

# Permanent Magnets Beyond Nd-Dy-Fe-B

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**Provision of a concise summary of recent developments of permanent magnet materials and the materials science underlining them toward realizing permanent magnets beyond the current Nd-Dy-Fe-B is attempted, and approaches to solving the remaining fundamental issues are discussed. Focused are two promising groups of materials: the ThMn<sub>12</sub>-type Fe-rich Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>12</sub>-based materials and the Nd<sub>2</sub>Fe<sub>14</sub>B-based materials. Materials science based on atomistic view of permanent magnet materials specifically developed for this purpose is required in order to break into a precise control of the microstructure in atomic levels with the aid of computational material engineering. Atomistic understandings of coercivity mechanism and differences in free energy associated with formation of non-equilibrium structures such as grain boundaries and interfaces with sub-phases are proposed to be essential.**

*Index Terms*—Atomistic micromagnetics, coercivity, computational thermodynamics, critical elements.

## I. INTRODUCTION

**P**ERMANENT magnets beyond Nd-Dy-Fe-B are sought for because of the predicted rapid growth of the market for highly efficient energy conversion machines and devices, for which the Nd-Dy-Fe-B family is currently the only choice in terms of magnetic performance and mass productivity. The hard magnetic component of this class of permanent magnets is Nd<sub>2</sub>Fe<sub>14</sub>B and Dy has been used since the very early stage of developments [1] in order to improve the intrinsic coercivity by augmenting the magnetic anisotropy field with formation of a pseudo binary compound (Nd-Dy)<sub>2</sub>Fe<sub>14</sub>B. Under promising forecasts for rapidly expanding markets of Nd-Dy-Fe-B for relatively large machines, especially electric vehicles, regenerative electricity generations such as wind turbines and robots, which require high-coercivity specifications for securing large power density operations at elevated temperatures, high-coercivity grades that do not use extensive amounts of the critical elements such as Dy have been strongly demanded [2].

One of the possible approaches is to improve the coercivity of the Dy-free Nd-Fe-B by further improving microstructures of the materials. Conceivable another approach is to develop less-rare-earth or rare-earth-free permanent magnets of a competitive performance. A balanced usage of the entire rare earth elements is also required to avoid inflation of the Nd price on which the costs of the unused rare earth elements are added. Therefore, development of permanent magnets using the currently overproduced rare earths, namely, Ce and Sm, would be the third approach [3]. Alloying Ce, already used in some low-price commercial magnets indeed for this reason, always results in a reduction of the remanence ( $B_r$ ) of an anisotropic rare earth magnet and, hence, is not included in the scope of this paper.

In this paper, a concise summary of the recent developments toward the permanent magnets, which go beyond the current Nd-Dy-Fe-B magnets, and remaining issues to be overcome are proposed with emphases on Sm-Fe-based 1-12-type compounds, which are considered as promising candidates that potentially may outperform the Nd-Fe-B [4], and Nd-Fe-B materials superior to the current grades in terms of thermal stability.

## II. MATERIALS

### A. 1-12-Type Fe-Rich Compounds

It is relatively recent that the large magnetization exceeding that of Nd<sub>2</sub>Fe<sub>14</sub>B at and above room temperature was confirmed based on the magnetic measurements on anisotropic specimens of the rare earth-iron compounds of the ThMn<sub>12</sub>-type crystal structure. Hirayama *et al.* [4] showed that the large magnetization of Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>12</sub> for  $x$  from 0.1 to 0.2, which were epitaxially grown on V-buffered MgO(001) single-crystalline substrates, is primarily a consequence of the significant increase in Curie temperature due to the addition of Co: the saturation magnetizations of these compounds in the ground states are almost independent to the Co concentration in the range  $0 \leq x \leq 0.2$ . Therefore, these compounds will not be Co-free if the performance superior to that of Nd-Fe-B should be sought for. NdFe<sub>12</sub>N is Co-free but decomposes at temperatures above about 500 °C and its anisotropy field decays relatively strongly with increasing temperature [5]. To obtain the 1-12-type R-Fe compounds in the bulk form, partial substitutions of Sm and Fe with structure-stabilizing elements are still necessary with a penalty of reduced saturation magnetization [6], [7].

