Calculation of the Gilbert damping matrix at low scattering rates in Gd

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In rare-earth metals the magnetization dynamics is determined by the interplay between the magnetization $\mathbf{M}_{4f}$ of localized $4f$ electrons and the magnetization $\mathbf{m}$ of delocalized $5d6sp$ valence electrons, whereby both subsystems can deliver angular momentum to the lattice, thus producing damping. It is shown within the framework of a phenomenological version of the s-f model that the effective Gilbert damping parameter for $\mathbf{M}_{4f}(t)$ is given by $\alpha_{4f}^{eff}=\alpha_{4f}+\alpha_{5d6sp}/(1+M_{4f}/m)$, where α_{4f} is a direct $4f$ contribution and α_{5d6sp} describes the Gilbert damping for the valence magnetization. By a combination of the *ab initio* density-functional electron theory with the breathing Fermi-surface model it is shown that for a [0001] orientation of the magnetization the indirect valence contribution to α_{4f}^{eff} is comparable to the damping parameter of Co (which is considerably smaller than the one of Ni). Measurements of the damping at low temperatures and for Gd samples with high purity are required to figure out whether there is a considerable larger direct contribution α_{4f}.

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I. INTRODUCTION

In recent years there has been a steadily growing interest in the physics of fast[1] (typically nanosecond) and ultrafast[2] (several picosecond or femtosecond) dissipative magnetization dynamics. Examples for the fast time scale are the dynamics of domain walls in nanowires,[3] the magnetization reversal in nanomagnets,[3] and the dynamics of vortices,[4] and such processes are of potential use in advanced data processing devices. Ultrafast magnetization dynamics is induced by exposing a ferromagnetic film to a very intense femtosecond optical laser pulse, resulting sometimes[5] in a nearly complete quenching of the magnetization in a time T_1 of down to about 100 fs. This is believed to be the ultimate time scale for the macroscopic manipulation of the magnetization.

For both time scales the creation and relaxation of electron-hole pairs play an important role. On the nanosecond time scale the electron-hole pairs are generated by the nonadiabatic dynamics of the atomic magnetic moments itself[6,7] whereas for the femtosecond time scale the laser beam produces these quasiparticles.[2] During the relaxation of the electron-hole pairs via scattering of electrons at phonons or defects angular momentum is transferred from the electronic system to the lattice by the action of the spin-orbit coupling, and this leads to the damping of the magnetization dynamics.

For the nanosecond time scale the magnetization dynamics is usually described[8–11] by the following equation of motion:

$$\frac{d\mathbf{M}}{dt} = -\gamma(\mathbf{M}\times\mathbf{H}_{eff}) + \frac{1}{M}\mathbf{M}\times\underline{\underline{\alpha}}\frac{d\mathbf{M}}{dt} \qquad (1)$$

or on extensions of this equation including the effect of spin-polarized transport currents. In Eq. (1) the first term describes the precession of the magnetization $\mathbf{M}$ around an effective field $\mathbf{H}_{eff}$ (γ is the gyromagnetic ratio). The second term represents the damping and $\underline{\underline{\alpha}}$ is the damping matrix (which has at most two different nonzero eigenvalues corresponding to two different eigenvectors) which, in general, depends on the momentary configuration of the magnetization in the whole sample. For a homogeneous magnetization this means that the damping depends on the momentary orientation of this magnetization in the crystal (orientational anisotropy of the damping). Furthermore, because of the matrix character of $\underline{\underline{\alpha}}$ the damping depends on the momentary orientation of $d\mathbf{M}/dt$ (rotational anisotropy). It has been shown[7] that the anisotropy of the damping is relevant for low electron scattering rates whereas it becomes isotropic at high scattering rates. Equation (1) reduces to the well-known Gilbert equation[12] when the matrix $\underline{\underline{\alpha}}$ is replaced by a constant damping scalar α. Furthermore if the momentary magnetization points into a high-symmetry direction of the crystal then the two eigenvalues of $\underline{\underline{\alpha}}$ are identical and the momentary equation of motion again has the form of a Gilbert equation.[10]

For the ultrafast time scale the magnetization dynamics is described by a phenomenological[2] or a microscopic[13,14] three-temperature model for the interaction between the electron, spin, and lattice subsystems. In the microscopic version of the three-temperature model[13,14] the transfer of angular momentum is accounted for by the spin-flip scattering of electrons at phonons, described by a probability a_{el} that an electron-phonon scattering event is accompanied by a spin flip of the involved electron. It is reasonable to assume that the same microscopic relaxation mechanisms are responsible both for the fast and the ultrafast magnetization dynamics.

