sciendo

ANNALS OF WEST UNIVERSITY OF TIMISOARA PHYSICS
Vol. LXV, 2023

DOI: 10.2478/awutp-2023-0013

MAGNETOCALORIC EFFECT IN FULL-HEUSLER Rh_2SmIn COMPOUND BASED ON RARE EARTHS USING DFT AND MONTE CARLO STUDIES

N.N. Koudjeti[1,*], B.N. Brahmi[1], Y. Kaddar[2], A. Zair[1], S. Bekhechi[1], A. Benyoussef[2]

[1]*Laboratory of Theoretical Physics, Faculty of Sciences, University Abu bekr Belkaid, B.P. 119, 13000, Tlemcen, Algeria*
[2]*Laboratory of Condensed Matter and Interdisciplinary Sciences (LaMCScI), Faculty of Sciences, Mohammed V University of Rabat,B.P. 1014, Morocco*

Article Info

Received: 24.10.2023
Accepted: 14.11.2023

Keywords:

Magnetocaloric applications, Full-Heusler, DFT, Exchange couplings, Monte Carlo simulation, RCP

Abstract

Magnetocaloric refrigeration is an integral part of technology and is under constant investigation. In this regard, the characterization of the magnetocaloric materials used is of major concern. In this study, we used different approaches to better understand the mechanisms underlying the magnetic and magnetocaloric properties of $Rh_2S\ mIn$ Full-Heusler. A physical model is suggested to explain the magnetic interaction within this material. Utilizing the density functional theory, exchange couplings and magnetic phase stability in Rh_2SmIn have been attempted as well in order to understand and clarify the various magnetic interactions in this compound. The magnetic and magnetocaloric properties were examined with Monte Carlo simulation (MCS) based on the Ising model. The transition temperature, magnetic entropy change, and relative cooling power (RCP) were computed and found to be in good agreement with experimental evidence. According to the results, $Rh_2S\ mIn$ is a good candidate to be used in magnetic refrigeration applications at high temperature.

1. Introduction

Refrigeration technology is becoming a necessity in our modern society. Where the choice of the best refrigeration technology depends on the environmental compatibility and energy efficiency. Until now the vapor compression refrigerators have been mainly used for cooling applications [1, 2, 3, 4]. However, the compressing and expanding processes of gas in these refrigerators are not very efficient due to the refrigeration accounts for 25% of residential and 15% of commercial power consumption. In addition, the usage of gases such as chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) are harming our living environment [5]. In this

regard, magnetic refrigeration (MR) technology, based on the magnetocaloric effect (MCE) is destined to become a very competitive cooling method because of its high energy efficiency and the absence of ozone-depliting gazes, compared to conventional refrigeration based on vapor compression [1].

Over the last few years, much attention has been devoted to the discovery of materials that can be exploited for magnetocaloric applications, such as intermetallics and rare earths. Heusler alloys represent intermetallic compounds with amazing physical properties. These alloys include more than 1500 compounds with magnetoelectronic (ME), magnetocaloric effect (MCE) [6, 7, 8, 9], magnetoresistance (MR), magneto-strain [10], exchange bias (EB) [11], magneto-optic (MO) [12] and elastocaloric effect (eCE) [13].

Heusler alloys are intermetallic compounds with the general formula *XYZ*, where *X, Y,* and *Z* are different elements in the periodic table [14]. They have attracted significant interest in recent years because of their interesting electronic and magnetic properties. The origin of the name Heusler is due to Fritz Heusler, who first synthesized these compounds in the 1903s [15]. Full-Heusler alloys have a cubic structure with the space group $Fm\bar{3}m$ ($N^{\circ}225$) [16] and are known for their excellent thermoelectric, magnetic [17, 18], magnetocaloric [19, 20, 21, 22].

That is why research in recent years has focused on the study of Heusler alloys as potential magnetocaloric materials for magnetic refrigeration. Several studies have reported very interesting results for Full-Heusler alloys, considered a promising platform for magnetocaloric applications, as expressed in Roy and al. (2021) [23] These authors investigated the magnetic and magnetocaloric properties of several Full-Heusler alloys and found that they exhibit significant magnetocaloric effects and high magnetic ordering temperatures, which allows them to be suitable for magnetic refrigeration, providing very promising results in this regard.

Other results with respect to the magnetocaloric properties of a Full-Heusler alloy revealed a large magnetocaloric effect, making it a potential candidate for magnetic refrigeration applications (Li and al. 2019) [24]. In this study, theoretical methods were used to investigate the magnetic and magnetocaloric properties of the alloy.

Many research initiatives have been devoted recently to the properties of all types of Heusler alloys $Ni_2\ MnGa$ [25], *Ni-Mn-Ga* and *Ni-Mn-Co-Sn* [26] and $Ni_{43}\ Mn_{46}S\ n_{11-x}Ti_x$ [27] with the objective of discovering various prop- erties for the different applications mentioned above. In this paper, we are interested in the Full-Heusler Rh_2SmIn compound by studying the magnetocaloric effect with DFT and Monte Carlo simulations. The paper is organized as follows: Section 2 contains the computational details. In Section 3, we provide the results and

discussion of our simulation, and we conclude in Section 4.

