Atomistic model study on thermodynamic properties of $(Nd_{1-x}Dy_x)_2Fe_{14}B$ and dysprosium substitution effect on coercivity in neodymium permanent magnets

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Abstract:

Neodymium (Nd) magnets ($Nd_2Fe_{14}B$) are key materials for achieving high energy conversion efficiency. The coercive force (field) of the magnets is often enhanced by adding dysprosium (Dy), particularly at high temperatures. To better understand the magnetic properties of Dy-substituted systems and the underlying mechanisms of coercivity enhancement, it is essential to investigate both the thermodynamic properties and dynamic behavior of $(Nd_{1-x}Dy_x)_2Fe_{14}B$ from a microscopic perspective.

To this end, we have recently developed an atomistic modeling approach [1–3]. This approach realistically incorporates the microscopic details of magnetic parameters and lattice structure while properly accounting for temperature effects, including thermal fluctuations, based on statistical mechanics. Using atomistic models with microscopic parameters estimated from first-principles calculations, we carried out a detailed investigation of the thermodynamic properties of $(Nd_{1-x}Dy_x)_2Fe_{14}B$. Our simulations successfully reproduced key experimental trends, including the temperature and field dependences of various properties, as well as changes in the spin-reorientation temperature. We present these findings along with magnetization profiles of the constituent atoms.

Furthermore, we explored the microscopic origin of the coercivity enhancement observed in Dy-substituted Nd magnets. Through an analysis of the crystal electric field energy of the rare-earth atoms in the Dy-substituted Nd magnet model, we found that the Dy atoms exhibit the anisotropy energy that remains stable with increasing temperature (Fig.1). This property significantly enhances coercivity, particularly at high temperatures [2,3]. Finally, we discuss future prospects for atomistic modeling, including its relationship to micromagnetic simulations and machine learning approaches.

References

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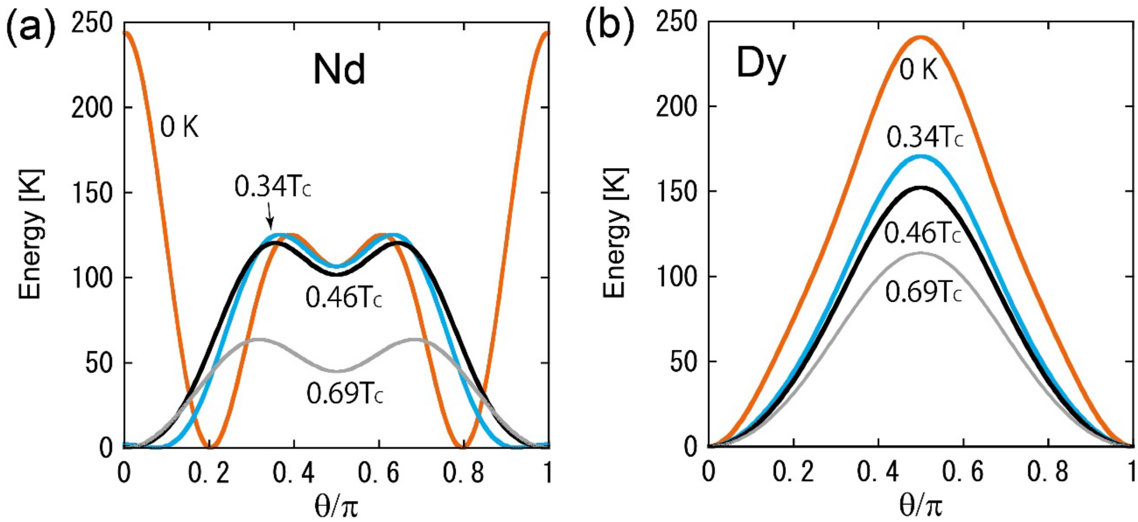

Fig. 1 Crystal electric field energy (a) for a Nd atom and (b) for a Dy atom at zero and finite temperatures.