There are many papers in which the quantities α and T_1 (or a_{el}) are measured or calculated for various materials and in which it is explored how these quantities can be modified, e.g., by doping with various atoms.[15] For the nanosecond time scale the investigations focus on the ferromagnetic $3d$ metals Fe, Co, and Ni and their compounds and alloys, whereas pure rare-earth metals have not been considered so far, most probably because they are magnetic only at temperatures lower than room temperature so that they are less relevant for technological applications. In contrast, for the demagnetization after femtosecond laser pulses there are several investigations also for the rare-earth metal Gd (Ref. 16) showing that in this material the laser-induced demagnetization is slower by three orders of magnitude than in ferromagnetic transition metals. In Gd magnetism is dominated by a

half-filled $4f$ shell with magnetic moment $7\mu_B$ which induces a smaller moment of about half a Bohr magneton in the $5d6sp$ valence band. Because the laser pulse excites electron-hole pairs in the valence band, it is assumed (see, e.g., Ref. 14) that the primary spin-flip processes appear by scattering of valence electrons and that the exchange coupling between valence electrons and $4f$ electrons is responsible for a simultaneous demagnetization of the $5d6sp$ and the $4f$ system. By analyzing the available experimental data within the microscopic three-temperature model it has been shown[14] that in spite of the drastically different demagnetization rates for $3d$ metals and Gd the spin-flip probabilities a_{el} for the $3d$ electrons and the $5d6sp$ electrons agree within a factor of about two. The different relaxation rates result from the fact that in the $3d$ metals the demagnetization completes at high electron temperatures (before electron-phonon equilibrium is achieved) whereas in Gd the electron temperature is drastically reduced during demagnetization, leading to a reduced demagnetization rate after an initial rapid decay.

In the present paper we consider the fast (i.e., Gilbert-type) dynamics for a homogeneous, i.e., position-independent magnetization $\mathbf{M}(t)=\mathbf{M}_{4f}(t)+\mathbf{m}(t)$ in Gd. As discussed above, $\mathbf{M}(t)$ is dominated by the $4f$ contribution $\mathbf{M}_{4f}(t)$ which induces a valence-electron magnetization $\mathbf{m}(t)$ via the exchange coupling between $4f$ electrons and $5d6sp$ valence electrons. Concerning the damping, angular momentum may be transferred to the lattice both from the $4f$ electrons (e.g., via phonon-modulated crystal-field interactions) and the $5d6sp$ valence electrons (e.g., by spin-dependent scattering of electrons at phonons or defects). Because the dynamics of $\mathbf{M}_{4f}(t)$ is coupled to the dynamics of $\mathbf{m}(t)$ via the exchange coupling between these two subsystems, the damping of $\mathbf{m}$ will also lead to a damping of $\mathbf{M}_{4f}$ and vice versa. It is one of the objectives of the present paper to consider (Sec. II A) the mutual interactions between $\mathbf{m}(t)$ and $\mathbf{M}_{4f}(t)$ within a phenomenological model, i.e., a classical version of the s-f model[17] (where the label "s" denotes the $5d6sp$ valence electrons). This model is the analog to the well-known s-d model (see, e.g., Refs. 18–20) for transition-metal ferromagnets or magnetic semiconductors (where the label s now denotes the sp valence states and "d" the d states of transition-metal atoms). In this model, Gilbert-type equations of motion are used for $\mathbf{m}(t)$ and $\mathbf{M}_{4f}(t)$ which include Gilbert damping terms with a damping scalar α_{5d6sp} and α_{4f}, respectively. The two equations are coupled via a respective exchange torque which contains the finite exchange interaction between $\mathbf{m}$ and $\mathbf{M}_{4f}$, i.e., we do not assume a rigid coupling between the two subsystems (in contrast to the approach of Ref. 14). Under certain approximations an effective equation of motion of Gilbert type is obtained where only the magnetization $\mathbf{M}_{4f}$ appears and where the mutual interaction between $\mathbf{M}_{4f}$ and $\mathbf{m}$ is reflected in an effective gyromagnetic ratio and in an effective damping scalar α_{4f}^{eff} which contains both α_{4f} and α_{5d6sp}. It will be shown that this approach is equivalent to the s-d model calculations of Ref. 20 where the Gilbert term in the equation for $\mathbf{m}$ is replaced by a Bloch-type relaxation term with a transverse relaxation time T_2, and a relation between α_{5d6sp} and an analog relaxation time $\tilde{T}_2$ is derived.

In the conventional s-d model the quantity T_2 is taken as a parameter. It is the second objective of the present paper (Sec. II B) to calculate α_{5d6sp}—which in a general situation has to be replaced by a damping matrix $\underline{\underline{\alpha}}_{5d6sp}$—by the *ab initio* density-functional electron theory within Kamberský's breathing Fermi-surface model.[6,7,9–11,21] This model holds for low scattering rates of electrons, i.e., for low temperatures and low defect concentrations. The damping matrix for Gd will be compared with the one for Co (Sec. III). In view of the drastically different electronic structures of these two materials it will be interesting to compare the two damping matrices both with respect to their magnitudes as well as with respect to their orientational and rotational anisotropies.

