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Theoretical Study Of Interfacial Damping In Perpendicular Anisotropy Superlattices Along Multiple Crystal Orientations

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Abstract

Damping, representing the loss of magnetic energy from the electrons to the lattice through the spin orbit interaction, is calculated for Co/Pt and Co/Pd superlattices grown along the (001), (111), and (011) orientations. The damping consists of two contributions: interfacial and, usually, bulk. The interfacial damping shows dependence on the superlattice orientation. The origin of the interfacial damping is due to both the distorted electronic states at the interface and the spin-orbit interaction in the weakly polarized non-magnetic Pt/Pd layers deposited on Co layers. The density of states around the Fermi level provides the spin-flip channels and closely correlates with the damping value. The damping shows asymmetry in the two transverse directions of the spin for spins at most angles. The damping for out-of-plane magnetization can be as much as 1.7 times larger than that of in-plane magnetization.

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I. INTRODUCTION

The determination of the ferromagnetic damping α is both a fundamental scientific problem and technologically important for spintronic devices. It reflects the elimination of the magnetic energy and determines the dynamics in magnetic systems, e.g. switching[1, 2]. The speed of the magnetic state change is generally proportional or inversely proportional to α based on the state manipulating method. In magnetic recording controlled by the magnetic field[3, 4], large α is preferred to increase the writing speed. In electrically manipulated spintronic devices[5, 6], the magnetic configuration could be changed by the spin torque effect that is produced by the electric current through the device. The minimization of α is required to increase the energy efficiency. Materials with small α substantially reduce the critical current required to switch the stored state.

The study of damping has recently shifted towards ferromagnetic thin metallic films[7–12]. Artificially layered magnetic metal structures, such as superlattices, are a topic of intense current interest because of their unusual surface properties and potential application in spintronic devices. These structures have demonstrated a variety of phenomena such as giant tunneling magnetoresistance[13–15], Ruderman-Kittel-Kasuya-Yosida (RKKY) coupling[16, 17] and most importantly, large perpendicular anisotropy(PMA). Transition-metal superlattices, such as Co/Pt[18, 19] and Co/Pd, deposited by molecular-beam epitaxy or sputtering are good candidates for PMA applications because they exhibit a very large PMA above 1×10^7 erg/cm³ and a moderate magnetization $M_s=800$ emu/cm³ in bulk, along multiple crystal axes. The large PMA guarantees the device stability over a large temperature range even at the nano-scale, in both high density magnetic recording and electrically manipulated spintronic devices. High PMA allows the extension of magnetic recording beyond the superparamagnetic limit and thus offers higher aerial densities. PMA materials substantially reduce the critical current for spin-torque switching relative to the usual in-plane magnetic anisotropy materials that are adversely affected by the demagnetization effect in a thin film structure. While the PMA is explored thoroughly both in experiment and theory, the damping α has not been fully investigated for superlattices. Both the anisotropy energy and damping in transition-metals superlattices is electronic in origin and predominantly results from the spin-orbit interaction(SOI). Despite the tendency for in-plane anisotropy caused by demagnetization energies, many short period magnetic multilayers exhibit a perpendicular

anisotropy, resulting from the influence of the interface. It has been found both experimentally and theoretically that the interfacial anisotropy is independent of the growth direction for Co/Pd superlattices[20–22], although the bulk contribution can vary according to magnetostrictive effects. However, the effect of the surface and the superlattice orientation on the damping is not clear yet. The investigation of the damping properties in various superlattices could give insight to the surface and growth orientation effect on damping, and enable optimization of superlattice structures exhibiting useful perpendicular anisotropy.

The mechanism of damping is described by the Kambersky model, representing the magnetic energy lost to the lattice through spin-orbit interaction. Calculation of α has been approached in torque-correlation theory, linear response theory, and scattering theory. It has been mostly explored in traditional bulk transition materials: Fe, Co and Ni. Enhanced damping is shown in $L1_0$ ordered/disordered FePt, CoPt alloys due to the obviously larger SOI strength ξ of Pt($\sim 0.5\text{eV}$) relative to the 3d transition metals such as Co and Fe. Experimental studies shows that high perpendicular anisotropy magnets including Pt exhibit large α , such as Co/Pt multilayers and ultrathin CoFeB/Pt. Materials containing Pd or ternary alloys substituting Pt with Pd always show reduced damping, which could partially be explained by the weaker SOI strength ξ of Pd($\sim 0.15\text{eV}$). However, the distorted electronic states at the interface of two materials might also cause a difference in damping, although this is rarely explored. Barati[23] calculates the interfacial effect for superlattices, oriented along the (001) direction; the extracted interfacial damping is negligible or negative, suggesting that surface effect helps minimize the energy dissipation, not consistent with experimental measurement. His layer distributed damping shows non-physical negative values, usually associated with non-conservation of magnetic energy. Besides, his bulk damping of Co is larger than 0.01, differing from experimental FMR data[24].

