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New calculations of Gilbert damping in ferromagnetic transition metals

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Abstract. Calculations of the Gilbert damping parameter alpha for bulk Ni are presented as a function of the spin-dependent Lorentzian broadening of the one-electron states. The Kambersky formula for alpha is used, correctly restricted to second order in the spin-orbit parameter so that intra band terms are suppressed, and the spin-dependent broadening is deduced from the recent calculations of electron lifetimes due to electron-phonon scattering by Carva et al. The calculated value of alpha for Ni at room temperature is in reasonable agreement with experiment.

1. Introduction

New calculations are presented of the Gilbert damping parameter $\alpha$ in bulk ferromagnetic transition metals which arises from spin-orbit coupling (SOC). We follow previous work [1, 2] by using the Kambersky formula [3] in which the effect of impurity and phonon scattering is simulated by a Lorentzian broadening $\Gamma$ of the one-electron states. However it has recently been shown [4] that the Kambersky formula is only valid to second order in the spin-orbit parameter $\xi$, so that the one-electron states in the formula must be calculated in the absence of SOC. Failure to apply this restriction, as in most existing calculations [1, 2], results in $\alpha$ diverging in the limit of a pure metal at $T = 0$ which corresponds to $\Gamma \to 0$. The striking difference at low $\Gamma$ between calculations of $\alpha$ with and without SOC in the band structure is shown for Fe and fcc Co in [2]. Qualitative comparison between calculations of this type and the observed temperature dependence of $\alpha$ [5] may be made with the reasonable assumption that $\Gamma$ increases with $T$ owing to phonon scattering. The observed rapid increase of $\alpha$ as $T$ decreases below 100K in Ni and hcp Co is often quoted [3, 1] in support of calculations using the Kambersky formula with SOC included in the band structure. However the observed temperature independence of $\alpha$ in Fe is in agreement with the calculation with SOC not included [2].

Here we report on new results for bulk Ni, which correctly exclude SOC in the band structure and use special techniques to calculate $\alpha$ down to the very low values of $\Gamma$ appropriate to a pure metal at low temperature. It is found that $\alpha$ increases as $\Gamma$ decreases to low values which is consistent with the observed temperature dependence. Additionally, in our calculations we include a spin-dependent broadening of electron states, obtained from first principles calculations of electron lifetimes due to electron-phonon scattering [6].


2. Calculation of the Gilbert damping constant

The calculation of the Gilbert damping constant proceeds from the Kambersky formula

\[
\alpha = \frac{\pi}{\mu_s} \sum_{n,m} \frac{1}{\Omega_{BZ}} \int dk |A_{nm}(k)|^2 L(\varepsilon_F - \varepsilon_n(k), \Gamma_n) L(\varepsilon_F - \varepsilon_m(k), \Gamma_m),
\]

which is the same as that used in [2], for bulk materials, when the temperature \( T = 0 \). Here \( \mu_s \) denotes the spin magnetic moment per atom (in units of the Bohr magneton \( \mu_B \)), \( \varepsilon_F \) is the Fermi energy, and the integral is over the three dimensional Brillouin zone of volume \( \Omega_{BZ} \). The sum is over all energy eigenstates \( n \), with energy \( \varepsilon_n(k) \) (which includes both majority and minority state electrons). The spin-orbit torque matrix element \( A_{nm} \), is given by

\[
A_{nm}(k) = \xi < k, n | S^-, H_{SO} | k, m >,
\]

where \( S^- = S_x - iS_y = \frac{1}{2} (\sigma_x - i\sigma_y) \) is the spin lowering operator and \( \xi H_{SO} \) is the one electron spin-orbit interaction with coupling constant \( \xi \). The Lorentzian functions are defined as

\[
L(\varepsilon_n, \Gamma_n) = (\Gamma_n/2\pi)/(\varepsilon_n^2 + \Gamma_n^2/4)
\]

where \( \Gamma_n \) is the spin-dependent electron-scattering rate.

It is important to realise that, as shown in [4], this expression for \( \alpha \) is only valid to second order in \( \xi \) and therefore, the eigenstates \( |k, n > \) must be calculated in the absence of SOC. In previous publications [3, 1] this point has been overlooked leading to non-zero diagonal (intra-band) terms \( A_{nm} \). Such terms give rise to the result that \( \alpha \) diverges as \( \Gamma \to 0 \), which corresponds to the unphysical prediction that Gilbert damping becomes infinite at \( T = 0 \) in a pure metal.

In this communication we calculate equation (1) within the tight-binding model, using s, p and d atomic orbitals, obtained by fitting \textit{ab-initio} energy bands of bulk metals [7]. Even within this relatively straightforward approach, the calculation of \( \alpha \) is computationally extremely demanding for small \( \Gamma \). This is because the Lorentzians become very narrow and hence the contribution to the integral over \( k \) becomes localised to a small region around the Fermi-surface in the three dimensional Brillouin zone. As a result, we typically require 800\(^3\) \( k \)-points for a tolerable convergence of the integral for \( \Gamma \geq 0.002\text{eV} \).

