

Magnetocaloric effect in $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ by Monte Carlo simulationsE. P. Nobrega,¹ N. A. de Oliveira,² P. J. von Ranke,² and A. Troper^{1,2}¹*Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, Rio de Janeiro 22290-180, RJ, Brazil*²*Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier 524, Rio de Janeiro 20550-013, RJ, Brazil*

(Received 24 April 2006; revised manuscript received 31 August 2006; published 27 October 2006)

In this work, we calculate the magnetocaloric effect in the series of compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$. We use the classical Monte Carlo simulation to deal with the $4f$ spin-spin interaction as well as the disorder at the rare-earth 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.

DOI: [10.1103/PhysRevB.74.144429](https://doi.org/10.1103/PhysRevB.74.144429)

PACS number(s): 75.30.Sg, 75.10.Dg, 75.20.En

I. INTRODUCTION

The magnetocaloric effect in rare-earth metals and their alloys has been intensively studied in the literature.¹⁻⁵ The series of compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ for $x \leq 0.5$ undergo first order transition from the ferromagnetic to the paramagnetic phase, together with a crystallographic transition from the orthorhombic phase (temperature below T_c) to the monoclinic one (temperature above T_c). In the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ with $x \leq 0.5$, the isothermal entropy changes upon magnetic field variation around the magnetic ordering temperature⁶⁻⁹ are very large as compared with that observed for metallic gadolinium. For $x > 0.5$ the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ always exhibit the orthorhombic phase and undergo a second order magnetic phase transition. The isothermal entropy changes (ΔS) upon magnetic field variation in the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ for $x > 0.5$ are comparable with the one found in metallic gadolinium. The structural, magnetic, and thermodynamical properties in the series of compounds¹⁰ $\text{Tb}_5(\text{Si}_x\text{Ge}_{1-x})_4$ are very similar to those observed in the series of compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$. In the doped compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ the orthorhombic phase and the second order magnetic phase transition occur in the whole range of Gd concentration. The magnetic ordering temperature in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ decreases from 336 K in Gd_5Si_4 to 225 K in Tb_5Si_4 . The magnetocaloric effect in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ has been experimentally studied¹¹ and experimental data of the isothermal entropy change (ΔS) and the adiabatic temperature change (ΔT_{ad}) upon magnetic field variations, as a function of Gd concentration, are available.

Despite the great deal of theoretical papers found in the literature, the theoretical description of the magnetocaloric effect in doped rare-earth compounds with disorder at the rare-earth sites has not yet been properly addressed. In order to calculate the magnetocaloric effect in rare-earth doped compounds such as $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$, which involve two types of rare-earth ions, we should go beyond the conventional molecular field theory. This is because the molecular field theory replaces the $4f$ spin-spin interaction by an interaction of the local spin with a mean field generated by the first nearest neighbors. Thus in the usual treatment of the $4f$ spin-spin interaction within the molecular field theory neither short range interactions, which are very important near the magnetic phase transition, nor the possibility of having

neighboring sites occupied by different types of rare-earth ions are considered. Very recently, we have used the classical Monte Carlo simulation^{12,13} to calculate the magnetocaloric effect in rare-earth compounds with only one type of rare-earth ions. In those papers, our results show that the Monte Carlo simulations explain quite well the experimental data of the magnetocaloric quantities ΔS and ΔT_{ad} . Moreover, the Monte Carlo calculations provides a good description of the specific heat capacity, even around the magnetic ordering temperature where the molecular field theory does not work well.

In the present work, we discuss the magnetic and thermodynamics properties as well as the magnetocaloric effect in the doped rare-earth compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$, which involve more than one type of rare-earth ions. In the particular case of such compounds the $4f$ spin-spin interaction should be treated beyond the conventional molecular field theory. Here, we use the classical Monte Carlo simulations^{14,15} where the occupation of a given rare-earth site by a Gd or Tb ion is randomly determined according to the Gd concentration. In order to calculate the energy of the system, we use a model of $4f$ -interacting spins and consider the z components of total angular momentum as quantum quantities, which can assume discrete values in the interval $-J \leq J^z \leq J$. For a given J^z , the transverse components J^x and J^y were randomly chosen under the condition $(J^x)^2 + (J^y)^2 = J^2 - (J^z)^2$. Within this approach we restrict the number of available states so that the upper limit of the magnetic entropy $S_{mag} = R \ln(2J+1)$ is reproduced, where R is the gas constant. In order to calculate the magnetocaloric quantities, i.e., the isothermal entropy change (ΔS) and the adiabatic temperature change (ΔT_{ad}) upon variation of the magnetic field, we take the electronic part of the entropy proportional to the temperature and consider the crystalline lattice entropy in the Debye approximation. The calculated magnetocaloric quantities ΔS and ΔT_{ad} for the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ are in good agreement with the available experimental data.¹¹

