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Local and nonlocal atomic contributions to unit-cell damping in near-adiabatic collinear magnetization dynamics

Jonas Seib, Daniel Steiauf, and Manfred Fähnle*
Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, D-70569 Stuttgart, Germany

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Recently a unified theory for the near-adiabatic magnetization dynamics in collinear and noncollinear systems has been presented [D. Steiauf *et al.*, Phys. Rev. B **78**, 020410(R) (2008)]. There, an equation of motion for atomic magnetic moments is derived which includes anisotropic and nonlocal atomic damping matrices. In the present paper the connection between damping for atomic and unit-cell magnetic moments in collinear systems is investigated. Using the unified theory, numerical values for the local and nonlocal atomic contributions to the unit-cell damping in collinear hcp-Co, bcc-Fe, and a Co layer are calculated. In addition, the damping matrix for the whole unit cell is calculated by a formerly established method, the torque-operator method. The results of the unified theory and of the torque-operator method which are based on different approximations agree very well.

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I. INTRODUCTION

In the last few years there has been extensive research activity, both experimental and theoretical, on the ultrafast magnetization dynamics in magnetically ordered materials. This research is important from a technological point of view, as it gives deeper insight into ultrafast switching processes of magnetic devices. From the viewpoint of fundamental research it is very interesting to get a better understanding of the fundamental equation of motion which underlies dissipative magnetization dynamics and to determine the character of damping parameters and the influence of material properties on these.[1,2]

It is common to subdivide magnetization dynamics into phenomena which appear on two different time scales.[3] In the near-adiabatic regime of more than several picoseconds, it is assumed that the electronic system is always close to the ground state with respect to the momentary magnetic configuration. Examples are the dynamics of domain walls[4] or field- and current-driven magnetization dynamics.[4,5] On the femtosecond time scale, for example, in ultrafast demagnetization experiments,[6] strong excitations from these ground states have to be taken into account.

On a phenomenological level the Gilbert equation[7] [Eq. (1)] is the generally used equation of motion for the magnetization $\mathbf{M}(\mathbf{r},t)$,

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

with the gyromagnetic ratio γ and the Gilbert damping scalar α. It is the simplest conceivable equation to describe a damped precessional motion as it consists of a term (first) causing precession around an effective field $\mathbf{H}_{\mathrm{eff}}$ and a damping term (second) which leads to relaxation of the magnetization toward the equilibrium parallel to the effective field. Recently there have been many attempts to find a more general equation of motion by the *ab initio* electron theory.[8–12]

The breathing Fermi-surface model[13] in combination with the *ab initio* electron theory is a successful way to describe damping in the near-adiabatic time regime.[8–13] It has been shown[12] that the breathing Fermi-surface model corresponds to intraband transitions in the torque-correlation model[14] which allows to calculate damping parameters for collinear (all atomic magnetic moments are parallel) magnetization in high-symmetry directions. The contribution of these intraband transitions, and so the damping in the breathing Fermi-surface model, depends on the temperature T like $1/T$ and so dominates in the low-temperature regime.

In the breathing Fermi-surface model, the dissipation is described by a relaxation time ansatz for the occupation numbers of single electron states. All electron-scattering processes are represented by a simple relaxation time τ for the occupation numbers; therefore the model does not investigate the influence of specific scattering mechanisms on damping parameters but of the electronic structure and the magnetic configuration.

Within the model it is possible to derive an equation of motion on an atomic scale which is of the same type as the Gilbert equation, which means that it consists of a precession and a relaxation term. In systems with collinear magnetization such an equation for the direction of the unit-cell magnetic moment has been published.[3,8,9,13] In this Gilbert-type equation the scalar Gilbert damping parameter α is replaced by a damping matrix $\mathbf{A}(\mathbf{e})$ which depends on the direction $\mathbf{e}$ of the magnetization. In Refs. 8 and 9 a strong dependence of the damping matrix on $\mathbf{e}$ has been shown for various systems, even vanishing damping occurs for specific orientations $\mathbf{e}$ under certain circumstances. An attempt to generalize the breathing Fermi-surface model to noncollinear magnetic configurations delivered an equation of motion with a nonlocal magnetization dependent damping matrix[10] $\mathbf{A}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\})$, where $\mathbf{R}$, $\mathbf{R}'$, and $\mathbf{R}''$ denote the positions of the atoms and $\{\mathbf{e}_{\mathbf{R}''}\}$ is the set of the orientations of the atomic magnetic moments $\mathbf{M}_{\mathbf{R}}=M_{\mathbf{R}}\mathbf{e}_{\mathbf{R}}$ at all sites $\mathbf{R}$. Quite recently a theory was able to unify damping in collinear and noncollinear systems and to tackle both situations on equal footing.[11] This has been done by a combination of the breathing Fermi-surface model with a variant of a magnetic force theorem[15] of the *ab initio* electron theory.

