June 8th, 2024

PhD contract offer

Subject: Model interfaces for redesign of Nd-Fe-B magnets.

General information

Workplace : Nancy
Type of contract : PhD Student contract / Thesis offer
Contract period : 3 years.
Expected date of employment : 1st October 2024
Proportion of work : Full time
Remuneration : 2135 €/month (gross).
Desired level of education : Master in Physics, Solid state chemistry or Material Sciences
Experience required : Master

Project description:

1. Introduction.

Rare-earth-element (REE) permanent magnets based on Nd-Fe-B are vital for use in electric vehicles and wind turbines, making them central to Europe's green-energy future. These materials have outstanding magnetic properties, based on the $Nd_2Fe_{14}B$ phase. However, the intrinsic properties of the tetragonal $Nd_2Fe_{14}B$ phase are massively under-exploited in a magnet and much effort is needed to translate them into better extrinsic magnet properties [1-4]. This is because Nd-Fe-B magnets are complex, multiphase materials, whose properties do not depend only of the intrinsic properties of the $Nd_2Fe_{14}B$ phase but also on the microstructure of the whole material and especially on the nature of the grain boundary phases formed during material processing. The $Nd_2Fe_{14}B$ phase itself has a high saturation magnetization and a large monocrystalline anisotropy, providing a high remanence (Br), reflected in the magnet "strength", and a high intrinsic coercivity (Hci), making it resistant to demagnetization. The overall performance of the magnet is described by the maximum energy product ((BH)max), which depends both on Br and Hci (see a chart of for various materials in Fig. 1).

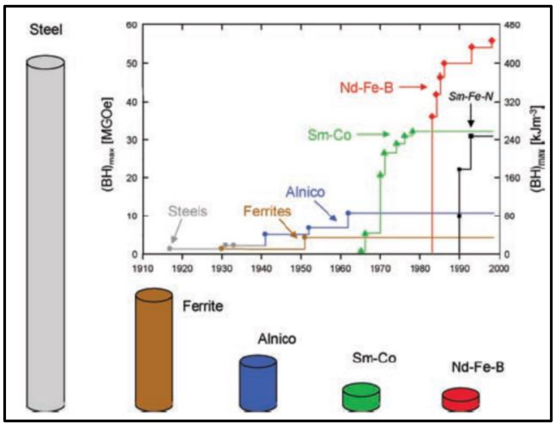

Figure 1: Development in the energy density ((BH)max) at room temperature of hard magnetic materials over the years. Adapted from [1].

However, in conventionally sintered magnets, the $Nd_2Fe_{14}B$ grains are microscopic. When exposed to a demagnetizing force, demagnetization begins at weaker regions normally at the grain interfaces with the grain-boundary phase before rapidly spreading, *i.e.* the nucleation model, with magnet coercivity being influenced by the chemical, structural, and magnetic properties of the grain surfaces and the grain boundaries. Despite all the efforts, the coercivities of Nd-Fe-B permanent magnets are only 20% of what is theoretically possible (*i.e.*, the Ha), meaning that significant improvements are possible. In this line, an idea is to develop Single-Grain Re-Engineered Nd-Fe-B Permanent Magnets by stripping $Nd_2Fe_{14}B$ grains and connected impurities from the existing Nd-rich phase and creating a new $Nd_2Fe_{14}B$/grain-boundary interface *in-situ* on fresh and recycled feedstocks. This process could allow for customizable REE content in the grain boundary and could reduce or even eliminate the need for heavy additional REE. The global project in which the PhD program will take place involves creating novel grain boundaries and interfaces based on micromagnetic simulations and computational thermodynamics. An important aspect will be to test these ideas by creating model interfaces using purposely grown $Nd_2Fe_{14}B$ single crystals and growing specific interface thin films. The methodology will be further extended to isolated single grains from recycled or fresh streams to develop a new form of Nd-Fe-B magnet by redesigning the magnet microstructure with innovative, single-grain *in-situ* grain-boundary engineering.

