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Gilbert damping and anisotropic magnetoresistance in iron-based alloys



L. Berger

Physics Department, Carnegie Mellon University, Pittsburgh, PA 15213, USA

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ABSTRACT

We use the two-current model of Campbell and Fert to understand the compositional dependence of the Gilbert damping parameter in certain iron alloys. In that model, spin-up and spin-down carriers have different resistivities ρ_{\uparrow} and ρ_{\downarrow} . We emphasize the part of the Gilbert parameter, called G_{sf} , generated by spin-flip interband processes. Both G_{sf} and the anisotropic magnetoresistance $\Delta\rho$ are proportional to the square of the spin-orbit parameter, and also proportional to ρ_{\uparrow} . In bcc alloys of iron with V, Cr, Mo, etc. solutes on the left of iron in the periodic table, ρ_{\uparrow} is increased by a scattering resonance (Gomes and Campbell, 1966, 1968). Then ρ_{\uparrow} , $\Delta\rho$, and G_{sf} all exhibit a peak at the same moderate concentration of the solute. We find the best fit between this theory and existing experimental data of Gilbert damping for Fe-V epitaxial films at room temperature (Cheng, 2006; Scheck et al., 2007). At room temperature, the predicted G_{sf} peak is masked by a background arising from non-flip intraband processes. At elevated temperatures, the peak is expected to become more prominent, and less hidden in the background.

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1. Introduction

The damping of the precession of the magnetization of a ferromagnet undergoing ferromagnetic resonance is called Gilbert damping. The damping rate is proportional to the precession frequency, and is characterized by the Gilbert parameter G , sometimes called λ [1]. The microscopic processes responsible for the existence of G in ferromagnetic metals are still not completely understood.

In the past, experiments were performed on polycrystalline samples, or on relatively thick single crystals [1] where the observed damping was affected by the skin effect and by exchange-conductivity effects which complicated the interpretation of the data. The availability of very thin epitaxial films [2], where the microwave field penetrates the sample fully, removes these complications.

Experiments on iron [3] and iron alloys are especially difficult because of the unusually small value of G . The present paper was prompted by the work of Cheng [4] on sputtered iron-vanadium epitaxial films of thickness 50 nm at room temperature, with vanadium concentration between 0 and 52 at%. We use also the G value [5] for a sputtered $Fe_{73}V_{27}$ epitaxial film of thickness 8 nm. More generally, the present theory applies to bcc alloys of iron with transition-metal solutes to the left of iron in the periodic table, such as Fe-V, Fe-Cr, and Fe-Mo.

One microscopic mechanism responsible for G in metals was proposed by Kambersky [6,7]. Electrons undergo transitions

between two states of the same spin while absorbing a quantum of spin wave. In this non-flip intraband mechanism, G is usually predicted to be inversely proportional to the electron momentum relaxation rate or, equivalently, to the electrical resistivity.

In an alternate mechanism, introduced by Turov [8], electrons jump between states of opposite spin. Early theories of this spin-flip interband mechanism were based on the s-d exchange model. A simpler and better kind of theory [9] uses only one kind of electrons. It predicts $\alpha = 1/(\omega_d \tau_{sr})$, where α is a dimensionless parameter related to G by the relation $G = \alpha \gamma M_s$, γ is the gyromagnetic ratio, \mathbf{M}_s the magnetization, ω_d the precession rate of a 3d electron spin in the intra-atomic d-d exchange field \mathbf{H}_{dd} , and τ_{sr} the 3d spin-relaxation time caused [10] by spin-orbit interaction.

In the latter theory, 3d electrons are assumed to be itinerant. The intra-atomic d-d exchange field \mathbf{H}_{dd} acting on a spin is generated by the spins of other 3d electrons. It is given by $\mathbf{H}_{dd} = -2J_{dd}\mathbf{S}/(g\mu_0\mu_B)$ where $J_{dd} \simeq 0.5$ eV is the d-d intra-atomic exchange integral, \mathbf{S} the average spin of a 3d atom, g the g -factor, μ_0 the vacuum permeability in the SI system of units, and μ_B the Bohr magneton. In ferromagnetic resonance, \mathbf{S} precesses under torques created by the total field \mathbf{H} which includes external, demagnetizing and anisotropy fields. As shown in the second paper of Ref. [9], a simple theory of the spin-flip interband processes can be developed, based on a classical equation of motion for \mathbf{S} . Typically, \mathbf{H}_{dd} is ten thousand times larger than \mathbf{H} . However, since it is antiparallel to \mathbf{S} , it exerts no Zeeman torque on it. A damping term of the Bloch form, resulting from the existence of τ_{sr} , is introduced into the equation of motion. Through that term, \mathbf{S} relaxes towards the instantaneous direction, called \mathbf{S}_0 , where it

