First-principles calculation of the nonadiabatic spin transfer torque in Ni and Fe

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The magnetization dynamics of a ferromagnet subjected to an electrical current are described by an extension of the Landau-Lifshitz-Gilbert equation that contains two additional terms, the adiabatic and nonadiabatic spin-transfer torques. First-principles calculations of the nonadiabatic spin-transfer torque parameter β for bcc iron and fcc nickel show that β is related to and typically of the same order as α, the damping constant, but is distinct from it. Calculations as a function of the ratio of spin-dependent scattering rates show that (1) the minimum of the damping constant as a function of scattering rate does not change significantly, and (2) when the polarization of the current approaches zero, β can become large but the implied domain-wall velocity does not.

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I. INTRODUCTION

More than thirty years ago, Berger[1] proposed using electrical currents in ferromagnetic metallic wires to move magnetic domain walls. Early experimental work[2,3] motivated by this idea was hampered by the fact that the smallest wires that could be fabricated required extremely large currents to move the walls. In the past decade, fabrication technology has developed sufficiently that domain walls could be moved with much more modest currents.[4–10] For more information, see the reviews[11,12] of experimental developments.

Berger[13] showed that the interaction between the electrical current and the textured magnetization patterns is mediated by the spin current that inevitably accompanies the charge current, and that the influence of spin currents could be accounted for by adding two additional terms to the Landau-Lifshitz-Gilbert equation of motion. This idea was developed further by several authors[14–16] and the labels adiabatic and nonadiabatic torque were introduced. For more information, see the reviews[17–19] of the theoretical developments.

The adiabatic spin-transfer torque has the form $-(\mathbf{v}_s \cdot \nabla)\mathbf{M}(\mathbf{r})$, where $\mathbf{M}(\mathbf{r})$ is the spatially varying magnetization and $\mathbf{v}_s$ is a spin velocity that is proportional to the current density and is discussed below. This torque arises when the electron moments stay aligned with the magnetization as they flow through a region of nonuniform magnetization.

The nonadiabatic spin-transfer torque is perpendicular to the adiabatic spin-transfer torque and the magnetization, so it has the form $-\beta\hat{\mathbf{m}}(\mathbf{r}) \times (\mathbf{v}_s \cdot \nabla)\mathbf{M}(\mathbf{r})$, where β is called the nonadiabatic spin-transfer torque parameter and $\hat{\mathbf{m}}$ is the direction of the magnetization. There are several contributions to the nonadiabatic torque. For thin domain walls, in which the domain-wall width is comparable to or smaller than the wavelength of the electrons at the Fermi energy, the electron spins cannot track the magnetization.[15,20–22] In this situation, there is a nonlocal correction to the adiabatic spin-transfer torque, part of which is along the adiabatic spin-transfer torque and part of which is perpendicular. This latter contribution is literally "nonadiabatic." For transition metals, this contribution is small in all but the narrowest domain walls and is typically neglected.[21] The contribution[14,16,23–25] of interest in the present work arises from processes that contribute to magnetic relaxation (damping). This contribution is literally *not* nonadiabatic because it persists in the adiabatic, or slowly varying, limit. However, the term nonadiabatic is typically used for this contribution and we follow that practice here.

While the adiabatic spin-transfer torque is thought to be well understood[1] and characterized,[26,27] the nonadiabatic contribution has been controversial. Several authors[28,29] have suggested that $\beta = \alpha$ in general. This suggestion is consistent with the behavior of particular models[23] and some experiments[9,10] but appears not to be generally correct.[24] The experimental situation remains unclear. Measurements on a wide variety of geometries, with a variety of materials, and using a variety of techniques find a wide spread in the values of β extracted from experimental measurements.[9,10,30–43] These values are typically obtained by comparing measurements of wall velocities with the predictions of behavior for simple models. One reason for the wide variation of extracted values may be that the velocities are influenced by the presence of disorder in the wires.[44]

Although the nonadiabatic spin-transfer torque is normally thought to be much smaller than the adiabatic spin-transfer torque ($\beta \ll 1$), it is important because it controls[14,16] the propagation of the domain walls at currents below the threshold for Walker breakdown.[45] In a smooth wire without magnetic damping, the adiabatic spin-transfer torque translates a domain wall without distortion at the velocity $\mathbf{v}_s$. Damping and the nonadiabatic spin-transfer toque modify this result[46] such that the domain wall distorts and the wall velocity is $(\beta/\alpha)\mathbf{v}_s$, where α is the Gilbert damping parameter.