2. Computational details

In our work, we are more inclined to investigate the magnetic properties of *Rh_2SmIn*.In fact, the magnetic moment of the titled compound is mainly due to the rare earth metal samarium (Sm). This atom has a spin of $S=\frac{5}{2}$ with values of : $\pm\frac{5}{2}$, $\pm\frac{3}{2}$, $\pm\frac{1}{2}$. To accurately predict the calculated close coupling parameters (J), we used the available data of *Rh_2SmIn* material from the quantum materials *(OQMD)* database. The structure of *Rh_2SmIn* adopts a space group of $Fm\bar{3}m$ as prototype ($L2_1$) Full-Heusler *Cu_2MnAl*, see table 1.

Table 1. Parameters values of Rh_2SmIn compound

Crystal structure	Values[a]
Space group	$Fm\bar{3}m$ (space groupe N°225)
Cell parameters	a=b=c=6.705 (Å)
	α=β=γ=90°

[a]*Source: https://oqmd.org/materials/entry/450181*

To present the magnetocaloric effect in our compound, we use the Ising Hamiltonian to describe the system:

$$H = -J\sum_{\langle ij\rangle} S_i S_j \; - g\mu_B B\sum_i S_i \qquad (1)$$

When a magnetic material is subjected to a sufficiently high magnetic field, the magnetic moments of the atoms become reoriented. If the magnetic field is applied adiabatically, the temperature of the material rises, and if the magnetic field is subsequently removed, the temperature decreases. This warming and cooling in response to the application and removal of an external magnetic field is called the MCE which is directly related to both the magnetic entropy change and the adiabatic temperature change. It is important to understand the relationship between these two quantities.

To perform the study of the magnetic properties and magnetocaloric behaviors of this alloy, we need to calculate the magnetization and the internal energy of this system. M is given by:

$$M = \frac{1}{N}\sum_i S_i \qquad (2)$$

$$E = \frac{1}{N}\langle H\rangle \qquad (3)$$

The change of entropy (S) of a magnetic material upon the application of a magnetic field (H) is related to magnetization (M) with respect to temperature (T) through the thermodynamic Maxwell relation:

$$\left(\frac{\partial S}{\partial B}\right)_T = -\left(\frac{\partial M}{\partial T}\right)_B \quad (4)$$

The magnetic entropy change, ΔS_M (T,B) is given by [29]:

$$\Delta S_M(\mathrm{T},\mathrm{B}) = S_M(\mathrm{T},\mathrm{B}) - S_M(T,0) = \int_0^B \left(\frac{\partial M(T,B)}{\partial T}\right)_B dB \quad (5)$$

In simple cases, the magnetic cooling efficiency of a magnetocaloric material could be evaluated by considering the magnitude of ΔS_M and its full-width at half-maximum (δT_{FWHM}) as follows [30]:

$$RCP = -\Delta S_M(\mathrm{T},\mathrm{B}) \times \delta \mathrm{T}_{\mathrm{FWHM}} \quad (6)$$

which stands for the so-called relative cooling power *(RCP)* based on the magnetic entropy change.

3. Results and discussions

The total and partial magnetic moments of different elements constituting *Rh_2SmIn* full Heusler are presented in Table 3. Such results are obtained by using the DFT method implemented in the wien2k code [31]. In fact, the samarium atoms defined the magnetic character in *Rh_2SmIn*. They occupied the middle of the edges and the center of the cubic unit cell. The *Wycoff* positions of *Rh_2SmIn* are shown in Table 2.

$$E_{AFM} = J\frac{ZS^2}{2} - BS \quad (7)$$

$$E_{FM} = -J\frac{ZS^2}{2} - BS \quad (8)$$

where E_{AFM} and E_{FM} are the energies of antiferromagnetic and ferromagnetic configurations, respectively. The number of the first nearest Sm neighbors atoms is equal to (Z = 12), whereas, the electronic number of the rare earth element Samarium is (Z_e = 62) with an electronic configuration of $[Xe]4f^6 6s^2$.The latter holds only 59 electrons $[Xe]4f^5$. Thus, in this

configuration, Sm^{3+} has, according to Hunds rule, a spin S=5/2. Our calculated values of E_{AFM} and E_{FM} are, respectively, -207108.77403786 *Ry* and -207108.78287137 *Ry*.

Table 2. Final postions [28]

	Postions			
Species	X	Y	Z	Charge
In	0.2500	0.2500	0.2500	11.406
Rh	0.0000	0.0000	0.0000	7.939
Rh	0.5000	0.5000	0.5000	7.939
Sm	0.7500	0.7500	0.7500	9.011

To obtain *J*, we used a combination between equations 7 and 8:

$$J = \frac{E_{AFM} - E_{FM}}{ZS^2} \tag{9}$$

The estimated value of the exchange parameter is J = 1.601 meV.

