Supporting Information for
Observation of large spin conversion anisotropy in bismuth

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No. 1 In situ RHEED patterns during the film growth

Figure S1 shows the in situ RHEED patterns of the MgO substrate, Ni, and Bi surfaces during film growth, where the incident electron beam was parallel to the [100] azimuth of the MgO substrate. Sharp streak patterns were observed in the region of thick Bi films (> 6 nm). These observations demonstrate that a sharp heteroepitaxial interface was obtained at Ni/Bi. While the spotty patterns observed in the thick Bi region show that the Bi surface was not atomically flat, these results show that all the layers were epitaxially grown. The RHEED pattern for Bi is consistent with the X-ray diffraction pattern in Fig. 1D and with a previous study (1) showing a rhombohedral (110) Bi (Bi(110)R) structure.

No. 2 XRD patterns before and after baking at device fabrication temperature

For the conventional lift-off process, substrates were baked after resist coating. To examine the influence of the baking on the samples, we carried out the XRD measurement after baking at 180°C for 270 sec. (90 sec × 3 times), same as the baking temperature in the device fabrication process. Comparing the result before baking, the XRD pattern did not change after baking (see Fig. S2). Therefore, we postulated that our Ni/Bi samples were not affected by baking in the device fabrication process.

No. 3 XRD patterns of Ni/Bi with and without substrate cooling during the Bi growth

We prepared Fe/Bi and Ni/Bi samples with and without substrate cooling during the Bi growth. The Ni/Bi with the substrate cooling is the sample mainly discussed in the main text. For the Fe/Bi samples, the substrate cooling changed crystal orientation of the Bi, Bi(111)R from the sample without cooling and Bi(110)R from the sample with cooling, as indicated by the XRD patterns (see Figs. 3A and 3B in the main text). On the other hand, Ni/Bi samples showed Bi(110)R for both conditions as shown in Fig. S3.

No. 4 Kittel equation considering magnetocrystalline anisotropy

The magnetization dynamics in a ferromagnetic thin film are described by the Landau-Lifshitz-Gilbert equation (2):

\[ \frac{dM}{dt} = -\gamma(M \times \mu_0 H_{eff}) + \frac{\alpha}{M_S} M \times \frac{dM}{dt}, \]  

where \( M \) is the magnetization, \( \gamma \) is the gyromagnetic ratio, \( \mu_0 \) is the vacuum permeability, \( \alpha \) is the Gilbert damping parameter, and \( M_S \) is the saturation magnetization of the ferromagnetic film. The effective magnetic field \( H_{eff} \) is described as \( H_{eff} = H + H_a + H_d + H_{rf} \), where \( H \) is the external magnetic field, \( H_a \) is the magnetic anisotropy field, \( H_d \) is the demagnetization field, and \( H_{rf} \) is the rf field. The first term represents the magnetization precession (field term), and the second term represents phenomenological magnetization damping to the saturation magnetization (damping term). This equation can be solved under the resonance condition, namely, ignoring the second term. Since the Ni film in our measurement was epitaxially grown on a single-crystal MgO substrate and became a single crystal, the magnetocrystalline anisotropy in Ni cannot be ignored. Then, Eq. [S1] is solved as follows (3):

\[ f_{res} = \frac{\mu_0 F}{2\pi} \sqrt{(H_{res} - 2H_1)(H_{res} + H_1 + M_{eff})}, \]  

where \( f_{res} \) (H_{res}) is the resonance frequency (magnetic field), and \( M_{eff} \) is the effective saturation magnetization, and \( H_1 \) is the magnetic anisotropy energy field. \( H_1 \) was estimated to be −13 mT and was independent of the Bi thickness. For single-crystal Fe, Eq. [S2] becomes as follows:

\[ f_{res} = \frac{\mu_0 F}{2\pi} \sqrt{(H_{res} + 2H_1)(H_{res} + 2H_1 + M_{eff})}. \]