II. THE METHOD

In order to calculate the magnetocaloric effect in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$, on the basis of Monte Carlo calculations, we start with the following energy:

$$E = - \sum_{il} \lambda_{il} \vec{J}_i^\alpha \vec{J}_l^\delta + \sum_i \zeta_i (\vec{r}_i \cdot \vec{J}_i^\alpha)^2 - \sum_i g \mu_B \vec{J}_i^\alpha \vec{H}, \quad (1)$$

where λ_{il} is the effective exchange interaction parameter, J_i^α (\vec{J}_i^δ) ($\alpha, \delta = \text{Gd or Tb}$) is the total angular momentum of rare-earth ions, and H is the applied magnetic field. The term $\zeta_i (\vec{r}_i \cdot \vec{J}_i^\alpha)^2$ represents the single ion anisotropy, where \vec{r}_i is the direction of the anisotropy and ζ_i is the anisotropic coefficient. The anisotropic term $\zeta_i (\vec{r}_i \cdot \vec{J}_i^\alpha)^2$ accounts for a reduction of the magnitude of the magnetization. In rare-earth systems the reduction in magnetic moment (quenching effect) is mainly due to the crystalline electric field (CEF) interaction. For rare-earth ions, the proper crystalline electric field interaction is described by higher order terms (fourth and sixth order terms) in angular momentum operators—Stevens Operators. Nevertheless, the inclusion of the proper CEF Hamiltonian together with the exchange and Zeeman interactions leads to a complex problem, which is in general solved in the conventional mean field approximation. In our Monte Carlo calculations, a simplification has to be introduced, since the quantization was performed only in the z component of the spin operator. It should be mentioned that the term $\zeta_i (\vec{r}_i \cdot \vec{J}_i^\alpha)^2$ does not reproduce the CEF anisotropy (such as the easy magnetic direction) as a proper CEF Hamiltonian. Nevertheless, the quenching effect can be controlled by our anisotropic second order term, which somehow mimics the crystalline electric field effect.

For a given temperature, the Monte Carlo method calculates the mean energy given in Eq. (1) by simulating different configurations of total angular momentum. Here we give a very brief description of the method: First we generate an orthorhombic unit cell containing Gd and Tb ions randomly distributed according to the Gd concentration. Then, we generate an initial configuration of total angular momentum, by drawing random numbers to establish the values of the components of the corresponding total angular momentum at each lattice site, taking into account if the site is occupied by Gd or Tb ions. We calculate the energy for this initial configuration (E_I) according to Eq. (1). We choose one particular site, whose occupancy (Gd or Tb) has already been determined, to change the values of the components of the corresponding total angular momentum. The components of the total angular momentum of the remaining ions into the crystalline lattice are kept unchanged. Then, we calculate the mean energy for this new configuration of total angular momentum (E_F) through Eq. (1). If $E_F < E_I$ the change in the components of the total angular momentum at the chosen site is accepted. If $E_F > E_I$, we calculate the probability factor $p = e^{-\beta(E_F - E_I)}$ and draw a random number r between 0 and 1. If $r < p$ the new configuration of total angular momentum is accepted. Otherwise, it is rejected and the initial configuration with energy E_I is preserved. Then, we move to the next site and repeat the entire process described before, until we sweep all N_S sites of the crystalline lattice. In the Monte Carlo method, the mean value of the energy $\langle E \rangle$ is obtained by

$$\langle E \rangle = \frac{1}{(N_c - N_0)} \sum_{i > N_0}^{N_c} E_i, \quad (2)$$

where “ i ” represents a given Monte Carlo step, N_c represents the total number of Monte Carlo steps, and N_0 is the number of Monte Carlo steps used for thermalization. A similar relation holds for the mean square energy $\langle E^2 \rangle$. The magnetic part of the heat capacity is calculated by

$$C_{\text{mag}}(T, H) = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}, \quad (3)$$

where k_B is the Boltzmann constant. The total heat capacity is given by $C = C_{\text{el}} + C_{\text{lat}} + C_{\text{mag}}$. Here $C_{\text{el}} = \gamma T$ is the contribution from the conduction electrons where γ is the Sommerfeld coefficient. C_{lat} is the contribution from the crystalline lattice, which in the Debye approximation is given by

$$C_{\text{lat}}(T) = 9RN_i \left[4 \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} \frac{x^3}{(e^x - 1)} dx - \frac{\Theta_D}{T} \frac{1}{(e^{\Theta_D/T} - 1)} \right], \quad (4)$$

