Estimation of magnetocaloric properties by using Monte Carlo method for AMRR cycle

Ryosuke ARAI[a,c], Ryo TAMURA[b], Akiko Saito[c], Hideki NAKAGOME[c], Takenori NUMAZAWA[a]

[a] National Institute for Materials Science, 3-13 Sakura, Tsukuba 305-0047 [b] National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044
[c] Department of Urban Environment System, Chiba University, 1-33 Yayoicho, Inage ward, Chiba 263-8522

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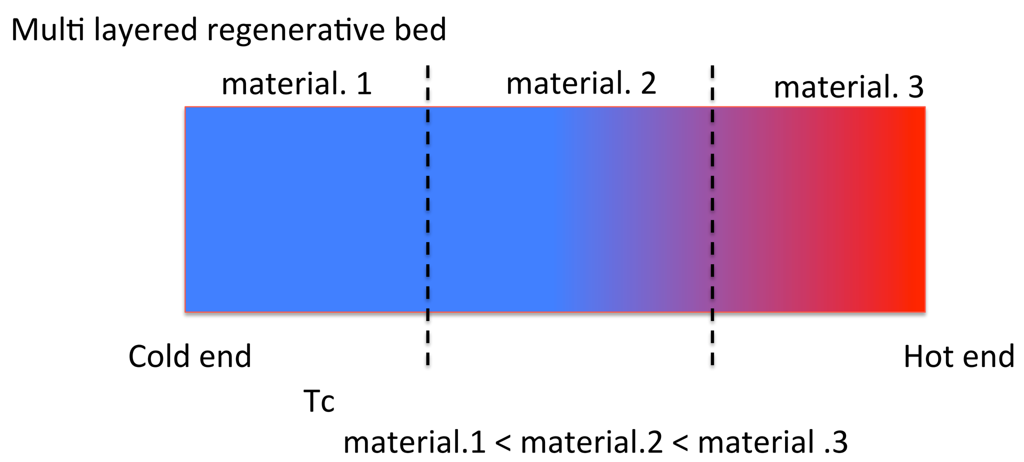
1. Introduction

To achieve wide refrigeration temperature range

Multi layer regenerative bed using some materials they have different Curie temperature



Selection of suitable materials and optimization of laminate configurations are essential to obtain good refrigerating performances. However, it is difficult to produce every kind of materials.

In this study, we examine through calculations the properties of Gd as the ferromagnetic material, which is a typical magnetocaloric material, and the impact on these properties when some of the Gd atoms are substituted for non-magnetic elements.

Objective

Estimating Curie temperatures, specific heat and magnetic entropy changes, using the Monte Carlo method for the material design.

2. Theoretical model

Potts-like model

Hamiltonian

$$\mathcal{H} = -\lambda_{ij} \sum_{\langle i,j \rangle} J_i J_j - g\mu_0 H^z \sum_i J_i$$