In the present paper, we apply the Kambersky model, within the tight binding(TB) method, to superlattices Co/Pd and Co/Pt growing in multiple crystal orientations. We identify the orientation dependent interfacial and bulk contribution to the total damping. We also check the damping dependence on the spin-orbit interaction strength of the non-ferromagnetic metal and infer the origin of the interfacial damping. We expand the damping calculation from the initial spin out-of-plane direction to spins at arbitrary angle and obtain the damping dependence on the spin orientation. Conclusions and discussion are presented at the end.

II. DAMPING MODEL

The superlattice configurations are multiple ferromagnetic 3d-transition metal monolayers deposited on various non-magnetic metal monolayers in the [001], [111] and [011] directions. We use periodic boundary conditions to evaluate the strength of the damping. The interfacial effect is included twice in the total damping, due to the two surfaces at the boundary. Thus we divide the extracted interfacial damping parameters by two to infer the interfacial damping. We use the tight binding method to calculate the electronic structure and obtain the damping values. The Slater-Koster TB parameters are taken from the calculations of Moruzzi et al., scaling with the d-band width as appropriate. By analogy with Kambersky's derivation of damping, we consider the damping tensor:

$$\alpha_{ij} = \frac{2\mu_B^2 g^2}{\gamma M \hbar} \sum_{n,m} \int \frac{d^3 k}{(2\pi)^3} \Gamma_{nm}^{ij}(k) W_{nm}(k), \quad (1)$$

$$\Gamma_{nm}^{ij}(k) = \langle n, k | [\sigma_i, H_{SO}] | m, k \rangle \langle m, k | [\sigma_j, H_{SO}] | n, k \rangle. \quad (2)$$

Here, i, j represents x, y , and z . H_{SO} and $\sigma_{i,j}$ are both expanded in the spin and orbit space through the Kronecker product of two distinct atoms. The matrix elements $\Gamma_{nm}^{ij}(k)$ measure transitions between states in bands n and m induced by the spin-orbit torque. When $n=m$, this intraband damping, i.e., relaxation from the non-equilibrated population, has a conductivity-like behavior. The opposite resistivity-like behavior corresponds to interband damping when $n \neq m$: it is caused by the SOI induced electron-hole relaxation combined with a magnon annihilation. Edwards [25] has argued that the intraband damping should be absent based on the direct calculation of the dynamical transverse susceptibility. The intraband absence removes the infinite divergence of damping at zero temperature and has significant effect on damping at low temperature. This will change our results slightly, as our calculations are near room temperature and the intraband damping has a negligible contribution to the total damping, as shown in Fig. 1. These scattering events are weighted by the spectral overlap of the phonons. The electron states are obtained within the static Hamiltonian H_0 , consisting of the spin-independent paramagnetic Hamiltonian H_{para} taken in the tight-binding approximation, the Hartree-Fock approximation of the ferromagnetic exchange Hamiltonian H_{HF} [26], and the SOI H_{SO} . Details of the computational method are published elsewhere[27, 28] and show that Pt and Pd are polarized. When the spin points in some highly symmetric directions, perpendicular to plane in superlattice oriented along

[001] axis, the damping tensor $\alpha_{xx} = \alpha_{yy}$ and thus is reduced to a scalar.

III. RESULTS & DISCUSSION

In a superlattice, the broken symmetry at the interface can be the dominant contribution to the total damping. Fig. 1 shows our prediction for the intrinsic damping constant of superlattices with different Co layer thickness. The superlattice is oriented along the [001] axis and the spin orientation is perpendicular to the plane. The wave vector \vec{k} sampling convergence of the damping computation is verified and \vec{k} sampling including 32^3 points is chosen to produce the required accuracy (relative error less than 2%) in the full Brillouin zone. The product of the damping and the layer number of Co is linearly dependent on the number of Co monolayers, in Fig. 1. $n\alpha = 2 * \alpha_{interface} + n\alpha_{bulk}$, where n is the number of Co layers, $\alpha_{interface}$ and α_{bulk} are the interfacial and bulk damping respectively. We are fixing the spin orientation to be perpendicular to plane even in the normally in-plane oriented thicker Co layers (this could be accomplished by an applied field), in order to extract the intrinsic interfacial damping. The interfacial damping extracted from the linear fitting for n Co/6 Pt and n Co/ 6 Pd is 0.18 and 0.019. The difference between the interfacial damping of two superlattices originates from the stronger SOI strength in Pt (0.5eV) than Pd (0.15eV). This interfacial source increases the amount of energy lost in the short-period superlattices significantly, compared to the bulk Co damping. The bulk damping is only determined by the Co intrinsic properties and not affected by the deposited non-magnetic monolayers. When the Co layer thickness is below around five monolayers, the damping shows an oscillatory behavior, and the damping increases abruptly at some Co layer thicknesses. This oscillation might be attributed to quantum well (QW) states with energies at the Fermi level. The occurrence of QW states in metallic films also leads to oscillations of interlayer exchange coupling and magnetic anisotropy with varying thickness of ferromagnetic films or nonmagnetic layers [17, 29–31]. The oscillation periods associated with QW states are related to the extremal radii of Fermi-surface sheets of Co films. The magnetic anisotropy (also caused by the spin-orbit interaction) of (001) fcc Co film oscillates with period around 2 monolayers, confirmed in earlier theoretical prediction [32] and recent experiment [30]. The anisotropy oscillation is dominant at the center of the 2D Brillouin zone where pairs of QW states are degenerate at the *Gamma* point. The oscillation periods