where N_i is the number of ions per formula unit R is the gas constant, and Θ_D is the Debye temperature. The total entropy of the compound is given by $S = S_{\text{el}} + S_{\text{lat}} + S_{\text{mag}}$, where $S_{\text{el}} = \gamma T$ is the contribution from the conduction electrons. S_{mag} is the contribution from the magnetic ions calculated from

$$S_{\text{mag}}(T, H) = \int_0^T \frac{C_{\text{mag}}(T, H)}{T} dT. \quad (5)$$

S_{lat} is the lattice contribution, which in the Debye approximation is given by

$$S_{\text{lat}}(T) = N_i \left[-3R \ln(1 - e^{-\Theta_D/T}) + 12R \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} \frac{x^3}{e^x - 1} dx \right]. \quad (6)$$

The isothermal entropy change (ΔS) and the adiabatic temperature change (ΔT_{ad}) upon magnetic field variation are calculated respectively from $\Delta S = S(T, H \neq 0) - S(T, H = 0)$ and $\Delta T_{ad} = T_2 - T_1$ under the adiabatic condition $S(T_2, H \neq 0) = S(T_1, H = 0)$.

III. RESULTS AND DISCUSSION

Now, we present our theoretical Monte Carlo calculations of the magnetocaloric effect in the series of compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$. The Landé factor and the total angular momentum were taken as $g=2$ and $J=7/2$ for Gd ions and $g=1.5$ and $J=6$ for Tb ions. We use a tridimensional cluster of $6 \times 6 \times 6$ orthorhombic unit cells with eight rare-earth ions (Gd or Tb) per cell, randomly distributed at the lattice sites, according to the Gd concentration. In order to establish the magnitude of the z components of the total angular momentum of the Gd and Tb ions at each lattice site we draw a

random number r such that $0 \leq r \leq 1$ and fix the value of J^z according to the following condition: if $(n-1)/(2J+1) < r \leq n/(2J+1)$ we take $J^z = -J + (n-1)$, where n is an integer number in the range $n=1, 2, \dots, (2J+1)$. The transverse components J^x and J^y were randomly established under the condition $(J^x)^2 + (J^y)^2 = J^2 - (J^z)^2$. The exchange interaction parameters λ_{ij} depend on the lattice parameters and on the type of ions occupying the neighboring sites. Therefore, it should depend on Gd concentration, since the lattice parameters in $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ get larger with increasing Gd concentration.¹¹ In a more rigorous treatment, the exchange interaction parameter should be self-consistently calculated in terms of the electronic structure of the compound. Here, for the sake of simplicity, we choose the exchange interaction parameter in order to adjust the experimental data of the magnetic ordering temperature. The exchange interaction parameters between Gd ions in the compound Gd_5Si_4 and between Tb ions in the compound Tb_5Si_4 were taken $\lambda_{\text{Gd-Gd}} = 1.189$ meV and $\lambda_{\text{Tb-Tb}} = 0.294$ meV. For the compound $(\text{Gd}_{0.9}\text{Tb}_{0.1})_5\text{Si}_4$ we take ($\lambda_{\text{Gd-Gd}} = 1.242$ meV, $\lambda_{\text{Tb-Tb}} = 0.284$ meV, and $\lambda_{\text{Gd-Tb}} = 0.41$ meV); for the compound $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ we take ($\lambda_{\text{Gd-Gd}} = 1.339$ meV, $\lambda_{\text{Tb-Tb}} = 0.284$ meV, and $\lambda_{\text{Gd-Tb}} = 0.41$ meV) and for the compound $(\text{Gd}_{0.5}\text{Tb}_{0.5})_5\text{Si}_4$ we take ($\lambda_{\text{Gd-Gd}} = 1.430$ meV, $\lambda_{\text{Tb-Tb}} = 0.294$ meV, and $\lambda_{\text{Gd-Tb}} = 0.41$ meV). Notice that the values of the exchange interaction parameters ($\lambda_{\text{Gd-Gd}}$, $\lambda_{\text{Gd-Tb}}$, and $\lambda_{\text{Tb-Tb}}$) in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ take into account the increase of the distance between Gd and Gd ions, Gd and Tb ions, and Tb and Tb ions, with increasing Gd concentration.¹¹ The anisotropic coefficients ζ for Gd and Tb ions in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ were taken respectively as $\zeta_{\text{Gd}} = 0.00$ meV and $\zeta_{\text{Tb}} = 0.0294$ meV for the whole range of Gd concentration. These values have been chosen in order to yield a very small reduction in the contribution from Tb ions to the total magnetization of the compound. The numerical simulation was performed using 4000 Monte Carlo steps for thermalization of the system and 3000 Monte Carlo steps to compute the average values of the physical quantities. In order to calculate the total specific heat capacity and total entropy, we use $\gamma = 5.4$ mJ/(mol K²) and $\Theta_D = 350$ K, which are consistent with the usual values found in the literature. Within these parameters we calculate the magnetization, the specific heat capacity and the magnetocaloric effect in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ for several values of Gd concentration.

