Materials Science of Permanent Magnets and Its Applications– The Output of Elements Strategy Initiative Center for Magnetic Materials (ESICMM)

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The materials science of permanent magnets that ESICMM pursues is for realization of the ultimate performance of hard magnetic materials and includes atomistic coercivity theory to make possible the true structural engineering based on atomistic understandings of structure-property relations. Also aimed at is a systematic thermodynamic basis for rational processing of the microstructure suggested from the theoretical studies. Multi-aspect structural analyses are the key elements for this purpose and theoretical and experimental searches for new compounds are another important element.

The atomistic theory of coercivity by now is able to compute the energy barriers of non-uniform magnetic reversals at finite temperatures, using atomistic spin models of hard magnetic compounds with the atomistic magnetic parameters and couplings obtained from the first-principles calculations[1]. The spin models are used also in stochastic micromagnetic simulations for time-dependent coercivity phenomena and in analyses of the influences of structural defects associated with surfaces and interfaces on the magnetic reversal behaviors. On the other hand, the size scale that finite element micromagnetic simulations, to which the atomistic simulations are to be connected, has reached to the micrometer realm with keeping mesh size comparable to the exchange length.

The thermodynamic basis of permanent magnets has grown from almost nonexistence to a state being able to assign the Nd-Fe-Cu-B-O system to discuss effects of microalloyed Cu and unavoidable impurity O on microstructural formation mechanisms, owing to combined experimental and computational construction of the data base for CALPHAD-type calculations. Dynamic aspects of non-equilibrium structural formation is investigated using the phase-field analyses, from which thermodynamic parameters such as diffusion constants and interfacial energies can be estimated.

Methods and techniques to analyze structure-property relations have acquired new members: First order recoil curve (FORC) analysis, X-ray scanning spectromagnetic microscope, and small angel neutron scattering, with which coercivity mechanisms can be studied from multiple aspects in addition to the STEM-EDS studies that have determined structure and chemistry of grain boundary (GB) phases[2], leading to advanced GB infiltration alloys for Dy-free Nd-Fe-B with less reduction in B_r.

The search of new hard magnets over both rare earth and non-rare-earth categories has added the $Sm(Fe\text{-}Co)_{12}$ compounds that have superior saturation magnetizations, anisotropy fields, and Curie temperatures[3] to the objective materials on each of which the ultimate performance shall be pursued.

Achievements mentioned above are credited to ESICMM Principal Investigators; T. Abe, Y. Gohda, K. Hono, T. Koyama, T. Miyake, T. Nakamura, T. Ohkubo, S. Okamoto, K. Ono, S. Miyashita, S. Sugimoto, YK. Takahashi, T. Teranishi, H. Tsuchiura, S. Tsuneyuki, and their colleagues.

Bibliography

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[3] Y. Hirayama, YK. Takahashi, S. Hirosawa, K. Hono, Scripta Mater. **138**, 62 (2017).

External links : http://www.nims.go.jp/ESICMM/research/index.html.