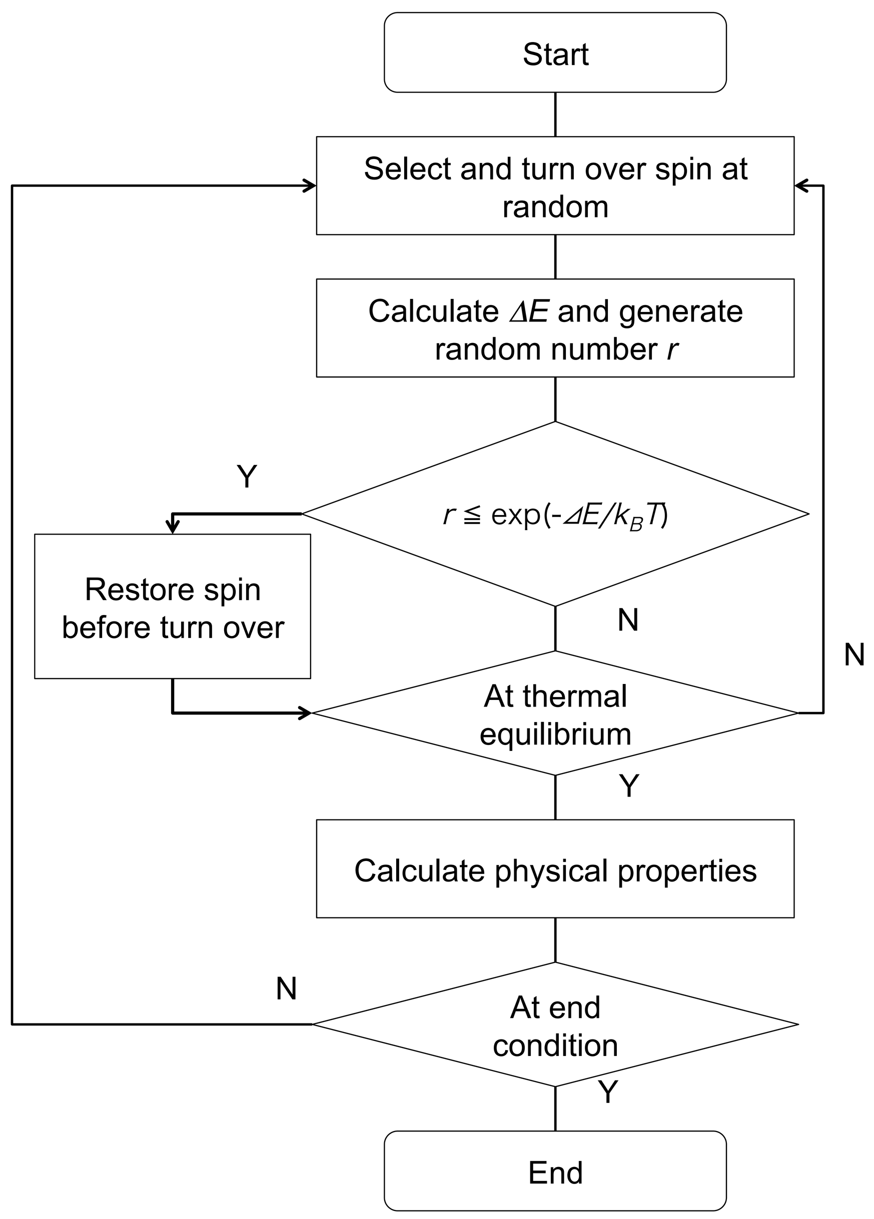
Where J is total angular momentum and takes { $-J$, $-(J-1)$, ⋯ , J }.
g is Lande's factor, μ_0 is Bohr magneton and H^z is external field.

Gd-R alloys

Gd-R alloys is materials such as some of the Gd atoms are substituted for non-magnetic atioms.

In order to express the substitution for non-magnetic elements, we assume crystal structure is same as Gd and some of the sites the lattice points are fixed at $J = 0$ at random. A value converted from the Curie temperature of Gd is used for λ_{ij}.

Algorithm of Monte Carlo method



3. Results and Discussion

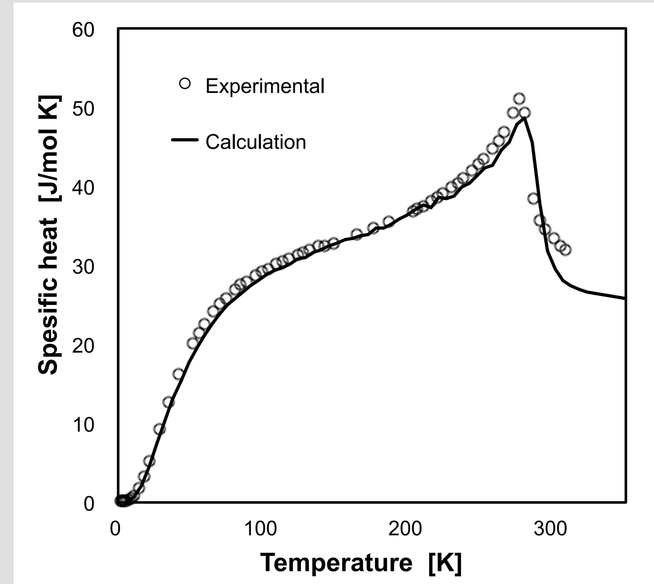
Calculation condition

Parameter	Value
Crystal structure	Hexagonal
Number of site	10^3
Concentration of non-magnetic site	0% and 3%
MCS (steady state)	4000 MCS
MCS (total)	8000 MCS
Number of iteration	30