Table 3. Magnetic moments

Elements	Magnetic moments (μ_B)
μ_{Int}	0.139
μ_{Rh}	-0.130
μ_{Sm}	5.323
μ_{In}	-0.010
μ_{Total}	5.191

The numerical results given below were performed using Monte Carlo simulation [33] and the Hamiltonian of our system is given by equation (1), including the calculated exchange coupling J.

Figure 1 shows the magnetization *M* and the susceptibility χ as a function of temperature with B = 0 (T). It is observed that at zero temperature, the magnetization M reaches the maximum value of M = 2.5 (we note that spins take the value of 5/2 in all states). When the temperature increases, the magnetization decreases continuously to reach zero at the Curie temperature Tc = 543K. The system thus, undergoes a second-order phase transition from the

ferromagnetic to the paramagnetic phase. In this figure, the magnetic susceptibility curve shows a peak corresponding to the Curie temperature Tc.

Next, in order to study the size effect (L), the simulations were performed with different values of L × L × L. Our calculations are done on a finite size set ranging from L = 8 to L = 48 for any lattice. Periodic boundary conditions were also used to approximate a realistic system. The magnetization M is shown in figure 2 for different sizes of our system as a function of temperature K. We can observe that the behavior of the magnetization is more susceptible to increasing with system size, and converges to zero at critical temperatures. The size effect is clearly shown while the second order transition occurs. Furthermore, the susceptibility in figure 3 increases with the rise of lattice size, reaching a maximum at the transition temperature.

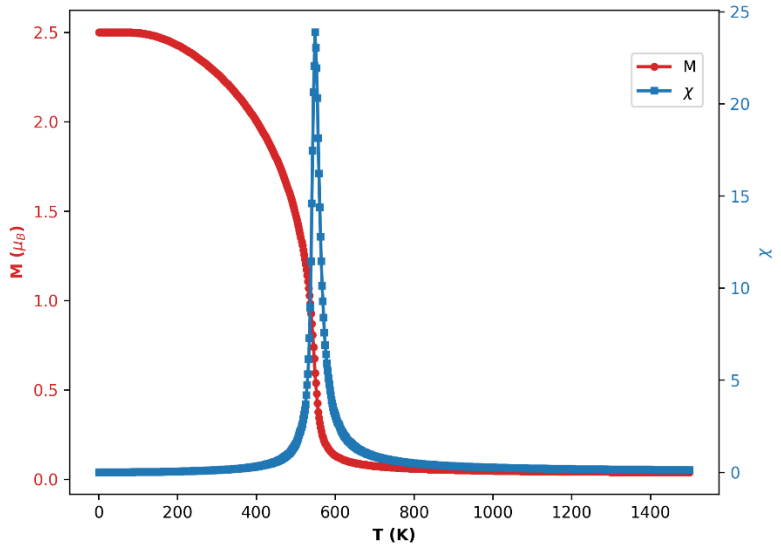


Figure 1. Magnetization M and Susceptibility χ versus the temperature of the full-Heusler Rh_2SmIn

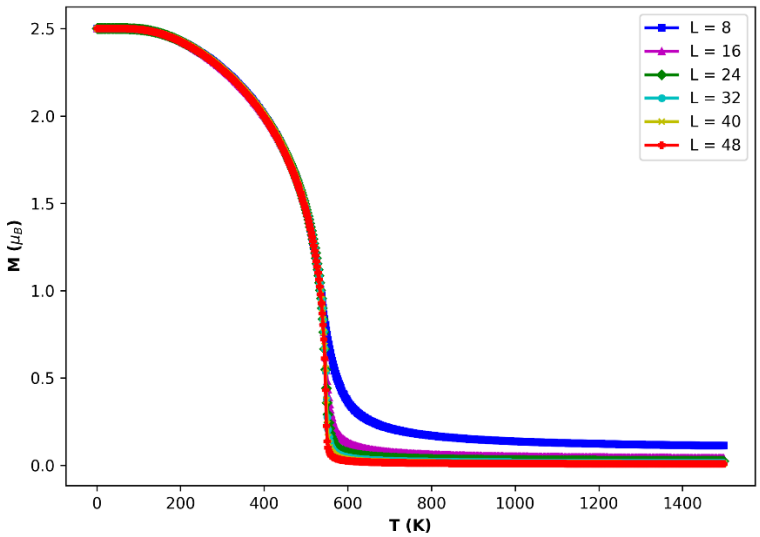


Figure 2. Size effect of Magnetization of the full-Heusler *Rh_2SmIn* versus the temperature

