

Magnetocaloric effect in the Laves phase pseudobinaries (Dy_{1-c}R_c)Al₂ (R = Er and Ho)

N.A. de Oliveira*, P.J. von Ranke

Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier 524, Rio de Janeiro 20550-013, RJ, Brazil

Received 29 March 2007

Available online 29 June 2007

Abstract

In this work we calculate the magnetocaloric effect in the Laves phase pseudobinaries (Dy_{1-c}Er_c)Al₂ and (Dy_{1-c}Ho_c)Al₂. We use a model Hamiltonian of interacting 4f-spins, including the crystalline electrical field interaction. The 4f spin–spin interaction is treated in an extended mean field approximation, in which the magnitude of the exchange interaction between 4f-spins depends on the type of rare earth ion is occupying the neighboring sites. The calculated isothermal entropy change and the adiabatic temperature change upon variations of the magnetic field are in good agreement with the available experimental data.

© 2007 Elsevier B.V. All rights reserved.

PACS: 75.30.Sg; 75.10.Dg; 75.20.En

Keywords: Magnetocaloric effect; Rare earth compounds; Spin Hamiltonians

1. Introduction

The magnetocaloric effect [1–5] is usually measured by the isothermal entropy change (ΔS) and by the adiabatic temperature change (ΔT_{ad}) under the application or removal of an external magnetic field. For usual ferromagnets, the magnetocaloric potentials ΔS and ΔT_{ad} usually exhibit maximum values around the magnetic ordering temperature and go smoothly to zero outside the region of the magnetic phase transition. For a given magnetic compound, the magnetic ordering temperature and consequently the temperature of the peak of the magnetocaloric potentials can be tuned either by applying pressure [6–8] or by doping the compound with suitable impurities [5,9,10]. A great deal of experimental works have been done in this direction and a lot of experimental data of the magnetocaloric potentials ΔS and ΔT_{ad} are available in the literature. However, the theoretical description of the magnetocaloric effect in rare earth

doped compounds is much more complex than the corresponding one in pure compounds. In order to theoretically discuss the magnetocaloric effect in doped rare earth compounds, let us separate them into two classes. In the first class of rare earth compounds doped with non-rare earth elements such as R(Al_{1-c}Ni_c)₂, the impurities play an important role in the magnetic ordering temperature, but they do not directly contribute to the magnetization. In this class of compounds, the theoretical description of the magnetocaloric effect can be done by using the conventional mean field theory because there is only one type of rare earth magnetic ions.

In the second class of rare earth compounds doped with another rare earth element such as (R_cR_{1-c})Al₂, the theoretical description is somewhat more complex. In such compounds the existence of more than one type of rare earth ions makes the theoretical description more difficult, because the internal molecular field depends on the environment of a given rare earth site. In the particular case of Er–Dy based compounds, the theoretical description [10] can be somewhat simplified because both Er and Dy have the same total angular momentum $J = \frac{15}{2}$.

*Corresponding author.

E-mail address: nilson@uerj.br (N.A. de Oliveira).

However, even in this case the crystalline electrical field is not properly described. In the general case, involving any type of rare earth element it is important to go beyond the conventional mean field theory to describe the neighborhood of the rare earth sites. Very recently, it has been developed a classical Monte Carlo calculations [11,12] to study the magnetocaloric effect in rare earth compounds described by a Hamiltonian of interacting spins. In that version of the classical Monte Carlo simulation a good description of the magnetocaloric effect in $R_5Si_2Ge_2$ ($R = Gd$ or Tb) and their alloys has been obtained. However, despite the good description of the experimental data, the classical Monte Carlo simulation has some intrinsic drawbacks: (i) It is not a quantum description, so that the crystalline electrical field interaction, sometimes so important in rare earth compounds, cannot be properly included in the calculations. (ii) It consumes much computer time. These points impose limitations to the use of the Monte Carlo simulations to other rare earth based compounds.

In this work we discuss the magnetocaloric effect in the Laves phase pseudobinaries $(Dy_{1-c}Er_c)Al_2$ and $(Dy_{1-c}Ho_c)Al_2$ by using a model of interacting 4f-spins, including the crystalline electrical field interaction. In the model, it is considered that the exchange interaction parameter between 4f-spins depends on the type of rare earth ion is occupying the neighborhood of a given site. The obtained results of specific heat and the magnetocaloric potentials ΔS and ΔT_{ad} are in good agreement with the available experimental data.

2. The method

In order to discuss the magnetocaloric effect in the compounds $(R^{\alpha}_{1-c}R^{\eta}_c)Al_2$ where R^{α} and R^{η} are rare earth elements, we start with the following Hamiltonian:

$$\mathcal{H} = - \sum_{il} \lambda_{il} \vec{J}_i^a \vec{J}_l^b - \sum_i g_i^a \mu_B \vec{H} \cdot \vec{J}_i^a + \sum_i \mathcal{H}_{(i)CF}^a \quad (1)$$

