Anisotropic magnetocaloric effect of CrI_3

Hung Ba Tran[1,2], Yu-ichiro Matsushita[1,2]

Tokyo Tech., Japan [1], Quemix Inc., Japan [2]

E-mail: tran.h.ag@m.titech.ac.jp

CrI_3 is considered to be a promising candidate for spintronic devices and data storage[1,2]. We derived the Heisenberg Hamiltonian for CrI_3 from density functional calculations using the Liechtenstein formula. Moreover, the Monte Carlo simulations were performed to analyze the effect of magnetic anisotropy energy on the thermodynamic properties. Our method successfully reproduced the negative sign of isothermal magnetic entropy changes when a magnetic field was applied along the hard plane. We found that the temperature dependence of the magnetocrystalline anisotropy energy is not negligible at temperatures slightly above the Curie temperature. We clarified that the origin of this phenomenon is attributed to anisotropic magnetic susceptibility and magnetization anisotropy. We also investigated the magnetic susceptibility that can be used for the characterization of the negative sign of the entropy change in the case of a hard plane. The competition of the magnetocrystalline anisotropy energy and external magnetic field at a low temperature and low magnetic field causes a high magnetic susceptibility as the magnetization fluctuates. Meanwhile, the anisotropy energy is suppressed as a sufficient magnetic field is applied along the hard axis, and the magnetization is fully rotated to the direction of the external magnetic field.

[1] Hung Ba Tran, Hiroyoshi Momida, Yu-ichiro Matsushita, Koun Shirai, and Tamio Oguchi, *Acta Mater*. **231**, 117851 (2022).

[2] Hung Ba Tran, Hiroyoshi Momida, Yu-ichiro Matsushita, Kazunori Sato, Yukihiro Makino, Koun Shirai, and Tamio Oguchi, *Phys. Rev. B* **105**, 134402 (2022).