Theoretical evaluation of perpendicular magnetic anisotropy of bct–Fe$_{50}$Co$_{50}$ stacked on Rh

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We studied the mechanism of the magnetic anisotropy in distorted bct–Fe$_{50}$Co$_{50}$ ordered alloys layered on Rh using a first principles calculation. For this purpose, we evaluated the uniaxial anisotropy constant $K_u$ and decomposed it into the bulk contribution $K_b$ and the interface contribution $K_{int}$. We discussed the origins of these contributions from the site–resolved $K_u$. The $K_b$ of the [Fe/Co]/Rh almost reproduces the $K_b$ of the bulk bct–Fe$_{50}$Co$_{50}$ in the case of both Fe/Rh and Co/Rh interfaces because the $K_b$ value at the inner layers of the [Fe/Co] is almost the same as that at the corresponding atoms in the bulk Co. As for $K_{int}$, it has a negative value in the two interface cases because the $K_{int}$ value of the Fe and Co atoms at the Rh interface is almost reduced to zero, which is primarily due to the collapse of the characteristic band structure in the [Fe/Co] ($c/a > 1$) by the mixing of electronic states with the Rh atoms.

Key words: first–principles calculation, hard magnetic material, thin film

1. Introduction

There has been a great demand for hard magnetic materials because of their prospects for application not only as strong permanent magnets but also in high–density magnetic storage devices. In order to fulfill this requirement, bct–FeCo alloys are one of the most promising candidates as a result of the theoretical prediction by the first–principles calculations 1). When the axial ratio between the $a$– and $c$–axes ($c/a$) is around 1.25, bct–Fe$_{50}$Co$_{100-x}$ alloy (0.5 ≤ $x$ ≤ 0.6) exhibits a large perpendicular magnetic anisotropy constant ($K_b$) about 700–800 μeV/atom, which is comparable to that of L10–FePt.

The large $K_b$ of the bct–FeCo is well explained by the approximate expression for the $K_b$ in terms of the 2nd–order perturbation of the spin–orbit interaction (SOI) as follows 2,3):

$$K_b = -\frac{1}{2\pi V} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \sum_{\epsilon} \text{Tr}[G^{\gamma}(\epsilon)H_{SO}\gamma G^{\gamma}(\epsilon)H_{SO}\gamma - G^{\gamma}(\epsilon)H_{SO}\gamma G^{\gamma}(\epsilon)H_{SO}\gamma],$$

(1)

where $V$ is the volume of the unit cell, $G^{\gamma}(\epsilon)$ is the one–electron retarded Green’s function excluding the SOI, and $H_{SO}\gamma$ is the SOI when the spin–quantization axis is along the $\mu$–axis and is defined as:

$$(H_{SO})_{\mu}(\theta, \phi) = \sum_{\xi} \xi, [U^{\gamma}(\theta, \phi)(I \cdot s)U(\theta, \phi)],$$

(2)

where $\xi, \xi$ is the strength of the SOI of the atoms located at site $i$, $I$ and $s$ are the orbital–angular– and spin–angular–momentum operators, respectively, and $U(\theta, \phi)$ is the rotation matrix of the spin quantization axis, where $\theta$ and $\phi$ together represent the direction of the $\mu$–axis, that is, $(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$.

In the absence of scattering events induced by alloy disorder, this equation can be expressed using the eigenstates and eigenenergies $E_{k, m, s}$ and $E_{k, n, s'}$ ($E_{k, n, s}$), as follows:

$$K_b = \frac{1}{V} \sum_{\epsilon} \sum_{\sigma \sigma'} \sum_{n, s, n', s'} |\langle k, n, \sigma | H_{SO} | k, n', \sigma' \rangle|^2 \left( \frac{E_{k, n, \sigma} - E_{k, n', \sigma'}}{E_{k, n, \sigma} - E_{k, n', \sigma'}} \right)$$

(3)