No. 5 Frequency and Bi thickness dependences of the ST-FMR measurement

Figure S4A on the next page shows the ST-FMR signals obtained from the Ni/Bi(7 nm) sample at various rf-current frequencies from 7 to 12 GHz. Clear resonance signals were observed, and the signals were symmetric between 45 and 225 degrees, indicating that there are negligible spurious effects such as thermal effects. The ST-FMR signal can be deconvoluted into symmetric and antisymmetric Lorentzian signals by fitting with Eq. [1] in the main text.
\[ V_{DC} = -C \left( S \frac{\Delta^2}{\mu_0 (H - H_{res})^2 + \Delta^2} + A \frac{\Delta \mu_0 (H - H_{res})}{\mu_0 (H - H_{res})^2 + \Delta^2} \right) + a \mu_0 H + b, \]  

where \( C \) is a coefficient concerning the anisotropic magnetoresistance, \( S \) is the symmetric component, \( A \) is the antisymmetric component, \( \Delta \) is the half-width at half-maximum of the spectrum, and \( a \) and \( b \) are coefficients of the linear background. Here, \( H_{res} \) and \( \Delta \) are related to the magnetization dynamics and are evaluated through the frequency dependence (see Figs. S4B and S4C). Since we used single-crystal fcc (001) Ni as the ferromagnetic layer, Eq. [S2] was used to fit the frequency \( f \) dependence of \( H_{res} \). The \( f \) dependence of \( \Delta \) can be fitted with the following equation (4): \( \Delta = \Delta_0 + \frac{1}{2} \text{f}_{\text{eff}} f \), where \( \Delta_0 \) is the frequency-independent scattering parameter and \( f \) is the Gilbert damping parameter. Both frequency dependences were well fitted, and thus, we can discuss the magnetic properties based on the ST-FMR measurement results.

The spin-charge conversion efficiency, \( \eta \), is in principle estimated from the ratio of \( S \) and \( A \) as follows:

\[ \eta = \frac{S}{A} \times \frac{\sqrt{1 - \frac{2H_{res}}{H_{eff}}}}{\sqrt{1 + \frac{H_{res} + M_{eff}}{H_{eff}}}} , \]  

where \( h \) is the Dirac constant, \( e \) is the elemental charge, \( b_\text{Ni} \) is the thickness of Ni, and \( b_\text{Bi} \) is the thickness of Bi. \( M_{eff} \) and \( H_1 \) can be estimated from the Kittel equation and the frequency dependence of the ST-FMR signal. Here, the contents of the root were modified for magnetic anisotropy. From the estimation of the above parameters and the use of Eq. [S5], we can estimate the spin-charge conversion efficiency of Bi. Here, we show the Bi thickness dependences of \( H_{res} \), \( M_{eff} \), \( H_1 \), and \( V_B = -CA \) and \( V_\delta = -CS \) (see Fig. S5).

No. 6 Estimation of the spin Hall angle of Bi considering the SOT in Ni

Considering the spin diffusion equation in the Ni/Bi layers and the SHE in the Ni layer, the spin current density at the Ni/Bi interface, which flows along the direction normal to the Ni/Bi interface with spins polarized transverse to the magnetization of Ni, can be expressed as follows (5):

\[ J_{s+} = \frac{\text{tanh}(\frac{\Delta \mu_0}{2h} b_\text{Bi} c_{\text{Bi}}) \theta_\text{Bi} + \text{tanh}(\frac{\Delta \mu_0}{2h} b_\text{Ni} c_{\text{Ni}}) \theta_\text{Ni}}{\text{coth}(\frac{\Delta \mu_0}{2h} b_\text{Bi} c_{\text{Bi}}) + \text{coth}(\frac{\Delta \mu_0}{2h} b_\text{Ni} c_{\text{Ni}})} \sin \phi , \]  