As the current increases, the distortion of the wall and its velocity increase. When the current exceeds the Walker breakdown current, the distorted wall becomes unstable causing the wall motion and the distortion to become cyclical. Above Walker breakdown, the domain-wall velocity approaches $\mathbf{v}_s$ as the current increases.

Much of the interest in understanding the nonadiabatic spin-transfer torque is driven by the hope that if a material

with a large β/α were found, it would be possible to move domain walls with much less current than is typically needed in present experiments. While it is true that the domain-wall velocity is $(\beta/\alpha)\mathbf{v}_s$ below Walker breakdown, it is also true that Walker breakdown occurs at lower currents as β/α becomes large, leaving the velocity at breakdown roughly constant.[46] Achieving the desired efficient and fast domain-wall motion also requires a way to suppress Walker breakdown.

In this paper, we present calculations of the nonadiabatic spin-transfer torque parameter based on our earlier calculations of the damping parameter[47] and subsequent formal derivations.[48] These calculations do not include the contributions to the nonadiabatic spin-transfer torque that are truly nonadiabatic, i.e., those that develop because the magnetization texture varies rapidly.[15,20–22] We treat the contribution to the nonadiabatic spin-transfer torque that follows from the same processes as the Gilbert damping. A number of authors[14–16,23–25] have calculated this contribution using free-electron-like Stoner models for the electronic structure. In earlier work,[48] in which we derived the formal expression evaluated here, we calculated the nonadiabatic spin-transfer torque for a few model systems, including a Kohn-Luttinger model for GaMnAs. The present calculations are based on first-principles models of the electronic structure.

In both the present work and our earlier calculations, the important spin-orbit contributions are already present in the electronic structure of the ideal bulk materials. The scattering in these models does not have a spin-orbit contribution separate from that of the host electronic structure. Other calculations of the nonadiabatic spin-transfer torque,[14–16,23–25] based on free-electron-like Stoner models, use the opposite approximation. In those models, there is no spin-orbit coupling in the host band structure, but defects cause spin-flip scattering. Such calculations provide great pedagogical value and may be important in samples in which there are defects with strong spin-orbit coupling. However, in typical transition metals and their alloys, it is important to treat models of the electronic structure that are complex enough to include the important spin-orbit coupling of the host material.

Our calculations do not include the class of spin-transfer torques that occur even in samples with a uniform magnetization. These have been discussed in materials that have spin-orbit coupling and are gyrotropic (optically active).[49–52] Similar torques occur in systems with spin-orbit coupling in which interfaces break inversion symmetry.[53] In fact, such torques are present in all bulk materials when the magnetization points in an arbitrary direction with respect to the crystal lattice. In that case, they are simply current-dependent corrections to the torque from the magnetocrystalline anisotropy. For the bulk systems that we treat, and for the high-symmetry directions we have chosen for the magnetization, the torques due to the magnetocrystalline anisotropy and its corrections are zero.

The present calculations and our earlier calculations of the damping parameter are based on phenomenological, spin-dependent scattering rates. Recent advances in calculations of the damping parameter based on scattering theory[54–56] or the coherent potential approximation[57] have moved beyond the necessity of a phenomenological lifetime for calculations of the damping parameter. These calculations have the advantage that they can be performed for the specific scattering mechanism that is believed to be important. In addition, they can be used to compute the properties of alloys, which are more commonly used in experiments. Preliminary calculations of the nonadiabatic spin-transfer torque parameter for a NiFe alloy have been reported.[58]

The rest of the paper is laid out as follows. Section II presents the formalism used in the calculations, Sec. IV gives the results, while Sec. III gives some numerical details about the calculations including a discussion of the numerical convergence. We find that although the damping parameter α and the nonadiabatic spin-transfer torque parameter β are of the same magnitude and can be described in terms of similar contributions, they are very different. In fact, we argue below that the product βv_s is a more appropriate parameter than β itself to characterize the nonadiabatic spin-transfer torque.

II. THEORY

Magnetic materials respond to time-dependent magnetic fields with damped magnetization dynamics. A model proposed by Heinrich and Kambersky[59–61] appears to provide a quantitative explanation for the measured damping in transition metals and their alloys.[47,55,56,62–65] In this model, the spin-orbit interaction mediates a transfer of energy and angular momentum between the magnetization and other electronic degrees of freedom. Electron-lattice scattering then transfers energy between the electronic and vibrational systems. Magnetic materials also respond dynamically when electrical currents flow through them, provided their magnetization is nonuniform. In the limit of a slowly varying (in space) magnetization, the nonadiabatic component of the spin-transfer torque can be thought of as a current-dependent correction to the damping.