In Fig. 1, we plot the total specific heat capacity for the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$, calculated in the absence of an external magnetic field. We can observe that our theoretical calculations, in which the magnetic part was calculated within the Monte Carlo simulation, are in good agreement with the available experimental data.¹¹ Moreover, we should emphasize that the present results obtained for the pure compounds Tb_5Si_4 and Gd_5Si_4 within the Monte Carlo calculations are better than the mean field ones, not shown in this paper, mainly around the magnetic ordering temperature where the mean field results do not agree with experiments. In Fig. 2, we plot the total specific heat capacity for the compound $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ in the absence of an external magnetic field (solid line) and for an applied magnetic field

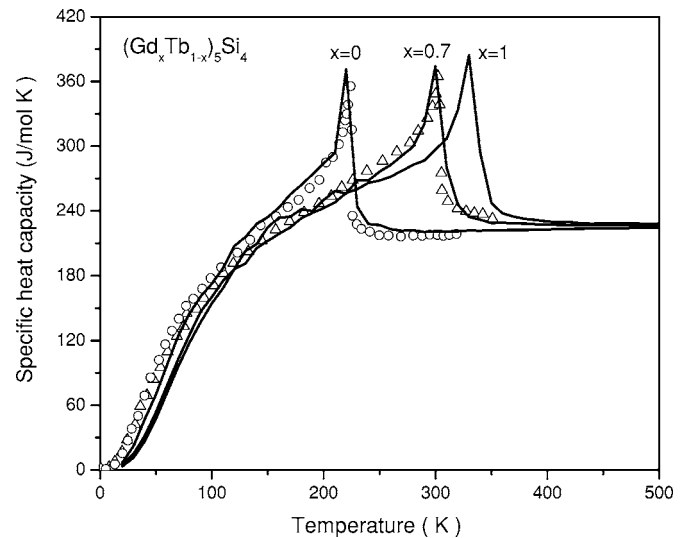


FIG. 1. Total specific heat capacity of $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ in the absence of an external magnetic field. Solid lines are the theoretical calculations whereas open circles and triangles are experimental data¹¹ for $x=0$ and $x=0.7$, respectively.

of 5 T (dashed line). From this figure we can also observe a good agreement between our theoretical calculations and the experimental data both for $H=0$ and $H=5$ T.¹¹ It is worth mentioning here that the experimental data of the specific heat for $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ could not be properly described by the conventional mean field theory, even far from the magnetic ordering temperature, because it does not consider the chemical disorder at the rare-earth sites. In Fig. 3, we plot the magnetic entropy for the compound $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ for $H=0$ (solid line), $H=5$ T (dotted line), and $H=7.5$ T (dashed line). Our theoretical calculations predict that the magnetic entropy in the compound $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ saturates around 88 (J/mol K). In Figs. 4 and 5 we plot the isothermal en-

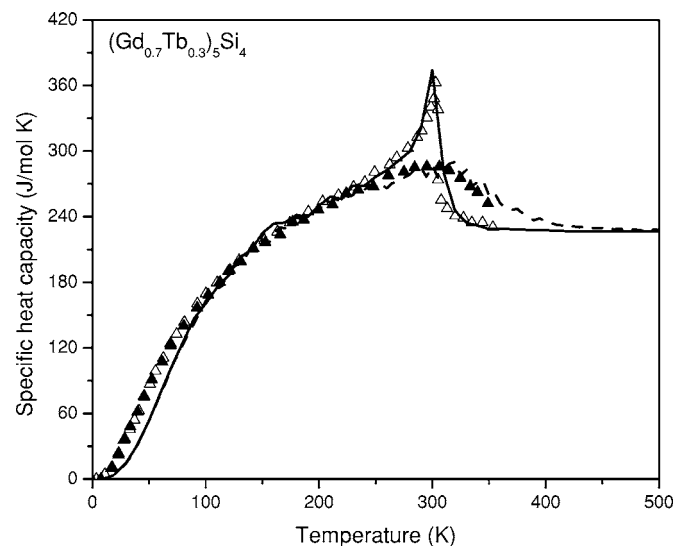


FIG. 2. Total specific heat capacity of $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$. Solid and dashed lines correspond to theoretical calculations for $H=0$ and $H=5$ T, respectively. Open and solid triangles are the corresponding experimental data.¹¹