where \( b_\text{Ni} \) is the thickness of Ni, \( \lambda_\text{Bi} \) (\( \lambda_\text{Ni} \)) is the spin diffusion length of Bi (Ni), \( \sigma_{\text{Bi}} \) (\( \sigma_{\text{Ni}} \)) is the electrical conductivity of Bi (Ni), \( j_{\text{C(Bi)}} \) (\( j_{\text{C(Ni)}} \)) is the electrical current density in Bi (Ni), and \( \theta_\text{Bi} \) (\( \theta_\text{Ni} \)) is the spin Hall angle of Bi (Ni). Here, we considered the magnetic field to be applied along the angle \( \phi = 45^\circ \) with respect to the current flow direction, and we neglected the interfacial spin-orbit coupling, spin precession during spin current diffusion (6), and the imaginary part because of the small influence on \( \xi_{DL} \) (7). Then, the damping-like torque efficiency \( \xi_{DL} \) considering the SHE in the ferromagnetic layer can be described as \( \xi_{DL} = j_{\text{C(Bi)}} / j_{\text{C(Ni)}} \sin \phi \). The spin-charge conversion efficiency can be expressed with \( \xi_{DL} \) as follows (8):

\[ \frac{1}{\eta} = \frac{1}{\xi_{DL}} \left( 1 + \frac{h}{\xi_{FL}} \right) = \frac{1}{\text{coth}(\frac{\Delta \mu_0}{2h} b_\text{Bi} c_{\text{Bi}}/\theta_\text{Bi}) + \text{coth}(\frac{\Delta \mu_0}{2h} b_\text{Ni} c_{\text{Ni}}/\theta_\text{Ni})} + \frac{h}{\xi_{FL}} \text{coth}(\frac{\Delta \mu_0}{2h} b_\text{Bi} c_{\text{Bi}}/\theta_\text{Bi}) , \]  

where \( \xi_{FL} \) is the field-like torque efficiency. Here, we assumed that \( \xi_{FL} / \xi_{DL} \) is independent of \( b_\text{Bi} \) because both torque efficiencies originate from the spin current described by Eq. [S6] and have the same \( b_\text{Bi} \) dependence. Therefore, the free parameters in Eq. [S7] were \( \theta_\text{Bi} \), \( \lambda_\text{Bi} \), and \( \xi_{FL} / \xi_{DL} \) in the fitting of the \( b_\text{Bi} \) dependence of \( \eta \). Figure S6 shows the calculation of the thickness dependence of \( \eta \) considering self-induced SOT in Ni for various \( \theta_\text{Bi} \). The values in the calculation of \( \eta \) are summarized in Table S1. In our calculation, \( \theta_\text{Bi} = 0.17 \), \( \lambda_\text{Bi} = 2.1 \) nm, and \( \xi_{FL} / \xi_{DL} \sim 0 \left( < 10^{-3} \right) \) were the best to reproduce our experimental results. Here, we used a typical conductivity of Bi in the fitting; however, higher conductivity than bulk conductivity has been reported in Bi thin films and Bi on metals (1, 9, 10). Figure S7 shows the fitting of \( \eta \) with various \( \theta_\text{Bi} \). \( \theta_\text{Bi} \) increased with increasing \( \sigma_{\text{Bi}} \) and was unchanged with decreasing \( \sigma_{\text{Bi}} \) (see Table S2). Therefore, the \( \theta_\text{Bi} \) estimated with typical parameters was close to the lower limit.
No. 7 Harmonic Hall measurement

The second harmonic Hall voltage $V_{2\omega}$ was measured with the Ni/Bi(11 nm) Hall bar. $V_{2\omega}$ was described as follows (17–19): 
$$V_{2\omega} = V_{\text{ANE}} + V_{\text{PHE}} + V_{\text{ONE}}$$ [S8]

where $V_{\text{ANE}}$ is the anomalous Hall voltage, $V_{\text{PHE}}$ is the planar Hall voltage, $V_{\text{ANE}}$ is the anomalous Nernst voltage, and $V_{\text{ONE}}$ is the ordinary Nernst voltage. For estimation of the fitting parameters, 1st harmonic measurements with $\theta = 0^\circ$ (anomalous Hall measurement) and $\theta = 90^\circ$ and $\phi = 0^\circ - 360^\circ$ (planar Hall measurement) were carried out (see Fig. S8A). We derived the amplitude of $V_{\text{ANE}}, V_{\text{PHE}} = 2.51$ mV, and the amplitude of $V_{\text{PHE}}, V_{\text{PHE}} = -0.72$ mV, at $t_{\text{Bi}} = 11$ nm, as shown in Figs. S8B and S8C.