Following earlier work,[48] expressions for the damping parameter and the nonadiabatic spin-transfer torque parameter are

$$\alpha_{\mathbf{q}} = \frac{\pi}{\Omega_c}\sum_{nm}\int\frac{d^3k}{(2\pi)^3}\alpha_{nm}(\mathbf{k},\mathbf{q}), \tag{1}$$

$$(\mathbf{q}\cdot\mathbf{v}_s)\beta_{\mathbf{q}} = \frac{\pi}{\Omega_c}\sum_{nm}\int\frac{d^3k}{(2\pi)^3}\alpha_{nm}(\mathbf{k},\mathbf{q}) \times(\tau_{m,k+q}\mathbf{v}_{m,k+q}-\tau_{n,k}\mathbf{v}_{n,k})\cdot e\mathbf{E}/\hbar\,, \tag{2}$$

$$\alpha_{nm}(\mathbf{k},\mathbf{q}) = |\Gamma^-_{nm}(\mathbf{k},\mathbf{q})|^2\int d\epsilon\, W_{nm}(\mathbf{k},\mathbf{q};\epsilon), \tag{3}$$

$$|\Gamma^-_{nm}(\mathbf{k},\mathbf{q})|^2 = |\langle n,k|[H_{so},\sigma^-]|m,k+q\rangle|^2\,, \tag{4}$$

$$W_{nm}(\mathbf{k},\mathbf{q};\epsilon) = \eta(\epsilon)A_{n,k}(\epsilon)A_{m,k+q}(\epsilon). \tag{5}$$

Here, $\mathbf{k}$ is the electron wave vector, $\mathbf{q}$ is the magnon wave vector, the subscripts m and n are electron band indices, Ω_c is the volume of the Brillouin zone, $\mathbf{v}_{n,k}$ is the velocity of the electron state, $\epsilon_{n,k}$ is its energy, and $\tau_{n,k}$ is its lifetime. $\mathbf{E}$ is the electric field in the material. The operator H_{so} is the spin-orbit Hamiltonian, and σ^- is the Pauli spin lowering operator. The electron spectral functions A_{nk} are approximated as Lorentzians centered at ϵ_{nk} with an effective width $\hbar/2\tau_{nk}$, where τ_{nk} is the electron scattering time. The derivative for the Fermi function, $\eta(\epsilon_{nk}) = -\partial f/\partial\epsilon_{nk}$ is sharply peaked for ϵ_{nk} near the Fermi level.

Equations (1) and (2) emphasize the similarity between α and β. Comparing them requires a calculation of $\mathbf{q}\cdot\mathbf{v}_s$. While an expression for $\mathbf{q}\cdot\mathbf{v}_s$ analogous to Eqs. (1) and (2) may be constructed,[48] it is significantly more difficult to evaluate numerically. We use a simpler expression valid in the absence of spin-orbit coupling.[48] In that limit, the spin velocity is

$$\mathbf{q}\cdot\mathbf{v}_s = \sigma_P \frac{qE}{en_s}, \tag{6}$$

where n_s is the dimensionless spin density and $\sigma_P = \sigma_\uparrow - \sigma_\downarrow$ is the spin-polarized conductivity. This approximation is justified because in transition-metal ferromagnets the spin-orbit energy is roughly two orders of magnitude smaller than the exchange energy. It can be shown that this velocity is

$$\mathbf{q}\cdot\mathbf{v}_s = \frac{\pi}{\Omega_c e n_s}\sum_n \int \frac{d^3k}{(2\pi)^3}\langle n^z_{nk}\rangle(\mathbf{q}\cdot\mathbf{v}_{nk})(\mathbf{v}_{nk}\cdot\mathbf{E}) \times \int d\epsilon\, W_{nn}(\mathbf{k},\mathbf{q};\epsilon)\,. \tag{7}$$

The velocities of individual electrons are $\mathbf{v}_{nk} = \partial\epsilon_{nk}/\hbar\partial\mathbf{k}$ and $\langle n^z_{nk}\rangle$ is the dimensionless z component of the spin of state $|n\mathbf{k}\rangle$ (here the magnetization is along the z direction). This expression is closely related to the conductivity for current in the $\hat{\mathbf{r}}_i$ direction in response to a field in the $\hat{\mathbf{r}}_j$ direction,

$$\sigma_{ij} = \frac{\pi}{\Omega_c}\sum_n \int \frac{d^3k}{(2\pi)^3}(\hat{\mathbf{r}}_i\cdot\mathbf{v}_{nk})(\hat{\mathbf{r}}_j\cdot\mathbf{v}_{nk}) \int d\epsilon\, W_{nn}(\mathbf{k},\mathbf{q};\epsilon)\,, \tag{8}$$

which can be derived from the Kubo formula for the conductivity. The current polarization is the ratio of the spin-polarized conductivity to the conductivity, $P = \sigma_P/\sigma$.