II. CALCULATIONAL PROCEDURES

A. Phenomenological s-f model

We now want to describe the mutual interaction between the two magnetic subsystems, the valence magnetization $\mathbf{m}$ formed by $5d6sp$ states (labeled by the symbol s) and the $4f$ magnetization $\mathbf{M}_{4f}$, by a phenomenological s-f model which is the counterpart to the s-d model, used for transition-metal ferromagnets and for magnetic semiconductors. We write down the equations of motion for $\mathbf{m}$ and $\mathbf{M}_{4f}$ which are coupled by the exchange interaction between the two subsystems.

In a homogeneous situation we suggest for the equation of motion for the valence-electron magnetization $\mathbf{m}(t)$ the following Gilbert-type equation:

$$\frac{d\mathbf{m}}{dt} = -\gamma(\mathbf{m}\times\mathbf{H}_m^{eff}) + \frac{1}{m}\mathbf{m}\times\underline{\underline{\alpha}}_{5d6sp}\frac{d\mathbf{m}}{dt} - \mathbf{T}. \tag{2}$$

In Eq. (2) $\mathbf{H}_m^{eff}$ is the effective field acting on $\mathbf{m}$ which is composed of the external field $\mathbf{H}^{ext}$, the anisotropy field $\mathbf{H}_m^{aniso}$ for the $5d6sp$ magnetization and the demagnetization field $\mathbf{H}^{demagn}$. The second term describes the damping. The third term is the torque density exerted by $\mathbf{M}_{4f}$ on $\mathbf{m}$ due to the exchange interaction between $4f$ electrons and $5d6sp$ electrons. It is modeled in the spirit of the s-d model[18] as

$$\mathbf{T} = -\frac{1}{\tau_{ex}M_{4f}}\mathbf{M}_{4f}\times\mathbf{m} \tag{3}$$

with

$$\tau_{ex} = \frac{\hbar}{SJ_{ex}}, \tag{4}$$

where J_{ex} is the $4f$-$5d6sp$ exchange coupling constant and $S=7/2$ is the total spin of the $4f$ shell of Gd.

For $\mathbf{M}_{4f}(t)$ we suggest again a Gilbert-type equation of motion

$$\frac{d\mathbf{M}_{4f}}{dt} = -\gamma(\mathbf{M}_{4f}\times\mathbf{H}_{4f}^{eff}) + \frac{1}{M_{4f}}\mathbf{M}_{4f}\times\alpha_{4f}\frac{d\mathbf{M}_{4f}}{dt} + \mathbf{T}. \tag{5}$$

The effective field for the $4f$ magnetization is $\mathbf{H}_{4f}^{eff}=\mathbf{H}^{ext}+\mathbf{H}^{demagn}$, there is no $4f$ anisotropy field[21] because of the

spherical $4f$ charge density of Gd. For simplicity, we describe the damping of $\mathbf{M}_{4f}$ by a scalar damping constant α_{4f}. The third term describes the torque density exerted by $\mathbf{m}$ on $\mathbf{M}_{4f}$.

Equations (2)–(5) represent a closed system of equations for $\mathbf{m}(t)$, $\mathbf{M}_{4f}(t)$ and hence for the total magnetization $\mathbf{M}(t)=\mathbf{M}_{4f}(t)+\mathbf{m}(t)$ which may be solved numerically for given initial conditions $\mathbf{m}(t=0)$ and $\mathbf{M}_{4f}(t=0)$. Because of the coupling between $\mathbf{m}$ and $\mathbf{M}_{4f}$, the damping matrix $\underline{\underline{\alpha}}_{5d6sp}$ will contribute to the effective damping of $\mathbf{M}_{4f}$ which is no longer determined exclusively by α_{4f}, and the damping scalar α_{4f} will contribute to the effective damping of $\mathbf{m}$ which is no longer determined exclusively by $\underline{\underline{\alpha}}_{5d6sp}$. In order to obtain a qualitative feeling for this, we determine the effective damping of $\mathbf{M}_{4f}(t)$ by a simple analytical calculation. In order to make such an analytical calculation feasible, we perform the following rough approximations. We assume that the third term in Eq. (2) is much larger than the first term which we therefore neglect completely. (The same approximation is made in the s-d model of Ref. 20.) Furthermore, we consider a situation where the momentary orientation of $\mathbf{m}$ is along a high-symmetry direction of the crystal so that the damping matrix $\underline{\underline{\alpha}}_{5d6sp}$ can be replaced[10] by a damping scalar α_{5d6sp}. Altogether, the equation of motion for $\mathbf{m}(t)$ then reads

$$\frac{d\mathbf{m}}{dt}=\frac{1}{m}\mathbf{m}\times\alpha_{5d6sp}\frac{d\mathbf{m}}{dt}-\mathbf{T} \tag{6}$$

which has to be solved together with Eqs. (3)–(5).

