Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Calculating Temperature Dependent Properties of 2D Magnets

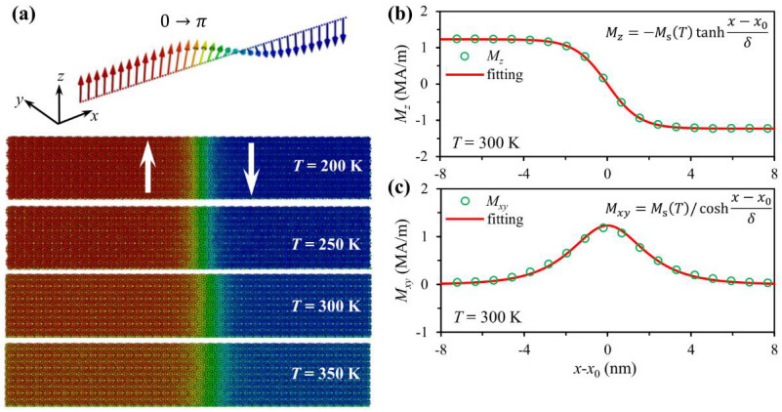

Figure 1: Calculated temperature dependent domain wall configuration in $Nd_2Fe_{14}B$.

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Project Term
2020 - 2021

Clusters
Lichtenberg Cluster Darmstadt

Software
VASP, VAMPIRE, OOMMF

Additional Software
MUMAX, MOOSE

Institute
Materials Science

University
Technische Universität Darmstadt

Introduction

Predicting the temperature dependent properties of magnetic materials is still challenging, which cannot be dealt with first-principle calculations and micromagnetic simulations alone. A multiscale scheme combining first-principles calculations, atomistic spin model simulations, and micromagnetic simulations should be utilized. The computation is across scale and is thus extremely expensive, requiring the computation source from high-performance computer (HPC).

Methods

We use a multiscale scheme which combines zero-K first-principles calculations, atomistic spin model simulations, and micromagnetic simulations.

Results

- We have predicted the temperature-dependent intrinsic magnetic properties of $Nd_2Fe_{14}B$ by multiscale simulation integrating ab initio calculations and atomistic spin model simulations.
- We have calculated the high-temperature magnetic properties of Nd-Fe-B permanent magnets with the consideration of microstructures by multiscale simulation integrating ab initio calculations, atomistic spin model simulations, and micromagnetic simulations.
- We have applied the temperature-dependent micromagnetic simulations combining phenomenological state of equation for the calculation of magnetocaloric effect in Co_2B magnetic materials.

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Discussion

Temperature-dependent magnetic properties of $Nd_2Fe_{14}B$ permanent magnets, i.e., saturation magnetization $M_s(T)$, effective magnetic anisotropy constants $K^{eff}i(T)$ (i = 1, 2, 3), domain-wall width $\delta_w(T)$, and exchange stiffness constant $A_e(T)$, are calculated by using ab initio informed atomistic spin model simulations. This work provokes a scale bridge between ab initio calculations and temperature- dependent micromagnetic simulations of Nd-Fe-B permanent magnets.

A computational scheme integrating the atomistic spin model (ASM) and micromagnetic simulations is proposed to predict the coercivity of Nd-Fe-B permanent magnets at high temperatures. With the ASM results as input, finite-temperature micromagnetic simulations based on the stochastic Landau-Lifshitz-Gilbert equation are performed to calculate the magnetic reversal and coercivity (H_c) at high temperatures.

We propose a calculation scheme which integrates micromagnetic simulations and the Arrott–Noakes equation for the investigation of the influence of microstructure and magnetocrystalline anisotropy on the magnetocaloric effect (MCE) in second-order magnetic phase transition materials. More extensive calculations with more complex microstructures, including different grain sizes, shapes, and orientations as well as different grain boundary properties have to be performed to gain further insight on the relation between microstructure and MCE.

Reference

Sabet, S.; Moradabadi, A.; Gorji, S.; Yi, M. et al. Impact of interface structure on magnetic exchange coupling in MnBi/FexCo1−x bilayers. Physical Review B 2018, 98 (17), 174440.
https://doi.org/10.1103/PhysRevB.98.174440

Yi, M.; Xu, B.-X.; Müller, R.; Gross, D.: Strain-mediated magnetoelectric effect for the electric-field control of magnetic states in nanomagnets. Acta Mechanica 2019, 230 (4), 1247–1256.
https://doi.org/10.1007/s00707-017-2029-7

Gong, Q.; Yi, M.; Evans, R.F.L.; Xu, B.-X.; Gutfleisch, O.: Calculating temperature-dependent properties of permanent magnets by atomistic spin model simulations. Physical Review B 2019, 99 (21), 214409.
https://doi.org/10.1103/PhysRevB.99.214409

Gong, Q.; Yi, M.; Xu, B.-X.: Multiscale simulations toward calculating coercivity of Nd-Fe-B permanent magnets at high temperatures. Physical Review Materials 2019, 3 (8), 084406.
https://doi.org/10.1103/PhysRevMaterials.3.084406

Yi, M.; Xu, B.-X.; Gutfleisch, O.: Computational study on microstructure evolution and magnetic property of laser additively manufactured magnetic materials. Computational Mechanics 64 (4), 917–935.
https://doi.org/10.1007/s00466-019-01687-2

Molina-Luna, L.; Wang, S.; Pivak, Y.; Zintler, A.; Pérez-Garza, H.H.; Spruit, R.G. ; Xu, Q.; Yi, M.; Xu, B.-X.; Acosta, M.: Enabling nanoscale flexoelectricity at extreme temperature by tuning cation diffusion. Nature communications 2018, 9 (1), 1-8.
https://doi.org/10.1038/s41467-018-06959-8

Yang, Y.; Ragnvaldsen, O.; Bai, Y.; Yi, M.; Xu, B.-X.: 3D non-isothermal phase-field simulation of microstructure evolution during selective laser sintering. npj Computational Materials 2019, 5, 81.
https://doi.org/10.1038/s41524-019-0219-7

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