Previous calculations of the damping parameter[47,64] using this formalism are limited by the use of a phenomenological electron lifetime. Here we make two modifications to somewhat mitigate this limitation. First, we plot the calculated results as a function of the calculated resistivity, found as the inverse of the conductivity, Eq. (8). While there is still an unknown parameter in the calculation, we now show the results as a function of a measurable quantity. A similar approach has been used in calculations based on scattering theory,[56] in which the resistivity and damping were both calculated as a function of the root-mean-square displacements of the atoms in the simulation cell from their equilibrium positions.

The second modification is that we generalize earlier calculations[47] of α to allow the lifetime to be spin dependent. The earlier calculations assume a universal electron lifetime τ for all electronic states; however, in real materials each electron state may have a unique scattering time. In ferromagnets, the most important variation is the difference between up-spin and down-spin lifetimes. Here, we define separate lifetimes for up- and down-spin electrons. Due to the spin-orbit interaction, each state is a mixture of up and down spin to varying degree. We define a lifetime for each state,

$$\left(\tau^{\text{eff}}_{n\mathbf{k}}\right)^{-1} = (\tau^\uparrow)^{-1}|\langle\psi_{n\mathbf{k}}|\uparrow\rangle|^2 + (\tau^\downarrow)^{-1}|\langle\psi_{n\mathbf{k}}|\downarrow\rangle|^2, \tag{9}$$

depending on the fractional admixture of both spin components in the wave function $\psi_{n\mathbf{k}}$. We calculate the electrical conductivity σ, spin-polarized conductivity σ_P, Gilbert damping parameter $\alpha_{\mathbf{q}}$, and the product of the nonadiabatic spin-transfer torque parameter and the spin-polarized conductivity $\beta_{\mathbf{q}}\sigma_P$ for several values of the ratio $r = \tau^\downarrow/\tau^\uparrow$.

III. COMPUTATIONAL DETAILS

All calculations were performed within the local spin-density approximation to the linearized augmented plane-wave implementation of density-functional theory.[66,67] Calculations begin from a calculated ground state electron density at the experimental lattice constant in the absence of the spin-orbit interaction. Quasiparticle wave functions and energies are constructed from this density by solving the Kohn-Sham equations in the presence of the spin-orbit interaction, with the exchange field in a specified direction. For each metal, the exchange field was set along the magnetocrystalline easy axis, which is the $\langle 001\rangle$ direction for Fe, the $\langle 0001\rangle$ direction for Co, and the $\langle 111\rangle$ direction for Ni. The magnon wave vector and current direction were set parallel to each other for each metal and in the $\langle 010\rangle$ direction for Fe, the $\langle 2\bar{1}\bar{1}0\rangle$ direction for Co, and the $\langle 10\bar{1}\rangle$ direction for Ni. Numerical details of the ground-state convergence,[68] treatment of the spin-orbit interaction,[69] and evaluation of the Gilbert damping parameter[47] have been published elsewhere. The computational details of the evaluation of the nonadiabatic spin-transfer torque parameter largely parallel those of the Gilbert damping parameter.

Integrations over k space were performed with the special points method[70] over the full Brillouin zone. The special points method requires an artificial temperature broadening of the Fermi level for numerical stability. Convergence was obtained with respect to this artificial broadening for a low-energy equivalent to approximately 100 K. While other k-space integration methods could be considered, none proved comparatively advantageous in previous calculations of the magnetocrystalline anisotropy energy,[69] leading to similar expectations for the nonadiabatic spin-transfer torque parameter since both quantities involve matrix elements related to the spin-orbit interaction.

Convergence with respect to the k-space integration is numerically more intensive for β as compared to either the damping parameter or the conductivity. The difference in the convergence properties of the α and β integrals can be readily seen from Eqs. (1) and (2). The former is a sum of positive definite terms that are large in the small fraction of k space near the Fermi surface. The latter, on the other hand, is a sum of terms that vary in sign over the same small region and so require a much denser sampling in k space. The convergence properties of β are illustrated in Fig. 1. For practical reasons, our k-space sampling was limited to $370^3 \approx 5\times10^7$ k points. For short lifetimes, i.e., large resistivities, the ratio $\beta\sigma_P/(\alpha\sigma)$ converges to within ±0.02, while for long lifetimes, i.e., small resistivities, it converges to within ±0.2, with worse convergence for yet lower resistivities. In contrast, the damping parameter converges to within $\pm1\times10^{-5}$ for all scattering rates and resistivities.