However the three-dimensional integral, over \((k_x, k_y, k_z)\), can be converted to a two-dimensional one, over \((k_x, k_y)\), by use of a novel trick. For each \((k_x, k_y)\), the positions of the Fermi-surface branches can be determined exactly by finding the eigenvalues of the matrix

\[
X = \begin{pmatrix}
0 & \mathbf{t}^{-1} \\
-\mathbf{t}^\dagger & (\varepsilon - \mathbf{u})\mathbf{t}^{-1}
\end{pmatrix}
\]

where \( \mathbf{u} \) is the tight-binding on-site potential and \( \mathbf{t} \) is the hopping matrix [8]. As a result, the peaks of the Lorentzians can be determined exactly and analytic approximations to the integral over \( k_z \) can be used. This results in a significant reduction in the number of \( k \)-points required to achieve convergence for small \( \Gamma \). For example, to obtain convergence for \( \Gamma \geq 0.002\text{eV} \), we now only require 800\(^3\) \( k \)-points.

3. Discussion of results

In figure 1, we see the effect of wrongly including the intra-band transitions in the calculation of \( \alpha \) for bulk Ni (black curve). In this figure, we take a spin-independent Lorentzian broadening \( \Gamma = \Gamma_\uparrow = \Gamma_\downarrow \), and as \( \Gamma \to 0 \), the value of \( \alpha \) is seen to dramatically increase (without limit) below \( \Gamma = 0.05\text{eV} \). On the other hand, the value of \( \alpha \) correctly calculated to second order in \( \xi \) (red curve) remains relatively flat but displays a slight minimum around \( \Gamma \approx 0.02\text{eV} \).

In figure 2 we plot our new results for \( \alpha \) over an enlarged scale, both with spin-independent (red curve) and with spin-dependent (black curve) \( \Gamma \) included. The spin dependent values of \( \Gamma \) at the Fermi surface are obtained from the spin resolved electron lifetimes \( \tau_\sigma = \{ \tau_\uparrow, \tau_\downarrow \} \), given
in references [6] and [9], by using the relation $\Gamma_\sigma = \hbar/2\tau_\sigma$. We observe that even without the intra-band terms $\alpha$ begins to increase for $\Gamma \leq 0.02\text{eV}$.

![Figure 1. $\alpha$ against scattering rate for bulk Ni, with and without intra-band terms included. Here $\Gamma = \Gamma_\uparrow = \Gamma_\downarrow$.](image1)

![Figure 2. $\alpha$ against scattering rate for bulk Ni, with and spin-dependent and spin-independent scattering. Here the horizontal axis denotes $\Gamma = \Gamma_\uparrow = 0.53\Gamma_\downarrow$.](image2)

We note that, using the results of references [6] and [9] for bulk Ni, room temperature corresponds to a value of $\Gamma_\uparrow = 0.0029\text{eV}$. Hence our value of $\alpha$ at room temperature is predicted to be $\alpha_{RT} \approx 0.01$ (see figure 2). Experimental values for $\alpha$ can be deduced from the ferromagnetic relaxation frequencies $\lambda$ measured by Bhagat and Lubitz [5]. They find that for pure Ni at room temperature $\lambda \approx 2.3 \times 10^8 \text{ sec}^{-1}$, which corresponds to a measured value of $\alpha_{\text{expt}} \approx 0.025$, in reasonable agreement with our predicted result.

4. Conclusion
We have presented calculations of the Gilbert damping parameter $\alpha$ for bulk Ni as a function of the Lorentzian broadening $\Gamma$ of the one-electron states. These calculations are based on Kambursky’s formula, correctly evaluated to second order in the spin-orbit coupling parameter $\xi$, using both spin dependent and spin-independent values of $\Gamma$. In both cases we find that $\alpha$ increases below $\Gamma \approx 0.02\text{eV}$. We intend to calculate $\alpha$ at lower values of $\Gamma$ than conventionally possible, using a novel technique, in order to determine its predicted behaviour as $T \to 0$.

References
[1] K. Gilmore, Y.U. Idzerda and M.D. Stiles, Phys. Rev. Lett. 99 027204 (2007)
[2] E. Barati, M. Cinal, D. M. Edwards and A. Umerski, Phys. Rev. B 90 014420 (2014)
[3] V. Kambursky, Czech. J. Phys B 26 1366 (1976)
[4] D. M. Edwards, J. Phys. Condens. Matter 28 086004 (2016)
[5] S. M. Bhagat and P. Lubitz, Phys. Rev. B 10 179 (1974)
[6] K. Carva, M. Battiato, D. Legut and P.M. Oppeneer, Phys. Rev. B, 87, 184425 (2013).
[7] D. A. Papaconstantopoulos, Handbook of the Band Structure of Elemental Solids, Plenum, New York, 1986.
[8] A. Umerski, Phys. Rev. B 55 5266 (1997)
[9] We are grateful to K. Carva for supplying a corrected value of the spin-lifetime for majority Ni.