$V_{\text{ANE}}$ and $V_{\text{ONE}}$ can be described as follows:

$$V_{\text{ANE}} = wE_{\text{ANE}} = w \cdot (-\alpha_{\text{ANE}})\mu_0 M \left( \begin{array}{c} \sin \theta_0 \cos \phi_0 \\ \cos \theta_0 \\ \sin \theta_0 \sin \phi_0 \end{array} \right) \times \left( \begin{array}{c} 0 \\ 0 \\ \Delta T \end{array} \right), \quad [S9]$$

$$V_{\text{ONE}} = wE_{\text{ONE}} = w \cdot (-\beta_{\text{ONE}})\mu_0 H \left( \begin{array}{c} \sin \theta \cos \phi \\ \cos \theta \\ \sin \theta \sin \phi \end{array} \right) \times \left( \begin{array}{c} 0 \\ 0 \\ \Delta T' \end{array} \right), \quad [S10]$$

where $w$ is the width of the channel, $\alpha_{\text{ANE}}$ is the anomalous Nernst coefficient of Ni, $\beta_{\text{ONE}}$ is the ordinary Nernst coefficient of Bi, $\theta$ ($\theta_0$) is the polar angle of the magnetic field (magnetization), $\phi$ ($\phi_0$) is the azimuth angle of the magnetic field (magnetization), and $\Delta T$ ($\Delta T'$) is the temperature gradient perpendicular to the Ni/Bi interface in Ni (Bi). $H$ and $M$ are the magnetic field and magnetization. For the magnetic field in the plane of the Ni/Bi interface, we assumed $\phi_0 \sim \phi$ and $\theta_0 \sim 90^\circ$, and Eq. [S8] can be written as Eq. [2] in the main text (17–19):

$$V_{2\omega} = A(H) \cos \phi + B(H) \cos 2\phi \cos \phi$$

where $A(H)$ and $B(H)$ are the damping-like torque effective field and the field-like torque effective field, $H_{\text{DL}}$ is the Oersted field, and $H_{\text{FL}}$ is the out-of-plane anisotropy field. $H_{\text{DL}} = 440$ mT was estimated from anomalous Hall measurement results, from the crossing point of the linear fittings in the low magnetic field region and saturated region (Fig. S8B). $V_{\text{ANE}}$ and $V_{\text{ONE}}$ are the amplitudes of the anomalous Nernst voltage and ordinary Nernst voltage. Figure S9 on the next page shows the $\phi$ dependence of $V_{2\omega}$ for various magnetic fields.

The magnetic field dependence of the fitting parameters, $A(H)$ can be deconvoluted into the anomalous Hall effect (AHE), ANE, and ONE components, and we can derive $\mu_0 H_{\text{DL}} = 160$ $\mu$T, $V_{\text{ANE}} = 1.8$ $\mu$V, and $V_{\text{ONE}} = 35$ $\mu$V/T. From the magnetic field dependence of $B(H)$, $\mu_0 H_{\text{FLL}} + H_{\text{DL}}$ was estimated to be 29 $\mu$T (see Fig. 4 in the main text). Here, $H_{\text{FLL}} = \mu_0 H_{\text{DL}}/2w$ was estimated to be 28 $\mu$T. The damping-like torque efficiency $\xi_{\text{DL}}$ and the field-like torque efficiency $\xi_{\text{FL}}$ can be described with $H_{\text{DL}}$ and $H_{\text{FL}}$ as follows (8):

$$\xi_{\text{DL(LFL)}} = \frac{2\mu_0 M_{\text{S}}}{\mu_0 H_{\text{DL(LFL)}}} \frac{H_{\text{FL(LFL)}}}{H_{\text{Bi}}}, \quad [S12]$$

