Relevance of $4f$-$3d$ exchange to finite-temperature magnetism of rare-earth permanent magnets: an \textit{ab-initio}-based spin model approach for NdFe$_{12}$N

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A classical spin model derived \textit{ab initio} for rare-earth-based permanent magnet compounds is presented. Our target compound, NdFe$_{12}$N, is a material that goes beyond today’s champion magnet compound Nd$_2$Fe$_{14}$B in its intrinsic magnetic properties with a simpler crystal structure. Calculated temperature dependence of the magnetization and the anisotropy field agree with the latest experimental results in the leading order. Having put the realistic observables under our numerical control, we propose that engineering 5d-electron-mediated indirect exchange coupling between 4f-electrons in Nd and 3d-electrons from Fe would most critically help to enhance the material’s utility over the operation-temperature range.

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I. MOTIVATIONS

In the past three decades, Nd$_2$Fe$_{14}$B has been the champion permanent magnet compound. A drawback of Nd$_2$Fe$_{14}$B has been its relatively low Curie temperature and that some practical applications require replacements of Nd with heavy-rare-earth (HRE) elements such as Dy and Tb to enhance the high-temperature coercivity, which is roughly proportional to the anisotropy field. Since the HRE elements are less abundant, ways to achieve the equivalent magnetic properties to those of HRE-doped permanent magnets using only light rare-earth (LRE) elements have recently been sought after. Also the relevance of understanding and controlling the finite-temperature magnetism of 4f-3d intermetallics is appreciated ever more.

A possible solution was recently suggested\textsuperscript{1} by the material NdFe$_{12}$N stabilized in an almost bulk state\textsuperscript{2}, where a newly fabricated film sample that consists of more than hundred unit-cell layers shows superior intrinsic magnetization and anisotropy field to Nd$_2$Fe$_{14}$B. The materials family, RF$_{7-x}Fe_{12-x}N$ (R=rare earth), had actually been known for a long time\textsuperscript{3} where the nitroganation pulls up the Curie temperature by 100-200 K and the magnetic anisotropy is enhanced as well, but the achieved magnetic properties were not on a par with the champion magnet compound Nd$_2$Fe$_{14}$B partially due to the necessity for the presence of the third element T=Ti etc. to stabilize the particular crystal structure. Recent breakthrough\textsuperscript{4} made it possible to have NdFe$_{12}$ without the third element in a sample fabricated as a thick film and nitriding achieved the intrinsic magnetic properties that goes beyond Nd$_2$Fe$_{14}$B at high temperatures\textsuperscript{5}.

Thus we are motivated to theoretically address the finite-temperature magnetism of NdFe$_{12}$N. This would provide the prospect for its intrinsic magnetic properties, which serves to solve the high-temperature coercivity problem in LRE-based compounds. On the theory side, finite-temperature magnetism of rare-earth-based permanent-magnet materials poses a fundamentally challenging many-body problem: \textit{ab initio} predictions mostly focus on the ground-state properties and the finite-temperature magnetism was discussed at best on the basis of a mean-field theory of a simplified model on the basis of a molecular field acting on an isolated rare-earth magnetic moment\textsuperscript{6,7}. For comparison with experimentally observed magnetic anisotropy, contributions from 3d electrons are sometimes added in an \textit{ad hoc} manner. In principle, the theory of magnetism in 4f-3d intermetallics takes a description of the correlated electrons in 4f and 3d-orbitals, which may be done with a multi-orbital periodic Anderson model (PAM) with the conduction electrons composed of 5d-band out of the rare-earth elements, harboring two species of impurities, 3d and 4f, each with the different levels of on-site electronic correlation.

