First-principles investigation of the damping of fast magnetization precession in ferromagnetic 3*d* metals

J. Kuneš and V. Kamberský
Institute of Physics, Academy of Sciences, Cukrovarnická 10, CZ-162 53 Prague, Czech Republic
(Received 21 January 2002; published 6 June 2002)

Understanding of the damping of fast magnetization precession in ferromagnetic materials is important for technological applications, in particular for the development of fast magnetic memories. We use first-principles electronic structures together with the model of "breathing Fermi surface" to calculate the magnetic damping rates for ferromagnetic Fe, Co, and Ni. The numerical results are found to be in reasonable agreement with the experimental data at low temperatures; in particular, we find an order of magnitude difference between Fe and the other two studied materials.

DOI: 10.1103/PhysRevB.65.212411 PACS number(s): 76.60.Es, 71.20.Be, 76.50.+g, 75.10.Lp

Recently revived interest in the damping of fast magnetization precession is in a great part caused by the revival of projects of fast magnetic memories, stretching back to the period of intensive research in the 1950s and 1960s. The microscopic mechanisms of relaxing populations of electronic states, with energies depending on the direction of magnetization,[1,2] has recently been discussed in detail by Suhl.[3] Since much of the present applied research concerns metallic magnetic films, it is to recall that the interactions of macroscopic magnetization with the electronic degrees of freedom in 3*d* metals and oxides are fundamentally different. The "valence-exchange" process in metals is very fast, the 3*d* electrons are strongly delocalized, with band width of several eV. Therefore the proper description of the electronic degrees of freedom around the Fermi level is in terms of delocalized Bloch states. The fast "hopping" quenches the orbital moment of the Bloch states and the spin-orbit interaction appears as a perturbation on top of the kinetic and electrostatic energy. This basic picture has been used already in 1940 by Brooks[4] to estimate the magnetic g factors and magnetocrystalline anisotropy energy of 3*d* metals and it changed only quantitatively since then.

As a consequence of the spin-orbit coupling, the energies of the Bloch states $\epsilon_{\mathbf{k},\mu}$ depend on the direction of magnetization $\alpha=\mathbf{M}/M$. Hence quasistatic changes of α produce small changes of the shape ("breathing") of the Fermi surface,[5,6] connected with relaxation of populations $n_{\mathbf{k},\mu}$ to the actual equilibrium values. Such relaxation occurs through transitions between the Bloch states close to the Fermi level E_F, resulting from collisions with lattice defects (including phonons). The same mechanisms are responsible for the electric resistance. The damping of magnetic precession then results from the phase lag between the changes of α and the population response. Estimates of the damping rates, based on this picture, were done by one of the authors some time ago[7] as a formal analogy to the Clogston valence-exchange mechanism.[2]. We briefly describe the model.

Variation of the total electron energy density

$$E=\Omega^{-1}\sum_{\mathbf{k},\mu}\epsilon_{\mathbf{k},\mu}n_{\mathbf{k},\mu} \tag{1}$$

with α is equivalent to action of an effective field

$$\mathbf{H}=-(M\Omega)^{-1}\sum_{\mathbf{k},\mu}n_{\mathbf{k},\mu}\frac{\partial\epsilon_{\mathbf{k},\mu}}{\partial\alpha}, \tag{2}$$

where the k summation is over the first Brillouin zone (BZ). The nonequilibrium populations are approximately given as $n_\mu=f_\mu-\tau_\mu df_\mu/dt$, where $f_\mu=f(\epsilon_\mu)$, $f(\epsilon)$ is the Fermi function, and τ_μ is the lifetime of a state μ. The k index was omitted for simplicity. This approximation pertains to fast relaxation, relatively to the frequency of magnetic precession ($\tau_\mu df_\mu/dt\ll 1$ and $\tau_\mu d^2f_\mu/dt^2\ll df_\mu/dt$). At microwave frequencies it is realistic even in quite pure crystals at low temperatures. Since f_μ depends on t through $\epsilon_\mu[\boldsymbol{\alpha}(t)]$, the out-of-phase part of the effective field is obtained simply by the chain rule

$$H_i=-(M\Omega)^{-1}\sum_{\mathbf{k},\mu}\tau_{\mathbf{k},\mu}\left(-\frac{\partial f_{\mathbf{k},\mu}}{\partial\epsilon_{\mathbf{k},\mu}}\right)\frac{\partial\epsilon_{\mathbf{k},\mu}}{\partial\alpha_i}\frac{\partial\epsilon_{\mathbf{k},\mu}}{\partial\alpha_j}\frac{d\alpha_j}{dt}. \tag{3}$$

