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Theoretical investigation of the magnetocaloric effect of $La_{0.7}(Ba, sr)_{0.3}MnO_3$ compound at room temperature with a second-order magnetic phase transition

R. Tlili[a,*], A. Omri[a,b], M. Bejar[a], E. Dhahri[a], E.K. Hlil[c]

[a]Laboratoire de Physique Appliquée, Faculté des Sciences de Sfax, B.P. 802, Université de Sfax, Sfax 3018, Tunisia
[b]Faculté des Sciences et Techniques de Sidi Bouzid, Université de Kairouan, Campus Cité Agricole 9100, Kairouan, Tunisia
[c]Institut Néel, CNRS et Université Joseph Fourier, BP 166, F-38042 Grenoble cedex 9, France

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Abstract

In this paper, the prediction of magnetic and magnetocaloric properties of $La_{0.7}(Sr,Ba)_{0.3}MnO_3$ (LSBMO) compound have been conducted using a phenomenological model. Indeed, the investigation of magnetic properties has revealed that the sample exhibits a paramagnetic to ferromagnetic phase transition. Interestingly, the Curie temperature (T_C) was found to decrease from 322 to 300 K with the decrease of magnetic fields. Moreover, the magnetocaloric data displays a large value of the magnetic entropy change, 1.5 J kg^{-1} K^{-1} under an applied magnetic field change of 20 kOe, which increases with the increase of the applied magnetic field, making it a promising compound for ecologically-friendly magnetic refrigeration at room temperature. Finally, the construction of the universal curve of the magnetic entropy change proves that the studied manganite undergoes a second order magnetic phase transition.

Keywords: Phenomenological model; Curie temperature; Magnetocaloric effect; Specific heat change; Universal curve

1. Introduction

In recent years, magnetic materials exhibiting the so-called magnetocaloric effect in the vicinity of room temperature have received much attention in view of their possible practical applications [1–3]. The magnetocaloric effect (MCE) is the working principle of the magnetic refrigeration technology, which is more energy efficient and environmentally friendly compared to the conventional vapor-compression-based refrigeration. At present, the magnetic refrigeration around room temperature is of particular interest owing to the potential impact not only on energy savings but also on the environment (the desire to eliminate the chlorofluorocarbons present in high-temperature gas-cycle systems). The key in using magnetic refrigeration at room temperature is to seek the proper material, whose Curie temperature is near room temperature, and which can produce a large entropy variation when it goes through a magnetization–demagnetization process [4,5]. The MCE of $La_{0.7}Sr_{0.3}MnO_3$ compound, which posses a $|\Delta S_{max}|$ of 3.84 J kg^{-1} K^{-1} at 346 K under a magnetic field of 13.5 kOe, has been reported earlier by N. Luong et al. [6]. In this context, the main objective of the present work is to tune the magnetocaloric effect to room temperature with the substitution of 50% of Sr by Ba.

In the current work, theoretical work on magnetization versus temperature for the $La_{0.7}(Sr,Ba)_{0.3}MnO_3$ compound at different magnetic fields is presented. A phenomenological model for the simulation of magnetization dependence on temperature variation is used to predict magnetocaloric properties such as magnetic entropy change, relative cooling power and heat capacity change.

*Corresponding author. Tel.: +21696589919; fax: +21674676609.
E-mail address: tliliriadh96@yahoo.fr (R. Tlili).

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2. Theoretical considerations

Based on a phenomenological model, described in [7], the dependence of magnetization on the variation of temperature is presented by:

$$M = \left(\frac{M_i - M_f}{2}\right) tanh[A(T_C - T)] + BT + C \quad (1)$$

where:

- M_i/M_f is an initial/final value of magnetization at ferromagnetic–paramagnetic transition as shown in Fig. 1;
- B is magnetization sensitivity (dM/dT) at ferromagnetic state before transition;
- $A = \frac{2(B - S_C)}{M_i - M_f}$;
- S_C is the magnetization sensitivity $\frac{dM}{dT}$ at Curie temperature T_C;
- $C = \left(\frac{M_i + M_f}{2}\right) - BT_C$.