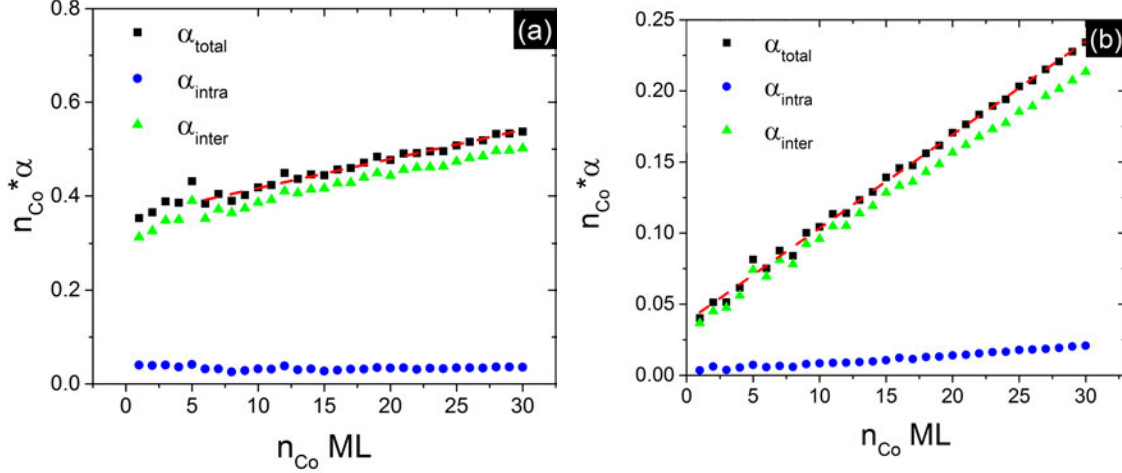


FIG. 1. The product of the number of Co layers and the damping constant versus the number of Co layers in superlattices (a) n Co/6 Pt and (b) n Co/ 6 Pd. The red dashed line is the linear fitting to the total damping constant. The dots in different shapes refer to the total, intraband and interband damping respectively.

for damping of (001) CoPd/CoPt are also around 2MLs, thus it might be the same QW states producing both the oscillation of anisotropy and damping.

The interfacial damping varies when superlattices orient along different axes. The linearity of $n\alpha$ remains for all oriented superlattices, shown in Fig. 2. When the spin direction is perpendicular to the plane, the bulk contribution to damping α_{bulk} is substantially independent of orientation, as expected for bulk Co. In contrast, $\alpha_{interfacial}$ shows larger values in [111] and [011] directions than [001] direction, especially for the Co/Pd superlattices, shown in Table I. The standard deviation of $\alpha_{interfacial}$ is 45% for Co/Pd, and $\sim 14\%$ for Co/Pt. In addition to the effect of the changing spin orientation, the interfacial damping is also affected by the altered atomic environment at the interface. The nearest and next nearest neighbours vary for superlattices oriented along distinct axes and modify the electronic states markedly, which results in a sensitive dependence of interfacial damping on the superlattice orientation. Furthermore, two sets of interfacial and bulk damping values are shown for spin in the [011] superlattice orientation, which reflects anisotropic ferromagnetic relaxation in the transverse in-plane directions. This anisotropic behavior is caused by the broken symmetry of the electronic states when spin is pointing in directions that are not high symmetric. This tensor behavior can be reduced to a scalar when the spin is in highly symmetric directions, for example, [001]-a fourfold or [111]-a threefold symmetric axis.

