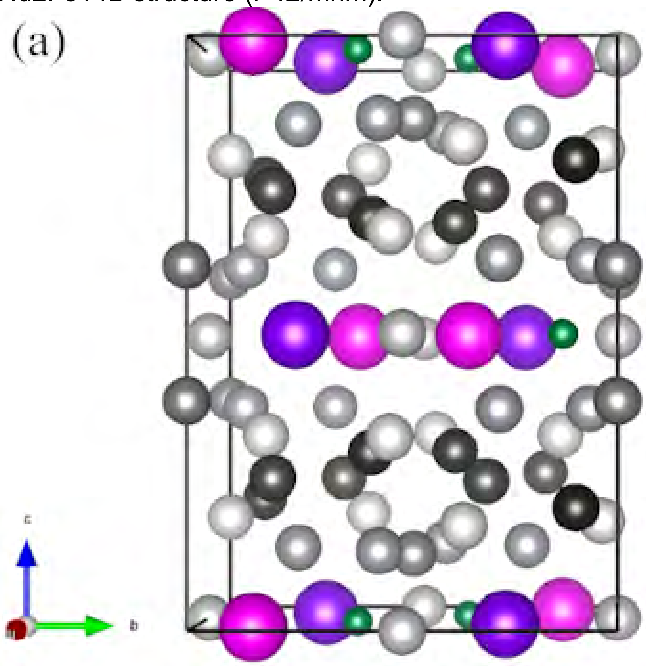
MS13-1-25 Development of cost-effective NdFeB permanent magnets by partial substitution of Ce and La #MS13-1-25

C.H. Kronbo [1], B.B. Iversen [1]
[1]Aarhus University - Aarhus (Denmark)

Abstract
$Nd_2Fe_{14}B$-based permanent magnets have been widely used for the last three decades as key components in many applications. We are working in collaboration with the global pump company Grundfos, who are using $Nd_2Fe_{14}B$-based permanent magnets in their motors driving their pumps, on developing $Nd_2Fe_{14}B$-based magnetic materials using low-cost, abundant materials such as Ce and La to substitute for Nd and thereby reducing the environmental footprint.
The crystal structure of $Nd_2Fe_{14}B$ is tetragonal with space group $P4_2/mnm$ and has six distinct Fe sites, two distinct Nd sites and one B site. The atomic structure, seen in Figure 1a, is layered with the atomic layers arranged perpendicular to the *c*-axis. The magnetic structure of $Nd_2Fe_{14}B$ adopts a ferromagnetic ordering at room temperature with the easy axis parallel to the *c*-axis. $Nd_2Fe_{14}B$ possesses a theoretical energy product as large as 64 MGOe and a Curie temperature of 585 K [1] which arise from exchange coupling between the magnetic moment of the rare-earth elements and the transition metals. Substituting Nd with other rare-earth elements such as Ce, or La creates isomorphic structures to the pure $Nd_2Fe_{14}B$ [2] but yield changes to the magnetic properties. Substitution with Ce and La is inevitably accompanied with magnetic dilution due to inferior intrinsic magnetic properties of $(Ce,La)_2Fe_{14}B$ but on the other hand reduces the environmental footprint. Ce in $Ce_2Fe_{14}B$ is in a mixed valence state (Ce^{3+}/Ce^{4+}) giving it one unpaired electron in the 4*f* orbital in the 3+ state and zero unpaired electrons in the 4+ state thus Ce needs to be in the 3+ state to contribute to the magnetic properties. It has been found that the Ce valence state is highly dependent on its steric environment and can be manipulated towards the favorable Ce^{3+} by co-substitution with La [3, 4].
Using synchrotron powder X-ray diffraction we are investigating substitution of Nd with Ce and La and an example of a diffractogram measured at Spring8 in Japan is shown in Figure1b. Using Rietveld refinement we are among other things looking at site occupancies to determine how Ce and La substitutes into the crystal structure. Comparing the crystallographic data with magnetic properties will enable us to find the optimal substitution stoichiometry for keeping a usable magnetic performance for applications.

References
[1] Sagawa, M., et al., *New material for permanent magnets on a base of Nd and Fe (invited)*. Journal of Applied Physics, 1984. 55(6): p. 2083-2087. [2] Herbst, J.F., *$R_2Fe_{14}B$ materials: Intrinsic properties and technological aspects*. Reviews of Modern Physics, 1991. 63(4): p. 819-898. [3] Poenaru, I., et al., *Ce and La as substitutes for Nd in $Nd_2Fe_{14}B$-based melt-spun alloys and hot-deformed magnets: a comparison of structural and magnetic properties.* Journal of Magnetism and Magnetic Materials, 2019. 478: p. 198-205. [4] Jin, J., et al., *Manipulating Ce Valence in $RE_2Fe_{14}B$ Tetragonal Compounds by La-Ce Co-doping*: Resultant Crystallographic and Magnetic Anomaly. Scientific Reports, 2016. 6(1): p. 30194.

Nd2Fe14B structure (P42/mnm).



PXRD measured at Spring8, Japan (0.49009 Å)