The denominator of this equation contains the energy difference between the occupied and unoccupied bands, which indicates that $K_b$ is mainly dominated by the electronic states near $E_F$. In bct–FeCo alloys, when $c/a$ is increased from 1, the energies of $d_\sigma^2$, $d_{\sigma'}^2$, and $d_{\sigma'}^2$ become close, and these energies undergo cross–over at the $\Gamma$ point around $c/a = 1.25$. In the case of an appropriate composition of bct–Fe$_{50}$Co$_{100-x}$ (0.5 ≤ $x$ ≤ 0.6), $E_F$ exists near the crossing point, and the giant $K_b$ arises near the $\Gamma$ point 1,4). Therefore, the $K_b$ in bct–FeCo is sensitive to the composition of elements and the lattice distortion.

One potential approach to fabricate the distorted FeCo alloys in real systems is to employ lattice mismatch between a bcc–FeCo alloy and a substrate. Using this technique, an artificial thin film of distorted bct–FeCo has been demonstrated on various substrates, such as Pt, Pd, Ir, Rh and FePt 4,5). Recently, Luo et al. succeeded in fabricating a Fe$_{50}$Co$_{50}$ ordered alloy with a strong perpendicular magnetization on a Rh substrate 6). In their experiment, Fe and Co mono–layers (MLs) were alternately stacked on Rh substrates. They confirmed that the $d\sigma$ value of the [Fe/Co] layer maintains a constant value of $d\sigma = 1.20$ from the 6th ML to the 12th ML of the [Fe/Co] layer. In this range of layers where $c/a$ remains constant, the obtained $K_b$ was decomposed into the bulk contribution $K_b$ and the interface contribution $K_{int}$ by means of fitting to the following phenomenological equation 7,8):

$$K_u = K_{mu} \times t_{FM} + K_{int},$$

(4)

where $t_{FM}$ is the thickness of the ferromagnetic film. In the graph of $K_u \times t_{FM}$ as a function of $t_{FM}$, $K_u$ and $K_{int}$ correspond to the slope and intercept, respectively. The

Journal of the Magnetics Society of Japan Vol.39, No.2, 2015 37
In section 2, we explain our calculation method for evaluating \( K_u \) and \( K_{int} \) and the site-resolved form of \( K_v \) based on 2nd-order perturbation of the SOI. In section 3.1, we show results for the \( K_v \) and \( K_{int} \) values, which are estimated from our calculated values of \( K_u \) and we compare them with the experimental results obtained in Ref. 9. In section 3.2, we present the site-resolved \( K_v \) and discuss the effect of the \( K_v \) value at each Fe and Co atom on the estimated \( K_u \) and \( K_{int} \) in section 3.1. In section 3.3, we perform a detailed analysis of the influence of the Rh substrate on the \( K_u \) of each Fe and Co atom, especially near the Rh substrate.

2. Calculation method

We adopted the tight-binding linear muffin-tin orbital method (TB-LMTO) under the local spin density functional approximation (LSDA), and we introduced the SOI Hamiltonian in the Pauli approximation. In the unit cell of our calculation object, we assumed 3 layers of Rh and a stack of \( N(N = 3, 5, 7) \) alternating layers of Fe and Co. Figure 1 shows the unit cell of the \([\text{Fe/Co}]/\text{Rh} \) bilayer, one of our calculation targets. As for the atom position at the interface, we took into account the two cases (that is, either Fe or Co atoms are located at the Rh interfaces) so that we can investigate the interface effect for each type of atoms. It should be noted that the \([\text{Fe/Co}]/\text{Rh} \) structure in the previous experiment \(^9\) is obtained by means of the molecular beam method, where the atom position is precisely controlled. Then we considered these two interface types without discussion of the formation energy in each interface type. For the lattice distortion of each atomic layer, the Rh layer is fixed in an fcc structure, which corresponds to the bct structure with \( \alpha a = \sqrt{2} \) in Fig. 1. In the \([\text{Fe/Co}] / \text{Rh} \) and Fe/Co layers, we determined the lattice distortion to be as follows: the in-plane (100) lattice constant of the \([\text{Fe/Co}] \) was adjusted to that of Rh in the (110) direction, and the volume of the \([\text{Fe/Co}] \) was preserved. Under this premise and using lattice constants for the ordered \([\text{Fe/Co}] \) alloy and for the Rh substrate of \( 2.85 \text{ Å} \) and \( 2.69 \text{ Å} \) respectively, we obtain a \( \Delta a \) of about 1.20 between the \([\text{Fe/Co}] / \text{Rh} \) and Fe/Co layers, which is consistent with the observed \( \Delta a \) of \([\text{Fe/Co}] \) films on Rh substrates \(^7,9\).

