

Monte Carlo calculations of the magnetocaloric effect in $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ compounds

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In this work, we use the Monte Carlo method to calculate the magnetocaloric effect in the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ for $x > 0.5$, where the magnetic phase transition is of second order. The isothermal entropy change and the adiabatic temperature change upon magnetic field variations are in good agreement with the available experimental data.

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I. INTRODUCTION

The magnetocaloric effect,¹⁻⁴ the ability of magnetic materials to heat up or cool down when placed in or removed from an external magnetic field, has great importance in the technology of magnetic refrigeration. The magnetocaloric effect in the series $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ has been experimentally studied in the whole range of concentrations.⁵⁻¹³ The phase diagram² shows that for $x > 0.5$ the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ have an orthorhombic phase and undergo a second order magnetic phase transition. In this range of concentrations, the isothermal entropy change (ΔS) and the adiabatic temperature change (ΔT_{ad}) upon magnetic field variations for the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ are comparable with the ones observed in pure gadolinium. For $x < 0.5$, the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ undergo a first order magnetic phase transition coupled with a crystallographic transformation from the orthorhombic to the monoclinic phase. As a result, the isothermal entropy changes upon magnetic field variations for the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ with $x < 0.5$, reach large values around the magnetic ordering temperature (T_C). For instance,⁵ around T_C , the peak in the isothermal entropy change for a magnetic field variation from 0 to 5 T in the compound $\text{Gd}_5\text{Si}_2\text{Ge}_2$ is about 20 J/(kg K).

Until recently, the theoretical descriptions¹⁴⁻²³ of the magnetocaloric effect in rare earth based compounds have been done by using a Heisenberg-like model Hamiltonian in which the spin-spin interaction is treated in the molecular field approximation. Within this framework, much of the experimental data of the magnetocaloric effect in rare earth based compounds has been explained. Despite the good description of the magnetocaloric quantities, the molecular field approach does not explain the experimental data of the magnetic part of the specific heat around the magnetic ordering temperature. At T_C , the magnetic specific heat calculated within the molecular field approximation goes abruptly to zero in disagreement with experimental data. This discrepancy between theory and experiment, which occurs because the molecular field theory does not take into account short range interactions, points out that we should go beyond the mean field approximation to understand the real physical mechanisms involved in the magnetocaloric effect in rare earth based compounds. In this work, we use the classical Monte Carlo simulation to calculate the magnetocaloric ef-

fect in the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$. We consider here, only the compounds within the concentration range $x > 0.5$ where there is only the orthorhombic phase and the magnetic phase transition is of second order. For compounds within the concentration range $x < 0.5$, where the magnetic phase transition is of the first order, we should consider the crystallographic transformation from the orthorhombic to monoclinic phase around the magnetic ordering temperature. Besides, we also should consider the magnetoelastic interaction. These considerations are somewhat more complex and are not in the scope of the present work. This paper is organized as follows. In Sec. II, we present the theory and we summarize the adopted Monte Carlo procedure as well as some molecular field results. In Sec. III, we discuss the numerical results, stressing the similarities and differences between the magnetocaloric quantities obtained within the Monte Carlo simulations and the ones obtained within the mean field approximation. Finally, Sec. IV is devoted to the conclusions.

II. THEORY

In order to describe the magnetocaloric effect in the compounds $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ for $x > 0.5$, we start with the following energy:

$$E = - \sum_{ij} \lambda_{ij} \vec{S}_i \cdot \vec{S}_j - \sum_i g \mu_B \vec{S}_i \cdot \vec{h}^{ext}, \quad (1)$$

where λ_{ij} is the exchange interaction parameter between neighboring sites, S_i is the spin of the Gd ions, and h^{ext} is the external magnetic field. It is worth mentioning here, that the classical Monte Carlo method for a system of interacting spins whose energy can be calculated from Eq. (1), has been largely used in the literature²⁴⁻²⁷ to obtain the magnetic properties of rare earth metals. In the present work, we are more interested in the calculation of the isothermal entropy change (ΔS) and the adiabatic temperature change (ΔT_{ad}) upon magnetic field variations. To obtain the magnetocaloric quantities ΔS and ΔT_{ad} , via the temperature dependence of the total entropy, it is absolutely necessary to reproduce the maximum experimental value of the magnetic entropy. It is well known that the classical Monte Carlo simulation for the Heisenberg Hamiltonian does not reproduce the saturation value of the magnetic entropy, $S_{mag} = R \ln(2S+1)$, where R is the gas con-

stant and the term $2S+1$ represents the number of available states, because the spins are treated as classical variables which can assume a continuous range of values. Thus, in order to reproduce the expected saturation value of the magnetic entropy we use in this work a Potts-like model,^{24,25} where the z components of the spins are considered as quantum quantities which can assume discrete values in the interval $-S \leq S^z \leq S$.

