCE near the second order transition temperature [11,12]. It has been reported that the DP $Br_2CrMo_{1-x}W_xO_6$ (x = 0, 0.2 and 0.5) shows, near T_C, a large MCE which decreases with the increasing of the substitution of Mo by W [13]. A large magnetic entropy change $(1.6J{\cdot}g^{-1}K^{-1})$ has been reported at $T_C = 285K$ in the sample $Br_2CRMo_{0.5}W_{0.5}O_6$ under a large applied magnetic field of $10kOe$. Other authors have reported a large MCE (with a magnetic entropy change of $1.32J{\cdot}Kg^{-1}K^{-1}$) at $T_C = 381K$ in the sample $Sr_2FeMo_{1-x}W_xO_6$ (x = 0.35) [14].

The DP Sr_2CrMoO_6 has been reported to crystallize in a cubic cell (space group symmetry: $Fm\bar{3}m$) with $a = 7.840$Å. Its calculated magnetic structure indicates that it's a half-metallic ferrimagnet with a Curie temperature $T_C^{exp} = 450K$ [15]. Thanks to its T_C above room temperature, this compound could find an application in magnetic refrigeration (in aerospace technology, metallurgy industry or automotive) or in domestic refrigeration and air-conditioning systems after special treatment (doping for instance) to bring its transition temperature very close to the room temperature. In this connection, this study has been conducted to predict the MCE at low fields in this DP by using a numerical simulation in the framework of Monte Carlo Simulation (MCS). The system has been taken as an Ising model involving super exchange and double exchange interactions and the interaction with an external magnetic field.

In the following section, a presentation of interactions taken into account in the adopted model is given. In section three, Monte Carlo simulation process and different physical quantities calculated through simulation are described. Section four is devoted to the presentation and the discussion of results. Conclusions are summarized in section five.

2. Simulated model

Sr_2CrMoO_6 DP belongs to the family of Cr-based DPs. Like the majority of compounds inside this class of materials [16–24], the DP Sr_2CrMoO_6 has a face centered cubic (fcc) crystal lattice of the rock salt structure containing two transition metal elements (*Cr* and *Mo*). Each transition metal ion is surrounded by an oxygen-octahedra. Accordingly, the main structure is composed of two sublattices having the same size and the same number of ions. Cr^{3+} ions interact with each other in the first sublattice via the double exchange (DE) coupling J_{Cr-Cr}, which is a next nearest neighbor (NNN) interaction coupling involving 12 NNN Cr^{3+} ions. Mo^{5+} ions interact with each other in the second sublattice via the DE coupling J_{Mo-Mo}, which is also a NNN interaction coupling involving 12 NNN Mo^{5+} ions. Ions of Cr^{3+} sublattice interact with ions of Mo^{5+} sublattice through the super exchange (SE) coupling J_{Cr-Mo}, which is a nearest neighbor (NN) interaction coupling involving 6 NN ions. The Hamiltonian hence, according to the Ising model, includes NN and NNN interactions terms and the term of energy related to the interaction with the external magnetic field:

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

$<i,j>$ denotes the NN and NNN spins at i and j sites. $S_i = \pm\frac{3}{2}, \pm\frac{1}{2}$ and $\sigma_i = \pm\frac{1}{2}$ are the respective spins of (Cr^{3+}, $3d^3$) and (Mo^{5+}, $4d^1$). N is the total number of ions in the whole system.

3. Monte Carlo simulation method

A MCS combined with a Metropolis algorithm has been performed in the framework of the Ising model above to predict the MCE in the DP Sr_2CrMoO_6. The system has been simulated as a cubic bulk with the size L = 64, which is larger than the thermodynamic limit determined previously at $L_{ThL} = 28$ for this class of materials [16–21]. Standard sampling method has been adopted to simulate the Hamiltonian given by Eq. (1). Cyclic boundary conditions have been imposed on the whole lattice and initial configurations has been randomly generated in a way Cr-spins $\pm\frac{3}{2}, \pm\frac{1}{2}$ are located randomly in i sites of the first sublattice, and Mo-spins$\pm\frac{1}{2}$ are located randomly in i sites of the second sublattice During the simulation, all sites in whole lattice are sequentially traversed at each MCS step and single-spin flips are attempted. A Metropolis algorithm enables to decide the acceptance or rejection of single spin flips. Data has been collected above an interval of MCS steps going from 1 to $3*10^6$ steps. The equilibrium has been reached after 1.810^5 steps, where averages of physical quantities have been computed. MCE is well known to be defined by the following physical quantities [25]:

Total magnetization per site is given by:

$$M = \frac{1}{N}\left\langle \sum_i S_i + \sum_i \sigma_i \right\rangle \quad (2)$$

Magnetic specific heat of Cr^{3+} and Mo^{5+} ions are given respectively by:

$$C_{Cr} = \frac{1}{K_BT}\left\{\left\langle E_{Cr}^2\right\rangle - \langle E_{Cr}\rangle^2\right\} \quad (3)$$

$$C_{Mo} = \frac{1}{K_BT}\left\{\left\langle E_{Mo}^2\right\rangle - \langle E_{Mo}\rangle^2\right\} \quad (4)$$

where, K_B is the Boltzmann's constant, T is the absolute temperature of the system and E is the internal energy per site defined as:

$$E = \frac{1}{N}\langle H\rangle \quad (5)$$

Thus, total Magnetic specific heat is given by:

$$C_M = \left\langle \frac{C_{Cr} + C_{Mo}}{2} \right\rangle \quad (6)$$

According to Debye model and Debye + Einstein model [26,27], total specific heat $C_{p,h}$ is composed of three terms; the first one is the electronic term, the second is the lattice term and the last one is the magnetic term. Thus, $C_{p,h}$ is given by:

Please cite this article in press as: O. El rhazouani, A. Slassi, Low field magnetocaloric effect in the double perovskite Sr_2CrMoO_6: Monte Carlo simulation, Computational Condensed Matter (2017), http://dx.doi.org/10.1016/j.cocom.2017.05.002