II. THEORETICAL RELATIONS

The unified theory[1,2,11] derives an equation of motion for the directions $\mathbf{e}_\mathbf{R}$,

$$\frac{d\mathbf{e}_\mathbf{R}}{dt} = -\gamma \mathbf{e}_\mathbf{R} \times \mathbf{H}_{\text{eff},\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}''}\}) + \mathbf{e}_\mathbf{R} \times \sum_{\mathbf{R}'} \mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\}) \cdot \frac{d\mathbf{e}_{\mathbf{R}'}}{dt}, \tag{2}$$

where $\mathbf{H}_{\text{eff},\mathbf{R}}(\{\mathbf{e}_{\mathbf{R}''}\})$ is the effective field at the atomic site $\mathbf{R}$, which depends on the whole configuration $\{\mathbf{e}_{\mathbf{R}''}\}$ of the atomic magnetic moments. In general, the effective field is composed of the external field, the exchange field, the anisotropy field, and the dipolar field. $\mathbf{R}'$ runs over all atoms and $\gamma = -2\mu_B/\hbar$ is the gyromagnetic ratio. The damping matrix $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\})$ is generally nonlocal in two respects. First, it relates the derivative $d\mathbf{e}_\mathbf{R}/dt$ at site $\mathbf{R}$ to the derivatives $d\mathbf{e}_{\mathbf{R}'}/dt$ at all other sites, and second, it depends not only on the orientation $\mathbf{e}_\mathbf{R}$ of the magnetic moment at site $\mathbf{R}$ but on the magnetic configuration $\{\mathbf{e}_{\mathbf{R}''}\}$ of the whole system,

$$\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\}) = -\frac{\gamma\tau}{M_\mathbf{R}} \sum_i \frac{\partial f_i}{\partial \varepsilon_i} \frac{\partial \varepsilon_i^{\text{HF}}}{\partial \mathbf{e}_\mathbf{R}} \frac{\partial \varepsilon_i^{\text{HF}}}{\partial \mathbf{e}_{\mathbf{R}'}}. \tag{3}$$

The damping matrix includes a factor τ which is a relaxation time for the occupation numbers of single electron states, introduced by the breathing Fermi-surface model, and a factor determined by derivatives of single electron energies $\partial\varepsilon_i^{\text{HF}}/\partial\mathbf{e}_\mathbf{R}$ which in turn depend on $\{\mathbf{e}_{\mathbf{R}''}\}$. The superscript "HF" implies that the derivatives are calculated by a variant of the magnetic force theorem[15] which uses the Harris-Foulkes functional[16] and which is described in Refs. 1 and 11. The index i runs over each single electron state with the occupation number f_i.

As described in Refs. 1 and 11 the unified theory is valid in the near-adiabatic regime. In a total adiabatic situation the electronic system is always in its ground state with respect to the momentary magnetic configuration $\{\mathbf{e}_{\mathbf{R}''}\}$. To describe the slightly nonadiabatic situation the theory introduces nonadiabatic occupation numbers of single electron states but keeps the adiabatic single electron energies and wave functions. The nonadiabatic occupation numbers relax toward the momentary Fermi-Dirac occupation numbers f_i with a relaxation time τ which is small compared to the characteristic time scale of the dynamics of the magnetic moments $\mathbf{M}_\mathbf{R}$. The adiabatic single electron wave functions and their energies ε_i depend on the directions $\mathbf{e}_\mathbf{R}$ of all magnetic moments. This is the origin of the nonlocal damping matrices $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}$ in the unified theory. In real materials the use of this property is only meaningful for length scales on which a coherent wave function exists. So it is only reasonable to calculate damping matrices $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}$ for pairs of magnetic moments $\mathbf{M}_\mathbf{R}$ and $\mathbf{M}_{\mathbf{R}'}$ with a distance $|\mathbf{R}-\mathbf{R}'|$ smaller than the electron mean-free path.