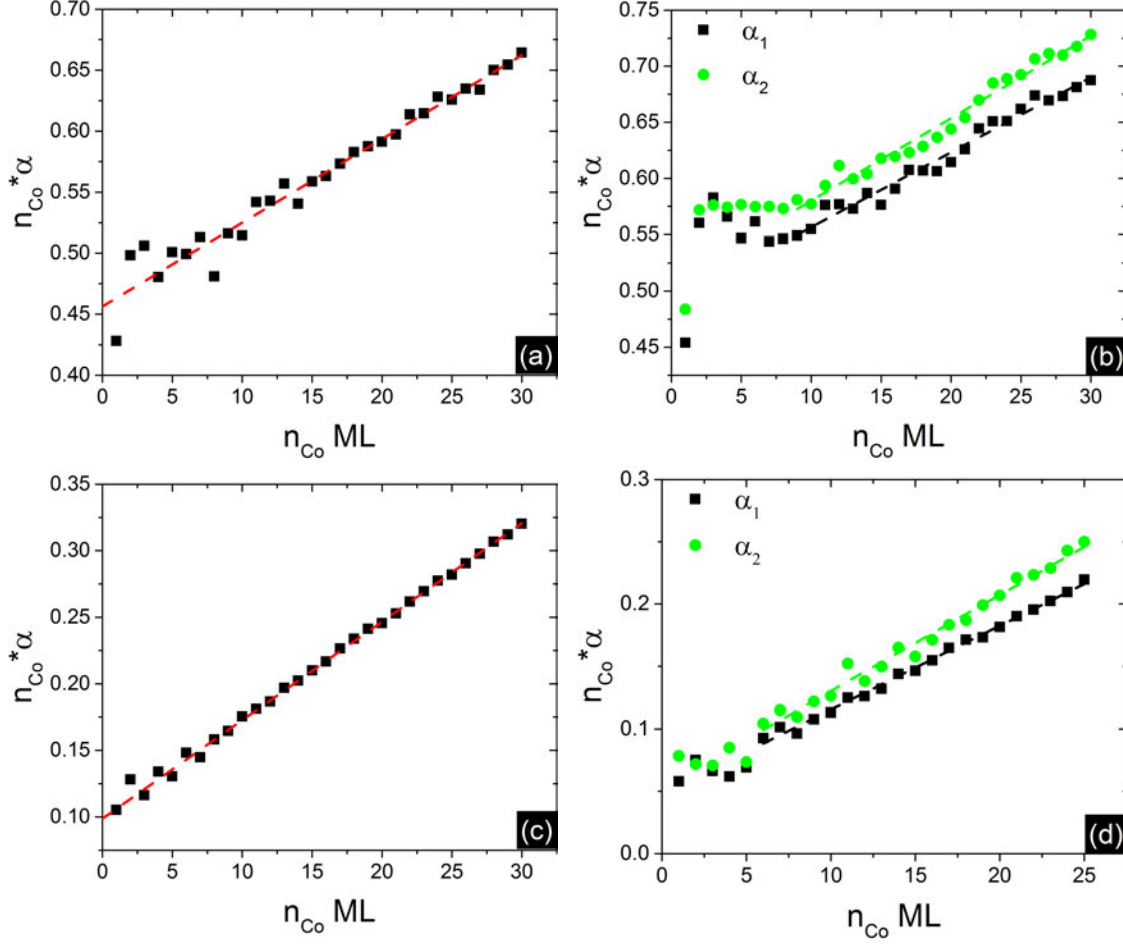


FIG. 2. The product of the number of Co layers and the damping constant versus the number of Co layers in superlattices of varying orientations (a) Co/Pt[111], (b) Co/Pd [111], (c) Co/Pt[011] and (d) Co/Pd [011]. The dashed lines are the linear fittings to the total damping constant. The superlattices are multiple Co layers deposited on six Pt or Pd layers. The spins are oriented perpendicularly to the planes. α_1 and α_2 in (c), (d) are the eigenvalues of the damping tensor.

The interfacial damping dependence on superlattice orientation is explained by the varying electronic state at the interface. We separate each layers' contribution to the damping by manually zeroing the SOI strength of all but one layer in the damping computation. Fig 3 shows that non-zero spin-orbit interaction in single magnetic or non-magnetic layers can enhance the damping, compared to the damping value 0.0055 of bulk fcc Co, particularly for the (111) orientations. This damping difference between (111) and (001) orientations is presumably caused by the interfacial electronic state at the Co layer adjacent to Pd/Pt layer, as confirmed by the contour map of the weighted d state in the 2D k-space, in Fig 4. The weighted d state is calculated by summing over all d states at one specific k point,

