Spin configuration of Ferromagnetic/antiferromagnetic Nano-composite Core/Shell Particles

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A systematic study of the spin configuration of ferromagnetic(core)/antiferromagnetic(shell) nanocomposite particles was carried out by two approaches: micromagnetic and atomistic simulations. The nano-composite particles considered have a spherical shape with the total diameter of 9.6 nm and are composed of a FM core with the diameter of 4.8 nm, which is covered by an AF shell. The cell size for simulation is chosen to be 0.4 nm, which is close to the lattice constant of both FePt and FeMn. The core parameters are $K_U = 7\times10^7$ erg/cc, $M_S = 1100$ emu/cc, $J_{FM} = 4\times10^{-14}$ erg and the shell ones are $K_{AF} = 1.3\times10^5$ erg/cc, $M_S = 800$ emu/cc, $J_{AF} = -1.2\times10^{-14}$ erg, where K_U is the uniaxial magnetic anisotropy of the FM, K_{AF} the uniaxial magnetic anisotropy of the AF, M_S the saturation magnetization, J_{FM} and J_{AF} the exchange integral of the FM and AF, respectively. The easy axis of both the core and the shell are chosen in the vertical direction. For the investigation of the effect of interlayer coupling, the exchange-coupling constant between FM and AF is varied from 10^{-16} to 10^{-14} erg. The influence of the uniaxial magnetic anisotropy (K_U) of the core on the spin structure is also investigated with K_U changing from 10^4 erg/cc to 7×10^7 erg/cc[1].

Figure 1 is the spin configuration of the core/shell particles with the variation of J_{FM-AF} obtained based on an atomistic model. It is interesting to note that multi-domains are present for all the J_{FM-AF} values, and that the spins at the interface between FM and AF is flopped to each other. This result by an atomistic model is consistent with that for a micromagnetic simulation. Fig.2 shows the spin distribution with various K_U values for $J_{FM-AF} = 4\text{x}10^{-14}$erg calculated based on both Micromagnetic and atomistic simulation. With this strong interlayer coupling, the spin structure obtained from both micromagnetic and atomistic models is similar, although there is a minor difference. This suggests that micromagnetic simulation is valid in the case of strong interlayer exchange coupling. Of interest in Fig. 2 is the changing of the easy axis of the core from horizontal to vertical direction as K_U increases. This can be explained by assuming that the spins of AF and FM favor to be perpendicular in the case of compensated AF as calculated by Koon[2]. Thus when K_U is small, the easy axis of the core is forced to be perpendicular to that of the shell. When K_U and K_{AF} are comparable, the strong coupling causes the FM spin tilted. When K_U is large, then the core anisotropy dominates, causing the spins of the core to be in vertical direction.

In summary, for a strong interlayer exchange coupling between FM and AF, the micromagnetic simulation result is consistent with the atomistic simulation result. However, in the case of weak interlayer exchange coupling the micromagnetic simulation predicts a multi-domain structure of the ferromagnet, being inconsistent with the atomistic simulation. The failure of micromagnetic simulation in describing the spin structure of the nano-composite particles might be interpreted in terms of the under-estimation of the exchange energy for rapid spatial fluctuations of the magnetization by the continuum exchange formalism or might be due to the cooling process procedure.

References: [1] Nguyen N.Phuoc, T.Suzuki, Roy Chantrell and Uli Nowak, *phys.stat.sol.(b)* 244, 4518 (2007).
[2] N.C. Koon, *Phys. Rev. Lett.* 78, 4865 (1997).

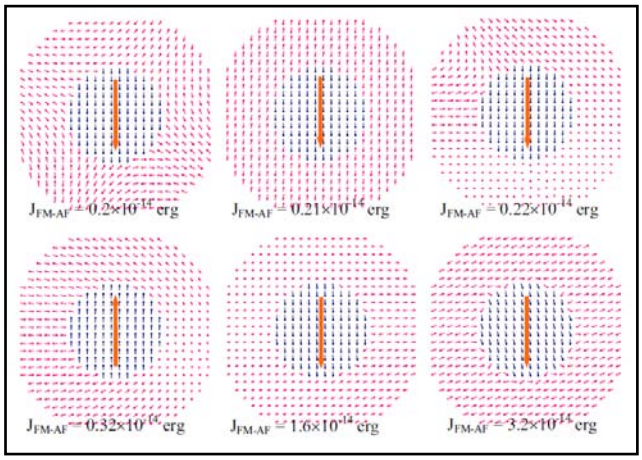

Fig.1 Spin configuration for a core(FM)/shell(AF) nano particles for various J_{FM-AF} values.

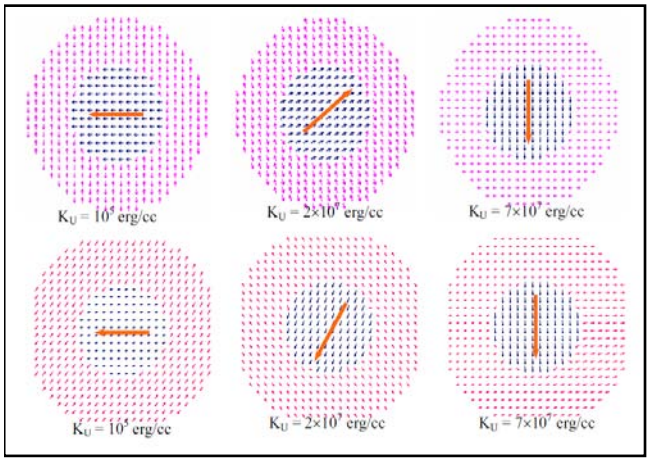

Fig.2 Spin configuration with various Ku based on Micromagnetic (upper) and atomistic simulation(lower).