This is to be compared with the damping field components in the macroscopic Gilbert equation

$$H_i=-\frac{\lambda}{(\gamma M)^2}\frac{dM_i}{dt}$$

in the form used by Bhagat[8] for ferromagnetic resonance (FMR). Here λ is the Landau-Lifshitz damping frequency and γ is the gyromagnetic ratio. As in Gilbert's original work[9] (and in Suhl's discussion[3]), the damping parameter λ appears to be a matrix, reflecting possible anisotropy. However, it is isotropic (scalar) in linear (low-power) FMR if $\boldsymbol{\alpha}$ precesses around a static $\mathbf{M}_0$ direction parallel to a high symmetry axis. At low temperatures, Eq. (3) further simplifies as $-\partial f_\mu/\partial\epsilon_\mu\approx\delta(\epsilon_F-\epsilon_\mu)$. Using the same effective lifetime τ for all the states we arrive at

$$\frac{\lambda}{\tau}=\gamma^2\Omega^{-1}\sum_{\mathbf{k},\mu}\left(\frac{\partial\epsilon_{\mathbf{k},\mu}}{\partial\alpha_j}\right)^2\delta(\epsilon_F-\epsilon_{\mathbf{k},\mu}), \tag{4}$$

where α_j is a component perpendicular to $\mathbf{M}_0$. As with other "fast relaxing" mechanisms, this model predicts an increase of the magnetic damping rate λ with decreasing scattering frequency τ^{-1}. The latter is to be identified with the Drude scattering frequency of itinerant electron states, which decreases roughly as T^2 with decreasing temperature, to a limit determined by the residual resistivity. In FMR, the "effective" τ is also limited by the mean "time of flight" of electrons in the electromagnetic skin depth and so the uniform relaxation model is not quantitatively correct in anomalous skin effect conditions.[10] To these limits, the model thus predicts $\lambda \sim T^{-2}$ behavior of the magnetic damping frequency at low temperatures.

Experimentally, a low-temperature increase of λ has been observed in FMR in pure single crystals of Ni (Refs. 8, 11–14) and (hcp) Co.[8] The factor λT^2 was evaluated for Ni from transmission experiments near the ferromagnetic antiresonance (FMAR), i.e., near the minimum of rf permeability and maximum rf penetration depth where the uniform relaxation model is applicable.[12] Comparison of low-temperature FMR results in Ni and Co indicated[8] that this factor is of the same order of magnitude in both systems. On the other hand, no low-temperature increase of λ has been found in analogous experiments performed on Fe single crystals.[15,16]

The aim of the present work is to evaluate the λ/τ ratio for Ni, Co, and Fe using Eq. (4) and the electronic structure from an *ab initio* calculation. For this purpose the full potential linearized augmented-plane-wave (FLAPW) method as implemented in the WIEN97 code[17] is used. Calculations of this ratio had already been performed[18] for Ni on the basis of a semiempirical (LCAO+OPW) band structure.[19] No attempt has been made so far to estimate theoretically the corresponding values for Co and particularly for Fe, where the absence of the low-temperature increase of λ arouses suspicion about applicability of the present model.

Alternatively, Eq. (4) also follows from a linear-response formulation[18,20] (as a particular contribution, in addition to damping caused by changing polarizations of the Bloch states). If the spin-orbit coupling is considered as a perturbation of a spin-polarized electronic structure,[4–6,17–21] written schematically as[21]

$$H_{SO}=\sum_j \xi_j \mathbf{L}_j \cdot \mathbf{S}, \tag{5}$$

where $\mathbf{S}$ is the spin and $\mathbf{L}_j$ the orbital angular momentum with respect to the lattice site j, then by geometrical arguments[22]

$$\frac{\partial \epsilon_{\mathbf{k},\mu}}{\partial \alpha_i}=\langle \mathbf{k},\mu | T_i | \mathbf{k},\mu \rangle, \tag{6}$$

where $\mathbf{T}$ is the transverse torque operator

$$\mathbf{T}=\alpha \times \sum_j (\xi_j \mathbf{L}_j \times \mathbf{S}). \tag{7}$$

