The Spontaneous Magnetization Enhancement by the Thermal Fluctuation in a Ferro-antiferromagnetic mixed system: an Atomistic Micromagnetic Simulation Study

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1. Introduction

The couplings between ferromagnetic (FM) and antiferromagnetic (AFM) materials offer interesting and technologically important phenomena such as an exchange bias effect [1]. Recently, Hong *et al.* [2] found a significant enhancement of the spontaneous magnetization (Ms) with temperature in the FM-AFM mixed phase, which is against the general behaviors of known magnetic materials. In this work, we investigate the temperature dependence of the spontaneous magnetization of a FM-AFM mixed system by using atomistic micromagnetic simulations.

2. Simulations

In order to mimic FM-AFM mixed phase, we adopted simple model system in which a FM spherical particle with radius ranging from 2 to 5 nm located inside AFM matrix as shown in Fig. 1(a). The calculation size of a whole system is 5×5×5 nm^3 with a periodic boundary condition along *x*, *y*, and *z*-axes. The face centered cubic (FCC) structure with 2.5 Å-lattice constant was used for both FM and AFM materials. The VAMPIRE package [3] was used to perform atomistic micromagnetic simulation with following material parameters: an atomic moment for both FM and AFM, 1.72 μ_B, the exchange constants J_{FM}= 12.2×10^{-21} J/link and J_{AFM}= 2.7×10^{-21} J/link, the atomic magnetocrystalline anisotropy K = 4.644×10^{-24} J/atom along an easy axis (*z*-axis). It should be noted that, in our atomistic simulations, all atoms are considered as the same material but the exchange interaction between atoms are different according to FM and AFM materials.

The Monte-Carlo method was used to consider the thermal fluctuation, and Ms value for a given temperature was obtained from the averaging of Ms during a hundred of Monte-Carlo calculation steps at a stable stage under a saturation magnetic field with 2 T along the easy axis (+*z* direction).

As shown in Figure 1, the Ms increases with the temperature for the case of FM spheres with D < 3nm, where the AFM interactions are dominant. Figure 2 reveals the physical mechanism of such a significant Ms increment in our simulations; at low temperature, the spin moments in a FM sphere are tilted largely from the applied field direction (+*z* direction) owing to the strong couplings with AFM spins at the interface. As increasing the temperature, the thermal fluctuations of AFM spins are getting larger and it gives rise to the weakening of the FM-AFM couplings. Consequently, FM spins are aligned along the applied field direction and it causes the enhancement of Ms with the temperature.

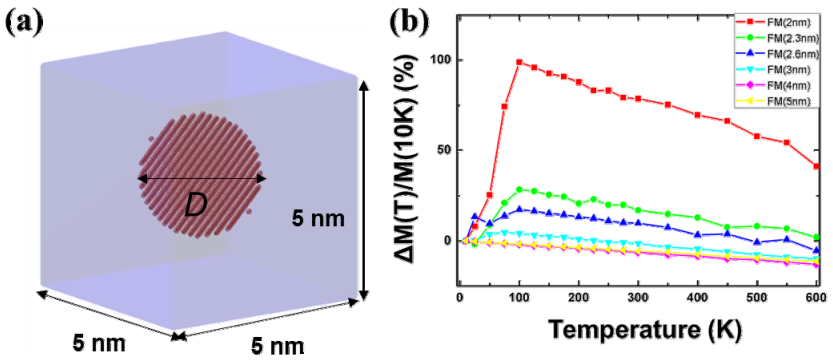

Fig. 1. (a) The model system with FM spherical particle of D = 2.6 nm. (b) The relative value of spontaneous magnetization changes as a function of the temperature.

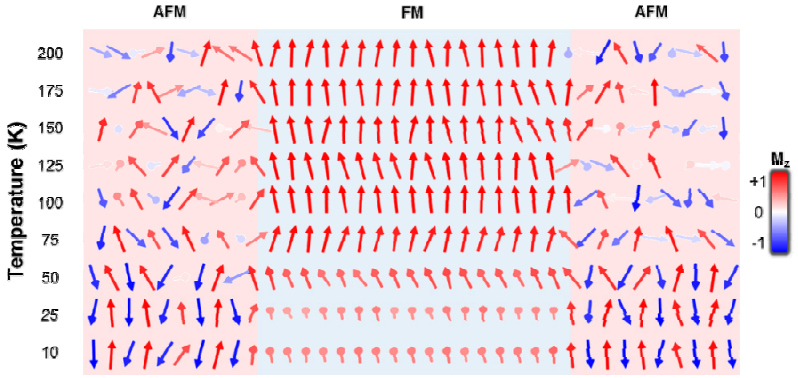

Fig. 2. Atomistic simulation results on the spin arrangement variation by the temperature for D = 2.6 nm.

3. References

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[3] R.F.L. Evans *et al.*, J. Phys. Condens. Matter **26** (2014) 103202.