Abstract Submitted
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Theoretical study of local magnetocrystalline anisotropy of ε-Fe_2O_3[1] DAISUKE HIRAI, Dept. Phys., Univ. Tokyo, SHINJI TSUNEYUKI, Dept. Phys., Univ. Tokyo and ISSP, Univ. Tokyo, YOSHIHIRO GOHDA, Dept. Mater. Sci. Eng., Tokyo Tech — Magnetocrystalline anisotropy (MCA) is positively correlated with corercivity that is one of important magnetic figures of merit for applications such as high-density magnetic recording media, high-frequency electromagnetic wave absorbers, and permanent magnets. In general, MCA is given for an entire phase of a material. In light of materials engineering, however, MCA information at respective atoms in crystals is useful to identify weak parts for possible nucleation cores of magnetic reversal and design the local MCA. Considering these facts, we examined the local MCA of hard magnetic materials on the basis of density functional theory and the second perturbation theory on spin-orbit interaction [1]. We studied the magnetic properties of ε-Fe_2O_3, which shows the largest coercivity among all the metal oxides [2]. Particularly, we tried to elucidate the effect of an oxygen vacancy on the magnetic properties. As a result, we clarified that the vacancy enhances both the magnetic moment and MAE.

[1] Z. Torbatian et al., Appl. Phys. Lett. 104, 242403 (2014);
[2] S. Ohkoshi *et al.*, Bull. Chem. Soc. Jpn. **86**, 897 (2013).

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