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

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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

Algorithm of Monte Carlo method

Potts-like model

Hamiltonian

\[ \mathcal{H} = -\lambda_{ij} \sum_{i,j} J_{i,j} - g\mu_B H \sum_i J_i \]

Where \( J \) is total angular momentum and takes \( \{ J , -J+1, \ldots, -J \} \). \( g \) is Lande’s factor, \( \mu_B \) is Bohr magneton and \( H \) is external field.

Gd-R alloys

Gd-R alloys is materials such as some of the Gd atoms are substituted for non-magnetic atom. 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 \( \lambda_{ij} \).

3. Results and Discussion

Calculation condition

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal structure</td>
<td>Hexagonal</td>
</tr>
<tr>
<td>Number of site</td>
<td>10^6</td>
</tr>
<tr>
<td>Concentration of non-magnetic site</td>
<td>0% and 3%</td>
</tr>
<tr>
<td>MCS (steady state)</td>
<td>4000 MCS</td>
</tr>
<tr>
<td>MCS (total)</td>
<td>8000 MCS</td>
</tr>
<tr>
<td>Number of iteration</td>
<td>30</td>
</tr>
</tbody>
</table>

We use \( \lambda \) that is calculated from experimental \( T_c \).

Result in Gd:

- Magnetic specific heat dependence on lattice size
- Specific heat
- Magnetic entropy change

Result in Gd-R:

- 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 the physical mechanisms to be reflected in the calculation.