Calculation of β also requires convergence with respect to evaluation of the band velocities and the magnitude of the magnon wave vector. The centered finite difference approximation was used to determine the electron velocities.

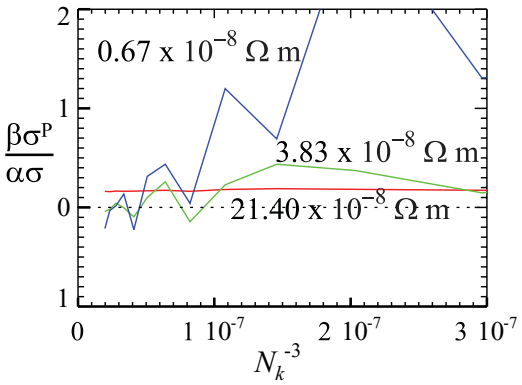

FIG. 1. (Color online) Nonadiabatic spin-transfer torque parameter for Fe as a function of k-space volume per sampling point. The curves are labeled by the values of the resistivity.

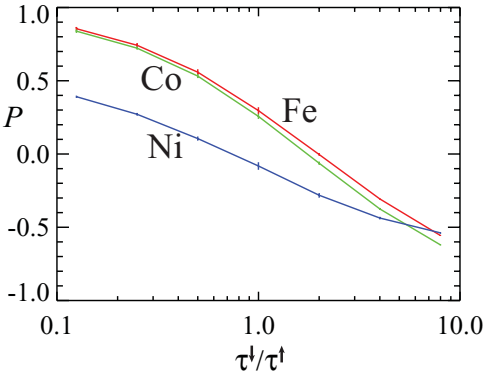

FIG. 2. (Color online) Polarization for bcc Fe (red), hcp Co (green), fcc Ni (blue) as a function of the ratio of lifetimes for the two spin channels, $r = \tau^{\downarrow}/\tau^{\uparrow}$. At each value of r, P is calculated for a range of $\tau^{\uparrow}$ and $\tau^{\downarrow}$ and the range of resulting values is indicated by the vertical bar at each data point.

Uncertainties due to the difference size and order of the method are smaller than those due to the k-space sampling. The definition of β is made in the limit as the magnon wave vector $\mathbf{q} \to 0$. The expressions for $\beta(\mathbf{q} \cdot \mathbf{v}_s)$ and $(\mathbf{q} \cdot \mathbf{v}_s)$ may be linearized with respect to $\mathbf{q}$ such that the magnitude of the magnon wave vector need not be specified; however we have evaluated these quantities with the magnon wave vector explicitly present. Results were calculated for a small wave vector of $q = 10^{-4}\,\pi/a$, where a is the lattice constant. Previous calculations of the q dependence of the Gilbert damping parameter show that it varies only weakly with q for such small values.[71]

IV. RESULTS

We calculate the conductivity σ, spin polarized conductivity σ_P, damping parameter α, and nonadiabatic spin-transfer torque parameter $\beta\sigma_P$ for a range of electron lifetimes with fixed ratios of minority to majority lifetimes $r = \tau^{\downarrow}/\tau^{\uparrow}$. We find that both the conductivity and the spin-polarized conductivity are proportional to the electron lifetime to better than 3% for each value of r computed. In most cases, the proportionality is much better. Calculations of the current polarization, $P = \sigma_P/\sigma$ are shown in Fig. 2. The current polarization does not go through zero for $r = 1$ because the projected densities of states and quasiparticle velocities are different for minority and majority electrons in all three materials. We computed the transport parameters for a series of $r = 0.125, 0.25, 0.5, 1.0, 2.0, 4.0$, and 8.0, but below only show the results for 0.5, 1.0, and 2.0. The results for the other values do not change any of the conclusions we draw.

Cobalt has been the subject of numerous transport measurements in the context of current-perpendicular-to-the-plane giant magnetoresistance.[72] Values of P that have been extracted from these measurements range from 0.38 ± 0.06 to 0.50 ± 0.08, which correspond to values of r between 0.6 and 0.8. Similar measurements exist for alloys of Fe, Co, and Ni, but do not exist to our knowledge for simple Fe and Ni. There have been extensive studies of the polarization of the resistivity of Fe, Co, and Ni with dilute impurities,[73] but the analysis was not extended to pure metals.

