Site preference of dopant elements in rare-earth permanent magnets

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Rare-earth permanent magnets (REPM's) fabricated on the basis of Nd-Fe-B alloys have a problem in temperature resistance of magnetic properties due to the relatively low Curie temperature at 585K of the main-phase compound $Nd_2Fe_{14}B$ and sometimes need expensive elements like Dy in industrial applications for traction motors of electric vehicles to supplement the high-temperature performance. It is desirable to raise the Curie temperature, enhance the temperature resistance of magnetic properties, or/and avoid expensive elements in REPM. While prospective $SmFe_{12}$-based REPM could provide an ideal answer to all of the above wished requests, addition of extra elements seems to be unavoidable to ensure the structural stability of the particular 1:12 crystal structure, among which one of the most typical ones is Ti, yielding $RFe_{11}Ti$ compounds. Here the best compromise in the tradeoff between ferromagnetism and structure stability is pursued. In order to estimate the best possible magnetic performance in the operation temperature range of the REPM compounds, we inspect from first principles the intrinsic magnetic properties and energetics for the site preference of dopant elements in $Nd_2Fe_{14}B$ [1] and in RFe_{12} (R=Sm and Nd) partly aided by experimental data obtained by neutron scattering experiments. We put a focus on the effect of dopant elements on the exchange couplings between rare-earth and Fe-group elements which basically put the most stringent constraint on the utility of the main-phase ferromagnet [2]. Contrasting trends between Ti and Co in the preferred sites are elucidated referring to the magnetic exchange couplings between dopant and host atoms. Implications of those numerically and experimentally observed trends on the robustness of localized magnetic moments on Fe all through the sample fabrication processes are discussed. The best compromise with $Sm(Fe,Co)_{11}Ti$ and $Nd(Fe,Co)_{11}TiN_x$ is inspected.

References

1) MM, preprint [arXiv:1812.10945].
2) MM, H. Akai, Y. Harashima, S. Doi, and T. Miyake, J. Appl. Phys. **119**, 213901 (2016).