$\xi_{\text{DL}}$ and $\xi_{\text{FL}}$ were estimated to be $2.7 \times 10^{-1}$ and $2.4 \times 10^{-3}$, respectively. Note that the spin Hall angle of Bi $\theta_{\text{S}} \sim \xi_{\text{DL}} = 0.27$ was very close to the that obtained from the ST-FMR measurement and the ratio of $\xi_{\text{CL}}/\xi_{\text{DL}} = 8.7 \times 10^{-3}$ obtained from the harmonic Hall measurement was very small, as in the results from the ST-FMR measurement (~ 0).

No. 8 Band structure of thin Bi(111)$_r$ and Bi(110)$_r$ films

Figure S10 on the next page shows the two-dimensional (2D) BZ for (A) Bi(111)$_r$ and (B) Bi(110)$_r$ films and their band structures (C) and (D), respectively, for 1 to 15BL. Density functional theory (DFT) calculations were performed using BAND software of Amsterdam Modeling Suite (20, 21). We used the fast inertial relaxation engine (FIRE) for geometry optimization (22). In the generalized gradient approximation (GGA) of DFT, the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional was used (23) together with double-zeta polarized basis sets and numerical orbitals with a large frozen core. The relativistic effects were taken into account by the noncollinear method.

For the Bi(111)$_r$ surface (Fig. S10A), the $\Gamma$-point in the 2D BZ corresponds to the $\Gamma$- and $T$-points in the bulk 3D BZ, where holes appear. The $M$-point in 2D corresponds to the $L$-point in
3D, where electrons appear. The bulk valence bands cross the Fermi energy at approximately the $\bar{\Gamma}$-point in the films with $\geq 7$BL. In contrast, the bulk conduction bands ($\bar{M}$-point) do not cross the Fermi energy in the films with $\leq 13$BL. These results agree well with the previous calculations below 10BL (24). Even in the 15BL film (~ 6 nm), the bulk electron density is extremely low, although the bulk conduction band crosses the Fermi energy. Although the numerical accuracy of the GGA calculation is not sufficient for the energy scale of a few meV (25), the GGA calculation can sufficiently capture the qualitative features for the current purpose. In fact, this evacuation of bulk electrons is consistent with the experimental observation by Hirahara et al. (10).

