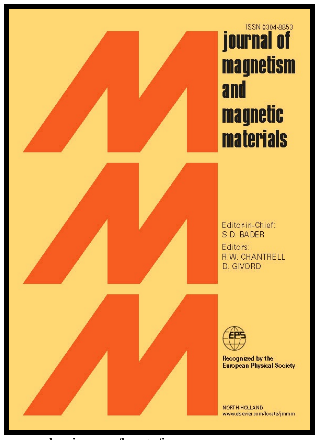

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PII: S0304-8853(16)32772-X
DOI: http://dx.doi.org/10.1016/j.jmmm.2016.10.127
Reference: MAGMA62040

To appear in: *Journal of Magnetism and Magnetic Materials*

Received date: 9 March 2016
Revised date: 26 August 2016
Accepted date: 25 October 2016

Cite this article as: Michael A. Susner, Benjamin S. Conner, Bayrammurad I Saparov, Michael A. McGuire, Ethan J. Crumlin, Gabriel M. Veith, Huibo Cao, Kavungal V. Shanavas, David S. Parker, Bryan C. Chakoumakos and Brian C Sales, Flux growth and characterization of Ce- substituted $Nd_2Fe_{14}B$ singl crystals, *Journal of Magnetism and Magnetic Materials* http://dx.doi.org/10.1016/j.jmmm.2016.10.127

Flux Growth and Characterization of Ce- Substituted $Nd_2Fe_{14}B$ Single Crystals

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Abstract

Single crystals of $(Nd_{1-x}Ce_x)_2Fe_{14}B$, some reaching $\sim 6 \times 8 \times 8$ mm^3 in volume, are grown out of Fe-(Nd,Ce) flux. This crystal growth method allows for large $(Nd_{1-x}Ce_x)_2Fe_{14}B$ single crystals to be synthesized using a simple flux growth procedure. Chemical and structural analyses of the crystals indicate that $(Nd_{1-x}Ce_x)_2Fe_{14}B$ forms a solid solution until at least $x = 0.38$ with a Vegard-like variation of the lattice constants with x. Refinements of single crystal neutron diffraction data indicate that Ce has a slight site preference (7:3) for the $4g$ rare earth site over the $4f$ site. Magnetization measurements at 300 K show only small decreases with increasing Ce content in saturation magnetization (M_s) and anisotropy field (H_A), and Curie temperature (T_C). First principles calculations are carried out to understand the effect of Ce substitution on the electronic and magnetic properties. For a multitude of applications, it is expected that the advantage of incorporating lower-cost and more abundant Ce will outweigh the small adverse effects on magnetic properties. Ce-substituted $Nd_2Fe_{14}B$ is therefore a potential high-performance permanent magnet material with substantially reduced Nd content.

Keywords:
Permanent Magnets, $Nd_2Fe_{14}B$, Rare Earth Magnets, Single Crystal Synthesis, Neutron Diffraction

PACS: 75.50.Cc, 75.50.Vv, 75.50.Ww, 71.20.Eh

1. Introduction

The reduction of critical materials present in consumer and industrial products in general, and in rare earth (RE) -based permanent magnets in particular, is a pressing concern due to increasing demand and a decline and/or uncertainty in the supply chain of these materials. Dysprosium, judged to be the most critical of these elements [1], is substituted onto the Nd site in $Nd_2Fe_{14}B$ (2-14-1) permanent magnets to increase the value of their coercive field and maximum operating temperatures [2, 3]. Depending on the application, the amount of Dy added can be large, in the range of 1.4-8.7 wt% [1]. The highest temperature applications, those that rely on the greatest quantities of dysprosium, are required by the rapidly emerging technologies of wind turbines, magnetically levitated transport, and traction motors for hybrid and electric cars [1].

Though Dy is indeed considered the most critical element, by many criteria Nd is not that far behind on the list of these crucial energy materials [1]. It is therefore imperative that new and innovative solutions are applied to the synthesis of permanent magnets that contain more abundant elements. To this end, recent work by Pathak *et al*. [4] has shown that partial substitution of Ce for Nd and Co for Fe (*i.e*. $(Nd_{0.8}Ce_{0.2})_2Fe_{12}Co_2B$) results in a permanent magnet with properties superior to those of Dy-substituted 2-14-1 magnets for temperatures above 450 K. However, these samples were fabricated as die-upset, hot-pressed, or melt-spun ribbons where the exhibited properties are dependent on such extrinsic factors as microstructure and secondary phases. Since 1) Ce is by far the most abundant of the rare earth elements and 2) these new magnets simultaneously eliminate the need for Dy and reduce the amount of Nd used, they

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