To estimate \( K_u \) and \( K_{int} \), we first calculate \( K_u \) from the force theorem \(^{20}\). After normalizing the energy difference to the volume of \([\text{Fe/Co}] \), which is proportional to the number of Fe and Co layers in the unit cell. We calculated \( K_u \) under the above condition, we performed a linear fit to \( K_u / \text{FM} \) as a function of \( \text{FM} \) by means of the least-squares technique. We estimated \( K_u \) and \( K_{int} \) from the slope and the intercept of the linear fit in eq. (4).

On the other hand, when we discuss the site-resolved \( K_v \), we employed the 2nd-order perturbation in terms of the SOI based on eq. (3). To evaluate \( K_v \) from each atom of the unit cell, we expand the \( |\kappa, n, \mu\rangle \) of eq. (3) in terms of the localized atomic basis \( |i, \mu, \sigma\rangle \), where \( i \) indexes the atomic sites, and \( \mu \) is the quantum number of the atomic

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Fig. 1 Unit cell of ordered \([\text{Fe/Co}] / \text{Rh} \) bilayer with Fe/Rh(Co/Rh) interfaces. We assumed the two types of interface cases where Fe or Co atoms are located on both sides of the Rh interface. \( \Delta a \) is fixed \( \sqrt{2} \) between the Rh/Rh layers and 1.2 between the Fe/Co and Fe(Fe)/Rh layers. We distinguish the same atoms of different positions by using the added parenthetical number. The distribution of the number of atoms reflects the mirror symmetry with respect to the a b plane containing the Co(Fe)(4) atom.
orbital. Applying this transformation, using the SOI Hamiltonian defined in eq. (2), and utilizing the relation for the matrix element of the SOI 21, \( K_u \) is decomposed into the contribution from each site and each combination of the spin–mixing via SOI, as follows:

\[
K_u^\sigma_\sigma' = -\frac{1}{8n^2} \sum_i \sum_{\mu \mu'} \sum_{\lambda \lambda'} \int_{-\infty}^{E_F} \text{d} \varepsilon \text{Im} \left( G_{i,j,\lambda,\mu}^\varepsilon G_{j,i,\lambda',\mu'}^{\varepsilon*} \right) \times (2\delta_{\sigma\sigma'} - 1)(\mu|\lambda|\mu') - (\mu|\lambda|\mu')(\lambda'|\lambda|\lambda'),
\]

which satisfies the relationship

\[
\sum_i \left( K_u^{1,1} + K_u^{1,1} + K_u^{1,1} + K_u^{1,1} \right) = K_u
\]

Table 1 Dependence of \( K_v \) in \([\text{Fe/Co}]_2/\text{Rh}_3\) for the two interface cases on the calculation method: the force theorem or the 2nd-order perturbation in terms of the SOI.

| Force theorem (Merg/cc) | 2nd-order perturbation (Merg/cc) |
|------------------------|----------------------------------|
| Fe/Rh                  | 29.1                             |
| Co/Rh                  | 17.1                             |