2. Main objectives of the PhD program.

The PhD program will focus on the most fundamental aspects of the above global project, by creating model interfaces from which the basic physical mechanisms at play can probably be better understood. An optimized grain boundary phase of the $Nd_2Fe_{14}B$ magnet will be suggested based on a computational thermodynamics approach for the prediction of intrinsic properties (saturation magnetization - Ms, Curie temperature - T_C, anisotropy constant - K1 and/or anisotropy field - H_a) to obtain the highest possible magnetocrystalline anisotropy and highest T_C with alloying elements. The proof-of concept of novel Nd-Fe-B permanent magnet with new grain boundary will be tested on model interfaces. For this purpose, the growth of high quality single crystals will be carried out, either by self-flux or by Czochralski methods, with dimensions of a few mm^2. Possible improvements in the sample sizes will be tested using alternative methods such as the floating zone crucible-free method. Crystals will be extracted and aligned using back-Laue X-ray diffraction. The low index (001) and (100) surfaces of single crystals will be examined under ultra-high vacuum conditions down to the atomic level. This is challenging as, despite the technological importance of the $Nd_2Fe_{14}B$ tetragonal phase, the literature on the surface science of this material is very limited. The first step will consist in the optimization of the surface preparation conditions in order to obtain atomically flat terrace and step surface morphology. The surfaces will be characterized by methods such as low-energy electron diffraction, scanning tunneling microscopy and photoemission spectroscopy. Then a model interface will be created by growing an ultra-thin film of the specific interfacial material on top of the bare $Nd_2Fe_{14}B$ substrate. The initial growth mode of the film along with its structure and chemistry will be determined at the surface for various conditions. An interface analysis (cross-sectional observation) will bring crucial information on the chemical distribution and possible phases formed as a function of the growth parameters and post-treatments. The resulting magnetic properties will be investigated at various length scales using different techniques, in collaboration with other partner's institutions. The detailed understanding of such model system will be crucial to implement the global strategy of Single-Grain Re-Engineered Nd-Fe-B Permanent Magnets at the industrial scale.

3. Methods.

Methods to be employed involve the synthesis of single crystals of the pure $Nd_2Fe_{14}B$ phase with large dimensions that are suitable for surface science experiments requiring ultra-high vacuum (UHV) conditions. Single crystals can be grown by the self-flux or by the Czochralski methods, with dimensions of a few mm^2. Improvements in the sample dimensions are foreseen using alternative methods such as the floating zone crucible-free method. Crystals will be extracted and aligned using back-Laue X-ray diffraction. The low index (001) and (100) surfaces of single crystals will be examined under UHV. Contamination-free surfaces will be prepared by cycles of Ar^+ sputtering followed by optimized annealing cycles at specific temperature in order to obtain atomically flat terraces separated by steps. The surface cleanliness and the near surface chemical composition (first few nanometers) will be determined by *in-situ* x-ray photoemission spectroscopy (XPS). The surface atomic structures will be investigated by low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM) down to the atomic level. Such atomically clean surfaces will serve as platforms to construct model interfaces. Thin films replicating the specific grain boundary phase will be deposited under UHV conditions by physical vapor deposition methods. Different growth parameters will be evaluated, including deposition flux, substrate temperature, post-treatments, etc.. Cross-section lamellae will be prepared and investigated by transmission electron microscopy in various modes. Physical properties of the model interfaces will be analyzed using different experimental methods, both in-house and at partner's institutions.

References:

[1] H. Sepehri-Amin, S. Hirosawa, K.Hono, "Advances in Nd-Fe-B Based Permanent Magnets", Ed. E. Brück, in Handbook of Magnetic Materials, Elsevier, Volume 27, 2018, Pages 269-372.

[2] Coey, J., "Perspective and prospects for rare earth permanent magnets". Engineering, 2020. 6(2): p. 119-131.

[3] K.Hono, H. Sepehri-Amin, "Prospect for HRE-free high coercivity Nd-Fe-B permanent magnets", Scripta Materialia 151 (2018) 6–13.

[4] Tang et al., "Unveiling the origin of the large coercivity in (Nd,Dy)-Fe-B sintered magnets", NPG Asia Materials (2023) 15:50.

Skills

Master in physics, materials science, or solid-state chemistry. A first experience in materials characterization would be appreciated. Proficiency in English, writing and oral communication.

Workplace

The project will take place at the Jean Lamour Institute that is among the largest French laboratories for material sciences (https://ijl.univ-lorraine.fr/). The institute is part of the CNRS (http://www.cnrs.fr/index.php) and the Université de Lorraine (http://www.univ-lorraine.fr/). The project involves three different research groups and state of the art equipments for thin film growth and surface characterization in ultrahigh vacuum (UHV), including a 70-meter long UHV tube connecting more than 20 different chambers (MBE, PLD, XPS, ARPES, RHEED, LEED, SAM, SEM, STM, etc..) as well as 2 standalone UHV multi-technique platforms (STM, LEED, XPS, UPS, etc..).

The Jean Lamour Institute is located in Nancy, a dynamic mid-size city with a population of > 200 000, including about 48000 students and 3700 professors and researchers.

Constraints and risks

No specific risk.
The position you are applying for is located in a sector relating to the protection of scientific and technical potential. It therefore requires, in accordance with the regulations, that your arrival be authorized by the competent authority of the Ministry of Higher Education, Research and Innovation.

Application

Interested candidates should apply before July 4th, 2024, through the CNRS website attaching a CV, motivation letter, and names of two or more researchers whom we may eventually contact:
https://emploi.cnrs.fr/Offres/Doctorant/UMR7198-MARTAI-112/Default.aspx?lang=EN
Short-listed candidates will be contacted for an interview as we receive their applications.

Further information:

• Vincent Fournée (CNRS Research Director) : vincent.fournee@univ-lorraine.fr
• Julian Ledieu (CNRS Research Director): julian.ledieu@univ-lorraine.fr