In this Hamiltonian the first term describes the spin–spin interaction between rare earth ions where λ_{il} is the exchange interaction parameter and $J_i^a(J_l^b)$ is the total angular momentum of rare earth ions where the labels $a = \alpha$ or η and $b = \alpha$ or η represent the two types of rare earth ions. The second term represents the Zeeman interaction between the rare earth momentum and the external magnetic field where (g^a) ($a = \alpha$ or η) is the Landé factor of the rare earth ion of a -type. The last term $\mathcal{H}_{(i)CF}^a$ describes the crystalline electrical field effect on the 4f multiplet of the rare earth ions of a -type. In the Lea Leask and Wolf notation [13], the crystalline electrical field for the cubic symmetry, has the form

$$\mathcal{H}_{(i)CF}^a = W_i^a \left[\frac{x}{F_4} (O_4^0 + 5O_4^4) + \frac{1 - |x|}{F_6} (O_6^0 - 21O_6^4) \right]^a \quad (2)$$

where O_n^m are the Stevens’ operators [14] and F_4 and F_6 are factors common to all the matrix elements. The parameter

W gives the crystal field energy scale and the parameter x gives the relative importance of the fourth and sixth order terms. The great difficult in dealing with the above Hamiltonian, is the presence of the disorder at rare earth sites. The usual mean field theory does not consider that the neighborhood of a given rare earth site is occupied by rare earth ions of different types. Here, we develop an alternative method, in which it is considered that the 4f spin–spin interaction depends on the type of rare earth ion is occupying the neighboring sites. We explicitly rewrite the Hamiltonian in Eq. (1) in the form

$$\begin{aligned} \mathcal{H} = & - \sum_{il} \lambda_{il}^{\alpha\alpha} \vec{J}_i^{\alpha} \vec{J}_l^{\alpha} - \sum_{il} \lambda_{il}^{\eta\eta} \vec{J}_i^{\eta} \vec{J}_l^{\eta} - \sum_{il} \lambda_{il}^{\alpha\eta} \vec{J}_i^{\alpha} \vec{J}_l^{\eta} \\ & - \sum_{il} \lambda_{il}^{\eta\alpha} \vec{J}_i^{\eta} \vec{J}_l^{\alpha} - g^{\alpha} \sum_i \mu_B \vec{H} \cdot \vec{J}_i^{\alpha} - g^{\eta} \sum_i \mu_B \vec{H} \cdot \vec{J}_i^{\eta} \\ & + \sum_i \mathcal{H}_{(i)CF}^{\alpha} + \sum_i \mathcal{H}_{(i)CF}^{\eta} \end{aligned} \quad (3)$$

In this Hamiltonian, the first term involves interaction only between rare earth ions R^{α} with exchange interaction parameter $\lambda_{il}^{\alpha\alpha}$, whereas the second term involves interaction only between rare earth ions R^{η} with exchange interaction parameter $\lambda_{il}^{\eta\eta}$. The third and fourth terms involve interaction between rare earth ions of different type, with exchange interaction parameter $\lambda_{il}^{\alpha\eta}$ and $\lambda_{il}^{\eta\alpha}$, respectively. We can write the above Hamiltonian as a sum of two coupled Hamiltonians, i.e.,

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2, \quad (4)$$

where

$$\begin{aligned} \mathcal{H}_1 = & - \sum_{il} \lambda_{il}^{\alpha\alpha} \vec{J}_i^{\alpha} \vec{J}_l^{\alpha} - \sum_{il} \lambda_{il}^{\eta\eta} \vec{J}_i^{\eta} \vec{J}_l^{\eta} - g^{\alpha} \sum_i \mu_B \vec{H} \cdot \vec{J}_i^{\alpha} \\ & + \sum_i \mathcal{H}_{(i)CF}^{\alpha}, \end{aligned} \quad (5)$$

$$\begin{aligned} \mathcal{H}_2 = & - \sum_{il} \lambda_{il}^{\alpha\eta} \vec{J}_i^{\alpha} \vec{J}_l^{\eta} - \sum_{il} \lambda_{il}^{\eta\alpha} \vec{J}_i^{\eta} \vec{J}_l^{\alpha} - g^{\eta} \sum_i \mu_B \vec{H} \cdot \vec{J}_i^{\eta} \\ & + \sum_i \mathcal{H}_{(i)CF}^{\eta}. \end{aligned} \quad (6)$$

Taking the mean field approximation for the spin–spin interaction, and using $\sum_l \langle \vec{J}_l^{\alpha} \rangle = Z_{\alpha\alpha} \langle \vec{J}^{\alpha} \rangle$ and $\sum_l \langle \vec{J}_l^{\eta} \rangle = Z_{\alpha\eta} \langle \vec{J}^{\eta} \rangle$ we get

$$\begin{aligned} \mathcal{H}_1 = & - \sum_i [\lambda^{\alpha\alpha} Z_{\alpha\alpha} \langle \vec{J}^{\alpha} \rangle - \lambda^{\alpha\eta} Z_{\alpha\eta} \langle \vec{J}^{\eta} \rangle - g^{\alpha} \mu_B \vec{H}] \vec{J}_i^{\alpha} \\ & + \sum_i \mathcal{H}_{(i)CF}^{\alpha}, \end{aligned} \quad (7)$$

where $Z_{\alpha\alpha}$ and $Z_{\alpha\eta}$ are the numbers of the nearest neighboring sites occupied by rare earth ions R^{α} and R^{η} , respectively. The Hamiltonian (\mathcal{H}_1) describes a sublattice of rare earth ions R^{α} under the action of effective molecular fields $\langle J^{\alpha} \rangle$ and $\langle J^{\eta} \rangle$ generated by the ions R^{α} and R^{η} in the neighborhood of a given site. A similar relation holds for

Download English Version:

<https://daneshyari.com/en/article/1804014>

Download Persian Version:

<https://daneshyari.com/article/1804014>

[Daneshyari.com](https://daneshyari.com)