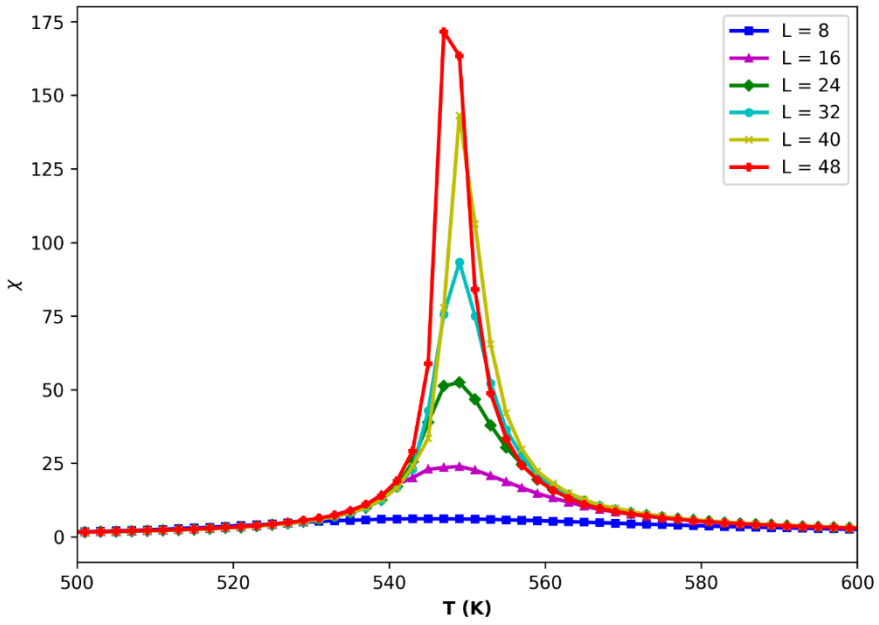


Figure 3. Size effect of Susceptibilty in full-Heusler *Rh_2SmIn* versus the temperature

Thus, in order to evaluate the magnetocaloric effect in *Rh_2SmIn*, the entropy changes were calculated for various magnetic fields from 1T to 6T with a step of 1T. This one is shown in figure 4 for system size L = 16 × 16 × 16. For a magnetic field of 6T, it is clearly seen that the entropy mutation is maximal at -4.6 J/kg.K around 543K. This maximum value grows with an augmentation of the magnetic field B. As well, for cooling applications, a material exhibiting a wide peak of $-\Delta S_M$ is much better than a material exhibiting a sharp peak of magnetic entropy change. The wide temperature distribution materials are favored for MC applications [34]. In the figure's inset, it can be observed that the change in entropy ΔS_M exhibits a wide peak around Tc. This behavior makes *Rh_2SmIn* more suitable for magnetic cooling. whereas the narrower peak in ΔS_M stipulate a less favorable situation for magnetic cooling properties. Within this context, we are comparing different experimental values of magnetic entropy change for other compounds from the Heusler family. This comparison is displayed in Table 4. We note that ΔS_M of *Rh_2SmIn* is better compared with *$Co_2Cr_{0.25}Mn_{0.75}Al$* [35] and close to *Fe_2CoAl* [36] but our Tc is lower than all of them. The properties of compounds gathered in Table 4 reveal that a giant magnetocaloric effect was obtained by *Co_2FeAl* [37] Heusler, hencefor, a sharp peak in ΔS_M was identified at high Tc, which induces less effectiveness and low efficiency, particularly in magnetic refrigeration. According to Table4, the value of ΔS_M of the *$Co_2Cr_{0.25}Mn_{0.75}Al$* is less than that found for *Rh_2SmIn*. However, the RCP values are closer to our result. On the other side, *Rh_2SmIn* has a weaker ΔS_M, but a higher RCP than *Fe_2CoAl*. From the point of view

of the Tc value, our investigated compound exhibits a closer temperature to the ambient one, which makes it more favorable for cooling refrigeration.