To do this, we subdivide $\mathbf{m}(t)$ according to

$$\mathbf{m}(t)=\mathbf{m}_0(t)+\delta\mathbf{m}(t). \tag{7}$$

Here

$$\mathbf{m}_0(t)=\frac{m_0}{M_{4f}}\mathbf{M}_{4f}(t) \tag{8}$$

is the $5d6sp$ magnetization which would appear in an adiabatic situation where $\mathbf{m}$ and $\mathbf{M}_{4f}$ are collinear due to the exchange coupling J_{ex}. In a nonadiabatic situation the valence-electron magnetization does not follow $\mathbf{M}_{4f}(t)$ adiabatically, giving rise to a contribution $\delta\mathbf{m}(t)$ which is perpendicular to $\mathbf{M}_{4f}(t)$. Inserting Eqs. (7) and (8) into Eqs. (3) and (6) and neglecting $d(\delta\mathbf{m})/dt$ as in the conventional s-d model[18] we find after some algebra

$$\mathbf{T}=-\frac{m_0}{M_{4f}}\frac{d\mathbf{M}_{4f}}{dt}+\frac{m_0}{M_{4f}^2}\mathbf{M}_{4f}\times\alpha_{5d6sp}\frac{d\mathbf{M}_{4f}}{dt}. \tag{9}$$

Inserting Eq. (9) into Eq. (5) yields

$$\frac{d\mathbf{M}_{4f}}{dt}=-\frac{\gamma}{1+m_0/M_{4f}}(\mathbf{M}_{4f}\times\mathbf{H}_{4f}^{eff})+\frac{1}{M_{4f}}\mathbf{M}_{4f}\times\alpha_{4f}^{eff}\frac{d\mathbf{M}_{4f}}{dt}, \tag{10}$$

i.e., a Gilbert equation with a renormalized gyromagnetic ratio $\gamma/(1+m_0/M_{4f})$ and an effective $4f$ damping scalar

$$\alpha_{4f}^{eff}=\frac{\alpha_{4f}}{1+m_0/M_{4f}}+\frac{\alpha_{5d6sp}}{1+M_{4f}/m_0}. \tag{11}$$

For the case $\alpha_{4f}=0$ the effective damping parameter for the $4f$ magnetization thus is given by

$$\alpha_{4f}^{eff}=\frac{\alpha_{5d6sp}}{1+M_{4f}/m_0}\approx\frac{m_0}{M_{4f}}\alpha_{5d6sp}. \tag{12}$$

Because the ratio m_0/M_{4f} is small, α_{4f}^{eff} is considerably smaller then α_{5d6sp}.

B. *Ab initio* calculation of α_{5d6sp}

As outlined in Sec. I, we do not consider α_{5d6sp} as an open parameter, but we calculate it by the *ab initio* density-functional electron theory. It has been shown in Ref. 22 that the damping in the $3d$ ferromagnets Fe, Co, and Ni is dominated by the excitation of electron-hole pairs caused by the magnetization dynamics and their subsequent relaxation due to electronic-scattering processes. We assume that the same holds for the damping in the $5d6sp$ subsystem of Gd. For this situation there are two contributions to damping,[6–8,22] a conductivitylike contribution which is proportional to the relaxation time τ for electronic-scattering processes and which results from electron-hole pairs generated in the same valence band ("intraband contribution"), and a resistivitylike contribution which is (for large τ) proportional to $1/\tau$ and which results from electrons and holes generated in different bands (interband contribution). Both contributions are included in Kamberský's torque correlation model,[23] and the conductivitylike contribution of this model is equivalent[6,22] to Kamberský's breathing Fermi-surface model.[9–11,24] We consider only the conductivitylike contribution which dominates[7,22] at large τ (low scattering rates), i.e., our calculations are based on the *ab initio* variant of the breathing Fermi-surface model described in full detail in Refs. 9–11, 22, and 25.

The breathing Fermi-surface model is valid if the characteristic time scale τ_m of the change in $\mathbf{m}(t)$ is much larger than the scattering time τ which describes the relaxation of the electronic occupation numbers. For τ_m/τ going to infinity the electronic system is at any time in its ground state with respect to the momentary orientation of $\mathbf{m}(t)$, and there is no damping at all. In this situation the adiabatic single-electron energies $\varepsilon_{j\mathbf{k}}$ of the valence electrons (j denotes the band index and $\mathbf{k}$ is the wave vector) depend on the momentary orientation of $\mathbf{m}$, and thus the adiabatic Fermi-surface changes in time (it "breathes"). In a nonadiabatic situation the momentary occupation numbers $n_{j\mathbf{k}}$ for the single-electron states lag behind the momentary adiabatic Fermi-Dirac occupation numbers $f_{j\mathbf{k}}$ which means that electrons and holes are formed with respect to the adiabatic situation.[7] The electronic-scattering processes then tend to restore the adiabatic situation, but because τ_m/τ now is still large but finite this requires time. The scattering processes which drive $n_{j\mathbf{k}}$ toward $f_{j\mathbf{k}}$ transfer in net angular momentum from the electronic system to the lattice and this produces damping.

