Large-scale simulation of $L1_0$ FePt nanoparticles toward magnetic recording

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$L1_0$ FePt nanoparticle has attracted much attention as a promising material for magnetic recording and nano-magnet applications. In magnetic nanoparticles, the magnetic anisotropy energy is the primary source to stabilize the magnetization against thermal fluctuation. The temperature dependence of the energy barrier in magnetic flips of the nanoparticles can be used to estimate the relaxation time of magnetic nanoparticles [1]. In this study, we perform a large-scale simulation for $L1_0$ FePt nanoparticles by combining first-principles calculations and Monte Carlo simulations. The exponential behavior of the Curie temperature of various nanoparticle sizes is quantitatively reproduced compared with the data observed in the experimental works. Moreover, the surface e ect on magnetic properties of $L1_0$ FePt nanoparticles is clarified by considering the magnetic profile in atomistic Monte Carlo simulations. Furthermore, the temperature and size dependence of the energy barrier for magnetic flips of $L1_0$ FePt nanoparticles is obtained in this work, demonstrating that the critical diameter of nanoparticles for long-term storage is 3.7 nm. Our work can be used as a guide to the experiment on developing the magnetic properties of nano-material applicable for magnetic recording.

[1] H. B. Tran, Y. Matsushita, "*Temperature and size dependence of energy barrier for magnetic flips in $L1_0$ FePt nanoparticles: First-principles study*", DOI: 10.2139/ssrn.4462256 (2023)