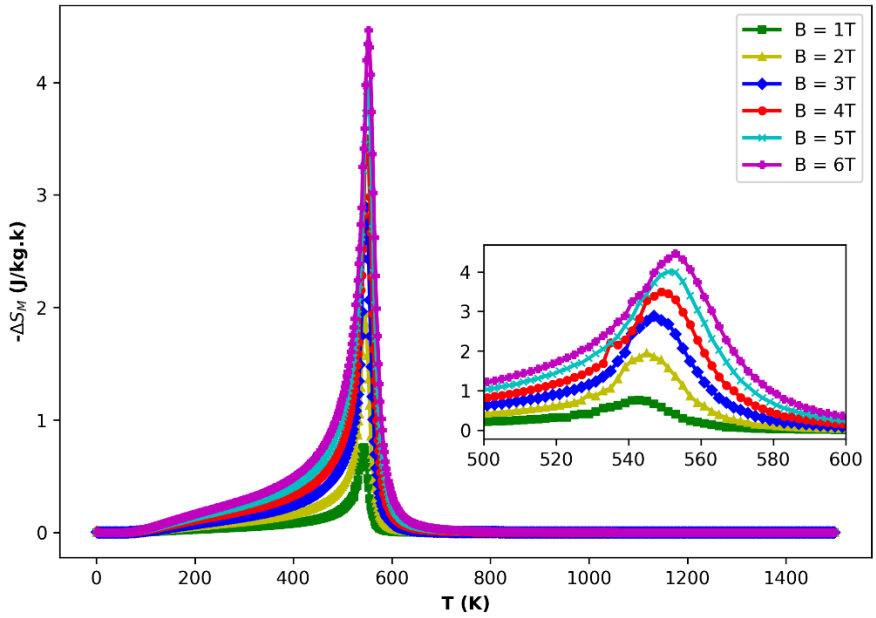


Figure 4. Magnetic entropy change for an external field ranging from 1T to 6T of *Rh_2SmIn*

Table 4. Comparaison of Rh_2SmIn with other compounds

Compounds	$-\Delta S_M$ (J/K.kg)	Applied magnetic field (T)	RCP (J/kg)	Tc (K)	Phase transition
Rh_2SmIn	4.46	6	163.4	543	Second order [This work]
Fe_2CoAl	2.45	2	44	830	Second order [36]
$Co_2Cr_{0.25}Mn_{0.75}Al$	3.5	9	285	720	Second order [35]
Co_2FeAl	15	1.4	89	1261	Second order [37]

The maximum susceptibility in figure 5 decreases markedly with increasing magnetic field. A slight shift is also shown in the position of susceptibility peaks, which occurs when B is raised. This means that Tc increases slightly as a function of B.

Based on equation (5), it is obvious that the variation of the magnetic entropy depends closely on the derivative of magnetization. In figure 6 -a), we illustrate the variation of the magnetic entropy according to the magnetic field exerted. We can see that ΔS_M rises with the growth of B, taking respectively the following values for B = 1, 2, 3, 4, 5, and 6T ΔS_M = 0.75, 1.95, 2.89, 3.5, 4.00, and 4.46 J/kg.K. Figure 6 -b) represents the relative cooling power *(RCP)* as a function of magnetic field, which is the most interesting parameter to evaluate potential magnetic refrigeration technologies. We find that the RCP increases rather linearly with increasing magnetic field, reaching a value of 169.97 J/kg. This linear variation of RCP as a

function of applied magnetic field was also observed in other works on compounds with ferromagnetic behavior, indicating significant heat conversion in the magnetic refrigeration cycle. This specific increasing nature of ΔS_M and RCP with B, along with the broader working temperature range, would be suitable for Ericsson-cycle refrigeration applications [38]. Hence, harnessing the magnetic and magnetocaloric properties of *Rh_2SmIn* Heusler alloy can be useful not only for spintronics, but also for magnetic refrigeration technology [39].