It may be noted that its diagonal elements are involved in the first order in the expression for the magnetocrystalline anisotropy energy,[21] where high precision integration is required since contributions of various occupied states compensate each other to a large extent. The expression for the magnetic damping involves only the squares of the torque matrix elements, thus only positive numbers are summed and the procedure is much less computationally demanding. The summation in Eq. (4) amounts to a modification of the computation of the density of states, performed by the Blöchl tetrahedron method.[23,17]

TABLE I. Damping ratios λ/τ from *ab initio* calculations

	$\lambda/\tau(10^{22}\ \mathrm{s}^{-2})$
fcc Ni [001]	1.2
fcc Ni [111]	1.0
hcp Co [0001]	1.6
bcc Fe [001]	0.14

The calculations were performed for experimental values of the lattice constants. The size of the LAPW basis is characterized by the product $R_{mt}K_{\max}=9.5$ of the atomic sphere radius and the plane-wave cutoff. The spin-orbit coupling was treated by the second variational step with the cutoff energy around 1 Ry above the Fermi level, which was checked to be high enough. The electronic structure was converged on a mesh of 1470 k points in 1/16 of BZ (and equivalently for Ni [111] and hcp Co where the irreducible part of BZ is 1/12). However already 405 irreducible k points are enough to get the charge density accurately. Evaluation of expression (4) is expected to be sensitive to the k point sampling. Therefore we performed a careful testing for bcc Fe, up to 10 500 k points in 1/16 of BZ. We found that for more than 3000 k points the accuracy of the BZ integration is better than 10%. Finally we remark that the calculations for Ni[001] and Ni[111] were performed on compatible k meshes and therefore their difference does not originate from the integration inaccuracies.

The main result appears to be the order-of-magnitude difference between the λ/τ ratio in bcc Fe and the other two systems. The results of the calculations are shown in Table I. The values obtained for Ni are in fair agreement with the previous numerical results[18] yielding $\lambda/\tau=0.9\times 10^{22}\,\mathrm{s}^{-2}$, for $\mathbf{M}$ along [001].

The difference between the results for Ni and Fe can be qualitatively explained from the band picture. The matrix elements (6) are zero in the nonrelativistic band structure with "quenched" orbital moments, they arise from the spin-orbit coupling. Large values, significant in the sum (4), occur in the vicinity of points or lines where nonrelativistic bands are degenerate at the Fermi level ϵ_F. The volume of these effective k-space regions increases with decreasing angle under which the nonrelativistic bands (and the Fermi surface sheets) cross. Such accidental low-angle crossing of two minority-spin Fermi surface sheets with high $3d$ contents is observed in Ni near the $\langle 110 \rangle$ planes in the BZ, and it gives the major contribution to the computed λ/τ in Ni. It also contributes to the well-known peak in minority-spin density of states at ϵ_F. These features are not present at ϵ_F in Fe. The symmetry degeneracies along 100 axes, found both in Fe and Ni and quoted previously[7] as a possible source of high λ/τ values, have negligible integral weight in the present results. We did not investigate in detail the origin of the high value for hcp Co.

Quantitative comparison with λ/τ deduced from experiment is straightforward in Ni where Heinrich *et al.*[12] analyzed in detail their results of FMAR transmission experiments in Ni crystals magnetized along [001]. The temperature dependence of λ between 300 and 77 K found in this analysis may be described as

$$\lambda=\left[1.1\times\left(\frac{300}{T[K]}\right)^2+1.2\times\left(\frac{T[K]}{300}\right)^2\right]\times10^8\ \ \mathrm{s}^{-1}.$$

While the second term increases with the temperature and corresponds to effects of relaxing polarizations,[20] the first term corresponds to the mechanism of fast relaxing populations. The calculated value of λ/τ shown in Table I corresponds to

$$\tau^{-1}=1.1\times\left(\frac{T[K]}{300}\right)^2\times10^{14}\ \ \mathrm{s}^{-1},$$

which is about a half of the scattering frequency of conduction electrons assumed by Heinrich *et al.* The authors also show that the FMAR analysis is not affected (more than by 10%) by the finite rf penetration depth.