The recent empirical estimation of saturation magnetization ( $J_s$ ) of (Sm<sub>1-y</sub>Zr<sub>y</sub>)(Fe<sub>0.8</sub>Co<sub>0.2</sub>)<sub>11.5</sub>Ti<sub>0.5</sub> is 1.54 T at room temperature for  $y = 0.2$ , which is inferior to that of Nd<sub>2</sub>Fe<sub>14</sub>B [8]. However, the intrinsic magnetic properties of the Sm-Zr-Fe-Co-Ti alloy at elevated temperatures above *ca.*, 100 °C are still attractive as shown in Fig. 1, in which the magnetic properties of typical hard magnetic

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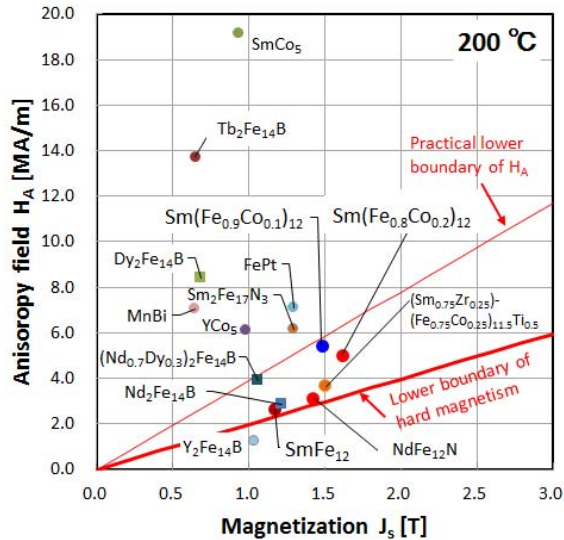


Fig. 1. Intrinsic magnetic properties of hard magnetic compounds at 200 °C based on various studies. This temperature is chosen as symbolic because high power-density machine inevitably operates at unfavorably high temperatures for permanent magnets. Red lines: lower boundary of hard magnetism corresponding to magnetic hardness factor ( $\kappa$ ) of unity and the practical lower boundary for  $H_A$  corresponding to  $\kappa = \sqrt{2}$ .

compounds at an elevated temperature of  $T = 200$  °C are mapped on the anisotropy field ( $H_A$ ) versus saturation magnetization ( $J_S$ ) coordinates. In order to overcome the self-demagnetizing energy, which is the magnetostatic energy proportional to  $J_S^2$ ,  $H_A$  needs to increase proportionally with  $J_S$  when a large  $J_S$  is pursued. In Fig. 1, the lower bound of hard magnetism follows the requirement proposed in [9] that the magnetic hardness factor  $\kappa = (\mu_0 H_A / 2J_S)^{1/2}$  needs to be larger than unity. The existing practical compounds, for instance,  $(\text{Nd}_{0.7}\text{Dy}_{0.3})_2\text{Fe}_{14}\text{B}$  used in the high-temperature grades of Nd-Dy-Fe-B sintered magnets, have anisotropy fields as large as about four times of  $J_S$ , corresponding to  $\kappa = \sqrt{2}$ , at operating temperatures [10]. Therefore, this may be considered as a practical lower boundary at the temperature considered.  $(\text{Sm}_{0.8}\text{Zr}_{0.2})(\text{Fe}_{0.8}\text{Co}_{0.2})_{11.5}\text{Ti}_{0.5}$  clears this boundary below about 110 °C [8], while  $\text{Sm}(\text{Fe}_{1-x}\text{Co}_x)_{12}$  almost does at 200 °C with  $x = 0.1$  and  $0.2$  (Fig. 1).

One of the conceivable ways for developing coercivity in the  $\text{Sm}(\text{Fe-Co})_{12}$ -based hard materials is the application of grain boundary modification by grain boundary diffusion (GBD) or grain boundary infiltration (GBI) processes, which have been successfully adopted to Nd-Fe-B permanent magnets. The difficulty in developing the  $\text{Sm}(\text{Fe-Co})_{12}$ -based systems is the well-known lack of a liquid phase [11] that could coexist with the 1-12 compound, which largely excludes the GBI technique with low-melting point alloys because it would result in the formation of undesired Fe-Co-rich ferromagnetic phases. However, GBD treatments at low temperatures have proved to be an effective way to produce a sizable coercivity ( $H_{cJ}$ ), about 600 kA/m, at room temperature in a textured multi-grain thin film  $\text{Sm}(\text{Fe}_{0.8}\text{Co}_{0.2})_{12}$  magnet with Cu diffusion at 400 °C [12].