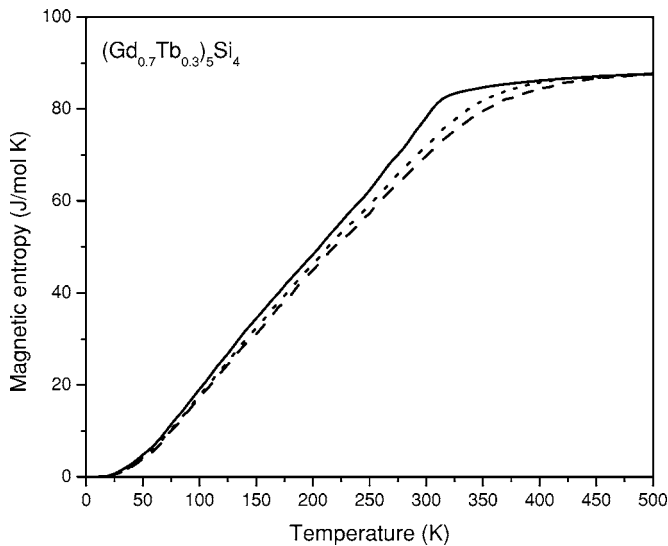


FIG. 3. Magnetic entropy of $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$. Solid, dotted, and dashed lines correspond to the theoretical calculations for $H=0$, $H=5$ T, and $H=7.5$ T, respectively.

entropy change and the adiabatic temperature change for the compound $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ upon magnetic field variation from 0 to 2 T, from 0 to 5 T, and from 0 to 7.5 T. From these figures, we can notice a good agreement with the Monte Carlo calculations and the experimental data.¹¹ Again we should stress that the experimental data of the magnetocaloric quantities ΔS and ΔT_{ad} for $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ could not be properly described by the conventional molecular field theory, because it does not consider the chemical disorder at the rare-earth sites.

In Fig. 6, we plot the magnetic entropy for the compound $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ ($x=0, 0.5, 0.9$, and 1.0) calculated in the absence of an applied magnetic field. From this figure we can

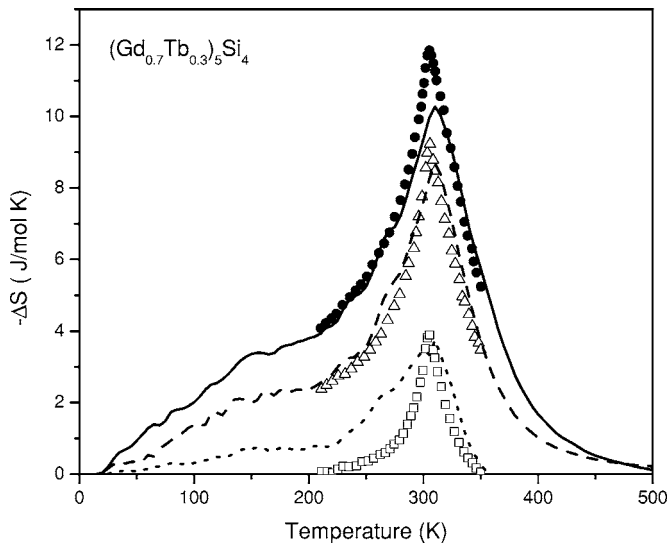


FIG. 4. Calculated isothermal entropy change for $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ upon magnetic field variations from 0 to 2 T (dotted line), from 0 to 5 T (dashed line), and from 0 to 7.5 T (solid line). Open squares, open triangles, and solid circles are the corresponding experimental data.¹¹