The low-temperature FMR data for Ni (Refs. 8,13) are, however, affected strongly, because FMR is measured around the maximum of rf permeability, i.e., minimum skin depth. At 80 K the ''effective'' λ measured in FMR is only one half of the value from FMAR, and at 25 K, in ''extreme anomalous'' conditions,[8,10,18] it is only 1/10 of the extrapolated FMAR value. Since only FMR data are available for Co and Fe, comparison with the present calculation may be only qualitative. The ''effective'' λ in Co is about three times lower than in Ni at very low temperatures,[8] while the calculated value of λ/τ is even somewhat higher. This may be plausibly explained by the significantly lower penetration depth in Co than in Ni, due to the higher magnetization and rf permeability in Co, and almost three times higher rf frequency used in the Co experiment.[8] In the Co and Fe experiments[8,15,16] the above criteria for the penetration depth were roughly the same but the ''effective'' λ in Co increased 5 times at 4 K from about $1.\times10^8\ \mathrm{s}^{-1}$ at 100 K, while in Fe it remained at $0.7\times10^8\ \mathrm{s}^{-1}$. This experimental difference is in accordance with the large difference found in the computed λ/τ for Co and Fe. It must of course be recalled that in the ''anomalous'' skin effect the Fermi surface integral (4) is not uniformly reduced but contains additional weight factors favoring the ''surf riding'' conditions for electrons.[10,18]

We conclude that the numerical results from the uniform relaxation model agree with the FMAR experiment in Ni with a reasonable assumption about the average electron lifetime, and at least qualitatively explain the differences found in low-temperature FMR results in Fe, Co, and Ni. Calculations based on previously indicated more general formulations[10,20] (taking into account off-diagonal elements of the population matrix, thus including the magnon wavelength for low electron scattering rates and interband polarizations for high rates) should provide a broader basis for comparison with experimental results.

We wish to thank P. Novák for his valuable comments. This work was supported by Grant No. A1010214 of the Academy of Sciences of the Czech Republic.

[1] H.P.J. Wijn and van der Heide, Rev. Mod. Phys. **80**, 744 (1950).
[2] A.M. Clogston, Bell Syst. Tech. J. **34**, 739 (1955).
[3] H. Suhl, J. Appl. Phys. **89**, 7448 (2001).
[4] H. Brooks, Phys. Rev. **58**, 909 (1940).
[5] J.C. Slonczewski, J. Phys. Soc. Jpn. **17**, 34 (1962).
[6] L. Hodges, D.R. Stone, and A.V. Gold, Phys. Rev. Lett. **19**, 655 (1967).
[7] V. Kamberský, Can. J. Phys. **48**, 2906 (1970).
[8] S.M. Bhagat and P. Lubitz, Phys. Rev. B **10**, 179 (1974).
[9] T. L.Gilbert, Ph.D. thesis, Illinois Institute of Technology, Chicago, 1956.
[10] V. Korenman and R.E. Prange, Phys. Rev. B **6**, 2769 (1972).
[11] S.M. Bhagat and L.L. Hirst, Phys. Rev. **151**, 401 (1966).
[12] B. Heinrich, D.J. Meredith, and J.F. Cochran, J. Appl. Phys. **50**, 7726 (1979).
[13] J.M. Rudd, K. Myrtle, J.F. Cochran, and B. Heinrich, J. Appl. Phys. **57**, 3693 (1985).
[14] W. Anders, D. Bastian, and E. Biller, Z. Angew. Phys. **32**, 12 (1971).
[15] S.M. Bhagat, J.R. Anderson, and L.L. Hirst, Phys. Rev. Lett. **16**, 1099 (1966).
[16] S.M. Bhagat, J.R. Anderson, and Ning Wu, Phys. Rev. **155**, 510 (1967).
[17] P. Blaha, K. Schwarz, and J. Luitz, WIEN97, Vienna University of Technology, 1997. [Improved and updated Unix version of the original copyrighted WIEN code, which was published by P. Blaha, K. Schwarz, P. Sorantin, and S. B. Trickey, in Comput. Phys. Commun. **59**, 399 (1990)].
[18] V. Kamberský, J.F. Cochran, and J.M. Rudd, J. Magn. Magn. Mater. **104-107**, 2089 (1992).
[19] E.I. Zornberg, Phys. Rev. B **1**, 244 (1970).
[20] V. Kamberský, Czech. J. Phys., Sect. B **26**, 1366 (1976).
[21] X. Wang, R. Wu, D.S. Wang, and A.J. Freeman, Phys. Rev. B **54**, 61 (1996).
[22] Rotation of the magnetization direction only changes the spin quantization axis, *i.e.*,, transforms the spin operator components in the crystal coordinate system or the $\xi\mathbf{L}$ components in the spin-quantization system (Refs. 18–21).
[23] P.E. Blöchl, O. Jepsen, and O.K. Andersen, Phys. Rev. B **49**, 16 223 (1994).