Within the breathing Fermi-surface model the damping term for $\mathbf{m}(t)$ is given by $1/m(\mathbf{m}\times\underline{\underline{\alpha}}_{5d6sp}d\mathbf{m}/dt)$ with[9–11]

$$\frac{m(\alpha_{5d6sp})_{\alpha\beta}}{\gamma\tau} = -\sum_i \frac{\partial f_{j\mathbf{k}}}{\partial \varepsilon_{j\mathbf{k}}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_\alpha}\bigg|_{\mathbf{e}} \frac{\partial \varepsilon_{j\mathbf{k}}}{\partial e_\beta}\bigg|_{\mathbf{e}} = Z. \quad (13)$$

In Eq. (13) the $\varepsilon_{j\mathbf{k}}$ are the adiabatic energies of the single-electron valence states and $f_{j\mathbf{k}}$ is the adiabatic Fermi-Dirac distribution function, both defined for the momentary orientation $\mathbf{e}(t)=\mathbf{m}(t)/m(t)$. The derivatives $\partial\varepsilon_{j\mathbf{k}}/\partial\mathbf{e}$ of the energies with respect to the orientation $\mathbf{e}(t)$ are calculated by a special variant of the magnetic force theorem,[26] for details see Ref. 11. In the band-structure calculation the $4f$ states are treated as open core states with appropriate constraints[21] which guarantee the correct localization of the $4f$ charge density and the correct $4f$ atomic moment of $7\mu_B$ for Gd. The valence states are determined by the tight-binding linear-muffin-tin-orbital method in the atomic-sphere approximation[27] in which spin-orbit coupling[28] has been implemented. The parameter τ is a phenomenological relaxation parameter which describes the relaxation of the nonadiabatic occupation numbers $n_{j\mathbf{k}}(t)$ toward the adiabatic Fermi-Dirac occupation numbers $f_{j\mathbf{k}}[\mathbf{e}(t)]$. It encompasses in an effective manner all the microscopic spin-flip scattering processes which are responsible for the transfer of angular momentum from the valence electrons to the lattice, for the given dynamical situation described by the breathing Fermi-surface model. Because the parameter τ is not known it is often approximated by the Drude relaxation time for the electrical resistivity, and therefore the breathing Fermi-surface contribution to damping which is proportional to τ [see Eq. (13)] is called conductivitylike contribution. The use of a single phenomenological Drude relaxation time is certainly not strictly valid. It has been shown[29] that while this approximation works well for the long lifetime limit, i.e., for the intraband terms described by the breathing Fermi-surface model, vertex corrections can be important in the short lifetime limit, where the interband terms dominate. Please note that the breathing Fermi-surface model describes explicitly (via $\partial\varepsilon_{j\mathbf{k}}/\partial\mathbf{e}$) only the change in the adiabatic Fermi surface with the dynamics of $\mathbf{e}(t)$ whereas it does not try to calculate the spin-flip scattering processes. In contrast, in the theories for the ultrafast magnetization dynamics the spin-flip probability a_{el} is determined explicitly.[30]

In former *ab initio* calculations the breathing Fermi-surface contribution to damping has been determined for the itinerant $3d$ ferromagnets Fe, Ni, and Co. In the present paper we consider the damping of the valence magnetization for the rare-earth metal Gd. It will be interesting to see how the damping in Gd compares to the one of Co (which has the same crystal structure), both concerning its magnitude as well as its orientational and rotational anisotropy.

III. DISCUSSION AND NUMERICAL RESULTS

A. Relation between the present *s-f* model and the conventional *s-d* model

In the conventional *s-d* model (which exists in different variants, see, e.g., Refs. 18–20) basically the same strategy is used as in the present *s-f* model. The total magnetization is again composed of a small valence part $\mathbf{m}$, originating from itinerant electrons and a large part $\mathbf{M}_d$ which is related to localized electrons, and $\mathbf{m}$ is again subdivided into an adiabatic part $\mathbf{m}_0$ and a nonadiabatic part $\delta\mathbf{m}$. Furthermore, again equations of motion for $\mathbf{m}$ and $\mathbf{M}_d$ are considered which are coupled by an exchange torque. The equation for $\mathbf{M}_d$ has the same form as Eq. (5) whereas in the equation for $\mathbf{m}$ the Gilbert term for the damping is replaced by a Bloch-type relaxation term

$$\mathbf{T}_{rel} = -\frac{\mathbf{m}-\mathbf{m}_0}{T_2}. \quad (14)$$

The quantity[20] T_2 (in Refs. 18 and 19 denoted as τ_{sf} and τ_{sr}^s, respectively) is called transverse spin-flip time,[20] spin-flip relaxation time,[18] or just spin-relaxation time.[19] It is the time which characterizes the decay of the transverse magnetization component $\delta\mathbf{m}=\mathbf{m}-\mathbf{m}_0$, i.e., a time characterizing the "macroscopic" quantity $\delta\mathbf{m}$. It should not be confused with the microscopic relaxation time τ for the electronic occupation numbers as introduced in Sec. II B, see below.