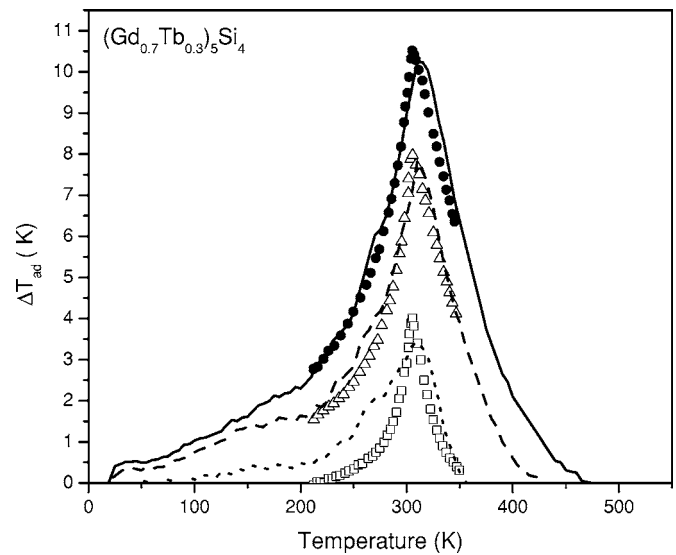


FIG. 5. Calculated adiabatic temperature change for $(\text{Gd}_{0.7}\text{Tb}_{0.3})_5\text{Si}_4$ upon magnetic field variations from 0 to 2 T (dotted line), from 0 to 5 T (dashed line), and from 0 to 7.5 T (solid line). Open squares, open triangles, and solid circles are the corresponding experimental data.¹¹

observe that the magnetic entropy in the compounds Gd_5Si_4 and Tb_5Si_4 saturates around 83 (J/mol K) and 103 (J/mol K) respectively. These values are consistent with the expected value given by $S_{\text{mag}}=R \ln(2J+1)$ per rare-earth ions. Our theoretical calculations show that for intermediate concentrations, the saturation values of the magnetic entropy in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ lie between the values obtained for the extreme limits of Tb_5Si_4 ($x=0$) and Gd_5Si_4 ($x=1.0$). It is worth mentioning that the saturation values of the magnetic entropy in the series of compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ for intermediate concentrations, which are automatically obtained by the numerical Monte Carlo calculations, are our theoretical prediction and need experimental data to be con-

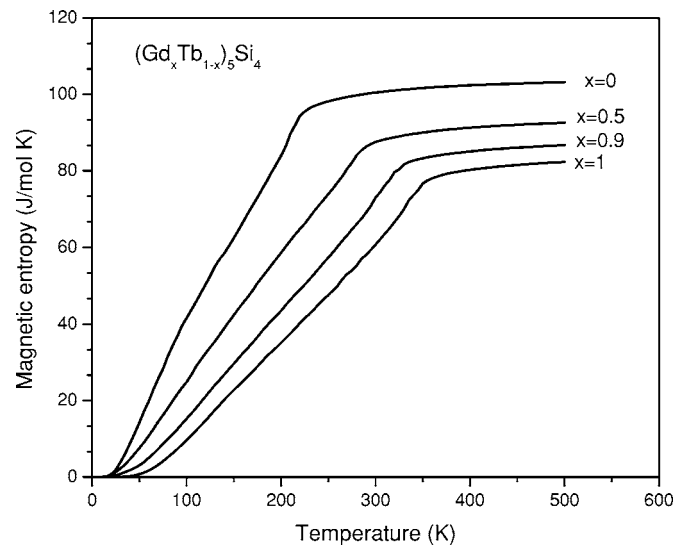


FIG. 6. Theoretically calculated magnetic entropy of $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ in the absence of an external magnetic field.

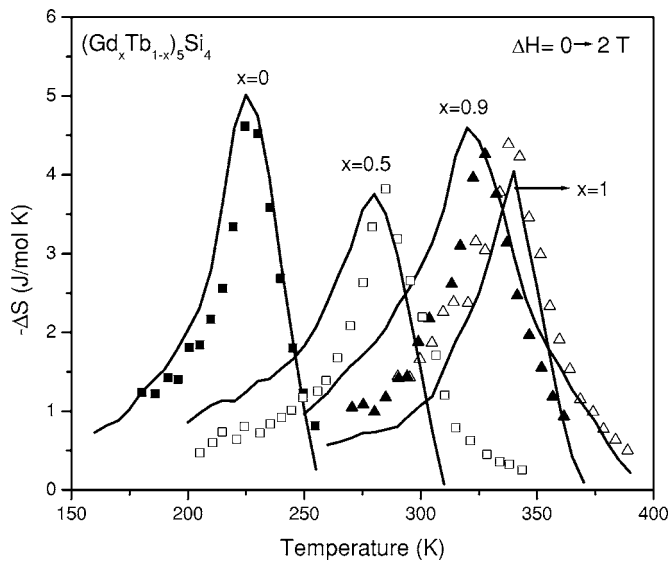


FIG. 7. Isothermal entropy change for $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ upon magnetic field variation from 0 to 2 T. The solid lines correspond to our calculations within the Monte Carlo simulation. Solid squares, open squares, solid triangles, and open triangles are the experimental data¹¹ for $x=0$, $x=0.5$, $x=0.9$, and $x=1.0$, respectively.