In order to meet the urgent practical needs and also to provide a guideline data for future realistic simulations of PAM with huge number of orbitals, we exploit the essence of a simplified model\textsuperscript{8} to describe only the low-energy effective physics of 4f-3d intermetallics with the model parameters determined as realistically as possible through \textit{ab initio} calculations: we define a multi-sublattice spin model with one group of the sublattices describing the 4f-originated localized magnetic moments and the other describing the 3d-magnetization; the spins reside on a realistic lattice that mimicks the crystal structure of the given target material NdFe$_{12}$N with the \textit{ab initio} input parameters. Note that the effective parameters, such as the strength of exchange couplings and crystalline electric fields, are determined as a consequence of the electronic states. They are target-material dependent, thus first-principles evaluation of the parameters is crucial for the quantitative modeling. Then we solve
the finite-temperature many-body problem with numerically exact Monte Carlo method to get the temperature dependence of magnetic observables and quantitatively compare with the latest experimental data. Our realistic lattice model is more realistic than were discussed in the previous works: The sublattice-specific character of each of the Nd and Fe atoms in the unit cell is taken into account on the basis of first principles, which is in contrast to a uniform molecular field imposed by Fe acting on rare-earth magnetic moments. Establishing the computational control of the intrinsic properties of magnetism of NdFe₁₂N, we discuss within our model how to manipulate it to enhance its practical utility most effectively.

II. THE REALISTIC-LATTICE SPIN MODEL

The spin model Hamiltonian defined on the lattice of the given crystal structure reads as follows.

\[ H = H_T + H_R + H_{RT}, \]

\[ H_T = - \sum_{(i,j) \in T} (2J_{ij}^{TT}) \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i \in T} D_{i}^{T} (S_{i}^{z})^{2}, \]

\[ H_R = - \sum_{m \in R} D_{m}^{R} (J_{m}^{z})^{2}, \]

\[ H_{RT} = \alpha_{RT} \sum_{(m,i), m \in R, i \in T} (2J_{mi}^{RT}) (g_j - 1) J_{m} \cdot \mathbf{S}_i \]

We have denoted the lattice points on which 3d (4f) magnetic moments reside by T (R), respectively. Here \( \mathbf{S}_i \) is a magnetic moment defined on site \( i \), \( J_{ij} \) is the exchange coupling between localized magnetic moments \( \mathbf{S}_i \) and \( \mathbf{S}_j \), and \( D_{i} \) encodes the single-ion magnetic anisotropy energy (MAE). Note that the summation \( \sum_{(i,j)} \) runs over each bond connecting the sites \( i \) and \( j \) only once. The 4f-part is described explicitly with the total magnetic moment \( \mathbf{J} = L + S \) with \( \mathbf{L} \) being the orbital moment. The spin moment can be extracted via \( \mathbf{S} = (g_j - 1) \mathbf{J} \) with \( g_j \) being Landé’s g-factor. Describing a 4f-moment of Nd³⁺ with a classical spin of length \( g_j \sqrt{J(J+1)} \) with \( J = 9/2 \) is semi-quantitatively justified within the scope of setting the target temperature range in 200 [K] \( \lesssim T \lesssim 500 \) [K], with the \( J \)-multiplets separated in the scale of 1000 [K]. The 4f-4f exchange coupling terms, \( J_{ij}^{RR} \), in the scale of \( O(1) \) [K] have been dropped because our target energy scale to be realistically described is motivated by the typical operating temperature range 200 [K] \( \lesssim T \lesssim 500 \) [K] of permanent magnets. Magnetic energy scales coming from \( J_{ij}^{RR} \)’s are at most \( \sim 0.1T \) and should be washed out.

The 4f-3d indirect exchange coupling as denoted by \( J_{mi}^{RT} \) in Eq. \( 1 \) comes from \( (5d)^m(3d)^n \) \( (m \lesssim 1 \) and \( n > 5) \) exchange which is antiferromagnetic and RE on-site 4f-5d direct exchange which is ferromagnetic. Overall \( J_{mi}^{RT} \) is an antiferromagnetic coupling between the spin component of 4f and 3d, which means 4f total moment and 3d magnetization are ferromagnetically coupled for Nd³⁺ with \( g_j = 8/11 \). The overall scale factor \( \alpha_{RT} \), tentatively set to be one, has been introduced to phenomenologically describe the indirect nature of the 4f-3d exchange coupling.