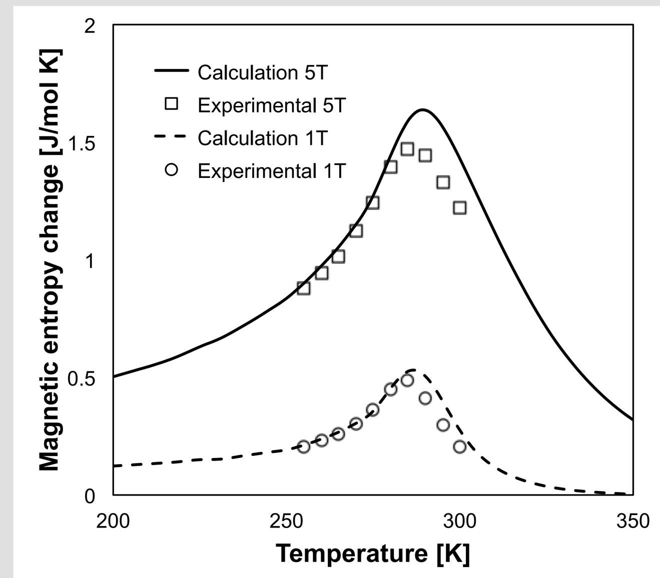
We use λ_{ij} that is calculated from experimental Tc

Result in $Gd_{97}Zr_3$

➢ Specific heat



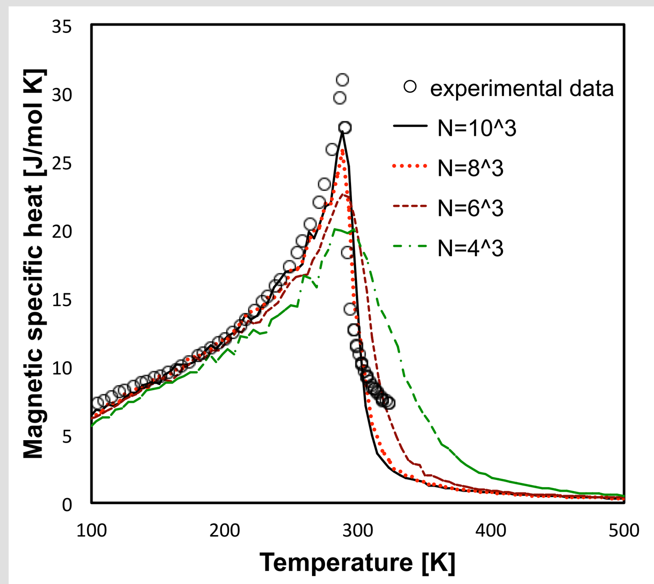
➢ Magnetic entropy change



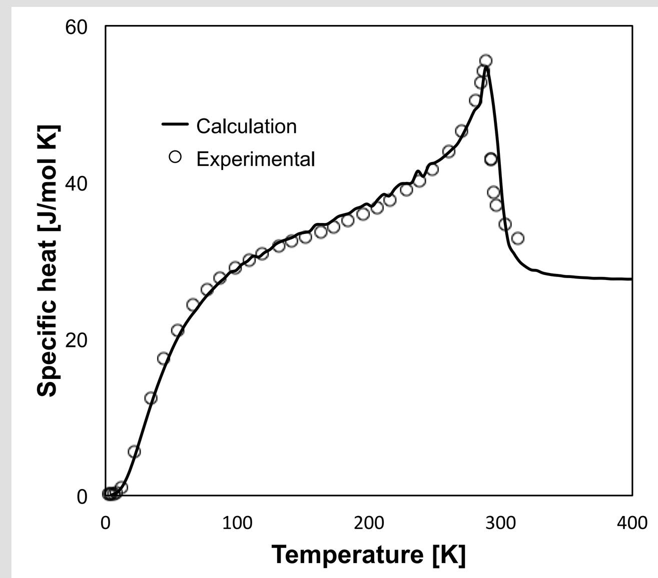
- Peaks of specific heat appear at somewhat higher temperature than experimental result.
- Calculated ΔS_M is bigger than experimental result.
- They are considered that influence of lattice constant by non-magnetic atoms