The Gilbert-type Eq. (2) of the present *s-f* model may be approximately cast into the form used in the conventional *s-d* model with the relaxation term in Eq. (14). To achieve this, we multiply Eq. (2) (omitting the first term and replacing $\underline{\underline{\alpha}}_{5d6sp}$ by α_{5d6sp}, see Sec. II A) from left with $\mathbf{m}$, solve for $\mathbf{m}\times d\mathbf{m}/dt$ and insert this quantity again in Eq. (2), yielding

$$\frac{d\mathbf{m}}{dt} = \frac{1}{\tau_{ex}M_{4f}(1+\alpha_{5d6sp}^2)}\mathbf{M}_{4f}\times\mathbf{m} + \frac{\alpha_{5d6sp}}{\tau_{ex}M_{4f}m(1+\alpha_{5d6sp}^2)}(m^2\mathbf{M}_{4f}-\mathbf{m}(\mathbf{m}\cdot\mathbf{M}_{4f})). \quad (15)$$

Using Eqs. (7) and (8) and the approximation $|\delta\mathbf{m}|^2\approx 0$, $|\mathbf{m}|\approx|\mathbf{m}_0|$, we find

$$\frac{d\mathbf{m}}{dt} = -\frac{\alpha_{5d6sp}}{\tau_{ex}(1+\alpha_{5d6sp}^2)}(\mathbf{m}-\mathbf{m}_0) - \frac{\mathbf{T}}{(1+\alpha_{5d6sp}^2)}. \quad (16)$$

Inserting Eqs. (7) and (8) into Eqs. (3) and (16) and neglecting $d(\delta\mathbf{m})/dt$ reproduces the Eqs. (9)–(11). Denoting the prefactor in front of $-(\mathbf{m}-\mathbf{m}_0)$ as inverse transverse spin-flip time $\tilde{T}_2$,

$$\frac{1}{\tilde{T}_2} = \frac{\alpha_{5d6sp}}{\tau_{ex}(1+\alpha_{5d6sp}^2)}, \quad (17)$$

then Eq. (16)

$$\frac{d\mathbf{m}}{dt} = -\frac{\mathbf{m}-\mathbf{m}_0}{\tilde{T}_2} - \frac{\mathbf{T}}{(1+\alpha_{5d6sp}^2)} \quad (18)$$

looks very similar to the corresponding equation of the *s-d* model [see, e.g., Eq. (5) of Ref. 20], except for the factor $1/(1+\alpha_{5d6sp}^2)$ in front of the exchange torque $\mathbf{T}$ [given by Eq. (3)]. This difference results from the fact that we start from the Gilbert-type Eq. (6) where the damping is proportional to the speed of change in the magnetization, $d\mathbf{m}/dt$, whereas in the *s-d* model the damping term in Eq. (14) is proportional to the difference $\mathbf{m}-\mathbf{m}_0$.

With Eqs. (17) and (12) we find (for the case $\alpha_{4f}=0$) a relation between α_{4f}^{eff} and $\tilde{T}_2$

$$\frac{1}{\tilde{T}_2}=\frac{\Omega\alpha_{4f}^{eff}\left(1+\frac{M_{4f}}{m_0}\right)}{1+(\alpha_{4f}^{eff})^2\left(1+\frac{M_{4f}}{m_0}\right)^2} \tag{19}$$

with $\Omega=1/\tau_{ex}=SJ_{ex}/\hbar$. This equation is the counterpart to Eq. (6) of Ref. 20 (which is slightly different from the corresponding equation of Ref. 18)

$$\alpha_d^{eff}=\Omega T_2[1+(\Omega T_2)^2]^{-1}\frac{m_0}{M_d}. \tag{20}$$

Although the forms of Eqs. (19) and (20) are different, they exhibit the same asymptotic behavior. For small α_{4f}^{eff}, Eq. (19) reduces to

$$\alpha_{4f}^{eff}=\frac{1}{\left(1+\frac{M_{4f}}{m_0}\right)\Omega\tilde{T}_2}, \tag{21}$$

which is equivalent to Eq. (1) given for α_d^{eff} in Ref. 19. For large ΩT_2 (i.e., small α_d^{eff}) Eq. (20) reads

$$\alpha_d^{eff}=\frac{1}{\frac{M_d}{m_0}\Omega T_2}, \tag{22}$$

which is also nearly equivalent to Eq. (21) because of $\frac{M_{4f}}{m_0}$, $\frac{M_d}{m_0}\gg 1$. In Ref. 20 this term is denoted as "spin-pumping contribution." The motion of the $4f$ magnetization pumps spin angular momentum into the system of valence electrons and this angular momentum is subsequently transferred to the lattice by electron-lattice scattering processes. For large $\alpha_{4f}^{eff}\sim\alpha_{5d6sp}$, when the dynamics of the valence magnetization $\mathbf{m}$ in Eq. (16) is dominated by the relaxation term, Eq. (19) reduces to

$$\alpha_{4f}^{eff}=\frac{\Omega}{\left(1+\frac{M_{4f}}{m_0}\right)}\tilde{T}_2, \tag{23}$$

and for $\frac{M_{4f}}{m_0}\gg 1$ this is again equivalent to the result found from Eq. (20) for the case of small ΩT_2, when the dynamics in Eq. (5) of Ref. 20 is dominated by the relaxation. We will see in Sec. III B that for Gd α_{4f}^{eff} is rather small. Therefore, our result for α_{4f}^{eff} represents the spin-pumping contribution to the effective $4f$ damping.