Allowing for spin-dependent lifetimes raises the question of whether allowing additional degrees of freedom changes the agreement found between experiment and earlier calculations of the damping parameter α that were based on spin-independent lifetimes.[47] Figure 3 shows calculations similar to those previously reported but for several values of the ratio of spin-dependent lifetimes. For Fe, the damping parameter α only depends weakly on r, but for Co α depends strongly on r. However, the agreement between experiment and the calculations found earlier[47] was based on comparing the minimum damping calculated as a function of lifetime to the minimum damping measured as a function of temperature. As seen in Fig. 3, the minimum calculated value of the damping does not vary strongly with r, suggesting that agreement between the calculations and experiment remains slightly better than a factor of 2.

Unfortunately, for the samples for which the damping was measured,[59,74] the temperature-dependent resistivity was not measured. Such measurements would be necessary to reliably compare the experimental results to those in Fig. 3 beyond comparing the minimum values. However, if we assume that those samples had typical values of the resistivity we can compare the temperatures at which the minima occur. For Co, the experimental minimum in the damping occurs around 100 K and the theoretical minima for $r = 0.5$ and 1.0 occur for resistivities close to $1.5 \times 10^{-8}\ \Omega\,\mathrm{m}$, which corresponds to a temperature close to 100 K.[75] We do not know the appropriate values of r for Fe or Ni, but we expect that $r < 1$ for Ni and $r > 1$ for Fe based on the argument that the lifetimes are inversely related to the densities of states for each spin channel. For Ni, the theoretical curves for $r < 1$ decrease from low resistivity until a resistivity significantly below the room-temperature value and then remain temperature independent for the range of resistivities treated. This behavior is consistent with experimental observations[74] that show an decrease in α from low temperatures to around 200 K and then no change up to 400 K. Experimentally, Fe is temperature independent below about 300 K and then slowly increases. While the flat behavior at low T is not expected from the calculations, it could be due to important contributions to the resistivity from temperature-independent sources such as impurities. The slow increase above room temperature is consistent with the calculated curves for $r > 1$.

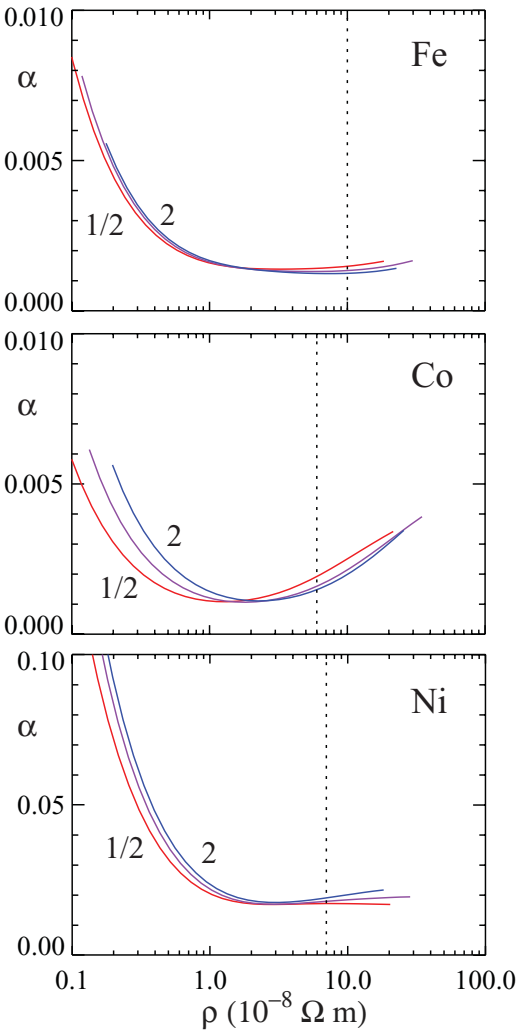

FIG. 3. (Color online) Damping constant versus resistivity for a series of ratios of spin-dependent scattering rates, $r = \tau^{\downarrow}/\tau^{\uparrow} = 2$, 1, 0.5. Dashed vertical lines indicate approximate room-temperature resistivities for each element.