In the following we consider the case of periodic systems. Then the summation in Eq. (2) runs over all atoms $\mathbf{R}'$ in the unit cell.

Equations (2) and (3) represent the equation of motion and the damping matrix for a general arbitrary configuration of the directions $\{\mathbf{e}_{\mathbf{R}''}\}$ of the atomic magnetic moments. In the case of a collinear configuration where all atomic magnetic moments $\mathbf{M}_\mathbf{R}$ have the same direction $\mathbf{e}_\mathbf{R} = \mathbf{e}$ and the same magnetization dynamics, which means $d\mathbf{e}_\mathbf{R}/dt = d\mathbf{e}/dt$, the equation of motion and the damping matrix simplify to

$$\frac{d\mathbf{e}}{dt} = -\gamma \mathbf{e} \times \mathbf{H}_{\text{eff}}(\mathbf{e}) + \mathbf{e} \times \mathsf{\mathbf{A}}(\mathbf{e}) \cdot \frac{d\mathbf{e}}{dt} \tag{4}$$

and

$$\mathsf{\mathbf{A}}(\mathbf{e}) = -\frac{\gamma\tau}{M} \sum_i \frac{\partial f_i}{\partial \varepsilon_i} \frac{\partial \varepsilon_i^{\text{HF}}}{\partial \mathbf{e}} \frac{\partial \varepsilon_i^{\text{HF}}}{\partial \mathbf{e}}, \tag{5}$$

with the magnitude M of the unit-cell magnetic moment. Equation (4) is the equation of motion for the direction $\mathbf{e}$ of the unit-cell magnetic moment which in a collinear system is the same as the direction of the atomic magnetic moments. For this case, in our theory the single electron energies ε_i depend on the orientation $\mathbf{e}$ via spin-orbit coupling which leads to an anisotropic damping matrix $\mathsf{\mathbf{A}}(\mathbf{e})$.[8,9] In Eq. (5) one can see that $\mathsf{\mathbf{A}}(\mathbf{e})$ is a symmetric 3×3 matrix. As $\mathbf{e}$ is a unit vector, the component of $\partial\varepsilon_i/\partial\mathbf{e}$ parallel to $\mathbf{e}$ is zero and the eigenvalue of $\mathsf{\mathbf{A}}(\mathbf{e})$ corresponding to the eigenvector parallel to $\mathbf{e}$ is also equal to zero. Therefore, the damping matrix has two nonzero eigenvalues $A_p (p=1,2)$, which correspond to two eigenvectors. Each of the two eigenvalues A_p describes the momentary damping which would occur if the momentary $d\mathbf{e}/dt$ in Eq. (4) was parallel to the respective eigenvector.

From Eq. (2), for collinear configuration and dynamics, and Eq. (4) one can derive a relation between the local damping matrix $\mathsf{\mathbf{A}}(\mathbf{e})$ for the unit-cell magnetic moment and the damping matrices $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''} = \mathbf{e}\})$ for the atomic magnetic moments,

$$\mathsf{\mathbf{A}}(\mathbf{e}) = \frac{1}{N} \sum_{\mathbf{R},\mathbf{R}'} \mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}(\mathbf{e}), \tag{6}$$

where $\mathbf{R},\mathbf{R}'$ run over all atoms in the unit cell and N is the number of these. We thereby denote the matrices $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}}$ as local contributions and the matrices $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}$ with $\mathbf{R} \neq \mathbf{R}'$ as nonlocal contributions to the damping matrix $\mathsf{\mathbf{A}}(\mathbf{e})$ of the unit-cell magnetic moment.