For the Bi(110)$_R$ surface (Fig. S10B), the $\bar{X}_z$-point in the 2D BZ corresponds to the $L$-points in the bulk 3D BZ. The $\bar{X}_z$-point in the 2D BZ corresponds to the $T$- and $L$-points in 3D BZ. The hole and electron carrier are completely mixed in the $k$-space for the Bi(110)$_R$ surface. According to previous (up to 8BL (26, 27)) and our present calculations (up to 15BL), the conduction band clearly crosses the Fermi energy for $\geq 3$BL. Contrary to the Bi(111)$_R$ surface, there is no clear indication of electron evacuation in the Bi(110)$_R$ surface.
Fig. S1. *In situ* RHEED images of the surface of the MgO substrate, Ni, and Bi.
Fig. S2. XRD patterns from the Ni/Bi before and after the baking.
Fig. S3. XRD spectra obtained from Ni/Bi with (w/) and without (w/o) substrate cooling during the Bi growth.
Fig. S4. (A) ST-FMR signals obtained from the Ni/Bi(7 nm) channel with various rf current frequencies \( f \). Solid lines indicate the fitting with Eq. [S4]. (B) Frequency dependence of the resonance field \( H_{\text{res}} \). The solid line indicates the fitting with the Kittel equation considering the magnetocrystalline anisotropy. (C) Frequency dependence of the full-width at half-maximum of the ST-FMR signal \( \Delta \). The solid line indicates the linear fitting, and we can extract the Gilbert damping parameter \( \alpha \) from its slope.
Fig. S5. Bi thickness dependence of (A) $H_{res}$, (B) $M_{eff}$, (C) $H_s$, and (D) $V_A = -CA$ and $V_S = -CS$. 
Fig. S6. Bi thickness $t_{\text{Bi}}$ dependence of the spin-charge conversion efficiency $\eta$ for various hypothetical spin Hall angles of Bi $\theta_{\text{Bi}}$ considering the self-induced SOT in Ni. The calculation well reproduces the data when $\theta_{\text{Bi}}$ equals 0.17.
Fig. S7. Bi thickness dependence of the spin-charge conversion efficiency $\eta$ and fitting of $\eta$ with various $\sigma_{\text{Bi}}$. 
Fig. S8. (A) Schematic image of the setup of the harmonic Hall measurement. (B) AHE measurement and (C) PHE measurement on the Ni/Bi(11.0 nm) Hall bar. The red solid lines indicate the fitting, linear for the AHE and cos $\phi$ for the PHE. $H_K$ can be estimated from the AHE as the crossing point of the linear fittings in the low magnetic field region and saturated region.
Fig. S9. Azimuth angle $\phi$ dependence of the second harmonic Hall voltage $V_{2\omega}$ for various magnetic fields. The red solid lines indicate the fitting with Eq. [S11].
Fig. S10. Brillouin zones for (A) Bi(111)\textsubscript{R} and (B) Bi(110)\textsubscript{R} and their band structures (C) and (D), respectively, up to 15BL computed by DFT. The horizontal dashed lines indicate the Fermi energy.
Table S1. Fitting constants in the calculation of $\eta$

| $\theta_{\text{h}}$ (11) | $\lambda_{\text{Ni}}$ (nm) (12, 13) | $\sigma_{\text{Ni}}$ (S/m) (11, 14) | $\sigma_{\text{Bi}}$ (S/m) (15) | $\mu_0 M_S$ (T) (16) |
|--------------------------|-------------------------------|---------------------------------|-------------------------------|---------------------|
| 0.07                     | 2.0                           | $8.0 \times 10^6$               | $2.4 \times 10^5$             | 0.61                |
Table S2. Fitting parameters in the calculation of $\eta$ for various $\sigma_{Bi}$