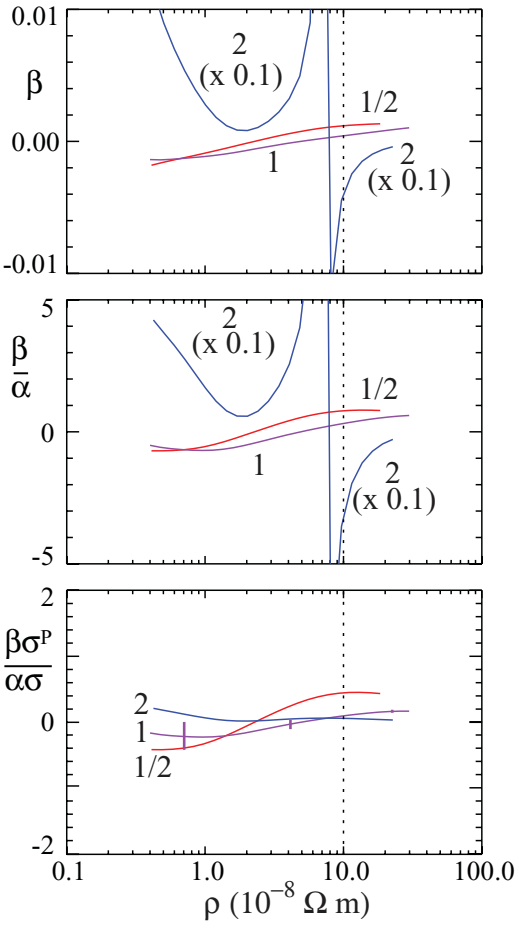

FIG. 4. (Color online) Spin-transfer torque parameter versus resistivity for several ratios ($r = 0.5$, 1.0, 2.0) of spin-dependent scattering rates for Fe. The top panel gives β, the middle panel β/α, and the bottom panel $\beta\sigma_P/(\alpha\sigma)$. The dashed vertical lines indicate the approximate room-temperature resistivity. In the top two panels, the results for $r = 2.0$ have been scaled down by a factor of 0.1. In the bottom panel, the vertical bars indicate the convergence estimates extracted from Fig. 1

We can qualitatively compare these results with those of Liu *et al.*[56] Here we calculate the resistivity as a function of the lifetimes; they do so as a function of the root-mean-square displacement of atoms, so a direct comparison is not possible. The results are qualitatively the same but differ in some details. The minimum values of the damping that they find are lower than those we find, but the values are comparable and the values of the resistivity at the minima are also comparable. The differences could be due to the different approaches for calculating the scattering.

Figures 4 and 5 give the calculated values of the nonadiabatic spin-transfer torque parameter for Fe and Ni respectively in the top panels (we were not able to numerically converge calculations for Co in a reasonable time). The middle panels give β/α and the bottom panels $\beta\sigma_P/(\alpha\sigma)$. These figures, particularly Fig. 4, illustrate a basic conclusion we can draw from these results: β and β/α are not the most meaningful descriptions of the nonadiabatic spin-transfer torque. For the case of Fe with $r = 2$, σ_P is close to zero but the combination $\beta\sigma_P$ need not be. The resulting value of β diverges as the current polarization approaches zero (near the room-temperature resistivity value), while the low-current domain-wall velocity, proportional to $\beta\sigma_P/(\alpha\sigma)$, remains constant. This suggests that $\beta\sigma_P$ as a quantity is a more fundamental characterization of the nonadiabatic spin-transfer torque than β itself, $\beta\sigma_P/\sigma$ is the most meaningful dimensionless characterization, and $\beta\sigma_P/(\alpha\sigma)$ is a useful characterization of the low-current domain-wall velocity.

The results for β/α in Figs. 4 and 5 make clear that α and β are of the same order (except when the polarization is close to zero) but are otherwise not closely related. They can have different signs and different orders of magnitude for specific combinations of scattering rates. However, there are common features between β and α. For low resistivities, the damping parameter α is dominated by the intraband contribution, which is proportional to $1/\rho$. For high resistivities, the interband contribution dominates. Similar behavior is seen for β, particularly for Ni. There is a low-resistivity contribution that is proportional to $1/\rho$ and a high-resistivity contribution

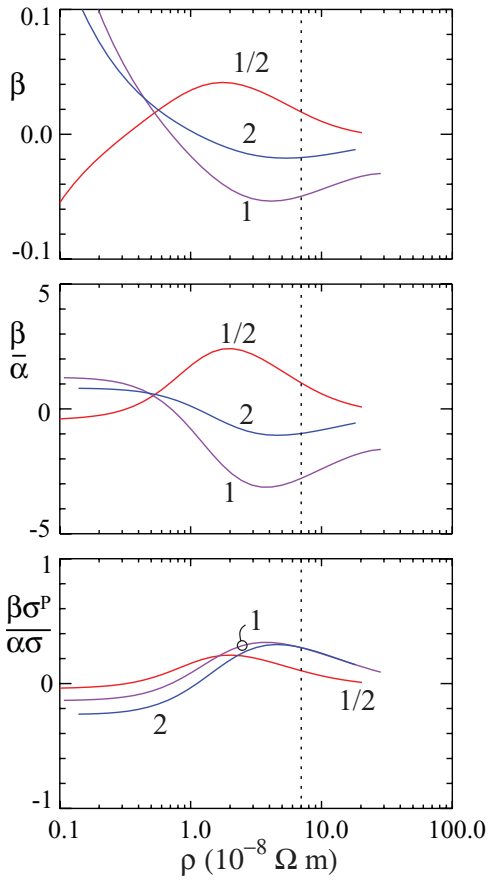

FIG. 5. (Color online) Spin-transfer torque parameter versus resistivity for several ratios ($r = 0.5, 1.0, 2.0$) of spin-dependent scattering rates for Ni. The top panel gives β, the middle panel β/α, and the bottom panel $\beta\sigma_P/(\alpha\sigma)$. The dashed vertical lines indicate the approximate room-temperature resistivity.

that has a more complicated dependence on resistivity. Since the sign of both terms in β is not fixed, the total can (and does) cross zero.