weighted by the band energy in the Lorentzian distribution centered at the Fermi level, similar to the damping computation. In the (001) superlattice orientation, the dominant k points contributing to damping in interfacial Co atom lie along diagonal lines, and show a non-monotonic behavior: the k points around the Γ point have less impact on the damping while the k points with magnitude 20% or 80% of the in-plane k basis vectors have ten times larger impact on the damping. For the interfacial Pt atom, the k points surrounding the Γ point contribute mainly to the damping. In contrast, for (111) interfacial Co atoms, the k points determining the damping are more uniformly distributed in the whole Brillouin zone. The most influential k points for the interfacial Pt atom are far away from the Γ point, opposite to the (001) superlattice. This interfacial electronic state is a mixture of electrons from both magnetic and non-magnetic metals. In the (001) superlattice, for the Co atom at the interface, the nearest neighbours (NN) are four Pd/Pt atoms and eight Co atoms, the next nearest neighbours (NNN) are one Pd/Pt atom and five Co atoms. In contrast for the (111) superlattice, the NN are three Pd/Pt atoms and nine Co atoms, the NNN

TABLE I. The table shows the extracted interfacial and bulk damping for Co/Pt and Co/Pd superlattices oriented in [001],[111] and [011] axes. The superlattices are multiple Co layers deposited on six Pt or Pd layers. The spins are oriented perpendicularly to the planes.

x Co/ 6 Pt		
	$\alpha_{interface}$	α_{bulk}
001	0.18	0.0062
111	0.23	0.0069
011	0.24	0.0067
	0.25	0.0073
x Co/ 6 Pd		
	$\alpha_{interface}$	α_{bulk}
001	0.019	0.0065
111	0.049	0.0074
011	0.024	0.0067
	0.026	0.0077

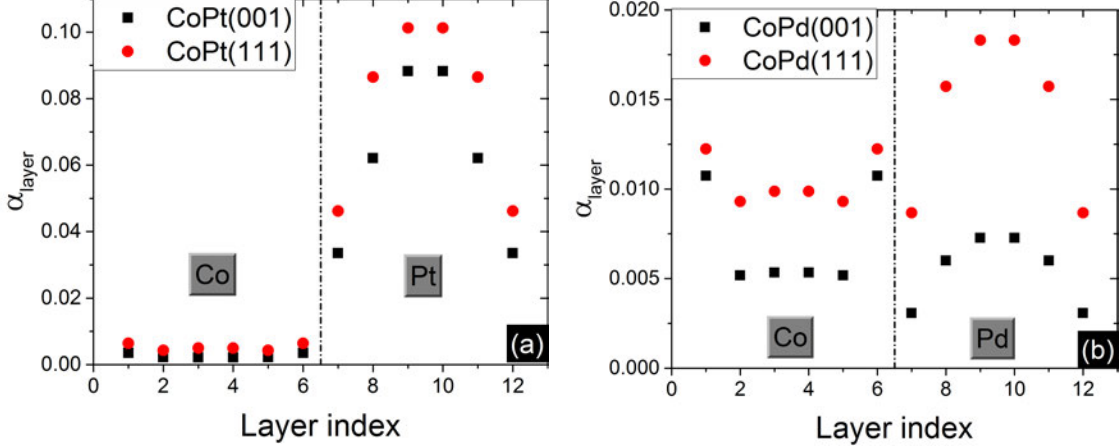


FIG. 3. Layer contribution to the Gilbert damping constant in superlattices in both (001) and (111) orientations. The superlattices are six Co monolayers deposited on (a) six Pt or (b) six Pd layers

are three Pd/Pt atoms and three Co atoms. The assorted surrounding atomic environment has distinct impact on the interfacial Co atoms, thus generating superlattice orientation dependent damping. We only focus on the d orbital states, because these states give the spin polarization and possess strong spin-orbit coupling.

The density of states (DOS) at the Fermi level has a significant impact on the damping because the spin scattering primarily happens in the electronic states around the Fermi level. We artificially shift the Fermi energy and separate the layer contribution to the damping. Fig 5 shows that the peak of the layer damping contribution is located at the same energy as the peak of DOS of each layer. Double peaks appear in the Co layers: one below the Fermi level around -0.05Ry and one above the Fermi level around 0.07Ry . The DOS peak of the interfacial Co monolayer is nearer the Fermi level than the DOS peak of the Co layer away from the interface. In the Pt atoms, a sharp peak in the damping is found near the Fermi level. In contrast to the Co layers, the interfacial Pt DOS peak is lower energy than the bulk DOS. The shape of the total damping is more complicated due to the mixture of the DOS of multiple atoms. The sharp change in the damping around the original Fermi level remains. The total damping varies by a factor of 40 near the Fermi level. Experimentally, tuning the damping could be accomplished by adding an amorphous agent such as B, that the DOS can be smoothed.