| $\sigma_{Bi}$ (S/m) | $\theta_{Bi}$ | $\lambda_{Bi}$ (nm) | $\xi_{FL}/\xi_{DL}$ |
|---------------------|--------------|---------------------|---------------------|
| $2.4 \times 10^4$   | 0.16         | 2.1                 | $\sim 0$            |
| $2.4 \times 10^5$   | 0.17         | 2.1                 | $\sim 0$            |
| $2.4 \times 10^6$   | 0.22         | 2.1                 | $\sim 0$            |
SI References
1. X.-X. Gong, et al., Possible p-Wave Superconductivity in Epitaxial Bi/Ni Bilayers. Chinese Phys. Lett. 32, 067402 (2015).
2. T. L. Gilbert, A phenomenological theory of damping in ferromagnetic materials. IEEE Trans. Magn. 40, 3443–3449 (2004).
3. C. Kittel, On the Theory of Ferromagnetic Resonance Absorption. Phys. Rev. 73, 155–161 (1948).
4. H. T. Nembach, et al., Perpendicular ferromagnetic resonance measurements of damping and Landé g-factor in sputtered (Co,Mn)1−xSix thin films. Phys. Rev. B 84, 054424 (2011).
5. M. Aoki et al., Anomalous sign inversion of spin-orbit torque in ferromagnetic/nonmagnetic bilayer systems due to self-induced spin-orbit torque. Phys. Rev. B 106, 174418 (2022).
6. A. Manchon, R. Matsumoto, H. Jaffres, J. Grollier, Spin transfer torque with spin diffusion in magnetic tunnel junctions. Phys. Rev. B 86, 060404 (2012).
7. K.-W. Kim, K.-J. Lee, Generalized Spin Drift-Diffusion Formalism in the Presence of Spin-Orbit Interaction of Ferromagnets. Phys. Rev. Lett. 125, 207205 (2020).
8. C.-F. Pai, Y. Ou, L. H. Vilela-Leão, D. C. Ralph, R. A. Buhrman, Dependence of the efficiency of spin Hall torque on the transparency of Pt/ferromagnetic layer interfaces. Phys. Rev. B 92, 064426 (2015).
9. M. Tokuda, et al., Spin transport measurements in metallic Bi/Ni nanowires. Appl. Phys. Express 12, 053005 (2019).
10. T. Hirahara, et al., Role of Quantum and Surface-State Effects in the Bulk Fermi-Level Position of Ultrathin Bi Films. Phys. Rev. Lett. 115, 106803 (2015).
11. Y. Omori, et al., Relation between spin Hall effect and anomalous Hall effect in 3d ferromagnetic metals. Phys. Rev. B 99, 014403 (2019).
12. A. Ghosh, S. Auffret, U. Ebels, W. E. Bailey, Penetration Depth of Transverse Spin Current in Ultrathin Ferromagnets. Phys. Rev. Lett. 109, 127202 (2012).
13. Y. Hibino, et al., Giant charge-to-spin conversion in ferromagnet via spin-orbit coupling. Nat. Commun. 12, 6254 (2021).
14. J. Xu, Y. Li, D. Hou, L. Ye, X. Jin, Enhancement of the anomalous Hall effect in Ni thin films by artificial interface modification. Appl. Phys. Lett. 102, 162401 (2013).
15. S. Xiao, D. Wei, X. Jin, Bi(111) Thin Film with Insulating Interior but Metallic Surfaces. Phys. Rev. Lett. 109, 166805 (2012).
16. B. D. Cullity, C. D. Graham, Introduction to magnetic materials, 2nd edition (John Wiley & Sons Inc., 2009).
17. M. Hayashi, J. Kim, M. Yamanouchi, H. Ohno, Quantitative characterization of the spin-orbit torque using harmonic Hall voltage measurements. Phys. Rev. B 89, 144425 (2014).
18. C. O. Avci, et al., Interplay of spin-orbit torque and thermoelectric effects in ferromagnet/normal-metal bilayers. Phys. Rev. B 90, 224427 (2014).
19. Z. Chi, et al., The spin Hall effect of Bi-Sb alloys driven by thermally excited Dirac-like electrons. Sci. Adv. 6, eaay2324 (2020).
20. G. te Velde, E. J. Baerends, Precise density-functional method for periodic structures. Phys. Rev. B 44, 7888–7903 (1991).
21. BAND 2021.1 (SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, https://www.scm.com/).
22. E. Bitzek, P. Koskinen, F. Gähler, M. Moseler, P. Gumbsch, Structural Relaxation Made Simple. Phys. Rev. Lett. 97, 170201 (2006).
23. J. P. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 77, 3865–3868 (1996).
24. Yu. M. Koroteev, G. Bihlmayer, E. V. Chulkov, S. Blügel, First-principles investigation of structural and electronic properties of ultrathin Bi films. Phys. Rev. B 77, 045428 (2008).
25. I. Aguilera, C. Friedrich, S. Blügel, Electronic phase transitions of bismuth under strain from relativistic self-consistent G W calculations. Phys. Rev. B 91, 125129 (2015).
26. J. I. Pascual, et al., Role of Spin in Quasiparticle Interference. Phys. Rev. Lett. 93, 196802 (2004).
27. G. Bian, et al., First-principles and spectroscopic studies of Bi(110) films: Thickness-dependent Dirac modes and property oscillations. Phys. Rev. B 90, 195409 (2014).