While the results presented here give large values for β/α in some regimes, particularly when σ_P approaches zero, these are unlikely to lead to a substantial reduction in the currents needed to move domain walls with useful velocities because the parameter important for the domain-wall velocity, $\beta\sigma_P/(\alpha\sigma)$, never gets large. Interestingly, this ratio is negative for a large range of values, implying that for those ranges of values and small currents (below Walker breakdown), the domain wall moves opposite to the direction of electron flow. While domain walls moving backward like this may seem unphysical, it is no different than any velocity different from $v_{DW}^{ad} = \sigma_P E/en_s$. For a wall moving at that velocity, the angular momentum supplied by the spin-polarized current exactly balances the rate of change of angular momentum in the magnetization due to the moving domain wall. For all other cases, angular momentum is transfered from the lattice to the magnetization through the combination of the damping and the nonadiabatic spin-transfer torque.

The results in Figs. 4 and 5 highlight the difficulties in calculating the nonadiabatic spin-transfer torque parameter. As compared to the Gilbert damping parameter, it is both more difficult to converge numerically and more sensitive to details of the scattering. The results from Fig. 1 show that for resistivities lower than about $0.6 \times 10^{-8}\ \Omega$ m, the convergence of the ratio $\beta\sigma_P/(\alpha\sigma)$ is comparable to the separation in values for different values of the ratio of scattering rates, r. For Ni, the convergence is better than for Fe and the ratio $\beta\sigma_P/(\alpha\sigma)$ approaches a constant for low resistivities as expected. For large resistivities, the convergence is much better, but the model becomes more suspect. At the upper limits of the curves in Figs. 4 and 5, the maximum width of a state, $\hbar/2\tau_{nk}$, is 0.3 eV, which is comparable to typical separations of the energy bands. When the widths of the states become comparable to their separation, this description of the electronic structure starts to break down.

In addition, strong disorder (large scattering rates) enhances the participation of high-energy particle-hole pairs in magnetic relaxation, thus rendering Eqs. (1) and (2) quantitatively unreliable.[76] In spite of all these difficulties, the results are sufficiently robust to draw the conclusions mentioned above. Unfortunately, between the numerical uncertainties and the sensitivity to the details of the scattering, quantitative predictions of the calculations will be difficult to test experimentally.

V. CONCLUSION

We compute the nonadiabatic spin-transfer torque parameter β for Fe and Ni and the damping parameter α for Fe, Co, and Ni. We generalize our earlier calculations of the damping parameter by allowing the electron lifetimes to be spin dependent and calculating the resistivity of the metals as a function of the same lifetimes. The latter allows for a potentially closer comparison with experiment when the resistivity is measured for the samples that are used to measure α and β. In this case, the unmeasured electron lifetimes are only needed implicitly. Fortunately, allowing the lifetimes to be spin dependent did not diminish the agreement found in the comparison of calculated damping parameters with those that have been measured.

The nonadiabatic spin-transfer torque parameter is of the same order of magnitude as the damping parameter, but is distinctly different. Because it is given by an integral over momentum space with an integrand that is peaked near the Fermi surface and varies in sign, the value of β is extremely dependent on details of the band structure and of the transport steady state. The calculation of the nonadiabatic torque gives $\beta\sigma_P$ directly; β is found by dividing by σ_P. However, we show that this construction can yield misleading results, particularly when the current polarization P is close to zero. The resulting value of β apparently diverges as the current polarization approaches zero, while the low-current domain-wall velocity [proportional to $\beta\sigma_P/(\alpha\sigma)$] remains constant. This suggests that $\beta\sigma_P$ is a more fundamental characterization of the nonadiabatic spin-transfer torque. For the dimensionless prefactor $\beta\sigma_P/(\alpha\sigma)$, which characterizes the domain-wall velocity, a value of 1 corresponds to one flipped spin per electron that passes through a domain wall. We find that it is less than 1 for Fe or Ni over the whole range of electron lifetimes we have considered.

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