Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Multiscale Simulations Toward Predicting Temperature Dependent Properties of Magnetic Materials

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2018 - 2019

Project Areas
Materials Science

Clusters
Lichtenberg Cluster Darmstadt

Software
VASP, OpenMX, VAMPIRE, OOMMF

Institute
FG Mechanik Funktionelle Materialien

University
Technische Universität Darmstadt

Introduction

Magnetic materials have been widely used in the modern society due to their intriguing functional properties. For example, permanent magnets with high coercivity, remanent magnetization, and energy product are not only the strategic materials for the energy turnaround, but also the essential components in modern wind turbines and hybrid vehicles. By using the spin or magnetism to store and process information, nanomagents are necessary for high-performance spintronics. The functional performance of magnetic materials is dependent on not only the intrinsic property but also the extrinsic microstructure. The interface charge mediated voltage control of magnetization is localized near the interface, but the voltage-induced magnetization switching behavior should be studied in the bulk level.

Methods

As an essential complementarity to the experimental study, the simulation work can provide fruitful information on designing experiments, optimizing microstructures, revealing the underlying mechanism, etc., and thus enhance the research efficiency. In this project, we perform atomistic simulations to make a better bridge between first-principles calculations and micromagnetic simulations and study the parameters transfer among different level simulations. In the proposal period, we

have performed first-principles and micromagnetic study in Nd-Fe-B magnets [1] and Sm-Co magnets [2], the charge/strain-mediated voltage control of magnetization switching dynamics [3,4], pure micromagnetic simulations on the magnetic reversal process in grain boundary diffused Nd-Fe-B magnets [5], as well as the atomistic spin simulations of temperature-dependent properties od $Nd_2Fe_{14}B$ and $Nd_2Fe_{14}B$/Fe [6].

Outlook

For the next year's proposal, we will continue to perform atomistic simulations to make a better bridge between first-principles calculations and micromagnetic simulations, with more focus on temperature dependent magnetic properties and magnetoelectric coupling.

Reference

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