Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Hyperfine fields of Fe in $Nd_2Fe_{14}B$ and $Sm_2Fe_{17}N_3$[1] HISAZUMI AKAI, Univ of Tokyo, MASAKO OGURA, Osaka Univ — High saturation magnetization of rare-earth magnets originates from Fe and the strong magnetic anisotropy stems from f-states of rare-earth elements such as Nd and Sm. Therefore the hyperfine fields of both Fe and rare-earth provide us with important pieces of information: Fe NMR enable us to detect site dependence of the local magnetic moment and magnetic anisotropy (Fe sites also contribute to the magnetic anisotropy) while rare-earth NQR directly give the information of electric field gradients (EFG) that are related to the shape of the f-electron cloud as well as the EFG produced by ligands. In this study we focus on the hyperfine fields of materials used as permanent magnets, $Nd_2Fe_{14}B$ and $Sm_2Fe_{17}N_3$ from theoretical points of view. The detailed electronic structure together with the hyperfine interactions are discussed on the basis of the first-principles calculation. In particular, the relations between the observed hyperfine fields and the magnetic properties are studies in detail. The effects of doping of those materials by other elements such as Dy and the effects of N adding in $Sm_2Fe_{17}N_3$ will be discussed.

[1]This work was supported by Elements Strategy Initiative Center for Magnetic Materials Project, the Ministry of Education, Culture, Sports, Science and Technology, Japan.

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Date submitted: 13 Nov 2014 Electronic form version 1.4