The former papers on the *ab initio* breathing Fermi-surface model (Refs. 1, 3, and 8–11) considered mainly collinear configurations and discussed the dependence of the damping matrix $\mathsf{\mathbf{A}}(\mathbf{e})$ on the direction $\mathbf{e}$. Thereby the torque-operator method[8,9,17] was used to calculate the derivatives $\partial\varepsilon_i/\partial\mathbf{e}$. In many technologically important situations, however, there are noncollinear configurations such as domain walls or vortices for which the nonlocality of $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}(\{\mathbf{e}_{\mathbf{R}''}\})$ may become essential. The focus of future calculations therefore will be on the discussion of this nonlocality. In the present paper a first step in this direction is made. To do this, we still consider a situation with collinear magnetic moments, but we consider periodic systems with two atoms in the unit cell so that the damping matrix $\mathsf{\mathbf{A}}(\mathbf{e})$ of the unit-cell magnetic moment is composed of the damping matrices $\mathsf{\mathbf{A}}_{\mathbf{R},\mathbf{R}'}$ of the two atoms in the unit cell, i.e., of local $(\mathbf{R} = \mathbf{R}')$ and nonlocal $(\mathbf{R} \neq \mathbf{R}')$ contributions. It should be noted that the calculation of the single contributions $\mathbf{A}_{\mathbf{R},\mathbf{R}'}$ to the unit-cell damping matrix $\mathbf{A}$ is not possible with the torque-operator method but only within the unified theory described above, and this is a big achievement of the unified theory.

Another objective of the present paper is to compare the results for the unit-cell damping matrix as obtained from the derivatives $\partial\varepsilon_i/\partial\mathbf{e}$, which are on the one hand determined by the torque-operator method and on the other hand by the magnetic Harris-Foulkes approach ($\partial\varepsilon_i^{\mathrm{HF}}/\partial\mathbf{e}$). Because both calculational methods involve approximations, it is interesting to see how well the corresponding results agree.

III. NUMERICAL RESULTS

In all calculations the derivatives of the energies ε_i are determined by the *ab initio* density-functional electron theory (DFT) in local-spin-density approximation, using the tight-binding linear-muffin-tin-orbital method in the atomic-sphere approximation[18] in which spin-orbit coupling[19] has been implemented. Lagrange constraining fields[20] are necessary to gain results according to the recent unified theory. For technical reasons, all calculations are performed without the orbital polarization term,[21] whereas in Ref. 9 this term has been used.[22]

The effective field appearing in Eq. (4) is in our calculations given by the anisotropy field caused by spin-orbit coupling and the interatomic exchange field. The external field is set to zero for technical reasons and to exclude external effects. No dipolar effects are included.

The derivatives $\partial\varepsilon_i/\partial\mathbf{e}$ are calculated for different prescribed directions of the magnetization. If the prescribed direction is not parallel to an equilibrium direction, the anisotropy field is present and the direction of the magnetization must be enforced by a constraining method.[20] In the torque-operator method, the direction of the magnetization is constrained by prescribing the direction of the spin-quantization axes. One self-consistent DFT calculation for each direction is necessary to calculate the derivatives $\partial\varepsilon_i/\partial\mathbf{e}$ from the expectation value of the torque operator as described in Ref. 9. In the unified theory, the direction of the magnetization is enforced by Lagrange constraining fields. Both self-consistent and one-shot Harris-Foulkes calculations are necessary to calculate the derivatives of the single electron energies ε_i numerically.

The investigated bulk materials are bcc-Fe and hcp-Co. A monatomic Co layer is realized by a supercell containing one layer of Co atoms and in addition empty atomic spheres. The numerical values are plotted in units of $M_{(\mathbf{R})}/\gamma\tau\cdot\mu_B^2/V\hbar^2$ as τ is a phenomenological parameter in the breathing Fermi-surface model which cannot be calculated *ab initio*. Please note that $M_{(\mathbf{R})}$ represents the value of the magnetic moment M of the unit cell for the plots of the unit-cell damping matrix, and for the curves of the atomic damping matrices it represents the value of the atomic magnetic moment $M_{\mathbf{R}}$. V represents the unit-cell volume.

A. hcp-Co

All calculations for hcp-Co were performed in the primitive two-atom unit cell. In Fig. 1 the eigenvalues of $\mathbf{A}(\mathbf{e})$ are plotted for different directions $\mathbf{e}$ of the magnetization calculated by the unified theory and the torque-operator method. Additionally the right-hand side of relation (6) is displayed. The eigenvalues of the single matrices $\mathbf{A}_{\mathbf{R},\mathbf{R}'}(\mathbf{e})$ are presented in Fig. 2.