Result in Gd

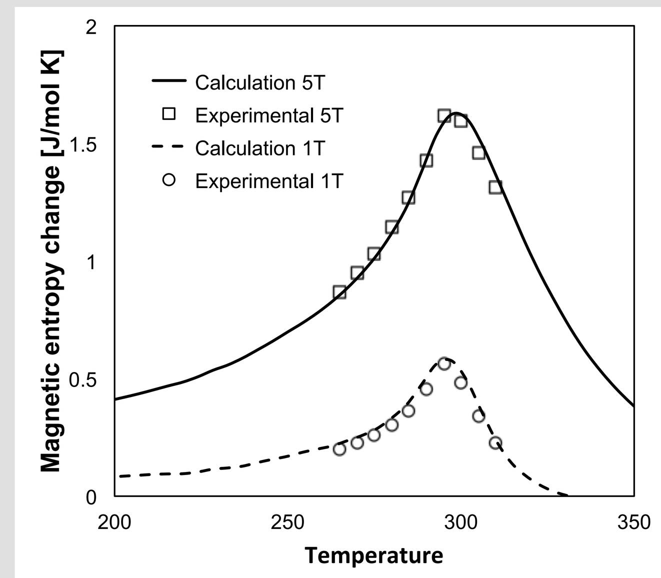
➢ Magnetic specific heat dependence on lattice size



➢ Specific heat



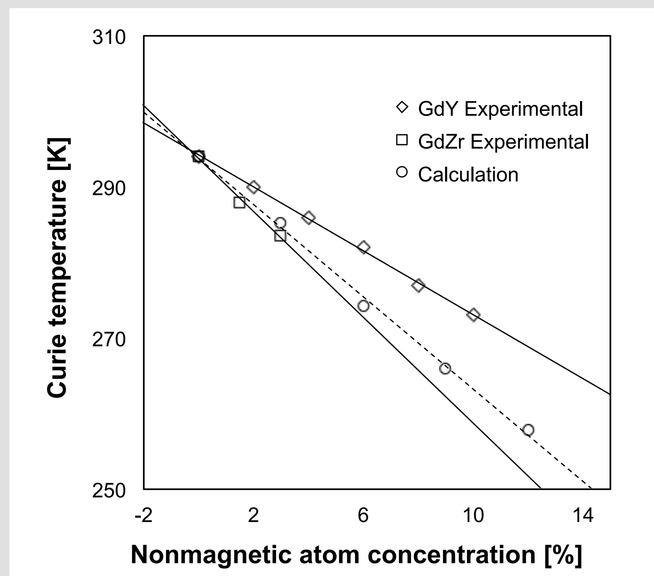
➢ Magnetic entropy change



- It is found that if the lattice size is more than 8^3, the calculated value generally agrees with the experimental value.
- Calculation results are in good agreement with experimental results

Result in other Gd-R alloys

➢ Curie temperature dependence on concentration of non-magnetic atoms



- In both of the experimental and calculated results, the Curie temperature shows a linear decrease with the increase of the non-magnetic element density x.
- The Zr substitution shows a bigger drop in the Curie temperature than Y with an increase in x.
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Conclusion

In this study we examined the estimation of physical properties of magnetic refrigeration materials using the Monte Carlo method. As a result, we obtained the following conclusions:

1) It could be confirmed that the magnetic refrigerant properties of Gd could be calculated with high accuracy with the Potts-like model of the hexagonal crystal system and the Monte Carlo method.
2) The magnetic refrigeration characteristics of Gd-R alloy could generally be reproduced by the calculation in which some of the sites on the lattice points were replaced randomly with non-magnetic sites.
3) In order to estimate the Curie temperature with high accuracy, it is essential to clarify its physical mechanisms to be reflected in the calculation.