The interfacial damping is closely correlated with SOI strength ξ because the source of the damping is the coupling between spin and lattice. It is shown that the interfacial

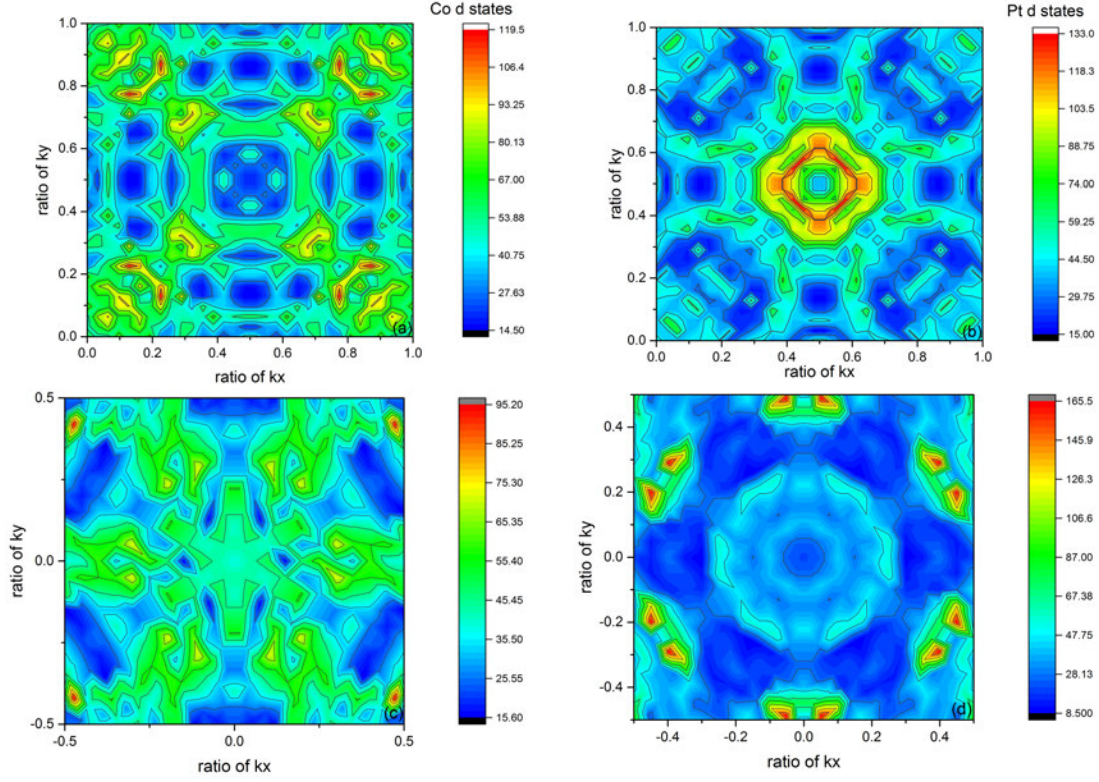


FIG. 4. Weighted d electronic states distribution in the Brillouine zone for the interfacial atoms (a) Co (b) Pt in the superlattice 6 ML Co/ 6 ML Pt in (001) orientation and (c) Co (d) Pt in the superlattice 6 ML Co/ 6 ML Pt in (111) orientation.

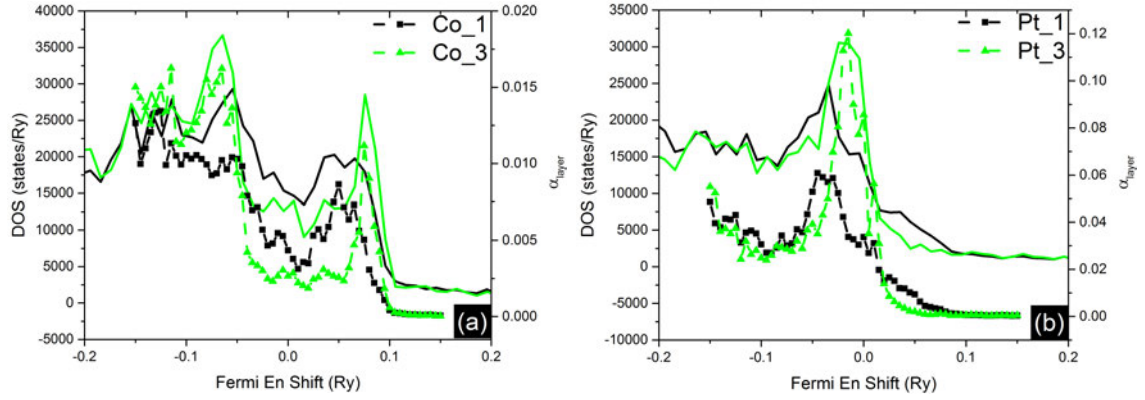


FIG. 5. The damping layer contribution versus the shifted fermi level of (a) Co MLs (b) Pt MLs. The index of the atom is based on the distance from the interface. 1 represents the interfacial atoms. The superlattice is six MLs Co deposited on six MLs Pt in (001) orientation. The properties of the other Co and Pt atoms in the superlattice are not shown due to the symmetry in the periodic boundary conditions.

