First-principles study in anisotropic magnetocaloric effect of AlFe₂B₂ beyond Callen-Callen theory Hung Ba Tran^{1,2}, Yu-ichiro Matsushita^{1,2} Tokyo Tech. ¹, Quemix Inc. ²

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It is well known that the temperature dependence of the effective magnetocrystalline anisotropy energy obeys the l.(l+1)/2 power law of magnetization in the Callen-Callen theory. Therefore, according to the Callen-Callen theory, the magnetocrystalline anisotropy energy is assumed to be zero at the critical temperature where the magnetization is approximately zero. This study estimates the temperature dependence of the magnetocrystalline anisotropy energy by integrating the magnetization versus magnetic field (*M*–*H*) curves, and found that the magnetocrystalline anisotropy is still finite even above the Curie temperature in the uniaxial anisotropy, whereas this does not appear in the cubic anisotropy case. The origin is the fast reduction of the anisotropy field, which is the magnetic field required to saturate the magnetization along the hard axis, in the case of cubic anisotropy. Therefore, the magnetization anisotropy and anisotropic magnetic susceptibility, those are the key factors of magnetic anisotropy, could not be established in the case of cubic anisotropy. In addition, the effect of magnetocrystalline anisotropy on magnetocaloric properties, as the difference between the entropy change curves of AlFe₂B₂ appears above the Curie temperature, which is in good agreement with a previous experimental study[1]. This is proof of magnetic anisotropy at slightly above Curie temperature.

[1] "Effect of magnetocrystalline anisotropy on magnetocaloric properties of AlFe₂B₂ compound" Hung Ba Tran, Hiroyoshi Momida, Yu-ichiro Matsushita, Kazunori Sato, Yukihiro Makino, Koun Shirai, and Tamio Oguchi, arXiv:2112.08154/1-23 (2021).