A. Derivation of the leading-order parameters

As shown in Fig. 1 the material NdFe₁₂N has a ThMn₁₂ crystal structure (space group \( I4/mmm \)) with Nd occupying the body-centered site of a tetragonal unit which incorporate 2 formula units. Around each Nd site, there are 4 Fe(8i) atoms which surround along the a-axis and b-axis. Four Fe(8j) atoms make a square right in the middle of Nd sites along the c-axis and nitrogen goes in the center of this square. Fe(8f) sites make a tetragonal box with the center occupied by Nd. Taking the ThMn₁₂ crystal structure as the starting point, the crystal structure is optimized from first principles. Then the crystal field parameters on Nd³⁺ are calculated on the basis of open-core description for the 4f-shell. Up to here the calculations are done with the \( ab \) \textit{initio} electronic-structure computational code package, QMAS \textsuperscript{15}. The parameters for the exchange-coupling are calculated with the \( ab \) \textit{initio} electronic-structure calculation code, Machikaneyama (AkaiKKR) \textsuperscript{16}, using the Korringa-Kohn-Rostoker Green’s function method, following the prescription proposed by Liechtenstein \textit{et al}.\textsuperscript{17}. Re-writing the term in Eq. \( 2 \) as \( J_{ij}^{TT} \mathbf{S}_i \cdot \mathbf{S}_j \equiv (S_i J_{ij}^{TT} S_j) \mathbf{e}_i \cdot \mathbf{e}_j \) with the vector \( \mathbf{e}_j \) denoting the direction of the magnetic moment on site \( i \), calculated exchange couplings \( (S_i J_{ij}^{TT} S_j) \) are summarized in Fig. \( 2(a) \) as a function of inter-site distance. As is the case for the champion magnet compound Nd₂Fe₁₄B \textsuperscript{18}, we find that the dominant Fe-Fe exchange couplings come from Fe...
pairs whose interatomic distances almost coincide with that in α-Fe. In our model we incorporate those dominant Fe-Fe exchange couplings, that can be classified into 8 classes on the realistic lattice for NdFe_{12}(N) to make a leading-order description. Comparing the calculated exchange couplings on the same bonds located on the equivalent positions in the unit cell between NdFe_{12} and NdFe_{12}N as shown in Fig. 2 (b), nitrogenation-enhanced exchange couplings are identified. Interestingly, we observe those bonds are located along a kagomé-lattice network spanned by Fe(8f) and Fe(8j), reminiscent of one-generation-back permanent-magnet materials represented by SmCo_{5} with the strong magnetic anisotropy. The other leading-order term in the overall Hamiltonian written as Eq. (1) is 4f single-ion MAE $D^{R}_{i} (J_{m_{i}})_{m}^{2}$, which also shows up in the energy scale of $O(10)$ [meV]. Rewriting the term in Eq. (3) as

$$ D^{R}_{i} (J_{m_{i}})_{m}^{2} = K^{R}_{m} (e_{m} \cdot n)^{2}, \quad (5) $$

with $n$ denoting the direction of the easy axis and $e$ the direction of the total magnetic moment $J_{m}$ on the rare-earth site $m$, a QMAS calculation gives $K^{Nd} = 5.8$ or $11.0$ [meV] (easy-axis) for NdFe_{12}N and $K^{Nd} = -3.0$ or $-2.3$ [meV] (easy-plane) for NdFe_{12} depending on the calculation setups. As a first step, we choose $K^{Nd} = 8.1$ [meV] for NdFe_{12}N and $= -2.8$ [meV] for NdFe_{12} within the range.

### B. Sub-leading parameters

We define $J^{RT}$ and $D^{T}$ in the overall Hamiltonian written as Eq. (1). Calculated antiferromagnetic exchange coupling between 5d-bands of Nd and 3d-bands of Fe are taken as they are to be the 5d-mediated $4f$-$3d$ coupling, assuming that intra-atomic direct exchange coupling is big enough to let the localized $4f$-moment and 5d-polarization work as a unified body. The results are summarized in Table I. The Fe-originated MAE in Eq. (2), which we will denote analogously to Nd-originated one in Eq. (5) as follows,