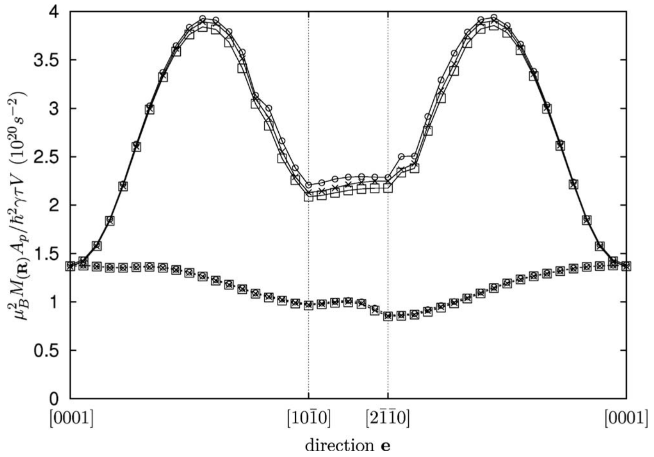

FIG. 1. hcp-Co: eigenvalues A_p of unit-cell damping matrix $\mathbf{A}(\mathbf{e})$ calculated with the unified theory (symbol ×) and the torque-operator method (symbol ○). Right hand side of relation (6) (symbol □). The two eigenvalues are given by the full and dashed lines, respectively.

B. bcc-Fe

To compare results for the unit-cell damping matrix $\mathbf{A}(\mathbf{e})$ of the unified theory with values obtained by the torque-operator method, eigenvalues of $\mathbf{A}(\mathbf{e})$ are calculated for different directions of $\mathbf{e}$ in the primitive one-atom unit cell. These are shown in Fig. 3.

Calculations in a two-atom unit cell are performed to obtain the eigenvalues of the atomic moment damping matrices $\mathbf{A}_{\mathbf{R},\mathbf{R}'}(\mathbf{e})$ within the unified theory. These are presented in Fig. 4 (lower curves). To test our results for these atomic damping matrices $\mathbf{A}_{\mathbf{R},\mathbf{R}'}(\mathbf{e})$, also the eigenvalues of the unit-

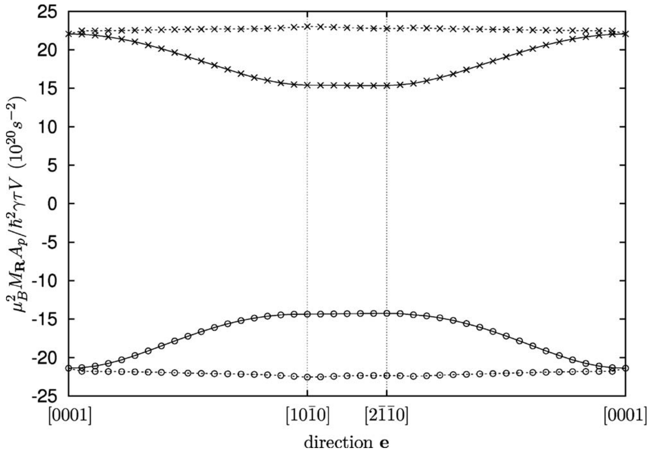

FIG. 2. hcp-Co: eigenvalues A_p of the atomic damping matrices: $\mathbf{A}_{\mathbf{R},\mathbf{R}'}=\mathbf{A}_{\mathbf{R}',\mathbf{R}}$ (symbol ○); $\mathbf{A}_{\mathbf{R},\mathbf{R}}=\mathbf{A}_{\mathbf{R}',\mathbf{R}'}$ (symbol ×). The two eigenvalues are given by the full and dashed lines, respectively.

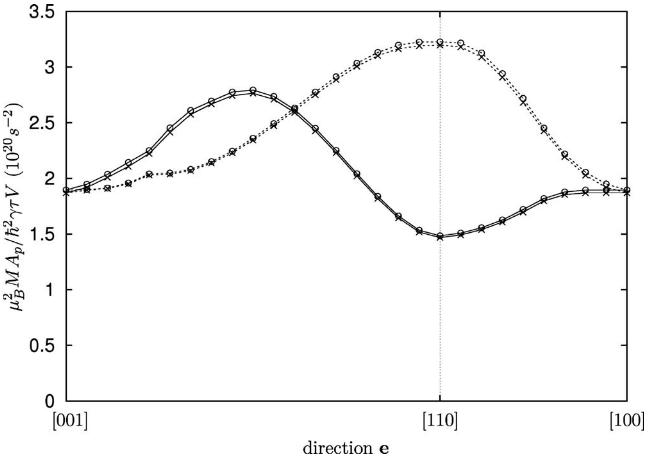

FIG. 3. bcc-Fe: eigenvalues A_p of unit-cell damping matrix $\mathbf{A}(\mathbf{e})$ calculated with the unified theory (symbol ×) and the torque-operator method (symbol ○). The two eigenvalues are given by the full and dashed lines, respectively.