The so-called rare-earth-free permanent magnets are largely excluded from Fig. 1 either because they have only small magnetization or because they do not clear the requirement for the lower bound of hard magnetism in the single-phase bulk forms (including films of sizable thickness of tens of nanometers). The anisotropic nanocomposite permanent magnets are also not included in this figure for the same reason. It may be noted that an anisotropic nanocomposite permanent magnets needs to be composed of hard magnetic phase with a significantly large magnetic anisotropy and a high Curie temperature, which are available only in a few Sm-based transition metal compounds such as  $\text{SmCo}_5$  and  $\text{Sm}_2\text{Fe}_{17}\text{N}_3$  in order to clear the requirements for magnetic hardness at this temperature [10]. The question is whether one can create an inherently unstable nanostructured material composed of an anisotropic nanocomposite consisting of a high-magnetization phase, e.g.,  $\text{Fe}_{0.7}\text{Co}_{0.3}$ , and one of these Sm-based intermetallic compounds assembled with a secondary phase that separates the nanocomposite material to prevent reversed magnetic domains from expanding throughout the material, maintaining a high degree of easy axis alignment and sharp interfaces in between. The 1-12-type Fe-rich  $\text{Sm}(\text{Fe-Co})_{12}$  compounds, having a reduced concentration of rare earth elements than the  $\text{Nd}_2\text{Fe}_{14}\text{B}$  type compounds (1/13 against 2/17) and a saturation magnetization as large as a hypothetical anisotropic Fe/ $\text{Nd}_2\text{Fe}_{14}\text{B}$  nanocomposite with Fe molar fraction of 50%, appear more attractive since the objectives of investigating the nanocomposite are readily achieved therein.

### B. Nd-Fe-B Beyond Nd-Dy-Fe-B

The  $\text{Nd}_2\text{Fe}_{14}\text{B}$ -based permanent magnets are the commercially available best permanent magnets for many applications including electricity-driven automobiles and large-scale generators as a result of quite fortunate features [13] that make the Nd-Fe-B system unique and advantageous over other materials; the existence of a low-melting point Nd-rich ternary liquid phase, absence of ferromagnetic equilibrium phases coexisting with tetragonal  $\text{Nd}_2\text{Fe}_{14}\text{B}$ , and the capability of the compound to be magnetically tuned by making mix crystals with other  $\text{R}_2\text{Fe}_{14}\text{B}$  compounds, e.g.,  $\text{Dy}_2\text{Fe}_{14}\text{B}$ .

To summarize the current situation, the present high-end Nd-Dy-Fe-B permanent magnets with large coercivity values are the materials that have been developed following the strategy of reduction of grain size and engineering of the grain boundary microstructures to reduce the usage of the heavy rare earth elements (HRE), namely, Tb and Dy, as much as possible [2], [14]. The coercivity enhancement due to the reduction of grain size of the main phase is now attributed, based on the micromagnetic simulations [15], [16], to a reduction of local demagnetization fields arising from the neighbor grains with reversed magnetization with decreasing the grain size. The grain boundary engineering has become the essential way to eliminate or significantly reduce the usage of HRE, and includes a simple enrichment of the Nd content in the magnet, Tb- or Dy- GBD at around 900 °C [17], [18], and GBI with low-melting point Nd-rich alloys at around 600 °C [19], [20]. GBI with Pr-based eutectic alloys has been