Table 2 Estimated result of \( K_v \) and \( K_{\text{int}} \) values, in \([\text{Fe/Co}]/\text{Rh}\) systems, which are obtained from the slope and the intercept of the linear fit in Fig. 2, respectively. \([\text{Fe/Co}]/\text{Rh}\) (Fe/Rh) and \([\text{Fe/Co}]/\text{Rh}\) (Co/Rh) represents the corresponding interface cases of \([\text{Fe/Co}]/\text{Rh}\). \([\text{Fe/Co}]/\text{Rh}\) (exp) is the estimated values from the experiment by Lao, and \( K_v \) of FeCo (bulk) denotes the \( K_v \) of the FeCo bulk with no Rh interface effect.

| \([\text{Fe/Co}]/\text{Rh}\) (Fe/Rh) | \( K_v \) (Merg/cc) | \( K_{\text{int}} \) (erg/cm²) |
|-----------------------------------|---------------------|-----------------------------|
| [Fe/Co]/Rh (Fe/Rh)              | 30.8                | -0.199                      |
| [Fe/Co]/Rh (Co/Rh)              | 25.4                | -0.913                      |
| [Fe/Co]/Rh (exp)                | 25.0                | 0.680                       |
| [Fe/Co]/Rh (bulk)               | 31.9                | -                           |

The site– and spin–dependent \( K_v \) values in terms of the SOI in \([\text{Fe/Co}]/\text{Rh}\) systems.

First, we compared the obtained \( K_v \) from the 2nd-order perturbation of the SOI with that from the force theorem. Table 1 shows this comparison for \([\text{Fe/Co}]/\text{Rh}\) for Fe/Rh and Co/Rh interface situations, respectively. We confirmed that the 2nd-order perturbation of the SOI is a good approximation for evaluating \( K_v \) for each of the two interface cases.

3. Results and discussions

3.1 Results for \( K_v \) and \( K_{\text{int}} \) under different \([\text{Fe/Co}]/\text{Rh}\) interface condition

At first, we examined the validity of eq. (4) using the calculated \( K_v \) based on the force theorem. Figure 2 shows the result of \( K_v \times t_M \) for various values of \( t_M \), which correspond to thickness of 3, 5, and 7 \([\text{Fe/Co}]\) MLs. The notations \((\text{Fe/Rh})\) and \((\text{Co/Rh})\) respectively represent the two possible interface conditions: a Fe layer that is adjacent to the Rh substrate and a Co layer that is adjacent to the Rh substrate. In the figure, the plotted data points and the line respectively represent the raw data and the linear fit obtained from the data. It can be seen that there is a good fit between the plotted data and the linear fit. Then, we determined \( K_v \) and \( K_{\text{int}} \) from the linear fit.

The \( K_v \) and \( K_{\text{int}} \) of the two interface conditions estimated from the line in Fig. 2 are shown as \([\text{Fe/Co}]/\text{Rh}\) (Fe/Rh) and \([\text{Fe/Co}]/\text{Rh}\) (Co/Rh) in table 2. \( K_v \) and \( K_{\text{int}} \) in FeCo (exp) represent the estimated values from the experimentally observed \( K_v \) of \([\text{Fe/Co}]/\text{Rh}\) 20, which consists of a Fe/Rh interface on one side and a Co/Rh interface on the other side. \( K_v \) of FeCo (bulk) represents the calculated \( K_v \) from the ideal bulk \([\text{Fe/Co}]/\text{Rh}\) with a \( K_{\text{int}} \) of zero. \( K_v \) in the case of the Fe/Rh interface is almost equal to that of FeCo (bulk). As for the Co/Rh interface case, \( K_v \) is nearly 80% of the value of \( K_v \) in FeCo (bulk). As a result, we can regard \( K_v \) as being mainly determined by the structure of \([\text{Fe/Co}]/\text{Rh}\)
and influenced comparatively little by the atom positions at the Rh interface. We also checked that the calculated $K_u$ is in good agreement with that of FeCo (exp). Conversely, for $K_{int}$, the results of both interfaces show negative values, which differs from the positive $K_{int}$ obtained through the experiment. In particular, $K_{int}$ of the Co/Rh interface has a large negative value of about $-0.9$ erg/cm$^2$, which is comparable to the $K_u$ of $-9$ Merg/cc, which occurs when $\\bar{n}_{m}$ is 1 nm.