$$ D^{T}_{i} (S^{T}_{m})_{m}^{2} = K^{T}_{i} (e_{i} \cdot n)^{2} \quad (6) $$

comes in the order $O(0.1)$ [meV] as referring to the past experimental measurements done for YFe_{11}Ti. In the present modeling we just incorporate $K^{Fe} = 0.1$ [meV] uniformly on all Fe sites as a phenomenological setting which should be sufficient to describe the magnetic properties around the room temperatures and slightly higher. Higher-order terms in addition to $K^{Nd}$ in Eq. (5) can be suspected in principle for which we have also calculated and saw that they are an order of magnitude smaller than the leading-order ones. Within the present scope to pick up the leading-order behavior of finite-temperature observables, we have dropped the higher-order contributions to the single-ion magnetic anisotropy of Nd.

### C. Methods

Having defined the realistic model basically from first principles for NdFe_{12}(N), the temperature dependence of the magnetic properties are calculated using the classical Monte Carlo method with the Metropolis local updates. We do one of the most plain local updates, that is, picking up lattice sites stochastically and proposing uniformly on the spherical spin space up to the stochastic decision referring to the energy difference as calculated by the spin model Hamiltonian defined as Eq. (1). Effective one-lattice sweep, i.e. with the stochastic choice of the lattice
III. RESULTS

With the prescription for the construction of the realistic-lattice spin model, calculated temperature dependence of magnetization and anisotropy field are shown in comparison with the experimental data. Model parameter dependence of the overall calculated temperature dependence is inspected to draw our main conclusion: $4f$-$3d$ exchange couplings $J_{mi}^{RT}$ in Eq. (4) dominates the observables in the operation temperature range i.e. around the room temperature or higher.

A. Magnetization

Calculated temperature dependence of magnetization $M(T) \equiv \sqrt{M_x^2 + M_y^2 + M_z^2}$ for the bulk, the Nd-sublattice, and the Fe-sublattice of NdFe$_{12}$N is shown in Fig. 3(a). Calculated Curie temperature falls in the same range as the experimentally claimed one. Considering the possible presence of $\alpha$-Fe-originated noise in the experimental data and neglect of all next-nearest-neighbor exchange interactions in our model which should have lowered the computational magnetic-ordering energy scale, the agreement is satisfactory. Also we see that the system-size dependence is negligible in our focus temperature range, which up to $T = 500$ [K] at most. Comparing the calculated temperature dependence of magnetization between NdFe$_{12}$ and NdFe$_{12}$N as shown in Fig. 3(b), we see that the experimentally observed nitrogenation-triggered enhancement in the Curie temperature by $\sim 200$ [K] is well reproduced.

We note that Nd in NdFe$_{12}$ has the easy-plane magnetic anisotropy which would compete against the easy-axis anisotropy from at least a part of the Fe sublattices. Here we just track the origin of the difference in the Curie temperature between NdFe$_{12}$ and NdFe$_{12}$N to the nitrogenation-enhanced exchange couplings as demonstrated in Fig. 2. Further studies on the outcome of the competing anisotropies in NdFe$_{12}$ is separated for future work.

B. Anisotropy field

Calculated magnetization curves with the externally applied magnetic field parallel and perpendicular to the easy axis in NdFe$_{12}$N (which is c-axis) at $T = 348$ [K] is shown in Fig. 3(a). The anisotropy field $H_a$ is identified as a crossing point of the two curves with a linear fit. Our numerical measurement just follows the experimental way to determine $H_a$. Thus determined anisotropy field $H_a(L,T)$ with the $L$-dependence being saturated out within the statistical error bars is plotted as a function of temperature in Fig. 3(b) in comparison to the recent experimental data. In the operation temperature range, a leading-order numerical control seems to be achieved.
We inspect which parameter dominates which part of the temperature dependence of the observables comparing with the latest experimental data. One of the most important practical utilities of permanent magnets lies in the coercivity that is roughly proportional to the anisotropy field of the parent material or the main phase, and the main issue here is to figure out how to sustain the anisotropy field at high temperatures. Calculated MAE and the main issue here is to figure out how to sustain the anisotropy field of the parent material or the main phase, lies in the coercivity that is roughly proportional to the