damping increases monotonically with the SOI strength of Pd/Pt, as shown in Fig 6. The interfacial damping persists when spin-orbit interaction in Pd/Pt $\xi_{Pd/Pt}$ equals zero. This implies that the interfacial damping is caused by both the SOI in the non-magnetic elements (Pd/Pt) introduced by electronic state mixture and the broken symmetry of the electronic state of magnetic element Co at the interface. The [001] and [111] interfacial damping from broken symmetry is 0.01 while the [011] orientation has damping 0.02 in both Co/Pt and Co/Pd systems. Compared to the interfacial damping at the original SOI strength of non-3d transition elements, the SOI from Pd ($\xi_{Pd} = 0.15eV$) has a minor effect on the interfacial damping, while the broken symmetry at the interface is the dominant source in Co/Pd system. For the SOI values beyond $\xi = 0.15eV$, the interfacial damping increases distinctly for stronger SOI in the non magnetic transition elements. This suggests that the damping could be tuned by depositing heavy metals (Ta, W etc.) for larger damping or light metals (Mn, Cu) for smaller damping, to adjust the performance of spintronic devices. For Co/Pt system, the interaction from Pt ($\xi_{Pt} = 0.5eV$) significantly affects $\alpha_{interface}$, enhancing the $\alpha_{interface}$ more than ten times, compared with the unavoidable contribution from the interfacial broken symmetry. The minor discrepancy between $\alpha_{interfacial}$ dependence in Co/Pt and Co/Pd might be caused by the subtle difference of the similar band structures between the two separate superlattice systems. The computation confirms that the bulk damping is not affected by the SOI in non-magnetic elements and is determined by the property of Co layers.

The total damping exhibits asymmetric behavior in the transverse directions for most spin orientations. A tensor is necessary to describe damping. Only in very highly symmetric directions, e.g. spin pointing along the perpendicular to plane axes in superlattices oriented in [001] and [111] directions, a tensor can be reduced to a scalar. Moreover, the tensor is dependent on the spin orientation. In both superlattices (Co/Pd, Co/Pt) oriented in [001], the damping tensor shows more marked difference between different spin directions than found for the other superlattices oriented in [011] and [111] directions, as shown in Fig. 7. The ratio of the maximum to minimum damping eigenvalues $\alpha_{max}/\alpha_{min}$ is 1.69 for Co/Pd and 1.21 for Co/Pt in the [001] orientation, while for the other two orientations, the maximum ratios are 1.03 ([111]) and 1.21 ([011]). Furthermore, the interfacial broken symmetry source is more sensitive to the spin orientation variation, rather than the SOI source in non-magnetic metals, as shown in the difference of the two systems Co/Pd and

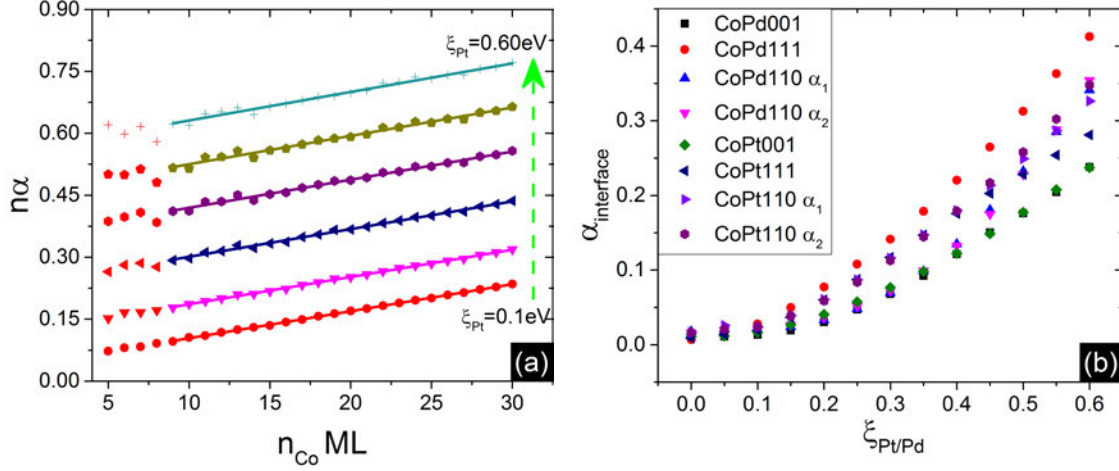


FIG. 6. (a) The product of the number of Co layers and the damping constant versus the number of Co layers in superlattice Co/Pt[111]. The ξ_{Pt} varies in the range of 0.1eV to 0.60eV with a step of 0.1eV. (b) the summary of the interfacial damping vs the SOI strength in non-magnetic material in superlattices oriented in various directions. The superlattices are multiple Co layers deposited on six Pt or Pd layers.