### Table 3 Site-resolved $K_u$ based on eq. (5) for [Fe/Co]$_3$/Rh$_{1}$ in the Fe/Rh and the Co/Rh interface cases, and the corresponding $K_u$ of the bulk FeCo for comparison.

| [Fe/Co]/Rh (Fe/Rh) | $K_u$ (10 eV/atom) | $m_u$(µm) |
|---------------------|-------------------|------------|
| Fe(1)               | 0.162             | 2.55       |
| Co(2)               | 3.48              | 1.59       |
| Fe(3)               | 1.44              | 2.64       |
| Co(4)               | 4.05              | 1.59       |
| Rh(1)               | 1.33              | 0.304      |
| Rh(2)               | -0.182            | 0.078      |

| [Fe/Co]/Rh (Co/Rh)  | $K_u$ (10 eV/atom) | $m_u$(µm) |
|---------------------|-------------------|------------|
| Co(1)               | -0.514            | 1.59       |
| Fe(2)               | 0.823             | 2.64       |
| Co(3)               | 3.94              | 1.58       |
| Fe(4)               | 1.52              | 2.65       |
| Rh(1)               | -0.287            | 0.376      |
| Rh(2)               | -0.486            | 0.114      |

| [Fe/Co] (bulk)      | $K_u$ (10 eV/atom) | $m_u$(µm) |
|---------------------|-------------------|------------|
| Fe                  | 1.35              | 2.63       |
| Co                  | 3.85              | 1.59       |

and influenced comparatively little by the atom positions at the Rh interface. We also checked that the calculated $K_u$ is in good agreement with that of FeCo (exp). Conversely, for $K_{int}$, the results of both interfaces show negative values, which differs from the positive $K_{int}$ obtained through the experiment. In particular, $K_{int}$ of the Co/Rh interface has a large negative value of about $-0.9$ erg/cm$^2$, which is comparable to the $K_u$ of $-9$ Merg/cc, which occurs when $\\bar{n}_{m}$ is 1 nm.

### 3.2 Discussion for the values of $K_u$ and $K_{int}$ in [Fe/Co]/Rh in terms of the $K_u$ contribution from the individual site and atom.

Next, we divided the $K_u$ of [Fe/Co]/Rh systems into contributions from each of the atomic sites by means of the 2nd-order perturbation in terms of the SOI, which is determined by the sum of the distortion effect of the [Fe/Co] and the interface effect induced by the Rh substrate.

Table 3 exhibits the site-resolved $K_u$ (eV/atom) of [Fe/Co]$_3$/Rh$_{1}$ for the two interface cases and the corresponding $K_u$ of bulk FeCo. We also show the magnetic moment $m_u$(µm) at each site. The number of each atom in [Fe/Co]/Rh denotes the positions of the atoms in Fig. 1.

When focusing on the site-resolved $K_u$ in bulk FeCo, the result indicates that both Fe and Co atoms make a positive contribution to $K_u$, and the $K_u$ contribution from the Co atom is about three times larger than that from the Fe atom. In [Fe/Co]/Rh systems, one can find that the $K_u$ contribution from each Fe or Co atom that is two atomic layers away from the Rh interfaces is nearly equal to that of the same atoms in bulk FeCo; this finding is valid under both of the interface cases. This result indicates that the effect on $K_u$ in Fe and Co atoms caused by the mixing of electronic states with those of Rh substrate is limited to a depth of only one or two layers from the interface. As a result, we confirmed that the $K_u$ of the [Fe/Co]/Rh system almost reproduces the $K_u$ of the bulk FeCo for each of two interface cases if the number of [Fe/Co] layer exceeds 5 MLs, where the center layer of [Fe/Co] is three layers away from the Rh interface: this number of layers corresponds to about a 0.8-0.85 nm thickness of [Fe/Co].