cell damping matrix $\mathbf{A}(\mathbf{e})$ of the two-atom unit cell have been calculated within the unified theory and they are plotted together with the right-hand side of relation (6) in Fig. 4 (upper curves). The curves with the crosses (×) in Fig. 3 on the one hand and the upper curves with the crosses (×) in Fig. 4 on the other hand should be identical. They slightly differ in absolute value and shape because both *ab initio* calculations are not converged with respect to the density of k points in the sampling of the Brillouin-zone integration due to the computational effort. Even when using about the same density of k points for the two calculations the results may differ because the k-point meshes for the one- and two-atom unit cells are not equivalent.

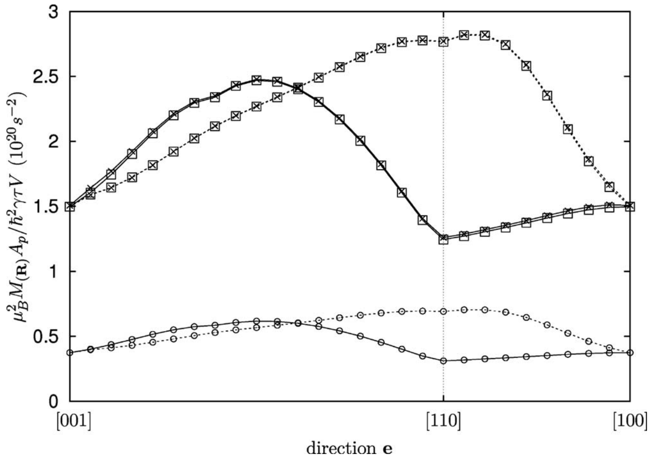

FIG. 4. bcc-Fe: eigenvalues A_p of the two-atom unit-cell damping matrix $\mathbf{A}(\mathbf{e})$ (symbol ×). Eigenvalues A_p of the atomic damping matrices: $\mathbf{A}_{\mathbf{R},\mathbf{R}'}=\mathbf{A}_{\mathbf{R}',\mathbf{R}}=\mathbf{A}_{\mathbf{R}',\mathbf{R}'}=\mathbf{A}_{\mathbf{R},\mathbf{R}}$ (symbol ○). Right hand side of relation (6) (symbol □). The two eigenvalues are given by the full and dashed lines, respectively. As the magnetic moment M of the unit cell is twice the atomic magnetic moment $M_{\mathbf{R}}$, an additional factor of 2 arises so that Eq. (6) is fulfilled.

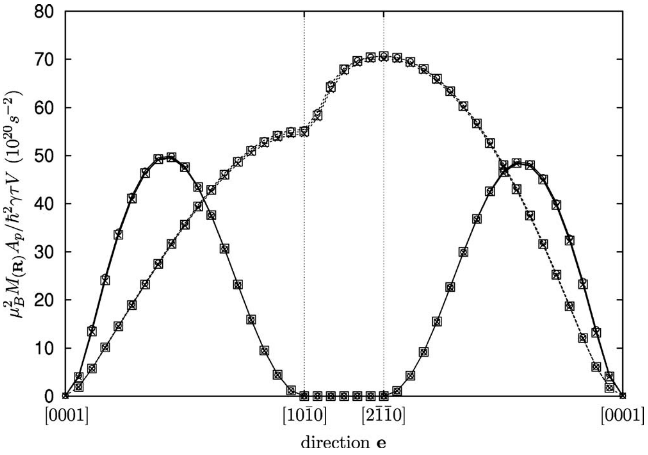

FIG. 5. Co layer: eigenvalues A_p of unit-cell damping matrix $\mathbf{A}(\mathbf{e})$ calculated with the unified theory (symbol ×) and the torque-operator method (symbol ○). Eigenvalues A_p of atomic damping matrix $\mathbf{A}_{\mathrm{Co,Co}}$ (symbol □). The two eigenvalues are given by the full and dashed lines, respectively.

