Magnetocaloric Effect in La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ Manganite Via Mean Field Theory

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Abstract: This study investigates the magnetocaloric effect of La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite, with a primary focus on leveraging the mean-field theory as a powerful tool for analysis. By applying this theoretical framework, alongside the Law of Approach to Saturation (LAS), key parameters such as saturation magnetization (M_0), total angular momentum (J), gyromagnetic factor (g), and exchange parameter (λ) were determined. The mean-field theory proved essential for simulating the isothermal magnetization M(H,T) and the magnetic entropy change $-\Delta S_M(T)$ curves, providing a comprehensive understanding of the material's magnetocaloric behavior. Despite its simplifications, the mean-field approach serves as a crucial starting point for modeling complex magnetic systems and offers valuable insights into the material's thermodynamic properties.

Keyword: Mean-field theory, Entropy, Magnetization, Simulation, Manganites.

1. INTRODUCTION

The magnetocaloric effect (MCE) describes a material's temperature alteration when exposed to a magnetic field. Applying a magnetic field aligns the magnetic dipoles in the material, reducing entropy and causing a temperature increase [1, 2]. Conversely, when the field is removed, the dipoles return to a disordered state, raising entropy and resulting in cooling [3-5]. This phenomenon underpins magnetic refrigeration, a cooling technology known for its energy efficiency and environmentally friendly attributes as compared to traditional refrigeration systems that depend on harmful refrigerant gases [6-10].

Second-order magnetic materials play a pivotal role in the MCE because of their continuous and gradual magnetic phase transitions, offering significant advantages for magnetic refrigeration [11-13]. Unlike first-order materials, which experience abrupt entropy and temperature changes, second-order materials transition smoothly near their Curie temperature, T_c [14, 15]. The importance of these materials stems from their key attributes, such as the lack of magnetic and thermal hysteresis. This property prevents energy loss in the form of heat during magnetization and demagnetization cycles, enhancing the overall efficiency of cooling systems. Additionally, their gradual transitions enable consistent and predictable performance, making them well-suited for practical applications. The adjustable magnetocaloric properties of second-order materials also allow for optimized cooling over a wider temperature range, addressing a critical challenge in scaling up energy-efficient cooling

technologies for routine use. Near T_c, thermodynamic and magnetic properties exhibit specific behaviors characterized by critical exponents, which quantify changes in magnetization, specific heat, and magnetic susceptibility [16]. Among magnetic materials. manganites stand out for their significant contribution to the MCE due to their versatile magnetic and electronic properties, which can be tailored through compositional adjustments and doping. Jiang et al. [17] recently investigated the crystal structure and magnetic properties of $La_{0.7}Sr_{0.3-x}Sm_xMn_{0.95}Ni_{0.05}O_3$ (x = 0, 0.05, 0.10, 0.15) manganites. Synthesized using the Pechini sol-gel method, the effects of substituting Sr^{2+} with Sm³⁺ on structure and magnetism were systematically studied. Rietveld refinement confirmed that all samples maintained a rhombohedral structure before and after substitution, with increasing doping resulting in an enlarged cell volume. The T_c was observed to decrease progressively with doping, falling to 323 K, 300 K, 220 K, and 186 K. The relative cooling power (RCP) peaked at 297.39 J kg⁻¹ under a 5 T magnetic indicating significant potential field. for room-temperature magnetic refrigeration applications.

Theoretical models have greatly enhanced the understanding of various material properties, often complementing experimental findings [18-20]. These models are essential for analyzing material behavior under different magnetic field (H) and temperature (T) conditions. For instance, some models simulate isothermal magnetization M(H,T) and magnetic entropy change $-\Delta S_M(H,T)$. Offering a cost-efficient alternative to extensive experimental studies. By solving equations of state numerically, researchers can generate predictive data and uncover valuable insights into the MCE without the need for resource-intensive experiments. As a result, numerous theoretical approaches have emerged, each striving to accurately

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replicate the MCE and validate their predictions against experimental results. This drive for precision has made modeling the MCE a focal point of scientific inquiry. In this study, we employed mean-field theory to investigate the MCE in La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite. Using a scaling approach, mean-field parameters were determined, and isothermal magnetization M(H,T) and magnetic entropy change $-\Delta S_M(T)$ curves were successfully simulated.

