



CEA – Saclay, 91191 Gif-sur-Yvette Cedex

**Service de Physique de l'Etat Condensé - UMR 368**

**VISIO SÉMINAIRE**

**Mercredi 20 janvier 2021 à 11h**

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## **Challenges to the coercivity of Nd-Fe-B magnet**

The magnet, i.e., the permanent magnet, is a familiar material, and plays important roles in many products such as electric motor and recording material. Analyses on its mechanism and improvements of the performance have been studied extensively. In particular, it is very important to study its temperature dependence. However, when we study the problem by methods of current physics, there are difficult problems. Here we introduce our trials on this problem for the high-performance Nd<sub>2</sub>Fe<sub>14</sub>B magnet, and study various types of hysteresis phenomena.

First, we constructed an atomistic Hamiltonian to take into account the temperature property [1]. With it, we calculated various thermodynamic quantities such as the magnetization and anisotropy energies by standard methods of statistical physics and confirmed the model can reproduce experimental results. Moreover, the domain wall profiles and the spectrum of FMR (ferromagnetic resonance) were also studied. As a merit of the atomistic model, we can find anisotropy due to the crystal structure and also atom-specific ordering properties.

The important property of magnets is the coercivity. Although we have studied quantum effects on the metastability [2], coercivity of classical magnets is still a challenging problem. In contrast to the above-mentioned thermodynamic quantities, we do not have theoretical formula for coercivity, and thus so far only little study has been done on the quantitative estimation of the coercivity at finite temperatures. Coercivity is a kind of spinodal phenomena. In systems of short-range interaction, however, there is no spinodal singularity at finite temperatures due to the nucleation. Therefore, we must study “spinodal-like” phenomena [3]. We first studies this problem in nano-size grains by the stochastic LLG equation [4] and also by a method using the free-energy landscape obtained by Wang-Landau method [5]. We obtained the strength of field at which the relaxation time of the magnetization is 1s (a definition of coercivity), and its temperature dependence. For larger grains, the dipole-dipole interaction plays a role and the so-called multidomain magnetic structure appears. To study such cases, we developed a modified SCO (stochastic cutoff) method and studied coercivity in such systems [6]. The magnet is an ensemble of grains. Trials for such complicated case is also introduced.



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