C. Co layer

The calculations for the hexagonal monatomic Co layer are performed in the supercell formalism. The supercell consists of a Co atom and five empty atomic spheres stacked above, so that an hcp stacking appears for the periodically repeated supercell. The periodic structure represents hexagonal monatomic Co layers separated by vacuum. Here, also the eigenvalues of the unit-cell damping matrix $\mathbf{A}(\mathbf{e})$ are calculated by the unified theory and the torque-operator method. Additionally, the eigenvalues of the atomic damping matrix $\mathbf{A}_{\mathrm{Co,Co}}(\mathbf{e})$ are calculated for different $\mathbf{e}$, which is again only possible in the unified theory. The results are plotted in Fig. 5.

IV. DISCUSSION AND CONCLUSIONS

In all investigated materials, the unit-cell damping matrix is calculated by the unified theory and the torque-operator method, and very good agreement between both methods is achieved. This agreement in collinear systems, where a comparison is possible, is an important step forward to establish the unified theory, which tackles both collinear and noncollinear systems on equal footing.

The atomic damping matrices $\mathbf{A}_{\mathbf{R},\mathbf{R}'}$ occurring in the atomic equation of motion (2) are calculated in collinear systems. For hcp-Co the primitive unit cell contains two basis atoms and therefore it is possible to calculate both the unit-cell damping matrix and the atomic damping matrices for the primitive unit cell. For bcc-Fe the primitive unit cell contains only one atom and therefore a nonprimitive supercell has to be used for which again both the unit-cell damping matrix and atomic damping matrices can be calculated. It is interesting that in hcp-Co $\mathbf{A}_{\mathbf{R},\mathbf{R}'\neq\mathbf{R}}$ and $\mathbf{A}_{\mathbf{R},\mathbf{R}}$ have different signs (see Fig. 2), whereas in bcc-Fe both matrices are identical (see Fig. 4, lower curve). One can show that this is a consequence of the lattice symmetry in these materials. In bcc-Fe the relation $\partial\varepsilon_i/\partial\mathbf{e}_{\mathbf{R}}=\partial\varepsilon_i/\partial\mathbf{e}_{\mathbf{R}'\neq\mathbf{R}}$ for the derivatives of single electron energies ε_i holds if the single electron states are Bloch states, as they are in our calculations where the label i stands for a band index and a wave vector $\mathbf{k}$. In hcp-Co this relation is not valid. The difference between $\mathsf{A}_{\mathbf{R},\mathbf{R}'\neq\mathbf{R}}$ and $\mathsf{A}_{\mathbf{R},\mathbf{R}}$ has the consequence that $d\mathbf{e}_{\mathbf{R}}/dt$ and $d\mathbf{e}_{\mathbf{R}'}/dt$ deliver different contributions to the total damping at the atomic site $\mathbf{R}$, even in a collinear configuration and dynamics. However, this does not lead to an atomic damping matrix which is different at the two basis atoms of Co, as the total damping matrices at site $\mathbf{R}$ and site $\mathbf{R}'$ are equal ($\mathsf{A}_{\mathbf{R},\mathbf{R}}+\mathsf{A}_{\mathbf{R},\mathbf{R}'}=\mathsf{A}_{\mathbf{R}',\mathbf{R}'}+\mathsf{A}_{\mathbf{R}',\mathbf{R}}$). This is reasonable because the two basis atoms are crystallographically equivalent. Nevertheless, if we consider a noncollinear dynamics in a momentary collinear configuration, as it occurs, e.g., during the excitation of a spin wave, then different time derivatives ($d\mathbf{e}_{\mathbf{R}}/dt \neq d\mathbf{e}_{\mathbf{R}'}/dt$) of the directions of the atomic magnetic moments lead to different total damping at site $\mathbf{R}$ and site $\mathbf{R}'$.

Our numerical results fulfill theoretical relation (6) when comparing the right-hand side consisting of the damping matrices $\mathsf{A}_{\mathbf{R},\mathbf{R}'}(\mathbf{e})$ for the atomic moments with the left-hand side which is the unit-cell damping matrix $\mathsf{A}(\mathbf{e})$. This is shown for hcp-Co in Fig. 1 and bcc-Fe in Fig. 4 (upper curves).

The unit cell of the Co-layer calculations contains one Co-atom and five empty atomic spheres which represent vacuum separating the Co layers. Figure 5 shows that the atomic damping matrix $\mathsf{A}_{\mathrm{Co,Co}}(\mathbf{e})$ is nearly equal to the whole unit-cell damping matrix. So the empty atomic spheres, which mathematically could in principal deliver further terms on the right-hand side of Eq. (6) (because the tails of the magnetization density localized in the Co layer leak to some extent into the empty atomic spheres), have nearly no contribution to damping.