firmed. From the curves of the total entropy versus temperature for $H=0$, $H=2\text{T}$, and $H=5\text{T}$, not shown in this paper, we calculated both the isothermal entropy change and the adiabatic temperature change upon magnetic field variations from 0 to 2 T and from 0 to 5 T. The calculated isothermal entropy changes in the compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ ($x=0, 0.5, 0.9$, and 1.0) upon magnetic field variations from 0 to 2 T and from 0 to 5 T are shown in Figs. 7 and 8, respectively. From these figures, we can observe an overall agreement between our theoretical calculations and the experimental

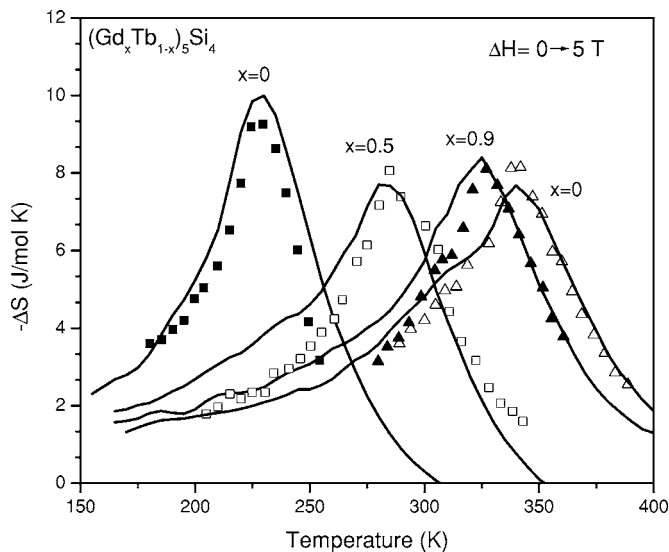


FIG. 8. Isothermal entropy change for $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ upon magnetic field variation from 0 to 5 T. The solid lines correspond to our calculations within the Monte Carlo simulation. Solid squares, open squares, solid triangles, and open triangles are the experimental data¹¹ for $x=0$, $x=0.5$, $x=0.9$, and $x=1.0$, respectively.

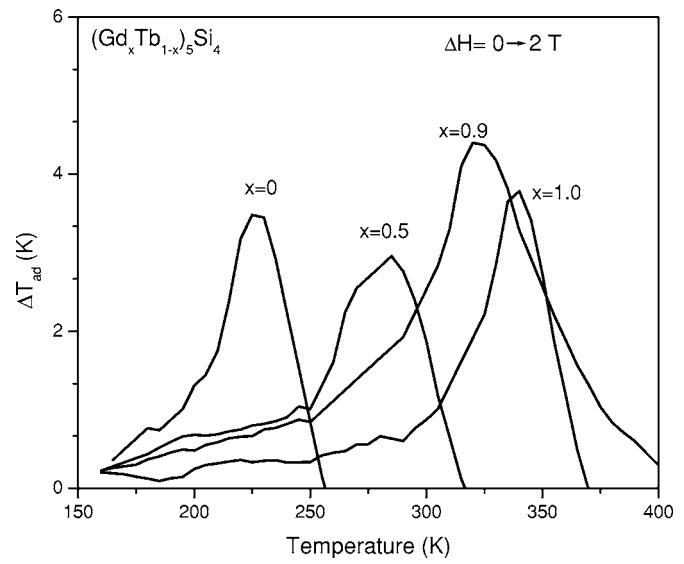


FIG. 9. Adiabatic temperature change for $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ upon magnetic field variation from 0 to 2 T. The solid lines correspond to our calculations within the Monte Carlo simulation.

data.¹¹ Some discrepancies between theory and experiments observed in these figures can be ascribed to the numerical fluctuations inherent to the Monte Carlo method. The corresponding adiabatic temperature changes upon the same magnetic field variations are shown in Figs. 9 and 10, respectively. Notice the good agreement between our calculations and the available experimental data for $x=1$. In order to check our theoretical calculations of the adiabatic temperature change as a function of Gd concentration further experiments are necessary.