\[ J_{\text{RT}} \] 

in determining the realistic magnetic anisotropy energy scale at finite temperatures, through a close comparison between calculated results and the \( J_{\text{RT}} \) written as Eq. 4 for the magnetic properties of NdFe\(_{12}\)N in the operation temperature range, we further pin-down the role of \( J_{\text{mi}} \) in determining the realistic magnetic anisotropy energy scale at finite temperatures, through a close comparison between calculated results and the

\[ J_{\text{mi}} = \frac{K^{\text{Nd}}}{K^{\text{Fe}}} \]

initio determination of the exact nature of Fe-sublattice-dependent MAE is under way.

Numerically manipulating the 5d-mediated 4f-3d indirect exchange coupling, \( J_{\text{RT}} \), we observe how the calculated temperature dependence of the magnetization and the anisotropy field in NdFe\(_{12}\)N is affected as shown in Figs. 6 (a) and (b), respectively. The anisotropy field is more significantly affected by \( J_{\text{RT}} \) than the magnetization especially around \( T \sim 300 \) [K]. This is a numerical demonstration that a small enhancement in \( J_{\text{RT}} \), which may be realized by the conduction-band engineering in 4f-3d intermetallics, can already lead to a considerable improvement.

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Fig. 6. $J^{RT}$-dependence of the calculated temperature dependence of (a) magnetization and (b) anisotropy field for NdFe$_{12}$N. Given values from the ab initio electronic-structure calculations are tabulated in Table I.

In Fig. 6 it is seen that the experimentally observed slope and the downward convexity of the temperature dependence of the anisotropy field for NdFe$_{12}$N is closest to the calculated $H_a(T)$ with $\alpha_{RT} = 0.25$. Also the experimental anisotropy field near the liquid-nitrogen temperature seems to come close to 14 [T], which suggests possible systematic underestimate in our calculated magnetic anisotropy which falls below 10 [T] in the limit $T \to 0$. The $ab\ initio$ estimation for the crystal-field coefficients for the estimation of the uni-axial magnetic anisotropy energy indeed involves a certain uncertainty.

An improved data collapse between theory and experiment in the lowest temperature range of $H_a(T)$ can be observed by manually setting $K^{Nd} = 2K^{Nd}_0$. As shown in Fig. 7 the slope of the temperature dependence up to the room-temperature range is well reproduced. The upper shift of the calculated $H_a(T)$ on the high-temperature side of the operation temperature range can be adjusted by a manual scaling of $J^{RT}$ with an overall factor of 4/3 to match the Curie temperature. This can be considered as an effective renormalization of the 3d-3d exchange couplings imposed by the discarded longer-range part in the exchange couplings.

Thus an inspection of the experimental temperature dependence of magnetization and anisotropy field leads to a set of model parameters for a quantitative description of the experimental finite-temperature data. Based on the obvious relevance of $J^{RT}$ for the Curie temperature and $K^{RT}$ for $H_a(T = 0)$, it is seen that $J^{RT}$ determines the slope of $H_a(T)$ near $T \gtrsim 0$.

In such parameter set, the $4f$-3d exchange couplings come close to a quarter of the tabulated numbers which were $1 \sim 2$ [meV] as seen in Table I. In the language of the two-sublattice model where an isolated $4f$-electron magnetic moment is put into the sea of 3d-electron magnetization via a molecular field $H_m$, the molecular field can be written in terms of our lattice model language as follows.

$$H_m = \alpha_{RT} J^{RT} S \times z_{Nd}$$

where $z_{Nd}$ is the coordination number around the Nd magnetic moment which is in the present case $z_{Nd} = 20$ within the nearest neighbor. Plugging in the realistic numbers $\alpha_{RT} \sim 0.25$, $J^{RT} \sim 2$ [meV], $S \sim 2$ [$\mu_B$] the magnitude of the exchange field is found to be $H_m \sim 40$ [meV] = 700 [T] which gives the same order as was found in the experimental analyses $H_m \sim 450 - 600$ [T] by neutron. $\alpha_{RT} = 1$ corresponds to $H_m$ beyond 1000 [T] thus is out of the realistic scale. The smallness of the realistic number in the factor $\alpha_{RT}$ presumably reflects the indirect nature of the $4f$-3d exchange.