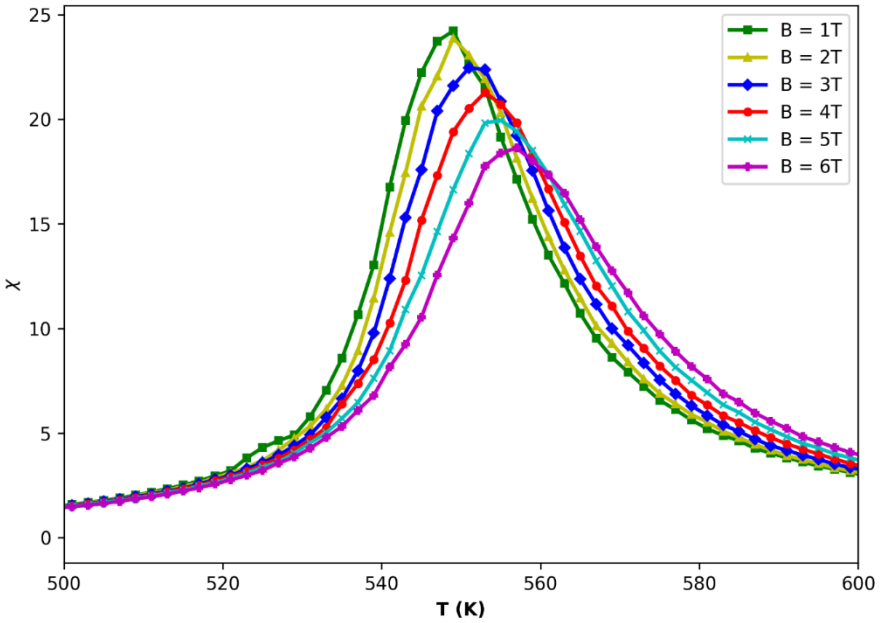


Figure 5. Magnetic contribution to the susceptibilty χ of *Rh_2SmIn*

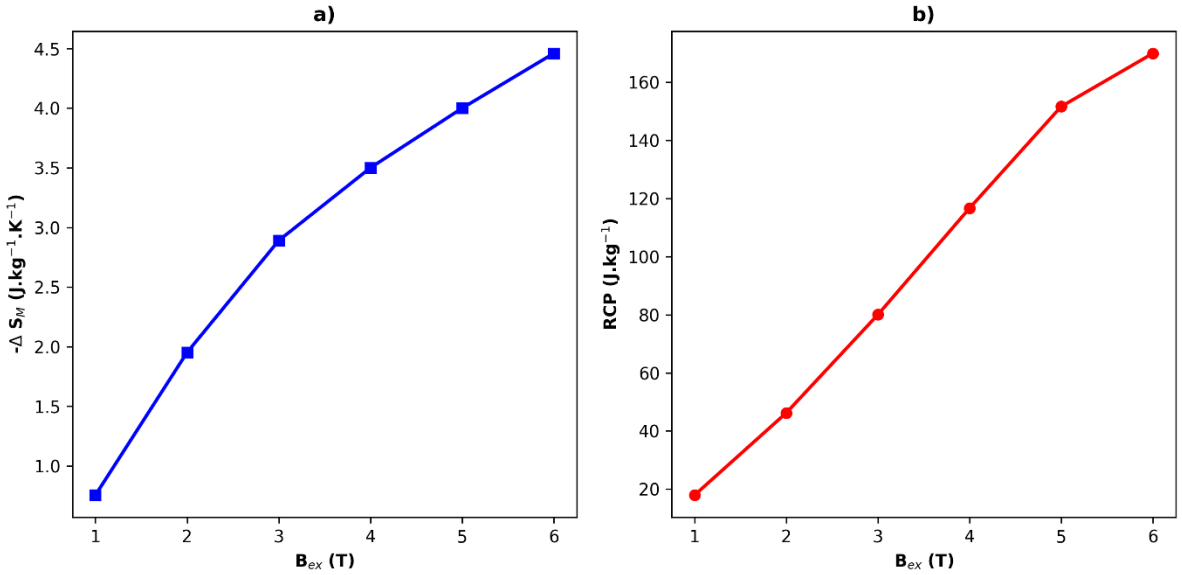


Figure 6. a) Maximum of the magnetic entropy change for different value of magnetic field of *Rh_2SmIn* and b) Relative cooling power RCP versus external magnetic field of *Rh_2SmIn*

4. Conclusion

In this work, we report a theoretical study of the magnetic behavior and magnetocaloric effect of Rh_2SmIn material by using both DFT and Monte Carlo simulations. Our results show that the magnetic properties are due mainly to samarium ions. Moreover, the most stable phase is ferromagnetic, with an exchange coupling of J = 1.601 meV. According to the deduced value of J, we performed Monte Carlo simulations and proved that the alloy shows a second order phase transition at a critical temperature around Tc = 543 K. The maximum entropy change was obtained near Curie temperature equal to -4.46 J/K.kg under a magnetic field variation of 6 T. While the corresponding RCP reaches a value of 169.97 J/kg. According to our results, Rh_2SmIn is a good candidate for magnetic cooling at high temperatures. We believe that this theoretical study can provide a foundation for experimentalists to invest in this compound and further, explore its potential for achieving excellent MCE.

Acknowledgements

The authors acknowledge the Laboratory of Theoretical Physics (LPT), for providing favorable conditions for the simulations, and data analysis. Professor Abdeljalil Rachadi (Laboratory of Condensed Matter and Interdisciplinary Sciences (LaMCScI), Mohammed V University of Rabat, Morocco) is gratefully acknowledged for his significant contribution and fruitful discussions.

References

[1] D. Guo, L. M. Moreno-Ramırez, Jia-Yan Law, Y. Zhang, V. Franco, *Excellent cryogenic magnetocaloric properties in heavy rare-earth based HRENiGa$_2$ (HRE= Dy, Ho, or Er) compounds*, Science China Material 66(1) (2023) 249–256

[2] B.G. Shen, J.R. Sun, F.X. Hu, H.W. Zhang, Z.H. Cheng, *Recent progress in exploring magnetocaloric materials*, Advanced Materials 21(45) (2009) 4545–4564

[3] Y. Zhang, *Review of the structural, magnetic and magnetocaloric properties in ternary rare earth Re2T2X type intermetallic compounds*, Journal of Alloys and Compounds, 787 (2019) 1173–1186

[4] J.Y. Law, L.M. Moreno-Ramırez, J.S. Blazquez, V. Franco, A. Conde, *Gd+GdZn biphasic magnetic composites synthesized in a single preparation step: Increasing refrigerant capacity without decreasing magnetic entropy change*, Journal of Alloys and Compounds, 675 (2016) 244–247

[5] M.H. Phan and S.-C. Yu, *Review of the magnetocaloric e_ect in manganite materials*, Journal of Magnetism and Magnetic Materials, 308(2) (2007) 325–340