To conclude, we tackled unit-cell damping in magnetically collinear systems by two theoretical approaches which are based on different approximations, and we found very good agreement. Furthermore, we calculated the local and nonlocal contributions of atomic damping matrices to the unit-cell damping matrix for supercells containing two atoms. This was only possible with one of the two theoretical approaches, the so-called unified method. After this successful treatment of collinear systems by the unified theory the next step will be to calculate the nonlocal damping matrices for noncollinear magnetic configurations.

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*faehnle@mf.mpg.de

[1] M. Fähnle, D. Steiauf, and J. Seib, J. Phys. D **41**, 164014 (2008).

[2] In Eq. (10) of Ref. 1 a × for a cross product is missing because of a printing error. Equation (13) of Ref. 11 and Eq. (2) in this paper show the correct equation of motion.

[3] M. Fähnle and D. Steiauf, in *Handbook of Magnetism and Advanced Magnetic Materials*, edited by H. Kronmüller and S. Parkin (Wiley, New York, 2007), Vol. 1, p. 282.

[4] M. Kläui and C. A. F. Vaz, in *Handbook of Magnetism and Advanced Magnetic Materials*, edited by H. Kronmüller and S. Parkin (Wiley, New York, 2007), Vol. 2, p. 879; L. Thomas and S. Parkin, *Handbook of Magnetism and Advanced Magnetic Materials* (Wiley, New York, 2007), p. 942.

[5] B. Van Waeyenberge, A. Puzic, H. Stoll, K. W. Chou, T. Tyliszczak, R. Hertel, M. Fähnle, H. Brückl, K. Rott, G. Reiss, I. Neudecker, D. Weiss, C. H. Back, and G. Schütz, Nature (London) **444**, 461 (2006).

[6] B. Koopmans, Nature Mater. **6**, 715 (2007).

[7] T. L. Gilbert, Ph.D. thesis, Illinois Institute of Technology, Chicago, 1956.

[8] J. Kuneš and V. Kamberský, Phys. Rev. B **65**, 212411 (2002); J. Kuneš and V. Kamberský, Phys. Rev. B **68**, 019901(E) (2003).

[9] D. Steiauf and M. Fähnle, Phys. Rev. B **72**, 064450 (2005).

[10] M. Fähnle and D. Steiauf, Phys. Rev. B **73**, 184427 (2006).

[11] D. Steiauf, J. Seib, and M. Fähnle, Phys. Rev. B **78**, 020410(R) (2008).

[12] K. Gilmore, Y. U. Idzerda, and M. D. Stiles, Phys. Rev. Lett. **99**, 027204 (2007).

[13] V. Kamberský, Can. J. Phys. **48**, 2906 (1970).

[14] V. Kamberský, Czech. J. Phys., Sect. B **26**, 1366 (1976).

[15] P. Bruno, Phys. Rev. Lett. **90**, 087205 (2003).

[16] J. Harris, Phys. Rev. B **31**, 1770 (1985); W. M. C. Foulkes and R. Haydock, Phys. Rev. B **39**, 12520 (1989).

[17] X. Wang, R. Wu, D. S. Wang, and A. J. Freeman, Phys. Rev. B **54**, 61 (1996).

[18] O. K. Andersen and O. Jepsen, Phys. Rev. Lett. **53**, 2571 (1984).

[19] C. Ederer, M. Komelj, M. Fähnle, and G. Schütz, Phys. Rev. B **66**, 094413 (2002).

[20] P. H. Dederichs, S. Blügel, R. Zeller, and H. Akai, Phys. Rev. Lett. **53**, 2512 (1984); R. Singer, M. Fähnle, and G. Bihlmayer, Phys. Rev. B **71**, 214435 (2005).

[21] O. Eriksson, M. S. S. Brooks, and B. Johansson, Phys. Rev. B **41**, 7311 (1990).

[22] The orbital polarization term leads to different absolute values of the damping matrix if one compares the results in Ref. 9 with the present results for the different systems. Please also note that M in the axis label in Ref. 9 is the magnetization, whereas here M is the magnetic moment of the unit cell and $M_{\mathbf{R}}$ is the atomic magnetic moment.