In conclusion, in this work we report on the theoretical calculations of the magnetocaloric effect in the doped compounds $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ using a model of localized $4f$ spins,

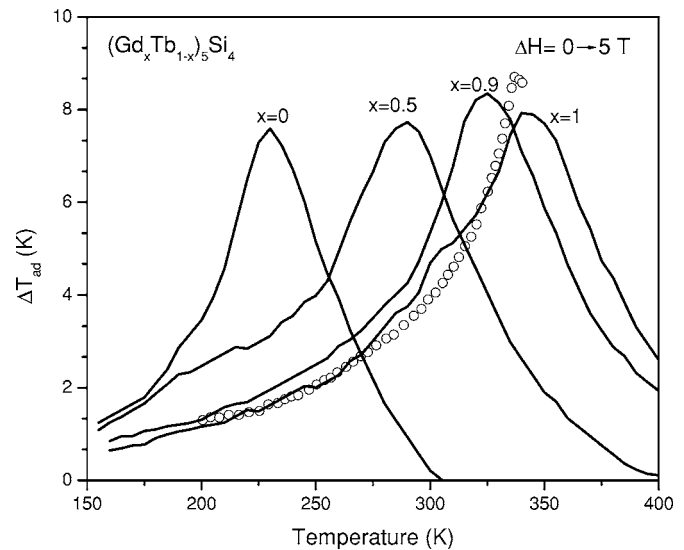


FIG. 10. Adiabatic temperature change for $(\text{Gd}_x\text{Tb}_{1-x})_5\text{Si}_4$ upon magnetic field variation from 0 to 5 T. The solid lines correspond to our calculations within the Monte Carlo simulation. Open circles are the experimental data (Ref. 11) for $x=1.0$.

where the $4f$ spin-spin interaction was treated in the Monte Carlo simulation. The theoretically calculated magnetocaloric quantities ΔS and ΔT_{ad} are in good agreement with the available experimental data.¹¹ It should be emphasized that, unlike the conventional molecular field theory, which does not consider disorder at the rare-earth sites, the present Monte Carlo calculations provide a proper description of the magnetic and thermodynamic properties as well as the magnetocaloric effect in rare-earth doped compounds involving more than one type of rare-earth ion. The present Monte

Carlo calculations can also be used for calculating the magnetocaloric properties of others doped rare-earth compounds undergoing a second-order magnetic phase transition.

ACKNOWLEDGMENTS

We acknowledge partial financial support from the Brazilian agencies CNPq and FAPERJ. This work was also financed by PRONEX No. E-26/171.168/2003.

-
- ¹K. A. Gschneidner, Jr. and V. K. Pecharsky, *Annu. Rev. Mater. Sci.* **30**, 387 (2000).
- ²V. K. Pecharsky and K. A. Gschneidner, Jr., in *Intermetallic Compounds for Magnetic Refrigeration in Intermetallic Compounds—Principles and Practice*, edited by J. H. Westbrook and R. L. Fleischer (Wiley, New York, 2002), Vol. 3, Chap. 25.
- ³A. M. Tishin, *Handbook of Magnetic Materials* (North-Holland, Amsterdam, 1999), Vol. 12, pp. 395–524.
- ⁴A. M. Tishin and Y. I. Spichkin, *The Magnetocaloric Effect and Its Applications*, 1st ed. (Institute of Physics, Bristol and Philadelphia, 2003).
- ⁵K. A. Gschneidner, Jr., V. K. Pecharsky, and A. O. Tsokol, *Rep. Prog. Phys.* **68**, 1479 (2005).
- ⁶V. K. Pecharsky and K. A. Gschneidner, Jr., *Phys. Rev. Lett.* **78**, 4494 (1997).
- ⁷V. K. Pecharsky and K. A. Gschneidner, Jr., *J. Magn. Magn. Mater.* **167**, L179 (1997).
- ⁸V. K. Pecharsky and K. A. Gschneidner, Jr., *Appl. Phys. Lett.* **70**, 3299 (1997).
- ⁹W. Choe, V. K. Pecharsky, A. O. Pecharsky, K. A. Gschneidner, Jr., V. G. Young, and G. J. Miller, *Phys. Rev. Lett.* **84**, 4617 (2000).
- ¹⁰L. Morellon, P. A. Algarabel, M. R. Ibarra, J. Blasco, B. Garcia-Landa, Z. Arnold, and F. Albertini, *Phys. Rev. B* **58**, R14721 (1998).
- ¹¹Y. I. Spichkin, V. K. Pecharsky, and K. A. Gschneidner, Jr., *J. Appl. Phys.* **89**, 1738 (2001).
- ¹²E. P. Nóbrega, N. A. de Oliveira, P. J. von Ranke, and A. Troper, *Phys. Rev. B* **72**, 134426 (2005).
- ¹³E. P. Nóbrega, N. A. de Oliveira, P. J. von Ranke, and A. Troper, *J. Phys.: Condens. Matter* **18**, 1275 (2006).
- ¹⁴D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge University Press, Cambridge, UK, 2000).
- ¹⁵M. E. J. Newman and G. T. Barkenma, *Monte Carlo Methods in Statistical Physics* (Clarendon Press, Oxford, 1999).