[6] A. Lebouc, M. Almanza, J. P. Yonnet, U. Legait, J. Roudaut, *Réfrigération magnétique etat de l'art et développements récents*, in ´Symposium de G´enie Electrique 2014´ (2014)

[7] R. Chellakumar, T. S. Deiva Malar, A. N. Rawther, K. Ravichandran, *Soft ferromagnetic Co2MnAl full Heusler alloy particles with high curie temperature for spintronics device applications*, Journal of Superconductivity and Novel Magnetism, 36 (2023) 547–557

[8] L. Qin, Y. Li, X. Zhang, L Li, *Tunable magnetic properties and magnetocaloric response of Mn0.5 Fe0.5NiGe alloys by heat treatments*, Solid State Communications, 353 (2022) 114885

[9] G. Kadim, R. Masrour, A. Jabar, E.K. Hlil, *Room-temperature large magnetocaloric, electronic, and magnetic properties in La0.75Sr0.25MnO3 manganite: Ab initio calculations and Monte Carlo simulations*, Physica A: Statistical Mechanics and its Applications, 573 (2021) 125936

[10] Z.Y. Wei, E.K. Liu, Y. Li, X.L. Han, Z.W. Du, H.Z. Luo, G.D. Liu, X.K. Xi, H.W. Zhang, W.H. Wang, G. H. Wu, *Magnetostructural martensitic transformations with large volume changes and magneto-strains in all-d-metal heusler alloys*, Applied Physics Letters, 109(7) (2016) 071904

[11] S. Arumugam, S. Ghosh, A. Ghosh, U. Devarajan, M. Kannan, L. Govindaraj, K. Mandal, *Effect of hydrostatic pressure on the magnetic, exchange bias and magnetocaloric properties of* $Ni_{45.5}Co_2Mn_{37.5}Sn_{15}$, Journal of Alloys and Compounds, 712 (2017) 714–719

[12] F. Hosseinzadeh, A. Boochani, S. Mohammad Elahi, Z. Ghorannevis, *GdPtBi heuslerene: mechanical stability, half-metallic, magneto-optic, and thermoelectric properties by DFT*, Philosophical Magazine, 102(10) (2022) 887–901

[13] Yi Shen, Z. Wei, W. Sun, Y. Zhang, E. Liu, J. Liu, *Large elastocaloric effect in directionally solidified all-d-metal heusler metamagnetic shape memory alloys,* Acta Materialia, 188 (2020) 677–685

[14] C. Felser and A. Hirohata, *Heusler alloys*. *Properties, Growth, Applications,* Springer, (2015) DOI https://doi.org/10.1007/978-3-319-21449-8

[15] F. Heusler, W. Starck, E Haupt, *Magnetisch-chemische studien*, Verh. Dtsch. Phys. Ges, 5 (1903) 219–232.

[16] T. Graf, C. Felser, S.S.P. Parkin, *Simple rules for the understanding of heusler compounds*, Progress in solid state chemistry, 39(1) (2011)1–50

[17] R. Kainuma, Y. Imano, W. Ito, Y. Sutou, H. Morito, S. Okamoto, O. Kitakami, K. Oikawa, A. Fujita, T. Kanomata, K. Ishida, *Magnetic-field-induced shape recovery by reverse phase transformation*, Nature, 439(7079) (2006) 957–960

[18] Y. Kaddar, H. Zaari, A. Rachadi, A. Benyoussef, A. El Kenz, M. Balli, *Theoretical study of the electronic structure, magnetic and magnetocaloric properties of the* $DyMn_2O_5$ *multiferroic*, Journal of Magnetism and Magnetic Materials, 530 (2021)167890

[19] A. Aryal, A. Quetz, S. Pandey, I. Dubenko, S. Stadler, N. Ali, *Magnetocaloric effects and transport properties of rare-earth (R=La, Pr, Sm) doped $Ni_{50-x}R_xMn_{35}Sn_{15}$ Heusler alloys*, Journal of Alloys and Compounds, 717 (2017) 254–259

[20] P. Xu, L. Hu, Z. Zhang, H. Wang, L. Li, *Electronic structure, magnetic properties and magnetocaloric performance in rare earths (RE) based Re_2BaZnO_5 (RE= Gd, Gy, Ho, and Er) compounds*, Acta Materialia, 236 (2022) 118114

[21] N.A. De Oliveira and P. J. von Ranke, *Theoretical aspects of the magnetocaloric effect*, Physics Reports, 489(4-5) (2010) 89–159

[22] S. Idrissi, H. Labrim, S. Ziti, L. Bahmad, *Characterization of the equiatomic quaternary heusler alloy ZnCdRhMn: structural, electronic, and magnetic properties*, Journal of Superconductivity and Novel Magnetism, 33 (2020) 3087–3095