In order to calculate the mean energy for a given temperature, we use the following algorithm:^{24,25}

(i) Generate randomly an initial spin configuration and calculate the energy of the initial configuration (E_I) according to Eq. (1).

(ii) Select a particular site ' i ' and change at random the value of the z component of the local spin momentum.

(iii) Calculate the energy for this new configuration (E_F) according to Eq. (1).

(iv) If $E_F < E_I$, accept the new configuration with energy E_F and go to step (viii).

(v) If $E_F > E_I$, calculate the probability factor $p = e^{-(E_F - E_I)/k_B T}$, where k_B is the Boltzmann constant.

(vi) Generate a random number r such that $0 < r < 1$.

(vii) If $r < p$, accept the new spin configuration with energy E_F , otherwise preserve the old spin configuration with energy E_I .

(viii) Move to the next site, change at random the value of the z component of the local spin momentum, and return to step (iii).

(ix) Repeat the entire process until all the lattice sites are swept.

The whole process described before constitutes just one Monte Carlo step. For a Monte Carlo step, the energy of system is the energy of the last generated spin configuration, (E_i) where the label ' i ' represents the number of a given Monte Carlo step. For a given temperature, the mean energy $\langle E \rangle$ and the mean square energy $\langle E^2 \rangle$ are calculated by

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

$$\langle E^2 \rangle = \frac{1}{(N_c - N_0)} \sum_{i > N_0}^{N_c} E_i^2, \quad (3)$$

where N_c represents the total number of Monte Carlo steps and N_0 is the number of Monte Carlo steps used for thermalization. For one Monte Carlo step, the average of the spin per lattice site is calculated by summing the spins throughout the lattice sites of the last spin configuration and dividing by the number of sites, i.e.,

$$\langle S \rangle_i = \frac{1}{N_S} \sum_{k=1}^{N_S} S_k. \quad (4)$$

Here the label ' i ' represents the Monte Carlo step and the label ' k ' represents the lattice sites. N_S represents the number of lattice sites and S_k is the spin at each lattice site. For a given temperature, the mean value of the spin per lattice site

is calculated by summing the averages of all Monte Carlo steps

$$\langle S \rangle = \frac{1}{(N_c - N_0)} \sum_{i > N_0}^{N_c} \langle S \rangle_i, \quad (5)$$

where the average $\langle S \rangle_i$ is by Eq. (4). At a given temperature, the average magnetization per ion is calculated by $M/ion = g\mu_B \langle S \rangle$, where the average $\langle S \rangle$ is calculated by Eq. (5). The magnetic part of the heat capacity for a given temperature is calculated by

$$C_{mag}(T, h^{ext}) = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}. \quad (6)$$

The total heat capacity is given by $C = C_{mag} + C_{el} + C_{lat}$, where C_{mag} is the magnetic part calculated in Eq. (6); C_{el} is the contribution from the conduction electrons and (C_{lat}) is the contribution from crystalline lattice. The contribution from the conduction electrons is taken as $C_{el} = \gamma T$, where γ is the Sommerfeld coefficient. Here we take C_{lat} in the Debye approximation, which is given by²⁸

$$C_{lat}(T) = 9RN_i \left[4 \left(\frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} \frac{x^3}{(e^x - 1)} dx - \left(\frac{\theta_D}{T} \right) \frac{1}{(e^{\theta_D/T} - 1)} \right], \quad (7)$$

where N_i is the number of ions per formula unit; $R = 8.31$ J/mol K is the gas constant and θ_D is the Debye temperature. In the same way, the total entropy of the compound is given by $S = S_{mag} + S_{el} + S_{lat}$. The contribution from the magnetic ions is given by

$$S_{mag}(T, h^{ext}) = \int_0^T \frac{C_{mag}(T, h^{ext})}{T} dT, \quad (8)$$

where C_{mag} is the magnetic heat capacity calculated in Eq. (6). The contribution from the conduction electrons is taken as $S_{el} = \gamma T$. The contribution from the crystalline lattice, also taken in the Debye approximation, is given by^{17,18}

$$S_{lat}(T) = N_i \left[-3R \ln(1 - e^{-(\theta_D/T)}) + 12R \left(\frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} \frac{x^3}{e^x - 1} dx \right]. \quad (9)$$

Here, we suppose that only the magnetic part of the entropy and the magnetic heat capacity depend on the applied magnetic field. This is a very reasonable approximation for compounds undergoing a second order magnetic phase transition. For compounds with first order magnetic phase transition, an extra term to account for the magnetoelastic coupling should be included in the energy given in Eq. (1).

