Japan Geoscience Union Meeting 2011
(May 22-27 2011 at Makuhari, Chiba, Japan)

SEM001-04 会場:301B 時間:5 月 26 日 09:19-09:36

Mean-field and micromagnetic models for nanoscale magnetism based on ilmenite-hematite solid solutions
Mean-field and micromagnetic models for nanoscale magnetism based on ilmenite-hematite solid solutions

Karl Fabian[1*], Suzanne A. McEnroe[1], Peter Robinson[1], Valera P. Shcherbakov[2]
Karl Fabian[1*], Suzanne A. McEnroe[1], Peter Robinson[1], Valera P. Shcherbakov[2]

[1]Geological Survey of Norway, [2]Geophysical Observatory Borok, Russia
[1]Geological Survey of Norway, [2]Geophysical Observatory Borok, Russia

Lamellar magnetism was proposed as a new type of magnetic remanence, carried by uncompensated magnetic layers at interfaces between nanoscale exsolution structures of antiferromagnetic (AFM) hematite and paramagnetic ilmenite. A first experimental proof that the natural remanent magnetization (NRM) of a rock from Modum, Norway, is due to lamellar magnetism, resulted from cooling grains with the original NRM to 5 K, and then measuring their hysteresis loop. The observed large shift of the hysteresis curves showed that exchange bias develops from the untreated NRM. Therefore, the moments which carry the NRM participate in the exchange coupling at the hematite-ilmenite interfaces. The development of physical models to understand the detailed mechanisms of exchange bias and other unusual magnetic properties within homogenous or exsolved minerals of the ilmenite-hematite solid-solution series IlmX (X FeTiO3 (1-X) Fe2O3) is an important research topic. In a general case of isolated nanoparticles embedded in an antiferromagnetic matrix the mechanism of exchange bias originates from the formation of a (quasi)spherical domain wall inside the AF matrix when the particle moment rotates under the influence of an external magnetic field. Micromagnetic calculations show that for isolated nanodots the energy of this domain wall increases nearly quadratically with the deflection angle of the nanodot moment. By introducing the corresponding quadratic energy term in a modified Stoner-Wohlfarth model, a two-parameter family of hysteresis loops is obtained, depending on scaled anisotropy energy and field direction. In case of pure solid solutions, geometric mean-field models implement the varying Fe and Ti concentrations, and the random distribution of Fe ions in the solid solutions. The models either use statistical interactions between sites, whereby they effectively average over all possible configurations, or they describe specific random configurations. Statistical mean-field models are successful in predicting the ferromagnetic (FM) Curie temperatures TC and Ms(T) curves of the IlmX solid solutions. The results depend on the choice of interaction coefficients, which either have been determined by neutron diffraction measurements (Samuelson and Shirane, 1979), by Monte Carlo model fits (Harrison, 2006), or by density-functional theoretic calculations (Nabi et al., 2010) . A special class of mean-field modelling has been suggested by Ishikawa (1957), to estimate the size of interacting clusters in IlmX beyond the FM percolation threshold ($X > 87$), where global ferrimagnetic order breaks down, and only finite ferrimagnetically ordered clusters generate a pseudo-Langevin magnetization curve at temperatures between the FM Curie temperature and the antiferromagnetic Neel temperature TN. Using a numerical inversion method, it is possible to fit measured hysteresis loops of synthetic IlmX samples (X= 92, 97) by improved theoretical pseudo-Langevin curves which depend on cluster-size- and exchange-interaction- distributions. Due to frustrated exchange interactions, the IlmX system can show magnetic spin-glass behaviour at low temperatures, which cannot be modeled by mean-field methods. At T=0, however, the Heisenberg hamiltonian of the spin system has only a finite number of possible values and can be minimized by combinatorial optimization. This at least makes it possible to gain some limited insight into the magnetic behaviour at very low temperatures.

Apart from statistical mean-field models, it is also possible to investigate specific atomic configurations, each corresponding to some fixed Ilm X. These models contain several tens to hundreds of ilmenite unit cells (e.g. 3x3x3 or 5x5x5) with periodic boundary conditions. Their main advantage is that they permit visual inspection of the geometric configuration in relation to the magnetic behaviour.

キーワード: lamellar magnetism, micromagnetic modeling
Keywords: lamellar magnetism, micromagnetic modeling