[23] T. Kihara, T. Roy, X. Xu, A. Miyake, M. Tsujikawa, H. Mitamura, M. Tokunaga, Y. Adachi, T. Eto, T. Kanomata, *Observation of inverse magnetocaloric effect in magnetic-field-induced austenite phase of Heusler alloys $Ni_{50-x}Co_xMn_{31.5}Ga_{18.5}$ (x= 9 and 9.7)* Physical Review Materials, 5(3) (2021) 034416

[24] W. Zhu, Z. Zhu, D. Li, G. Wu, Li Xi, Q.Y. Jin, Z. Zhang, *Magnetization precession and damping in Co_2FeSi heusler alloy thin films*, Journal of Magnetism and Magnetic Materials, 479 (2019) 179–184

[25] Y. G. Yildiz and G. D. Yildiz, *Modeling of the magnetization and magnetocaloric effect in Ni2MnGa heusler alloy with the effective field theory*, Journal of Low Temperature Physics, 207(3-4) (2022) 171–180

[26] V. Basso, C. P. Sasso, K. P. Skokov, O. Gutfleisch, V. V. Khovaylo, *Hysteresis and magnetocaloric effect at the magnetostructural phase transition of Ni-Mn-Ga and Ni-Mn-Mo-S n heusler alloys,* Physical Review B, 85(1) (2012) 014430

[27] H. Wang, Y. Li, Y. Yao, J. Xu, Z. Han, Y. Fang, L. Zhang, C. Zhang, B. Qian, X. Jiang, *Effect of Ti doping on the phase transitions, magnetocaloric effect, and exchange bias in $Ni_{43}Mn_{46}Sn_{11-x}Ti_x$ Heusler alloys*, Journal of Magnetism and Magnetic Materials, 498(2020) 166216

[28] B. N. Brahmi, N. N. Koudjeti, S. Dergal, S. Bekhechi, R. Boudefla, H. Ez-Zahraouy, *Theoretical prediction of structural, electronic, and magnetic properties of Rh_2YIn (Y= Nd, Sm) full-heusler alloys*, Journal of Superconductivity and Novel Magnetism, 31(10) (2018) 3091–3095

[29] J. I. Pérez-Landazábal, V. Recarte, V. Sánchez-Alarcos, J. J. Beato-López, J. A. Rodríguez-Velamazán, J. Sánchez-Marcos, C. Gómez-Polo, E. Cesari, *Giant direct and inverse magnetocaloric effect linked to the same forward martensitic transformation*, Scientific Reports, 7 (2017) 1–8

[30] K.A. Gschneidner Jr, V.K. Pecharsky, A.O. Pecharsky, C.B. Zimm*, Recent developments in magnetic refrigeration*, Division of Construction and Functional Materials, 315 (1999) 69–76

[31] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran, L. D. Marks, *WIEN2k - An Augmented PlaneWave + Local Orbitals Program for Calculating Crystal Properties*, revised edition WIEN2k 23.1 (Release 01/16/2023)

[32] S. Amraoui, A. Feraoun, M. Kerouad, *Ab-initio and Monte Carlo studies of the multiferroic double perovskite Ba_2FeMnO_6,* Physica A: Statistical Mechanics and its Applications, 550 (2020) 124198

[33] A. Jabar and R. Masrour, *Magnetic properties of an olympicene structure: Monte carlo simulations,* Physica A: Statistical Mechanics and its Applications, 541 (2020) 123377

[34] K. Engelbrecht, C. R. H. Bahl, *Evaluating the effect of magnetocaloric properties on magnetic refrigeration performance*, Journal of Applied Physics, 108 (2010) 123918

[35] P. Nehla, V. Anand, B. Klemke, B. Lake, R. Dhaka, *Magnetocaloric properties and critical behavior of $Co_2Cr_{1-x}Mn_xAl$ Heusler alloys,* Journal of Applied Physics, 126 (2019) 203903

[36] A. Ahmad, S. Mitra, S.K. Srivastava, A.K. Das, *Structural, magnetic, and magnetocaloric properties of Fe_2CoAl Heusler nanoalloy,* Journal of Magnetism and Magnetic Materials, 540 (2021) 168449

[37] A. Ahmad, S. Mitra, S.K. Srivastava, A.K. Das, *Giant magnetocaloric effect in Co_2FeAl Heusler alloy nanoparticles*, Journal of Physics D: Applied Physics, 54 (2021) 385001

[38] H. Takeya, V. K. Pecharsky, K. A. Gschneidner, Jr., J. O. Moorman, *New type of magnetocaloric effect: Implications on low-temperature magnetic refrigeration using an Ericsson cycle*, Applied Physics Letters, 64 (1994) 2739–2741

[39] R. Wróblewski, K. Sielicki, M. Leonowicz, *Magnetocaloric properties of stacked $Ni_{50}Mn_{18.75x}Cu_{6.25+x}Ga_{25}$ (x= 0; 0, 25; 0, 5) polycrystalline alloys*, 7th International Conference on Magnetic Refrigeration at Room Temperature, Torino, Italy (2016)