E-mail address: lberger@andrew.cmu.edu

would have the lowest energy. The importance of \mathbf{H}_{dd} lies in the fact that it has an influence on \mathbf{S}_0 . Then, starting from Bloch-type damping, the final result is found to have a form consistent with Gilbert damping, i.e., with a damping rate proportional to the \mathbf{S} precession frequency ω around the field \mathbf{H} . The Gilbert damping parameter is predicted [9] to be $\alpha = 1/(\omega_d \tau_{sf})$, as stated above.

In the rest of the paper, we will denote by G_{nf} the non-flip intraband part of G , and by G_{sf} the spin-flip interband part. Combining the equations found in the previous paragraph with the formula $\omega_d = 2S_{J_{dd}}/\hbar$, we obtain

$$G_{sf} = C/\tau_{sf}, \quad C = \mu_0 g^2 \mu_B^2 n_{at} / J_{dd}. \quad (1)$$

Here, n_{at} is the number of atoms per unit volume. Calculation methods have been developed [11,12] which derive both G_{nf} and G_{sf} from the same formalism. As mentioned by the authors of Ref. [12], the lack of exact knowledge of electron momentum-relaxation rates in magnetic metals is an important obstacle to further progress. The so-called two-current model provides a partial solution to that problem.

2. Two-current model and electrical resistivity in iron-based alloys

The two-current model was introduced by Campbell and Fert [13]. In that model, spin-up and spin-down charge carriers are assumed to each have unique and well-defined effective masses m_\uparrow, m_\downarrow , concentrations n_\uparrow, n_\downarrow , and momentum-relaxation times $\tau_\uparrow, \tau_\downarrow$. In earlier work [14], we used that model and spin-orbit interaction to build a theory of spin relaxation applicable to nickel and certain fcc nickel-based alloys. For reasons explained in that paper, the idea of spin mixing [13,15] was ignored. In the present section, we show how this theory must be modified to apply to bcc alloys of iron with transition-series elements on the left of iron in the periodic table, such as Fe-V, Fe-Cr, Fe-Mo, etc. The roles of spin-up and spin-down electrons are exchanged.

In nickel and many nickel alloys, the spin-up Fermi level is at a fixed location above the top of the spin-up 3d band, in a region with low density of states and high velocity characteristic of 4s electrons. Because of this [14], spin-up electrons carry most of the current, and ρ_\uparrow is much smaller than ρ_\downarrow .

Similarly, the spin-down Fermi level of iron and bcc iron alloys is fixed [16] in a narrow gap of the 3d band, with low density of states. Because of this, $1/\tau_\downarrow$ is small, and ρ_\downarrow is usually larger than ρ_\uparrow . One difference, however, is that the spin-down electrons at the Fermi level of iron have a stronger 3d character than the spin-up electrons of Ni and, therefore, a larger spin-orbit interaction. The spin-dependent resistivities $\rho_\uparrow, \rho_\downarrow$ and the measured resistivity ρ are given by

$$\rho_\uparrow = m_\uparrow / (e^2 n_\uparrow \tau_\uparrow), \quad \rho_\downarrow = m_\downarrow / (e^2 n_\downarrow \tau_\downarrow), \quad (2)$$

$$\rho^{-1} = \rho_\uparrow^{-1} + \rho_\downarrow^{-1}. \quad (3)$$

In 1966, Gomes and Campbell [17] recognized that the scattering potential created by a transition-metal solute atom in Ni, Fe, or Co is too strong for the first Born approximation to be valid for $d \rightarrow d$ scattering. For transition-metal solutes V, Cr, Mo, etc. on the left of iron in the periodic table, the potential is repulsive, and a scattering resonance is present [17] near the top of the spin-up 3d band of an iron alloy, close to the Fermi level. The direct effect of the resonance is to increase the spin-up 3d electron probability on the scattering solute atom, in a ratio r_F . Then, in turn, ρ_\uparrow is increased.

In the alloys considered here, the atomic moment is much larger on iron atoms than on solute atoms [18]. This provides [19] a direct experimental confirmation of the idea that electron

probabilities are different on the two kinds of site. Also, the resulting difference in exchange potential reinforces the resonance for spin-up electrons, and decreases it for spin down [20]. Therefore, for simplicity, we will assume that the scattering resonance is present only in the spin-up band.