As outlined in the introduction and in Sec. II B we do not consider $\tilde{T}_2$ as a free parameter but we determine this quantity from Eq. (13) where we calculate $\alpha_{4f}^{eff}=\alpha_{5d6sp}/(1+M_{4f}/m_0)$ by the *ab initio* density-functional electron theory. When we take into account (as we do) just the intraband contribution to α_{5d6sp} (which is proportional to the electronic relaxation time τ), then the "spin-pumping term" [given by Eq. (21)] yields $\tilde{T}_2\sim\frac{1}{\tau}$. In contrast, when we take just the interband contribution to α_{5d6sp} (which is proportional to $1/\tau$) then the spin-pumping term gives $\tilde{T}_2\sim\tau$. Accordingly, we find for the other limit given by Eq. (23) that $\tilde{T}_2\sim\tau$ ($\tilde{T}_2\sim\frac{1}{\tau}$) when we consider the intraband (interband) contribution to α_{5d6sp}. From this discussion it becomes clear that one should not try to denote one of the two limits given by Eqs. (21) and (23) as breathing Fermi-surface contribution. The breathing Fermi-surface contribution is the one for which α_{4f}^{eff} is proportional to the "microscopic" relaxation time τ, it is not necessarily related to the one for which α_{4f}^{eff} is proportional to the macroscopic relaxation time $\tilde{T}_2$.

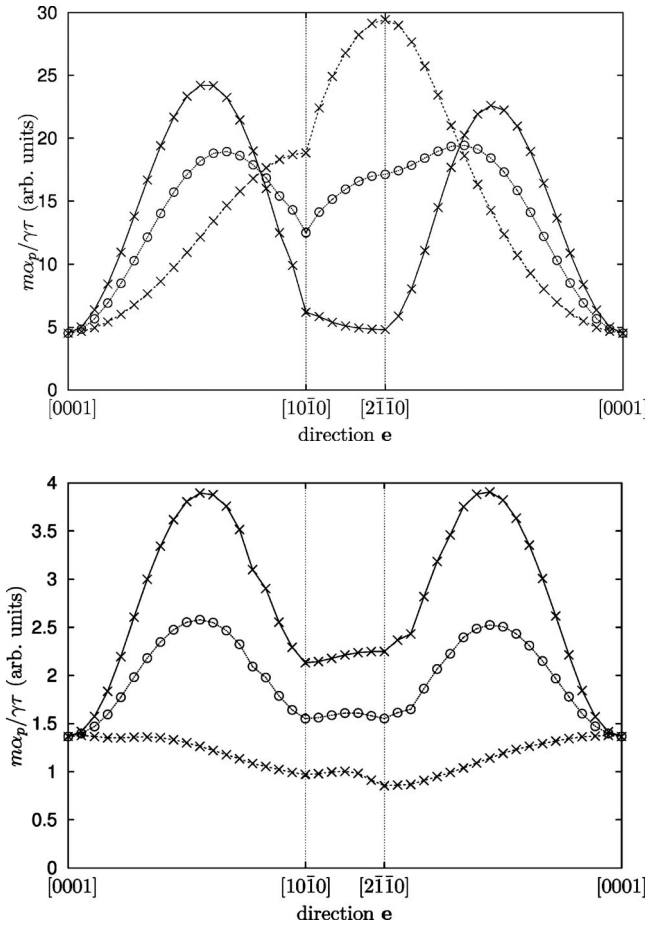

FIG. 1. The two eigenvalues α_p ($p=1,2$, symbols ×) of the matrix $m\underline{\underline{\alpha}}/\gamma\tau$ as function of the orientation of the magnetization in the crystal, and the arithmetic mean of the two eigenvalues (symbol ○), for Gd (top) and Co (bottom, from Ref. 25).

B. Numerical results for $\underline{\underline{\alpha}}_{5d6sp}$

As discussed in Sec. II B, the breathing Fermi-surface model describes explicitly only the driving force for the magnetic relaxation, i.e., the change in the adiabatic Fermi surface with the dynamics of $\mathbf{e}(t)$, whereas the scattering process itself is accounted for by a phenomenological relaxation parameter. When considering different materials such as Co and Gd, it makes sense to compare the right-hand side of Eq. (13) for the two materials because this side contains all the electronic information on the systems. Figure 1 rep-

resents the two eigenvalues α_p, $p=1$ and 2, of the matrices $Z^{\mathrm{Gd}}=m\underline{\underline{\alpha}}_{5d6sp}/\gamma\tau$ for Gd (top) and $Z^{\mathrm{Co}}=m\underline{\underline{\alpha}}_{3d4sp}/\gamma\tau$ for Co (bottom) for the valence electrons as function of the orientation of $\mathbf{e}(t)$ in the crystal. It becomes obvious that the degree of anisotropy of $\underline{\underline{\alpha}}$ is similar for the two materials. The eigenvalues of $m\underline{\underline{\alpha}}_{5d6sp}/\gamma\tau$ are a factor of about 3–10 larger for Gd with the more delocalized $5d$ states than for Co with the more localized $3d$ states.