V. CONCLUSIONS AND OUTLOOK

Ab initio modeling for the $4f$ and 3d magnetism coupled by 5d-electrons on the basis of the realistic spin-lattice model for the rare-earth permanent magnet materials NdFe$_{12}$N and NdFe$_{12}$ quantitatively captures the realistic energy scales in the leading order in the operating temperature range, 200 [K] $\lesssim T \lesssim 500$ [K]. Experimentally observed magnetic ordering and magnetic anisotropy energy scales are put under numerical control and we have shown that enhancing the $4f$-3d indirect...
exchange coupling would work most effectively to realize the magnetic properties of more practical use in the operation temperature range. Establishing a quantitative description starting with the simplified model would pave the way to more realistic simulations to explicitly incorporate the strongly-correlated nature of 4f-electrons embedded in the conduction-electron sea of 5d-electrons to comprehensively describe the finite-temperature physics starting from the range $T \approx 1$ [K] all the way to the Curie temperature close to 1000 [K].

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1M. Sagawa, S. Fujimura, N. Togawa, H. Yamamoto, and Y. Matsuura, J. Appl. Phys. 55, 2083 (1984).
2S. Hirosawa, Y. Matsuura, H. Yamamoto, S. Fujimura, M. Sagawa, J. Appl. Phys. 59, 873 (1986).
3K. Hono and H. Sepehri-Amin, Scr. Mater. 67, 530 (2012).
4T. Miyake, K. Terakura, Y. Harashima, H. Kino, and S. Ishibashi, J. Phys. Soc. Jpn. 83, 043702 (2014).
5Y. Hirayama, Y. K. Takahashi, S. Hirosawa, and K. Hono, Scr. Mater. 95, 70 (2015).
6Y. Hirayama, T. Miyake, and K. Hono, JOM 67, 1344 (2015).
7For a review, see e.g. J. Yang and Y. Yang, in Handbook of Advanced Magnetic Materials, Eds. Y. Liu, D. J. Sellmyer, and D. Shindo, Springer (2006).
8M. Yamada, H. Kato, H. Yamamoto, and Y. Nakagawa, Phys. Rev. B 38, 620 (1988).
9I. M. Cadogan, J. P. Gavigan, D. Givord, and H. S. Li, J. Phys. F: Met. Phys. 18, 779 (1988).
10R. J. Radwański, J. Mag. Mag. Mater. 62, 120 (1986); Z. Phys. B 65, 65 (1986); R. J. Radwański and J. J. M. Franse, Phys. Rev. B 36, 8616 (1987).
11M. D. Kuz’mín, Phys. Rev. B 46, 8219 (1992); M. D. Kuz’mín and J. M. D. Coey, Phys. Rev. B 50, 12533 (1994).
12M. Fähnle, K. Hummler, M. Liebs, and T. Beuerle, Appl. Phys. A 57, 67 (1993).
13R. Sasaki, D. Miura, and A. Sakuma, Appl. Phys. Express 8, 043004 (2015).
14R. Skomski, J. Appl. Phys. 83, 6724 (1998).
15Y. Harashima, K. Terakura, H. Kino, S. Ishibashi, and T. Miyake, JPS Conf. Proc. 5, 011021 (2015).
16http://qmas.jp
17http://kkr.phys.sci.osaka-u.ac.jp
18A. I. Liechtenstein, M. I. Katnelson, V. P. Antropov, and V. A. Gubanov, J. Mag. Mag. Mater. 67, 65 (1987).
19I. F. Herbst, Rev. Mod. Phys. 63, 819 (1991).
20A. Nikitin, I. S. Tereshina, V. N. Verbetskii, and A. A. Salmova, Fiz. Tverd. Tela (St. Petersburg) 40, 285 (1998).
21Y. Hirayama et al., JIM meeting 2015, and private communications.
22M. Loewenhaupt and I. Sosnowska, J. Appl. Phys. 70, 5967 (1991).