### 3.3 Detailed discussion of the effect of Rh-substrates on the $K_u$ of Fe and Co atoms in terms of spin-mixing and orbital-mixing via the SOI.

Next, we discuss the influence of the Rh substrate on the $K_u$ of Fe and Co atoms by analyzing the contributions of each spin-mixing combination via SOI based on eq. (5). Figure 3 shows the spin-resolved $K_u$ of Fe and Co atoms located at the Rh interface and at the center of the [Fe/Co] layer in the [Fe/Co]/Rh systems. We also show the corresponding values of $K_u$ for atoms in the bulk FeCo. For the $K_u$ of Fe and Co atoms at the center of the [Fe/Co] in the [Fe/Co]/Rh, we observe good correspondence with those values of the bulk FeCo in every spin-mixing element of the SOI, and we found that the coupling between the minority-spin states via the SOI had the largest contribution to the total $K_u$ of this site. On the other hand, as for the $K_u$ of Fe and Co atoms at the Rh interface, the contribution of the minority-spin states to $K_u$ is strongly attenuated with respect to that from the same atoms at the center of the [Fe/Co]. Furthermore, the $K_u$ induced from the SOI between majority-spin states and from that between the states off spin states increase and decrease, respectively. As a result, the total $K_u$ value is nearly offset by each spin-mixing contribution at the Rh interface, as shown in table 3.

To explain the mechanism of the change of each component of the spin-resolved $K_u$ in Fe and Co atoms at the Rh interface, we begin by showing in Figure 4 the $d$-orbital DOS of the Fe(Co) and Rh atoms at the interface and that of Fe(Co) atoms at the center of FeCo.
[Fe/Co] in [Fe/Co]7Rh3 for the case of the Fe/Rh(Co/Rh) interface. When focusing on the majority-spin DOS for the particular atom (Fe or Co) at the different positions, one can find the larger d-orbital states in the interface atoms around EF, which strongly contributes to the Ku of this atoms, as can be seen by examining the denominator of eq. (3). This increase in the DOS is triggered by the mixing of electronic states with those of the Rh atoms at the interface with a majority-spin DOS that has a peak at EF. This mixing is explained by the induced magnetic moment of Rh at the interface as shown in table 3.

Therefore, it is anticipated that the larger Ku(↑⇔↑) in the Fe and Co interface atoms originates from the interaction of electronic states with those of the Rh substrate. Furthermore, this increase of the majority-spin DOS near EF also strongly affects the Ku(↑⇔↓+↓⇔↑) because this Ku is dominated by the pair of states (the majority-spin state and minority-spin state) that couples via SOI near EF, as shown in eq.(3). On the other hand, as for the origin of the strong reduction of Ku(↓⇔↓) in Fig.3, the difference in minority-spin DOS near EF between that at the interface and that at the center of [Fe/Co] is relatively small and cannot explain the change of Ku(↓⇔↓) in Fe and Co atoms at the Rh-interface.

To further discuss Ku(↓⇔↓), we evaluate the contribution to this Ku from each orbital coupling between the μ and μ' states via SOI, which is defined by:

![Graph](image1)

**Fig. 3** spin-resolved Ku in the Fe and Co atoms at the Rh interface and the center of [Fe/Co] of [Fe/Co]7Rh3 for both Fe/Rh and Co/Rh interfaces. We also show the corresponding Ku of the Fe and Co atoms in bulk FeCo.

![Graph](image2)

**Fig. 4** d-orbital DOS near Ef in the Fe, Co, and Rh atoms at the interface and that in Fe and Co atoms located at the center of the [Fe/Co] in [Fe/Co]7Rh3 with Fe/Rh and Co/Rh interface cases.