2. RESULTS AND DISCUSSION

The mean-field theory is widely applied to investigate the MCE. In this way, magnetization values

are expressed in terms of the saturation magnetization amplitude, M_0 , which is moderated by the Brillouin function, B_I [21]:

$$M(H,T) = M_0 B_I(x), \tag{1}$$

with
$$x = \frac{Jg\mu_B}{k_B} \left(\frac{H+H_{exch}}{T}\right)$$
 and B_J is given as:
 $B_J(x) = \frac{2J+1}{2J} \operatorname{coth}\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J} \operatorname{coth}\left(\frac{1}{2J}x\right),$ (2)

Where $H_{exch} = \lambda M$, *J*, *g*, k_B , μ_B are the exchange magnetic field, the total angular momentum, the gyromagnetic factor, the Boltzmann constant and the Bohr magneton, respectively.



Figure 1: (a): Linear fits of $\frac{H}{T}$ vs. $\frac{1}{T}$ at various magnetization from 1 to 30 emu.g⁻¹. (b): Fitting of H_{exch} vs. M with $\lambda_1 M + \lambda_3 M^3$ function for La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite.



Figure 2: (a): The Law of Approach to Saturation (LAS) fitting M - H curves at various temperatures in the ferromagnetic region. (b): The Bloch's law fit to temperature dependent saturation magnetization for La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite.

lons beyond the mean-field level. Such enhancements would provide a more comprehensive understanding of the magnetic behavior at low fields and improve the accuracy of theoretical predictions. such as incorporating Monte Carlo simulations and local moment models, which could address the limitations of the mean-field approach in low-field regions.



Figure 3: The Brillouin function fits the scaling plots M(H,T) vs. $\frac{H+H_{exch}}{T}$ for La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite.

The magnetocaloric effect (MCE) describes a material's temperature alteration when exposed to a magnetic field. Applying a magnetic field aligns the magnetic dipoles in the material, reducing entropy and causing a temperature increase. Magnetic refrigeration technology based on Gd-based paramagnets is expected to be applied to refrigeration in extremely low temperatures, thereby reducing the consumption of liquid helium. Here, we obtained a compound, Gd3TeBO9 with high Gd3+ concentration through element substitution. The Gd3+ concentration in this

compound is as high as 2.4×1024 ions/kg, which is 33 % higher than the commercial Gd3Ga5O12 (GGG), and further magnetic tests show that Gd3TeBO9 has a large magnetic Overall, the fair agreement at high fields underscores the robustness of the Brillouin function in describing the material's macroscopic magnetic properties, while the low-field deviations point to the need for a more nuanced approach such as incorporating Monte Carlo simulations and local moment models, which could address the limitations of the mean-field approach in low-field regions.

Under a magnetic field variation from H_1 to H_2 , the magnetic entropy change $-\Delta S_M$ may be derived from the mean-field approach and the second Maxwell's relation as:

$$-\Delta S_M(T)_{H_1 \to H_2} = \int_{M|_{H_1}}^{M|_{H_2}} (f^{-1}(M)) dM$$
(7)

By solving Eq. (7), the theoretical values for $-\Delta S_M(T)$ were computed. These results were then compared with the values estimated using the Maxwell relation, as shown in Figure **4**(**b**). While the $-\Delta S_M(T)$ curves derived from the mean-field theory generally align with those obtained through the Maxwell relation, there are noticeable discrepancies when comparing the predictions experimental data. theoretical to Specifically, the mean-field approach tends to overestimate the magnitude of the entropy change and predicts peak values at higher temperatures than those discrepancy observed experimentally. This is particularly pronounced in materials undergoing second-order phase transitions, such as certain manganites. The observed shift in the predicted temperature range can be attributed to factors not included in the mean-field model, such as magnetic inhomogeneities, short-range ordering effects, and



Figure 4: Comparison between the experimental (symbols) and the mean-field generated curves (blue lines) (a) M(H,T) and (b) $-\Delta S_M(T)$ curves for La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite.

more complex magnetic interactions [25]. Despite these challenges, both the mean-field theory and Maxwell's relation continue to serve as valuable methods for analyzing the magnetocaloric effect.

3. CONCLUSION

In conclusion, this study successfully explored the MCE of La_{0.7}Sr_{0.3}Mn_{0.95}Ni_{0.05}O₃ manganite, utilizing the mean-field theory alongside the Law of Approach to Saturation (LAS) to evaluate key parameters (λ, J, g) and M_0). The mean-field theory played a critical role in simulating the isothermal magnetization M(H,T) and magnetic entropy change $-\Delta S_M(T)$ curves, offering valuable insights into the material's magnetocaloric behavior. However, it is important to acknowledge the limitations of the mean-field approach, which oversimplifies the interactions between spins and may not fully capture the complex behavior of real magnetic systems, especially in the presence of long-range interactions or spatial inhomogeneities. Despite these limitations, the mean-field theory provides a solid for initial modeling and framework а deeper understanding of the material's thermodynamic properties, paving the way for more advanced approaches in future studies.

CONFLICTS OF INTEREST

The authors have no conflicts of interest.

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