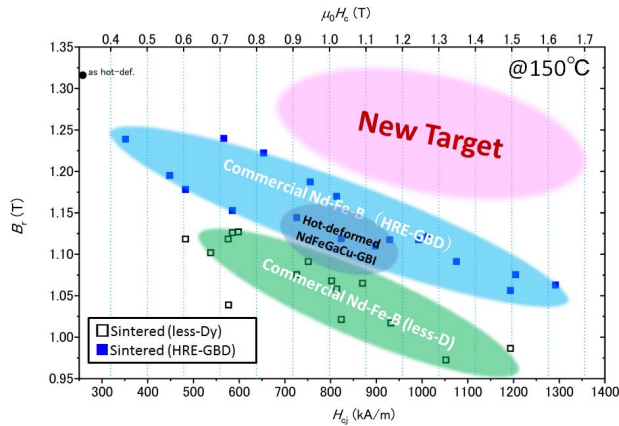


Fig. 2. Magnetic performance of anisotropic  $\text{Nd}_2\text{Fe}_{14}\text{B}$ -based permanent magnets at  $150^\circ\text{C}$  and the new target for the magnets beyond Nd-Dy-Fe-B. Square symbols: typical data provided in technical data sheets of several representative permanent magnet producers and the region depicted for hot-deformed hot deformed Nd-Fe-B magnets grain boundary infiltrated with an Nd-Fe-Ga-Cu alloy is based on Liu *et al.* [24].

shown to be more effective than with the Nd-based alloys to increase the coercivity at room temperature, but with a penalty of increased temperature dependence of coercivity, resulting in a smaller coercivity than the case of infiltration with the Nd-based alloys [21], [22]. These processes rely on the existence of a liquid phase along the grain boundaries.

The currently available magnetic performance of anisotropic Nd-(Dy)-Fe-B are shown in Fig. 2, in which typical technical data of sintered magnets provided by magnet producers are plotted for  $150^\circ\text{C}$ , which has become a typical operating temperature currently required for permanent magnets in hybrid electric vehicles (HEVs) after recent redesigning of the electric traction system for a usage of the less-Dy and Dy-free Nd-Fe-B magnets [23]. The minimal coercivity of these magnets operable at  $150^\circ\text{C}$  is about 1.6 MA/m at room temperature and the remanence around 1.4 T. In Fig. 2, recently reported results obtained by GBI of Nd-Fe-Cu-Ga alloys into hot-deformed Nd-Fe-B anisotropic magnets [24] are also shown. Small amount of Dy is still necessary for high-coercivity sintered magnets when required to be operable above  $150^\circ\text{C}$  in the conventionally designed motors for HEVs [25].

The current Nd-(Dy)-Fe-B materials are not ultimate, leaving a room for the development of Nd-Fe-B that goes beyond them: the current situation is unsatisfactory because the Nd-Fe-B grains are still exchange coupled along the lateral direction perpendicular to the  $c$ -axis in the most part because of their high concentration of Fe and Co [26], [27]. The crystal structure of the intergranular grain boundary phase also varies with the orientation of the interface from a crystalline fcc-type structure in the Nd-rich side parallel to the (001) surface of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  to amorphous on the Fe-rich side perpendicular to the (001) surface in the case of sintered magnets [26]. The mechanism how the chemical compositions and eventually the crystal structures are determined is not entirely clear, although it may be conceived naturally that this may be related to the layered structure of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  consisting of Nd-containing atomic planes separated by pure Fe blocks

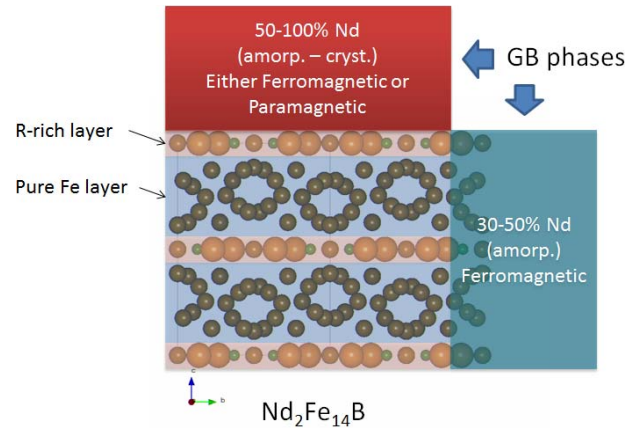


Fig. 3. Schematic of the relation between the crystal orientation of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  and the chemical compositions and crystal structures of the intergranular Nd-rich phase.