For the sake of comparison, between our Monte Carlo calculations and the mean field ones, we also calculate the magnetocaloric effect within the molecular field approximation. In the molecular field approximation, the magnetization is also calculated by $M/ion = g\mu_B \langle S \rangle$, where the average $\langle S \rangle$,

associated with relation (1), is calculated in terms of the Brillouin function. The magnetic entropy associated with the energy (1), in the molecular field approach is given by^{17,18}

$$S_{mag}(T, h^{ext}) = N_m R \left[\ln \sum_m e^{-\beta E_m} + \frac{1}{k_B T} \frac{\sum_m E_m e^{-\beta E_m}}{\sum_m e^{-\beta E_m}} \right], \quad (10)$$

where N_m is the number of magnetic ions per formula unit and E_m are the energy eigenvalues for a Heisenberg model Hamiltonian. In the absence of the crystalline electrical field, the magnetic entropy can also be written as

$$S_{mag}(T, h^{ext}) = N_m R [\ln Z - x S B_S(x)], \quad (11)$$

where $Z = \sum_m e^{-\beta E_m}$ is the partition function; B_S is the Brillouin function, and $x = g \mu_B [h^{ext} + \lambda \langle S \rangle / g \mu_B] / k_B T$, where λ is the exchange interaction parameter. The magnetic heat capacity can be numerically obtained from the thermodynamic relation $C_{mag} = T \partial S_{mag} / \partial T$. In the theoretical calculations of the magnetocaloric quantities ΔS and ΔT_{ad} where the spin-spin interaction is treated within the molecular field approximation, the electronic entropy and heat capacity are also considered as $S_{el} = \gamma T$ and $C_{el} = \gamma T$, respectively. The lattice heat capacity and the lattice entropy are also given by Eqs. (7) and (9), respectively.

III. NUMERICAL RESULTS

The calculations presented so far are quite general and can be used to calculate the magnetocaloric effect in rare earth based compounds, whose energy can be written in the form of Eq. (1). In this work, we apply the Monte Carlo method to calculate the magnetocaloric effect in $Gd_5(Si_x Ge_{1-x})_4$ for $x > 0.5$, where the magnetic phase transition is of second order. We use a tridimensional cluster of $5 \times 5 \times 5$ orthorhombic cells with eight Gd atoms per cell and consider only next neighbors interactions. Notice that in the Monte Carlo calculations only the magnetic ions (Gd) are considered in the crystalline structure. However, it is very important to mention that Ge and Si ions play a fundamental role in the determination of the magnetic ordering temperature, which depends on the exchange interaction parameters λ_{ij} . For a given concentration, the exchange interaction parameters λ_{ij} , which take into account the distance between the neighboring sites occupied by Gd ions, were chosen to correctly reproduce the experimental data of the magnetic ordering temperature. The Landè factor was taken as $g=2$ and the spin momentum of Gd as $S=7/2$. In order to establish the magnitude of the z component of the spin momentum of the Gd ions at each lattice site, we proceed as follows: We draw a random number r such that $0 < r < 1$ and fix the value of S^z according to the following scheme: $S^z = -3.5$ if $0 \leq r \leq 0.125$; $S^z = -2.5$ if $0.125 < r \leq 0.25$; $S^z = -1.5$ if $0.25 < r \leq 0.375$; $S^z = -0.5$ if $0.375 < r \leq 0.5$; $S^z = 0.5$ if $0.5 < r \leq 0.625$; $S^z = 1.5$ if $0.625 < r \leq 0.75$; $S^z = 2.5$ if $0.75 < r \leq 0.875$; and $S^z = 3.5$ if $0.875 < r \leq 1.0$. For a given temperature, we perform Monte Carlo simulation using 5000 Monte