Scattering theory provides [21,22] a formula for $1/\tau_1$ valid even when the first Born approximation fails. We consider a spin-up 3d electron in an initial Bloch-wave state ϕ_{km}^+ of wave vector \mathbf{k} and symmetry index $m=1-5$. It is an energy eigenstate in the absence of scattering. This Bloch wave encounters the potential $V(\mathbf{r})$ of the crystal containing scattering solutes located at random locations. The relaxation rate to similar outgoing spin-up 3d Bloch waves $\phi_{k'm'}^+$ is [21]

$$\begin{aligned} 1/\tau_1 &= (2\pi/\hbar) | \langle \phi_{km}^{sc+} | (V(\mathbf{r}) - \bar{V}) \phi_{k'm'}^+ \rangle |^2 D_1(E_F), \\ \phi_{km}^+ &= u_{km}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} / \sqrt{\Omega}, \quad \phi_{k'm'}^+ = u_{k'm'}(\mathbf{r}) e^{i\mathbf{k}'\mathbf{r}} / \sqrt{\Omega}, \\ \phi_{km}^{sc+} &= (n_{at} \Omega)^{-1/2} \sum_{\mathbf{l}} C_{\mathbf{l}km}^+ \phi_m^{at}(\mathbf{r} - \mathbf{l}). \end{aligned} \quad (4)$$

Here, ϕ_{km}^{sc+} is [21] what has become of the incoming Bloch wave ϕ_{km}^+ after entering the region of the scatterers. It is not a plane wave anymore. The structure of this scattering state includes an enhanced value of the electron probability $|C_{\mathbf{l}km}^+|^2$ at location \mathbf{l} if that location is that of a solute atom. Also, D_1 is the spin-up density of states, Ω the crystal volume, $\phi_m^{at+}(\mathbf{r})$ a spin-up 3d atomic state. Finally, the so-called virtual-crystal potential \bar{V} is [23] some real-valued average of $V(\mathbf{r})$ over the crystal which has the periodicity of the crystal lattice. The Bloch functions are defined as eigenstates of a hamiltonian where \bar{V} is the potential energy. In Eq. (4), the value of the matrix element must still be averaged over equilibrium distributions of both \mathbf{k}, m and \mathbf{k}', m' .

For each value of the solute concentration x , Nordheim [23] chose the value of \bar{V} so that the coherent forward scattering amplitude would vanish. In that manner, he was able to show that the $T=0$ resistivity of a concentrated alloy $B_{1-x}A_x$ is proportional to $x(1-x)$ at $T=0$. The resistivity is maximum for $x=0.5=50\%$. Nordheim's formula was based on the first Born approximation, valid in the absence of resonances, and we use it for ρ_\downarrow :

$$\rho_\downarrow = A_\downarrow x(1-x) + \rho_\downarrow^{ph}. \quad (5)$$

Here, A_\downarrow is a constant, and ρ_\downarrow^{ph} an additional constant term we have added to represent phonon and defect scattering in films at $T \geq 0$.

In Ref. [19], we derived an analytic expression which extends the Nordheim expression to the case where the Born approximation fails because of a resonance. The original derivation was based on an equation similar to the present Eq. (4), except that the equivalent of ϕ_{km}^+ was of 4s character. The derivation is still valid. We use this for ρ_\uparrow :

$$\rho_\uparrow = \frac{A_\uparrow x(1-x)}{[x/|C_B|^2 + (1-x)/|C_A|^2]^2} + \rho_\uparrow^{ph}, \quad |C_A| = [1 + (1-x)(r_F^{-1} - 1)]^{-1/2}, \quad |C_B| = [1 + x(r_F - 1)]^{-1/2}. \quad (6)$$

Here, C_A and C_B are the average spin-up electron amplitudes on A and B atoms, with $r_F = |C_A|^2/|C_B|^2$. Eq. (6) reduces to the Nordheim formula of Eq. (5) in the special case $r_F = 1$ where the resonance is absent. According to Eq. (6), ρ_\uparrow has a peak [19] at a concentration $x \approx (1 + r_F)^{-1}$. If $r_F \gg 1$, this x is much less than 50 at%. The coherent potential approximation gives [24] results similar to those of Eq. (6) but without a general analytic expression for the resistivity.

By analyzing existing data for $\Delta\rho$ and ρ in Ni-Fe, Ni-Co, Ni-Mn, Muth and Christoph [25] showed that ρ_\downarrow has a large peak at a moderate concentration of solute in nickel. By a similar analysis

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