(Fig. 3). Micromagnetic analysis using the model structures assuming various magnetic parameters for the intergranular grain boundary phase shows the exchange decoupling along the lateral direction should result in a considerable improvement in coercivity [28].

Alloying Ga in some specific cases is reported to result in improvements in coercivity via formation of all non-ferromagnetic grain boundary phases including a relatively Fe-rich  $\text{Nd}_6\text{Fe}_{13}\text{Ga}$ -type phase that is non-ferromagnetic at room temperature and above [29]–[31]. Unfortunately, this phase forms as a relatively thick intergranular phase (*ca.*, 20 nm thick in comparison to 2 nm in the conventional sintered magnets) by consuming a part of  $\text{Nd}_2\text{Fe}_{14}\text{B}$ , resulting in a decrease in saturation magnetization. The decrease in magnetization is, however, equivalent to that which occurs by alloying Dy in the conventional grades of sintered Nd-Fe-B, justifying the usage of Ga for the sake of eliminating Dy without significantly deviating from the conventional performance line on the  $B_r$  versus  $H_{cJ}$  map.

A new target of permanent magnets beyond Nd-Dy-Fe-B that are operable at or above  $150^\circ\text{C}$  shown in Fig. 2 may be reached with  $\text{Nd}_2\text{Fe}_{14}\text{B}$  by taking into account the reversible temperature coefficient of  $J_S$  of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  and a minimal but tuned degree of imperfection in texture, which helps to avoid the sharp decrease in coercivity [32] as the texture approaches the perfection. One of the promising approaches is to form a very thin (a few nanometers) magnetically harder shell enriched with Dy or Tb on the surface of Dy-free  $\text{Nd}_2\text{Fe}_{14}\text{B}$  to minimize the usage of the HRE [33]. Eliminating excessive volume fraction of non-ferromagnetic phases such as Nd-metallic phases and oxides at the triple junctions is another key issue. The target performance may be reachable also with the  $\text{ThMn}_{12}$ -type Fe-rich  $\text{Sm}(\text{Fe-Co})_{12}$  family of compounds described in the previous section. The development of coercivity is the key challenge in the either cases, for which an atomistic control of the grain boundary microstructures, particularly, atomic arrangements that influence the local anisotropy and exchange stiffness of the rare earth atoms will be required.

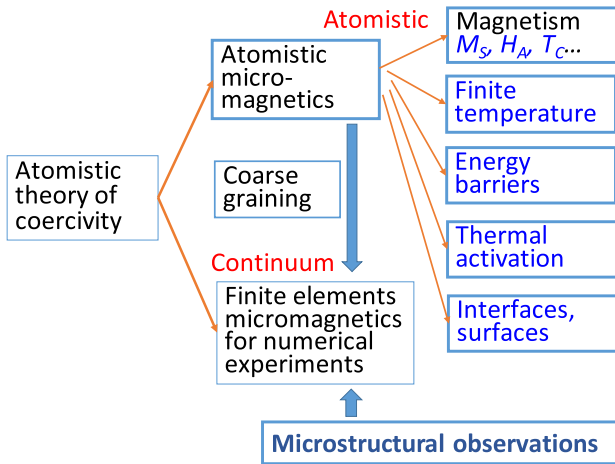


Fig. 4. Fundamental components in atomistic understanding of coercivity and steps in the atomistic levels.

### III. ATOMISTIC APPROACHES

#### A. Atomistic Micromagnetics

While structural investigations with a nearly atomic resolution are available currently, the information is not fully utilized in elucidation of coercivity of a macroscopic bulk magnet at present because there is no link between the atomistic information and the conventional micromagnetic theories that are based on the continuum picture of magnetic materials. The atomistic understanding of coercivity becomes important because the defects of atomic scales are not yet identified nor characterized in spite that the magnetization reversal is believed to start from local magnetic defects of atomistic scales with the assistance of thermal energy. To describe such phenomena, several steps in the atomistic level need to be established and then connected to conventional continuum simulations as shown in Fig. 4.