The figure represents in addition the arithmetic mean of the two eigenvalues which (to a very good approximation) determines the linewidth of a ferromagnetic resonance experiment.[31] For a situation for which the breathing Fermi-surface model is valid (i.e., for slow magnetization dynamics and low scattering rates) the linewidth of the ferromagnetic resonance in Co and Gd should be anisotropic, i.e., it should depend on the orientation of the dc field in the sample.

In the following we assume that the relaxation times τ for Gd and Co are similar. Because the valence moment of Gd is about a factor of three smaller than the one of Co, the damping constant $\alpha_{5d6sp}=\gamma\tau Z^{\mathrm{Gd}}/m$ then is a factor of 10–30 larger than the parameter $\alpha_{3d4sp}^{\mathrm{Co}}$ of Co. According to Eq. (12), and taking into account $M_{4f}/m_0 \gg 1$ and $m \approx m_0$, the indirect contribution of the valence electrons to α_{4f}^{eff} is given by

$$\alpha_{4f}^{eff,indirect} = \frac{\gamma\tau}{M_{4f}} Z^{\mathrm{Gd}}, \tag{24}$$

which is $\alpha_{4f}^{eff,indirect} \approx (0.7-2.3)\alpha_{3d4sp}^{\mathrm{Co}}$. The lower limit holds for the [0001] orientation of the magnetization. Altogether, we thus predict that for this orientation the indirect contribution of the valence states to the effective $4f$ damping parameter is comparable to the one of Co, which—in turn—is considerably smaller[22] than the damping parameter of Ni.

IV. CONCLUSIONS

In the rare-earth metals the magnetization dynamics is determined by the interplay between the localized $4f$ electrons and the delocalized $5d6sp$ valence electrons, whereby both electronic subsystems can deliver angular momentum to the lattice and can thus produce damping. Within a special variant of the classical s-f model, Gilbert-type equations of motion for the $4f$ magnetization $\mathbf{M}_{4f}(t)$ (with a damping scalar α_{4f}) and for the valence magnetization $\mathbf{m}(t)$ (with α_{5d6sp}) are written down, which are coupled by exchange torques. For a homogeneous situation an effective Gilbert equation just for $\mathbf{M}_{4f}(t)$ is derived with an effective damping parameter $\alpha_{4f}^{eff}=\alpha_{4f}+\alpha_{5d6sp}/(1+M_{4f}/m)$.

Our s-f model is similar to the conventional s-d model for itinerant ferromagnets apart from the fact that in the s-d model the damping is not described by a Gilbert term but by a Bloch-type relaxation term with a transverse spin-flip relaxation time T_2. It is shown that the Gilbert damping term of our s-f model can be cast into a Bloch-type relaxation term with a spin-flip relaxation time $\tilde{T}_2$, and a relation between $\tilde{T}_2$ and α_{5d6sp} is derived. In the conventional s-d model the quantity T_2 is taken as an open parameter. Because we have the relation between $\tilde{T}_2$ and α_{5d6sp}, and because a well-established electronic theory for the Gilbert damping exists [the *ab initio* version of Kamberský's torque correlation model including a conductivitylike (breathing Fermi surface) and a resistivitylike contribution to damping], we are in the position to calculate α_{5d6sp} and hence $\tilde{T}_2$ and α_{4f}^{eff} on the electronic level.

We have calculated α_{5d6sp} (which, in general, has to be replaced by the matrix $\underline{\underline{\alpha}}_{5d6sp}$) by the *ab initio* density-functional electron theory for the case of low electronic-scattering rates for which the breathing Fermi-surface contribution dominates. The damping of the valence-electron magnetization of Gd is considerably larger than the one of the itinerant ferromagnet Co but exhibits a similar degree of orientational and rotational anisotropy.

Altogether, a complete microscopic theory for the contribution $\alpha_{5d6sp}/(1+M_{4f}/m)$ of the valence electrons to the effective damping parameter α_{4f}^{eff} of the $4f$ magnetization $\mathbf{M}_{4f}$ of Gd has been given. It is predicted that for a [0001] orientation of the magnetization this contribution is comparable to the damping parameter of Co (which is rather small). The total effective damping α_{4f}^{eff} is the sum of this valence-electron contribution and the direct $4f$ contribution α_{4f} which cannot be calculated within the framework of the present theory. Therefore, it would be highly interesting to measure the effective damping for a Gd sample at low valence scattering rates, i.e., for samples of high purity and at low temperatures. A measured damping parameter which is considerably larger than our calculated valence contribution would reveal the dominance of the direct $4f$ contribution α_{4f}.

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