First-principles study of Nd-magnet microstructure interfaces with the K computer

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It is indispensable to consider microstructure effects in evaluating the performance of permanent magnets, because the main phase of magnets, such as neodymium magnets, has a low density of intrinsic defects resulting in the absence of pinning for the domain-wall motion. Thus, the interface between the main phase and a subphase becomes a key to prevent the penetration of the domain wall into the main phase. In the present study, we investigate the atomic configuration and the local magnetic properties of the microstructure interfaces in the Nd-Fe-B magnets by large-scale first-principles calculations on the K computer.

The addition of Cu to Nd-Fe-B magnets has been demonstrated experimentally to be effective in enhancing the coercivity, where a lower melting temperature of Nd-Cu alloy results in the enhancement of the microstructure quality. However, direct effects of Cu atoms on the magnetic properties are not clarified. Thus, in this study, we performed large-scale first-principles calculations on the K computer using the OpenMX code to investigate the effects of Cu, in particular, on the local magnetic anisotropy [1,2]. As the subphase, we considered the NdO_x phase, where the Nd sublattice has the fcc structure. As Fig. 1 shows, we identified the stable Cu positions around the interface by comparing the formation energies. Moreover, we confirmed that the Cu becomes less stable in existing deep inside the main phase or the subphase. We also found that Cu atoms at a stable atomic position contribute to enhanced local magnetic anisotropy of the main-phase Nd atom close to Cu (Fig. 1).

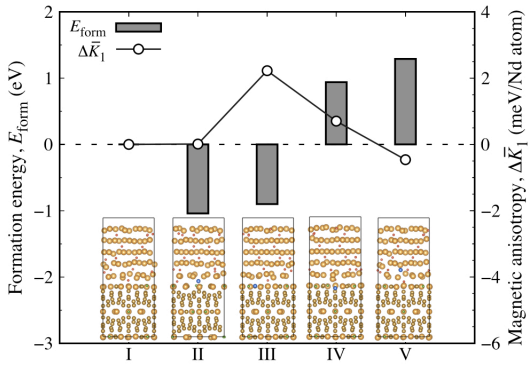

Fig. 1 : Formation energies and the changes in the Nd local magnetic anisotropy.

References

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