A classical Heisenberg-type spin model of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  was constructed and thermal averages of magnetic properties were computed and the finite temperature behaviors of magnetization and magnetic anisotropy were discussed as site-resolved properties related to atomistic microstructures [34], [35]. In the spin model, the ground state magnetic couplings and magnetic anisotropy of the itinerant 3d electrons are evaluated with the first-principles calculations and mapped to the localized atomic moment picture. This can be accepted as a sound approximation for the investigation of finite-temperature behaviors of the Fe and Co magnetic moments in hard magnetic compounds. The 4f electrons are treated as fully localized, and the magnetism of the rare earth atoms is assumed to follow the classic molecular field and crystal field theories. The temperature-dependent properties such as sub-lattice magnetization and magnetic anisotropy energy are calculated as a thermal average for which the Monte Carlo methods are used with some constraints in the case of, for instance, the direction-dependent magnetization. The spin model of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  contains  $6^3$  unit cells, thus 14 688 atoms to yield a negligible size dependence. By making the model large enough to incorporate a domain wall, energy barriers in non-uniform magnetization reversal involving domain

wall displacements may be obtained, and the temperature dependence of the critical field for nucleation of reversed magnetic domains can be discussed [36]. The spin models may be expanded to include local defects such as interfaces and local magnetism therein, which, in principle, can be obtained combining atomic resolution observations and first-principles calculations. In this way, the role of the atomistic defects, which is totally inaccessible in classic micromagnetic theories based on continuum models of magnetic substances, would be fully elucidated. It may be noted that occurrence of negative anisotropy constants at Nd atomic sites on (001) surfaces of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  [37] and their destroying impacts on coercivity [38] were discussed earlier. Their simulations were based on discretized Landau–Lifshitz–Gilbert (LLG) simulations but did not include the thermal activation effects.

At present, inclusion of thermal activation effects in a large-scale LLG simulations representing relevant structural models of real permanent magnets is possible only through the estimation of the energy barrier for magnetization reversal, which is to be compared with the  $25 k_B T$  barrier following the classical argument for a waiting time of the order of 1 s [39]. The time scale treatable with the atomistic stochastic LLG simulations is still in the sub-nanosecond range [35]. The current focal point is, therefore, the gap bridging from the atomistic theory to the continuum theory. In an approach, a number of atomic spins would be mapped into a macrospin corresponding to the magnetization of a cell of finite-element approximation used in the continuum model, magnetic parameters (i.e., the anisotropy constant and the exchange stiffness) of which are also mapped from the behavior of the atomistic spin model at a finite temperature of interest. In such investigations, explicit treatments of the thermal activation process in the atomistic micromagnetic calculations will be required in order to properly map the behavior to the micromagnetic motion of macrospins at the temperature [35]. Similar argument has been presented recently by Westmoreland *et al.* [40].

#### B. Formation of Interfaces and Their Magnetic Properties

Controlling the structural, compositional, and magnetic properties of interfacial regions between the matrix and grain boundary phases can be effectively aided by computational thermodynamic assessments that predict the possible phases and their compositions that would make thermodynamically stable interfaces with the matrix phase. This is the last piece in the fundamental steps in atomistic understanding of coercivity shown in Fig. 4. Macroscopic thermodynamic assessments to describe the sub-phases that coexist with the hard magnetic matrix phase are possible with the semi-empirical Calculations-of-Phase-Diagrams (CALPHAD)-type computations using the Gibbs energy functions of formation energy parameterized and stored in the database. However, data sets of phases relevant to rare earth permanent magnets are yet quite scarce. The parameters need to be determined based on experimental data such as heat capacity, heat of solution, and, more recently, microscopically analyzed concentrations of solutes in closed equilibrium

experiments using reactive crucibles [41] or reaction sintering [42] techniques.

