Mapping of theoretical approach in magnetics

– coarse graining theory–

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Nowadays, the objects for magnetics are spreading to various fields. Under those circumstance, the requirements to theoretical analysis increase, i.e. a simple modeling, numerical prediction, etc. Besides, the requests such as materials predictions based on the data base analysis called “materials informatics” or “material genome” become strong, too.

Generally, from a viewpoint of magnetics, it is necessary to understand the magnetization distribution and/or a magnetization process in devices and materials. In this sense, the micromagnetics theory is convenient to understand the side view of the phenomenalism. However, that theory is insufficient to define the exact property, because it does not include self-consistency of theory. To obtain the accurate magnetic property, the knowledge from a microscopic theory should be required.

For the discussion of magnetization state, the magnetic energy can be defined by following procedure,

1) Spin–spin interaction (including the exchange interaction, spin transfer) is evaluated within a framework of electric theory.
2) The magnetic anisotropy constant is evaluated within a framework of first principles calculation for certain materials.
3) The magnetic dipole interaction is generally evaluated by the numerical calculation of a classical spin model.
4) The thermo-dynamic behavior of magnetization is evaluated by the statistical average of a classical spin model.

Then, the obtained magnetic energies reflect onto the micromagnetics calculation. At this point, the atomistic calculation is ready to carry out.

However, to analyze the entire body of materials and devices, the atomistic calculation needs to expend too much computational resources. In this sense, it is required well defined coarse graining theory for connecting atomistic calculations and conventional micromagnetics calculations.

In terms of energy evaluation 3), the multipole expansion method naturally deals with the magnetic dipole interaction, in which the contribution from the distant part is averaged over a certain volume. For 4), the formulation of the Landau-Lifshitz-Bloch equation is suggested[1)], which includes the degree of freedom for permitting the expansion and

contraction of the magnetization vector. For 1), the method of single spin approximation[2)] is one of the candidate to deal with the exchange interaction between the textured grains. Finally, for 2), the conversion from a single site anisotropy to the expression of energy density form simply satisfies the coarse graining.

Reference

1) D. A. Garanin: "Fokker-Planck and Landau-Lifshitz-Bloch equations for classical ferromagnets", *Phys. Rev. B*, **55**, 3050 (1997)

2) S.-J. Lee, S. Sato, H. Yanagihara, E. Kita, C. Mitsumata: "Numerical simulation of random magnetic anisotropy with solid magnetization grains", *J. Magn. Magn. Mater.*, **323**, 28 (2011)