Supplemental Material for "Atomistic model analysis of the spin reorientation transition in $(Nd_{1-x}Dy_x)_2Fe_{14}B$ systems"

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1 Magnetic parameters of the atomistic model

1.1 Magnetic moments in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$

Figure S1 depicts the magnitudes of the magnetic moments $s = |\boldsymbol{s}|$ of the constituent atoms in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$, estimated by first-principles calculations using AkaiKKR (MACHIKANEYAMA code) [1]. We find that the differences in magnetic moments between the corresponding atomic species in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$ are minimal. It should be noted that for Fe and B atoms, $\boldsymbol{S}_i = \boldsymbol{s}_i$, while for Nd and Dy atoms, $\boldsymbol{S}_i = \boldsymbol{s}_i + \boldsymbol{\mathcal{J}}_i$, as explained in the main text.

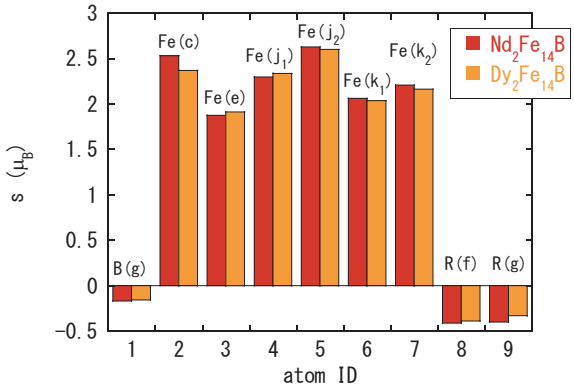

Figure 1: Magnetic moments of the constituent atoms in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$. R denotes Nd and Dy in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$, respectively.

1.2 Exchange interactions in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$

Figures S2(a) and S2(b) show the distribution of the exchange interactions $(2J_{ij}s_is_j)$ as a function of the interatomic distance (R), estimated using AkaiKKR for $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$, respectively. We observe that both systems exhibit similar distributions of exchange interactions, and the values are nearly identical. The exchange interactions between Nd atoms (Nd–Nd), between Dy atoms (Dy–Dy), and between B and Fe atoms (B–Fe) contribute only marginally.

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Figure S3 presents a comparison of the distributions of the exchange interactions ($2J_{ij}s_is_j$) as a function of the interatomic distance (R) for Fe–Fe and R–Fe bonds in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$.

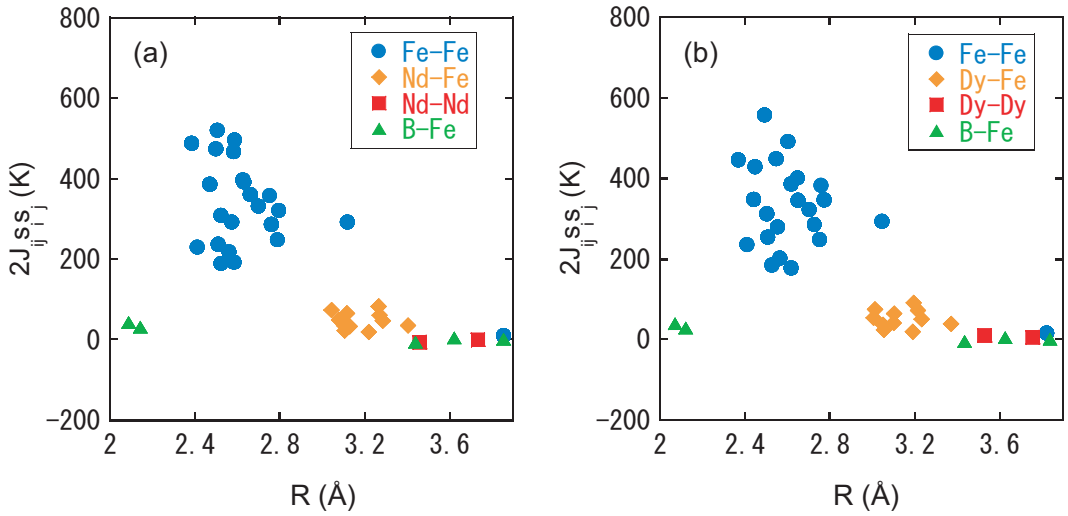

Figure 2: Distribution of the exchange interactions ($2J_{ij}s_is_j$) as a function of the interatomic distance (R) for (a) $Nd_2Fe_{14}B$ and (b) $Dy_2Fe_{14}B$.

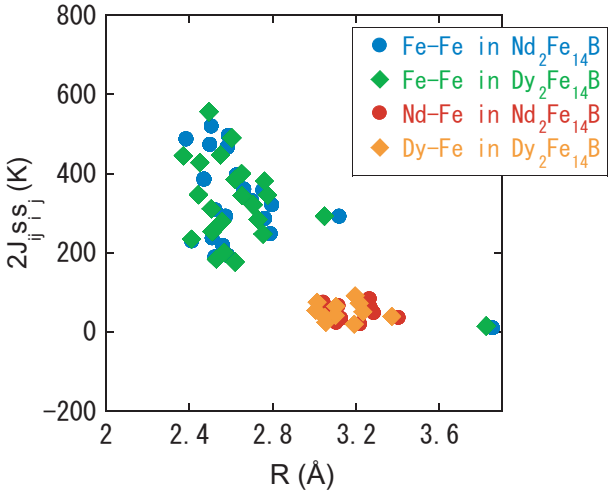

Figure 3: Comparison of the distributions of the exchange interactions ($2J_{ij}s_is_j$) as a function of the interatomic distance (R) for Fe–Fe and R–Fe bonds in $Nd_2Fe_{14}B$ and $Dy_2Fe_{14}B$.

1.3 Parameters of the crystal electric field energies for Nd and Dy atoms

The values of A_n^m for Nd atoms in $Nd_2Fe_{14}B$ and for Dy atoms in $Dy_2Fe_{14}B$ are listed in Table 1 and the corresponding values of $\langle r^n \rangle$ are shown in Table 2.

Table 1: A_n^m in units of Ka_0^{-n} [2].

	A_2^0	A_4^0	A_6^0
Nd	295	-12.3	-1.84
Dy	302	-12.7	-0.973

Table 2: Values of $\langle r^2 \rangle$, $\langle r^4 \rangle$, and $\langle r^6 \rangle$ in units of a_0^n, where a_0 is the Bohr radius [3].

	$\langle r^2 \rangle$	$\langle r^4 \rangle$	$\langle r^6 \rangle$
Nd	1.001	2.401	12.396
Dy	0.726	1.322	5.102

1.4 Anisotropy energies of Fe atoms

The anisotropy energies Ds^2 of Fe atoms in $R_2Fe_{14}B$, along with their site occupancies, are presented in Table 3.

Table 3: Anisotropy energies Ds^2 (K) of Fe atoms [4].

	Fe(c)	Fe(e)	Fe(j_1)	Fe(j_2)	Fe(k_1)	Fe(k_2)
$D(s)^2$ (K)	-24.8	-0.348	12.4	6.73	6.38	4.41
Site occupancies	4	4	8	8	16	16

References

[1] http://kkr.issp.u-tokyo.ac.jp/jp/

[2] M. Yamada, H. Kato, H. Yamamoto, and Y. Nakagawa, Phys. Rev. B 38, 620 (1988).

[3] A. J. Freeman and R. E. Watson, Phys. Rev. 127, 2058 (1962).

[4] Y. Miura, H. Tsuchiura, and T. Yoshioka, J. Appl. Phys. 115, 17A765 (2014).