An Nd-Fe-B permanent magnet is a multi-component system, e.g., Nd-Dy-Fe-Co-Al-Ga-Cu-B-O, even if minor impurities are neglected. A large portion of the data sets of even binary basic systems, such as Nd-O, Nd-Dy, and Dy-O, has been missing. Even for basic Nd-Fe-B and Nd-Dy-Fe-B systems, basic binary systems such as Fe-B and Nd-B had to be carefully re-assessed from various thermodynamic data [43]–[45]. It is only recent that the Nd-O system has been reinvestigated by Abe *et al.* [46], to include oxygen into CALPHAD assessment of Nd-Fe-B. They determined the Gibbs energy parameters with both empirical equilibrium measurements and first-principles calculations of formation energies. In their work, the Gibbs energies were assessed for relevant binaries to reach the five-components system, Nd-Fe-B-Cu-O, which is the basic system to describe any practical magnets based on Nd<sub>2</sub>Fe<sub>14</sub>B. It was found that the Nd-Fe-B-Cu-O system shows phase separation in the liquid phase in a composition range in which an Fe-rich liquid and an Nd-O-rich liquid phases are formed. Their work has made it possible to analyze the behavior of oxygen dissolved in the metallic Nd phase and in the Nd-rich liquid phase.

The anisotropic features in chemical compositions of the intergranular grain boundary phases and the partitioning of microalloyed elements such as Cu on the surface of Nd<sub>2</sub>Fe<sub>14</sub>B in grain boundaries are other two important issues that remain unexplained. Cu is known as one of the typical microalloying elements in Nd-Fe-B that brings about a strong effect of enhancing the coercivity upon post-sintering annealing process [47], [48]. Elucidation of free energy difference associated with formation of interfaces with sub-phases is a challenging problem: the first principles fully relaxed calculations of structures of interfaces in rare earth magnets have been limited to interfaces involving the Nd<sub>2</sub>Fe<sub>14</sub>B (001) surface. Differences in formation energy of structures composed of more than 200 atoms involving an Nd<sub>2</sub>Fe<sub>14</sub>B(001)/fcc-NdO<sub>x</sub> interface and one Cu atom located in various positions in the initial structures were investigated by Tatetsu *et al.* [49], [50]. They found that the interface having structures with the Cu atom at either an interstitial position at the interface and Fe (4e) site of Nd<sub>2</sub>Fe<sub>14</sub>B at the interface have lower formation energy than the structure without the Cu atom. This result is in accordance with the observation that Cu atoms segregate at the surface of Nd<sub>2</sub>Fe<sub>14</sub>B grains at the interface with Nd-rich phases in sintered Nd-Fe-B permanent magnets [51].

In construction of model structures of interfaces for more general cases that would appear in the Nd<sub>2</sub>Fe<sub>14</sub>B-based systems, molecular dynamics simulations have been employed by a few groups [40], [52], [53]. Notably, Kubo *et al.* [53] succeeded in constructing a model of angular-dependent interatomic potentials that reproduces the crystal structure of Nd<sub>2</sub>Fe<sub>14</sub>B and used it in an analysis of Nd<sub>2</sub>Fe<sub>14</sub>B/Nd interfaces. Direct first-principles calculations of atomistic magnetocrystalline anisotropy and exchange coupling parameters among the magnetic moments based on those model structures have not been attempted. Calculation of the

electronic structure and magnetic properties of the interfaces remains practically difficult and development of methods to deduce the statistically meaningful properties from an ensemble of model structures, each of which may not be energetically the most stable ones but represents one of thermodynamically possible structures, appears challenging but is required.

#### IV. CONCLUSION

Development of permanent magnets beyond the Nd-Dy-Fe-B anisotropic magnets requires extensive understanding of the materials science of permanent magnets. Development of Nd-Fe-B with performance beyond the commercially available grades may be possible with sophisticated grain boundary engineering in the atomistic scales. The Sm(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>12</sub>-based Fe-rich compounds with the ThMn<sub>12</sub>-type structure appear as one of the promising candidates for Nd-free anisotropic magnets, but a proper intergranular phase to compose a multi-phase microstructure to generate coercivity is still missing. The rare-earth-free hard magnetic materials have the intrinsic difficulty to outperform Nd<sub>2</sub>Fe<sub>14</sub>B because of their insufficiency in either the magnetocrystalline anisotropy or the spontaneous magnetization. To realize the permanent magnets beyond Nd-Dy-Fe-B, materials science, specifically developed for this purpose, is required in the atomistic resolutions in order to break into more precise control of the microstructures. The computational material engineering, in which atomistic understanding of the coercivity mechanism and estimation of free energy for non-equilibrium thermodynamic simulations are essential, will help to deal with the actual multi-component permanent magnet alloys.

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