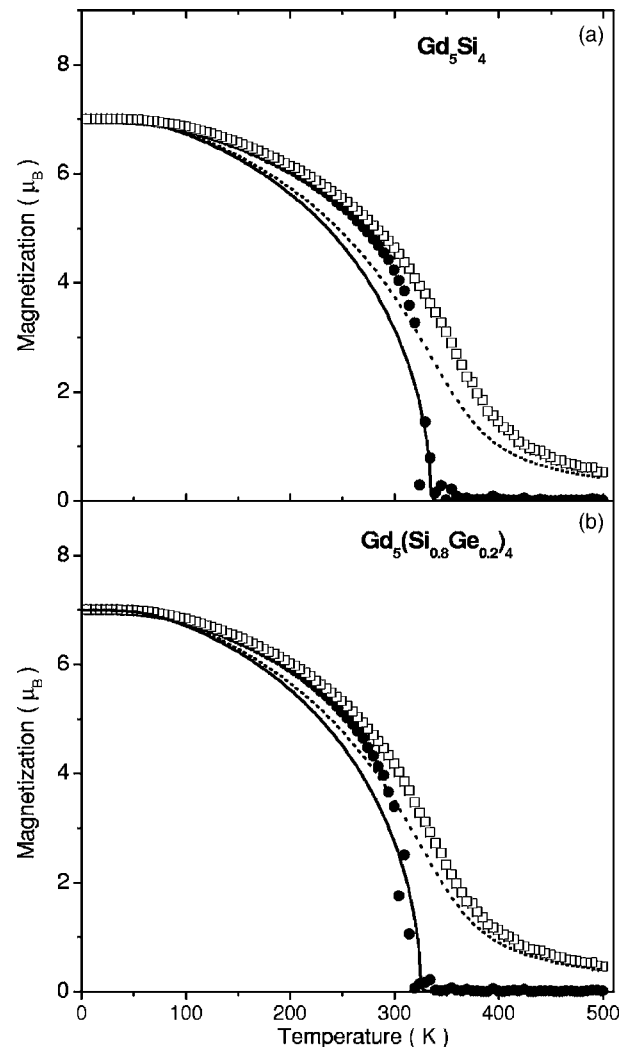


FIG. 1. Temperature dependence of the magnetization per Gd ions of the compounds Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b). The solid and dotted lines represent the calculations within the molecular field approximation for $h^{ext}=0$ and $h^{ext}=5$ T. Solid circles and open squares represent the curves obtained within the Monte Carlo simulation for $h^{ext}=0$ and $h^{ext}=5$ T.

Carlo steps, where 2000 were used for thermalization of the system and 3000 were used to compute the average values of the physical quantities. The mean values of the energy and spin were calculated from Eqs. (2)–(5). The magnetic part of the heat capacity was calculated using Eq. (6) and the magnetic entropy was obtained from Eq. (8). The electronic heat capacity was calculated using $\gamma=5.4$ mJ/(mol K²) and the lattice heat capacity and entropy were calculated using $\Theta_D=430$ K. The parameters γ and Θ_D are in the usual range of values used in the literature.¹⁴ For the sake of comparison, we also calculated the magnetocaloric quantities of the compounds $Gd_5(Si_{1-x}Ge_x)_4$ by using the magnetic entropy given by Eq. (10) obtained within the molecular field approximation.

In Fig. 1, we plot the magnetization of the compounds Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b) obtained within the Monte Carlo calculation for $h^{ext}=0$ T (solid circles) and $h^{ext}=5$ T (open squares). The solid and dotted lines represent