**Table 4** Orbital resolved Ku (meV/atom), which originated from the specific combination of orbital coupling via the SOI up to l=2, of the Fe and Co atoms at the interface and the center of the [Fe/Co] layer. The difference of Ku value between the inside layer and the interface layer in each atom is also shown.

| Orbital coupling via SOI | px–px | py–py | dα–dα | dβ–dβ | dα–dβ | dα–dβ | dα–dβ |
|--------------------------|-------|-------|--------|--------|--------|--------|--------|
| Fe (interface)           | 0.627 | -0.600| 1.72   | 10.1   | -2.35  | -1.78  | 6.24   |
| Fe (center)              | 0.878 | -0.896| 1.83   | 10.7   | -2.34  | -1.79  | 6.22   |
| Fe (interface) · Fe(center)| -0.251| 0.296 | -0.110 | -0.533 | -0.00676 | 0.00730 | -0.0182 |
| Co (interface)           | 0.786 | -0.785| 2.86   | 14.9   | -3.20  | -3.17  | 10.9   |
| Co (center)              | 1.13  | -1.14 | 2.51   | 18.1   | -3.25  | -2.97  | 10.8   |
| Co (interface) · Co(center)| -0.347| 0.356 | 0.345  | 3.25   | 0.0533 | -0.200 | -0.0362 |

Journal of the Magnetics Society of Japan Vol.39, No.2, 2015
Fig. 5 (a): Bloch spectral functions (BSFs) of minority-spin $d_{x^2}$ and $d_{xy}$ states of the Fe and Co atoms located at the Rh interface and the center of [Fe/Co] in [Fe/Co]/Rh for Fe-Rh and Co-Rh interfaces. (b): BSFs of the same orbits as (a) in the Fe and Co atoms of bulk FeCo. In both (a) and (b), the density of red and blue colors respectively represent the intensity of the density of states of $d_{x^2}$ and $d_{xy}$ minority-spin states. The SOI effect is disregarded when calculating all spectrums.

We performed a theoretical evaluation of the magnetic anisotropy in the ordered bct-FeCo/Co alloy (c/a = 1.2) alloys stacked on Rh, where two kinds of magnetic anisotropy occurs as a result of the distortion of [Fe/Co] layers and the interface effect of Rh substrate. First, we estimated the bulk anisotropy $K_u$ and the interface anisotropy $K_{i}$ by a linear fit to the theoretically obtained $K_u$. We found that the $K_u$ values of the [Fe/Co]/Rh system were close to the $K_u$ of the bct-FeCo alloy (c/a = 1.2) in both Fe/Rh and Co/Rh interfaces.

Conclusions

We performed a theoretical evaluation of the magnetic anisotropy in the ordered bct-FeCo/Co (c/a = 1.2) alloys stacked on Rh, where two kinds of magnetic anisotropy occurs as a result of the distortion of [Fe/Co] layers and the interface effect of Rh substrate. First, we estimated the bulk anisotropy $K_u$ and the interface anisotropy $K_{i}$ by a linear fit to the theoretically obtained $K_u$. We found that the $K_u$ values of the [Fe/Co]/Rh system were close to the $K_u$ of the bct-FeCo alloy (c/a = 1.2) in both Fe/Rh and Co/Rh interfaces.
and Co/Rh interface cases. This result was explained by the site-resolved $K_u$ in the Fe and Co atoms: the $K_u$ maintains a value similar to that of the bulk FeCo when the atoms are more than two atomic layers away from the Rh interface. This property is featured by the common characteristic pair of $d_{xy}$ and $d_{x^2-y^2}$ orbitals of minority-spin states near $E_F$, which results in the large positive $K_u$. As for $K_{int}$, it has a negative value in both of the two interface cases. From the site-resolved $K_u$, we found that the $K_u$ values of the Fe and Co atoms at the Rh interface were almost reduced to zero compared with the values of the same atoms at the center of the [Fe/Co]. This phenomenon is characterized by two changes of the electronic states in the Fe and Co atoms at the Rh interface: an increase of the majority-spin DOS near $E_F$ and a collapse of the specific band structure, which induces the large $K_u$ of the [Fe/Co], because of the strong coupling of electronic states with the Rh-substrate.

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