The changes of entropy, which result from spin ordering, are induced by the variation ($\Delta(\mu_0 H)$) of the applied field from 0 to $\mu_0 H$. In order to evaluate the MCE, they can be calculated using the following expression [8]:

$$\Delta S_M = \left\{ -A\left(\frac{M_i - M_f}{2}\right) sech^2[A(T_C - T)] + B \right\} \mu_0 H_{max} \quad (2)$$

The finding of a large magnetic entropy change is accredited to high magnetic moment and rapid change of magnetization near T_C. A result of Eq. 2, which is a maximum magnetic entropy change ΔS_{max} (where $T = T_C$) can be evaluated by the following equation [9]:

$$\Delta S_{max} = \left[-A\left(\frac{M_i - M_f}{2}\right) + B \right] \mu_0 H_{max} \quad (3)$$

Eq. 3 is important because the value of the magnetic entropy change allows evaluating the magnetic cooling efficiency. The relative cooling power is the negative of the product of the maximum magnetic entropy change and the full-width at half-maxima (δT_{FWHM}) can be carried out as follows [8,9]:

$$\delta T_{FWHM} = \frac{2}{A} sech\left[\sqrt{\frac{2A(M_i - M_f)}{A(M_i - M_f) + 2B}}\right] \quad (4)$$

The most meaningful parameter that provides a measure of the effectiveness of magnetic materials for the applications in magnetic refrigeration is the relative cooling power (RCP) [10–12]. RCP is a measure of the quantity of heat transferred by the magnetic refrigerant in one ideal cycle and it is expressed as follows:

$$\begin{aligned} RCP &= -\delta T_{FWHM} \times \Delta S_{max}(T, \mu_0 H_{max}) \\ &= \left(M_i - M_f - 2\frac{B}{A}\right)\mu_0 H_{max} \\ &\quad \times sech\left[\sqrt{\frac{2A(M_i - M_f)}{A(M_i - M_f) + 2B}}\right] \end{aligned} \quad (5)$$

The change of specific heat associated with a magnetic field variation from zero to $\mu_0 H$ is given by [13–15]:

$$\begin{aligned} \Delta C_p(T, \mu_0 H) &= C_p(T, \mu_0 H) - C_p(T, 0) \\ &= T\frac{\partial[\Delta S_M(\mathrm{T},\ \mu_0 \mathrm{H})]}{\partial T} \end{aligned} \quad (6)$$

According to this model, $\Delta C_p(\mathrm{T},\ \mu_0 \mathrm{H})$ can be rewritten as

$$\Delta C_p(\mathrm{T},\ \mu_0\mathrm{H}) = -\mathrm{TA}^2(M_i - M_f) sech^2[A(T_C - T)] tanh[A(T_C - T)]\mu_0 H_{max} \quad (7)$$

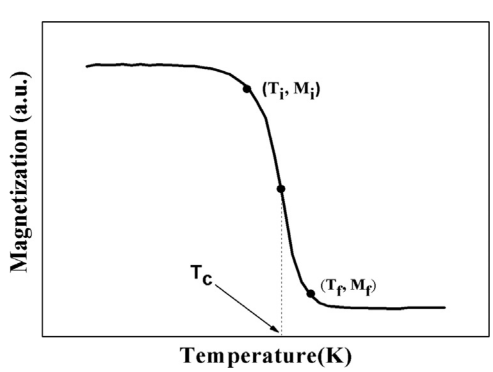

Fig. 1. Temperature dependence of magnetization for $La_{0.7}(Ba, Sr)_{0.3}MnO_3$ compound under constant applied field.

3. Simulation

In order to apply the proposed phenomenological model, numerical calculations were carried out with parameters as displayed in Table 1. Fig. 2 shows the temperature dependence of magnetization $M(T)$ in different applied magnetic fields for $La_{0.7}(Sr, Ba)_{0.3}MnO_3$ (LSBMO) compound. While the solid lines represent modeled data using model parameters given in Table 1, the symbols represent the experimental data. It is noteworthy to mention that there is a good agreement between the experimental and the calculated results. The $M(T)$ curves reveal that the LSBMO ($1 \le \mu_0 H \le 50$ kOe) sample exhibits a magnetic transition from ferromagnetic state to paramagnetic

Table 1
Model parameters for $La_{0.7}(Ba, Sr)_{0.3}MnO_3$ compound in different applied magnetic fields.

$\mu_0 H$ (kOe)	M_i (emu/g)	M_f (emu/g)	T_C (K)	B (emu g^{-1} K^{-1})	S_C (emu g^{-1} K^{-1})
1	30.5	8.48	300	−0.12	−0.93
5	32.17	12.82	303	−0.14	−0.72
10	34.36	13.63	309	−0.16	−0.62
20	36.86	12.13	315	−0.17	−0.54
30	37.61	17.76	313	−0.16	−0.45
40	38.15	18.68	318	−0.17	−0.41
50	38.43	19.56	322	−0.16	−0.41