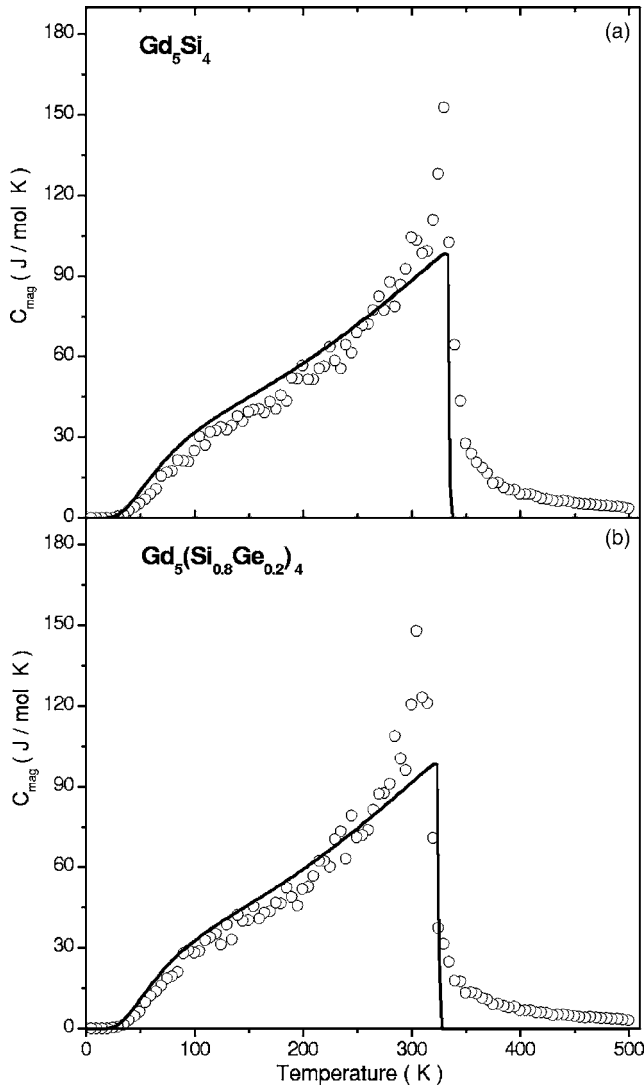


FIG. 2. Magnetic heat capacity of the compound Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b) calculated in the absence of an external magnetic field. Open circles represent the Monte Carlo calculations while the solid lines represent the molecular field calculations.

the magnetization curves obtained within the molecular field theory for $h^{ext}=0$ T and $h^{ext}=5$ T, respectively. We can observe that at low temperatures, the magnetizations obtained within the Monte Carlo calculation and the ones calculated in the molecular field approach agree quite well. However, around the magnetic ordering temperature, there are some deviations between them. This can be ascribed to the short range interactions which are not well considered in the mean field approach. In Fig. 2, we plot the magnetic heat capacity in the absence of an external magnetic field for the compounds Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b) obtained within the Monte Carlo calculation (open circles). The solid lines are the corresponding calculations obtained within the molecular field theory. From this figure, we can observe that the curves obtained with the Monte Carlo calculation and the ones obtained in the molecular field are very similar at low temperature. However, around the magnetic ordering temperature, the curves obtained in the molecular field approxi-

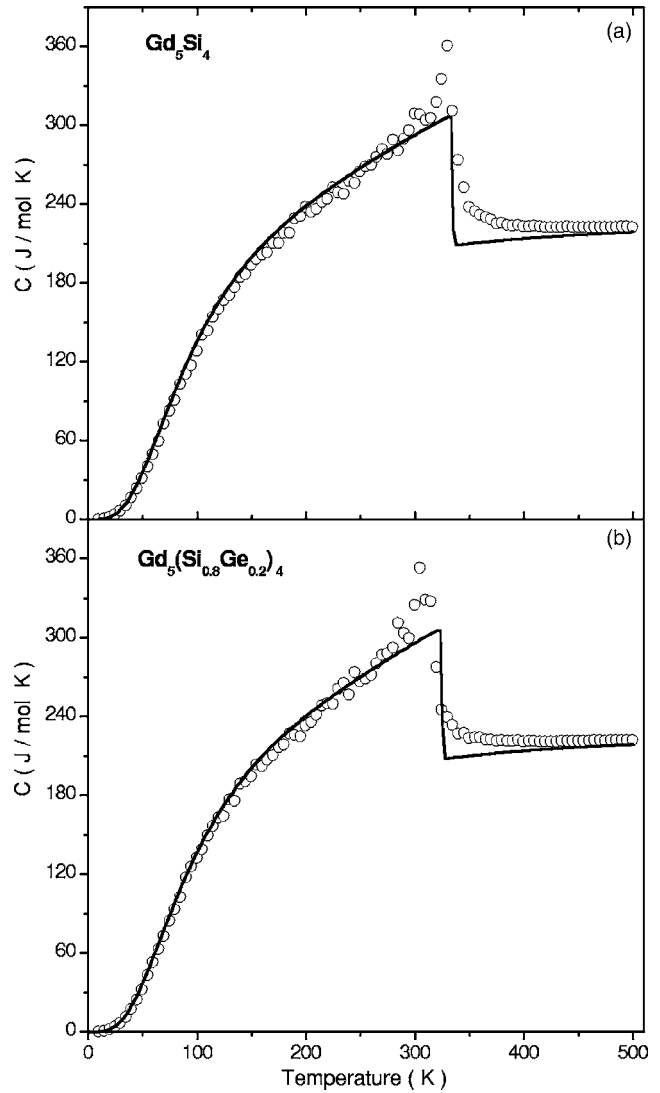


FIG. 3. Total heat capacity of the compound Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b) in the absence of an external magnetic field. Open circles represent the Monte Carlo calculations and the solid lines represent the molecular field calculations.

mation go abruptly to zero, whereas the ones obtained in the numerical Monte Carlo calculation go smoothly to zero, as it is usually observed experimentally in the literature.¹⁴ Again the failure of the molecular field theory around the magnetic phase transition is ascribed to the short range interactions which are not well considered in the mean field approximation.

In Fig. 3, we plot the total heat capacity ($C=C_{el}+C_{mag}+C_{lat}$) for the compounds Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b) calculated in the absence of an external magnetic field. In this figure, the open circles represent the total heat capacity where the magnetic part was obtained within the Monte Carlo calculation. The solid lines represent the total heat capacity where the magnetic part was calculated within the molecular field approximation. In this figure, we can observe that the curves obtained via the Monte Carlo calculation and the ones obtained within the molecular field theory agree quite well at low and high temperatures. Notice that the high

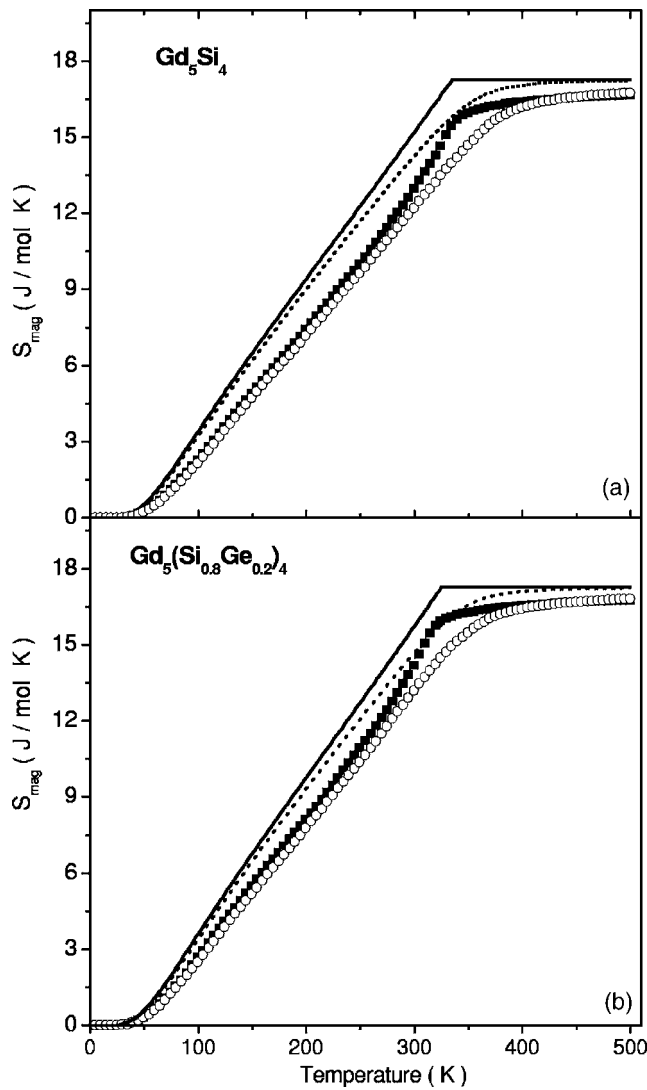


FIG. 4. Temperature dependence of the magnetic entropy of the compound Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b). Solid squares and open circles represent the Monte Carlo calculations for $h^{ext}=0$ and $h^{ext}=5$ T. The solid and dotted lines represent the molecular field calculation for $h^{ext}=0$ and $h^{ext}=5$ T.

temperature value is in good agreement with the Dulong-Petit law. However, some deviations occur around the magnetic ordering temperature, where the molecular field approach fails to describe the magnetic part of the heat capacity.

In Fig. 4, we plot the magnetic entropy for the compound Gd_5Si_4 (a) and $Gd_5(Si_{0.8}Ge_{0.2})_4$ (b) in the absence of an applied magnetic field and for an applied magnetic field of 5 T. Solid squares and open circles are the Monte Carlo calculations for $h^{ext}=0$ and $h^{ext}=5$ T, respectively. The solid and dotted lines represent the calculation of the mean field theory for $h^{ext}=0$ and $h^{ext}=5$ T, respectively. Notice that the saturation value of the magnetic entropy around 17 J/mol K is consistent with the expected value given by $S_{mag} = R \ln(2S + 1)$. We can observe that the curve obtained within the molecular field approximation for $h^{ext}=0$ exhibits a break around the magnetic ordering temperature. This type of be-

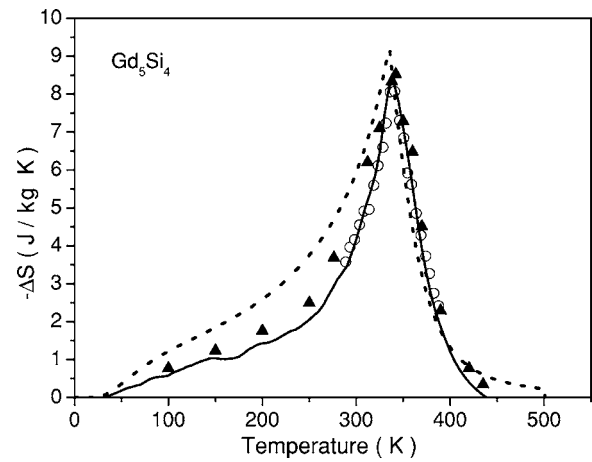


FIG. 5. Isothermal entropy change in the compound Gd_5Si_4 for a magnetic field variation from 0 to 5 T. The solid line and solid triangles correspond to the Monte Carlo calculations using the total entropy and Maxwell relation, respectively. The dotted line represents the molecular field calculations. Open circles are experimental data (Ref. 11).

havior is directly associated with the abrupt drop in the magnetic heat capacity. On the contrary, the corresponding curve obtained via the Monte Carlo calculation increases smoothly until it reaches the saturation value.

Using the temperature dependence of the total entropy for $h^{ext}=0$ and $h^{ext}=5$ T, we calculate both the isothermal entropy change and the adiabatic temperature change. For the sake of comparison, we also calculate the isothermal entropy change by using the Maxwell relation $\Delta S = \int (\partial M / \partial T) dh^{ext}$. In Figs. 5 and 6, we plot the isothermal entropy change under a magnetic field variation from 0 to 5 T for the compounds Gd_5Si_4 and $Gd_5(Si_{0.8}Ge_{0.2})_4$, respectively. Solid lines represent the calculations using the total entropy, whereas solid triangles represent the calculations using the Maxwell relation. In these figures, we also plot the isothermal entropy

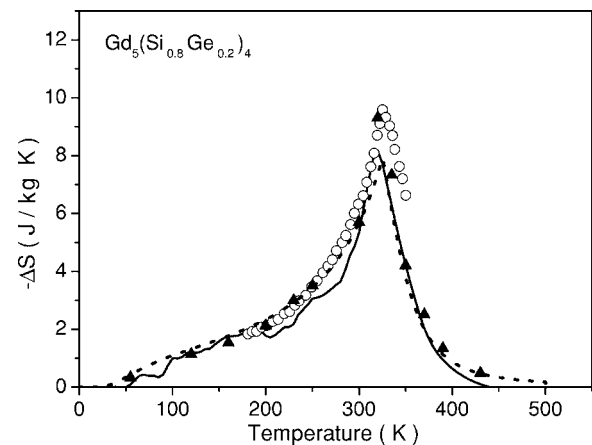


FIG. 6. Isothermal entropy change in the compound $Gd_5(Si_{0.8}Ge_{0.2})_4$ for a magnetic field variation from 0 to 5 T. The solid line and solid triangles correspond to the Monte Carlo calculations using the total entropy and Maxwell relation, respectively. The dotted line represents the molecular field calculations. Open circles are experimental data (Ref. 11).

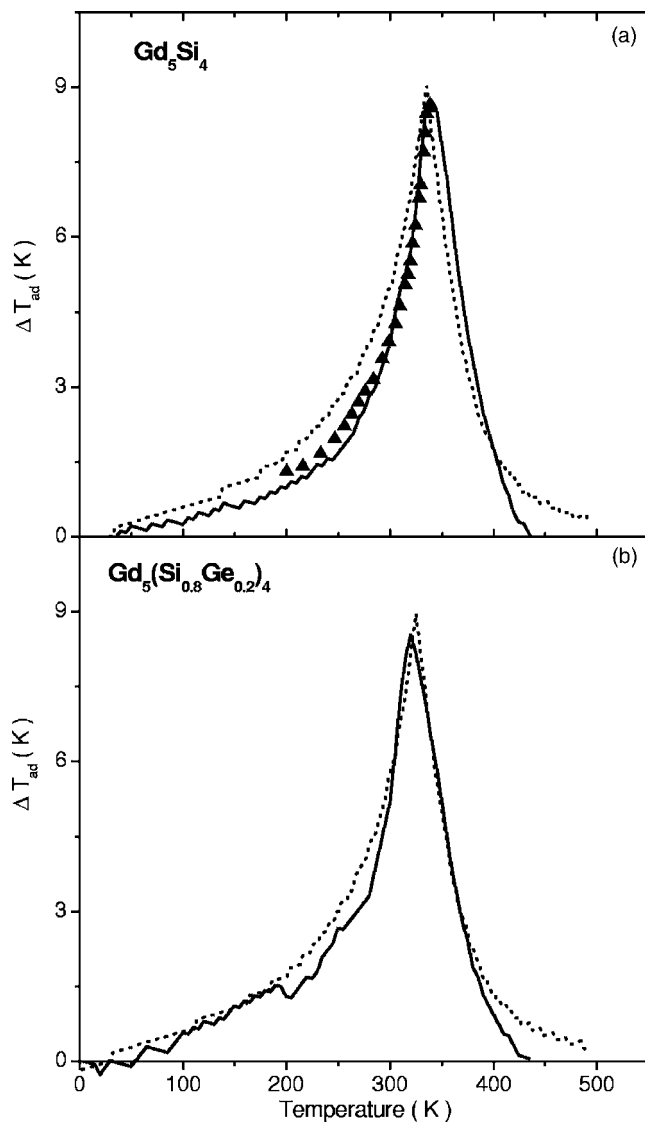


FIG. 7. Adiabatic temperature change in the compound Gd_5Si_4 (a) and $\text{Gd}_5(\text{Si}_{0.8}\text{Ge}_{0.2})_4$ (b) for a magnetic field variation from 0 to 5 T. The solid lines correspond to the Monte Carlo calculations, whereas the dotted lines represent the molecular field calculations. Triangles are experimental data (Ref. 11).

change obtained within the molecular field theory (dotted lines). From these figures, we can observe a better agreement between the Monte Carlo calculations (solid lines) and ex-

perimental data¹¹ (open circles). In Fig. 7, we plot the adiabatic temperature change for the compounds Gd_5Si_4 (a) and $\text{Gd}_5(\text{Si}_{0.8}\text{Ge}_{0.2})_4$ (b) obtained within the Monte Carlo calculations for a magnetic field variation from 0 to 5 T (solid lines). The results from the molecular field theory are shown by the dotted lines. From Fig. 7(a), we again observe a better agreement between the Monte Carlo calculations (solid line) and the available experimental data (triangles).¹²

IV. CONCLUSIONS

In this work, we report on the Monte Carlo calculations of the magnetocaloric effect in the compound $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ in the concentration range in which the magnetic phase transition is of second order. For the concentration range in which the first order magnetic phase transition takes place, the present calculation should be modified in order to incorporate the magnetoelastic coupling. It is worth mentioning that although the molecular field approximation fails to explain the magnetic heat capacity around the magnetic ordering temperature, the magnetocaloric quantities ΔS and ΔT_{ad} obtained within this mean field theory are very reasonable. Since the molecular field theory is much less time consuming than the Monte Carlo calculations, it can be used as a first attempt to obtain the trend of the magnetocaloric quantities in rare earth based compounds. However, for a more rigorous description of the physical mechanism involved in the magnetocaloric effect of rare earth based compounds, we should use the Monte Carlo calculations. Besides, the Monte Carlo simulation enables us to calculate the magnetocaloric effect in disordered systems containing more than one type of rare earth ions, where the molecular field theory is not a good approximation at all. The Monte Carlo method also enables us to simulate new rare earth based compounds which may exhibit sizeable magnetocaloric effect as well as to calculate the magnetocaloric effect in antiferromagnetic compounds. Therefore, this work on the theoretical calculations of the magnetocaloric effect based on the Monte Carlo simulation opens a brand new horizon in the theoretical study of the magnetocaloric effect in rare earth metals and their compounds.

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