Co/Pt.

IV. CONCLUSION

We identified the interfacial damping of superlattices Co/Pt and Co/Pd, considering typical experimental realizable orientations [001], [111] and [011]. The interfacial damping is related to the lattice orientation: [001] orientation exhibits lower interfacial damping than the other two orientations in both systems. This damping is caused by the broken symmetry at the interface and the spin-orbit interactions of the non-magnetic materials in the superlattice, thus the interfacial damping is inevitable as a consequence of generating high perpendicular anisotropy with ultra-thin film structures for use in spintronic applications. The damping is strongly correlated with the DOS around the Fermi level due to the spin scattering channel. It is also dependent on the spin orientation: the energy dissipation of out-of-plane magnetization could be 1.7 times larger than that of in-plane magnetization. This angular dependence damping could impact the spin dynamics, in both switching and spin oscillation, compared to the classical invariant damping constant.

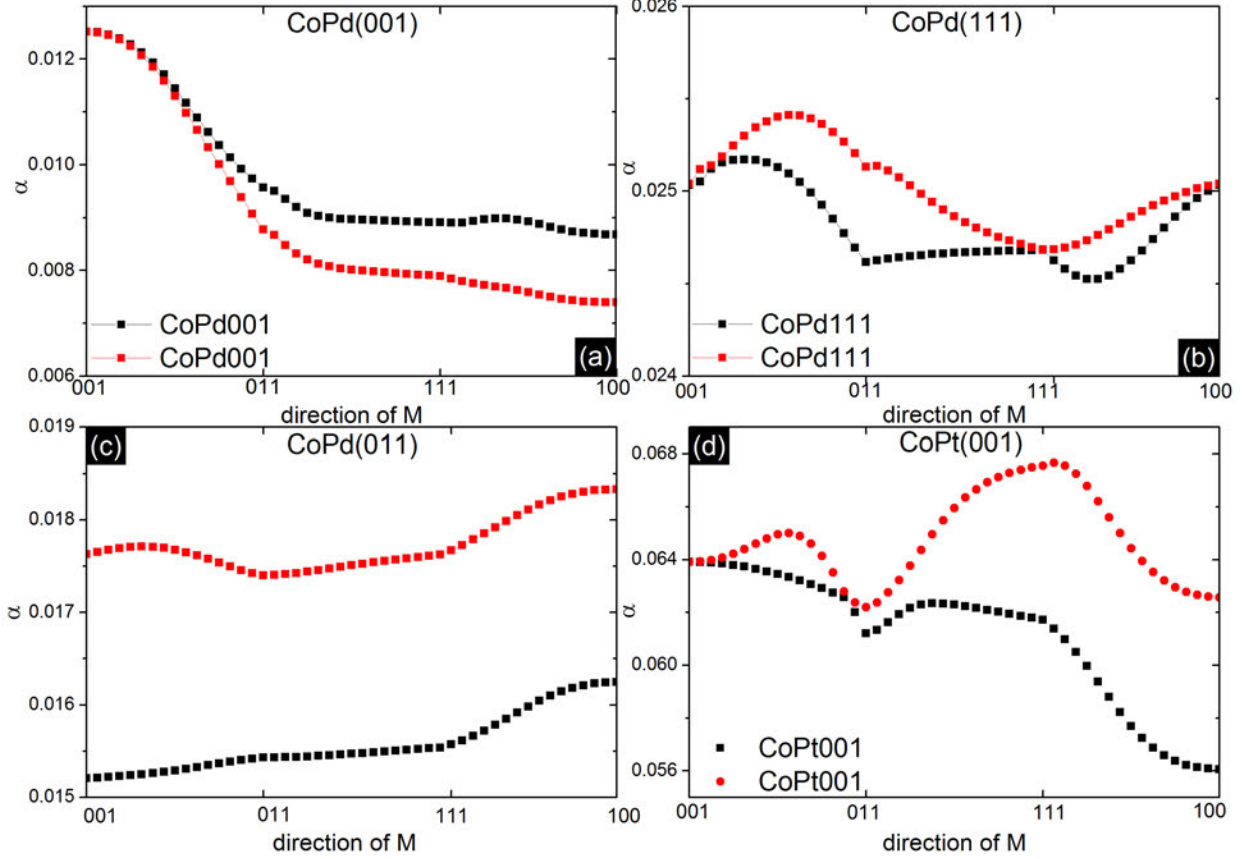


FIG. 7. The eigenvalues of the damping tensor versus the spin orientation in superlattice (a) Co/Pd[001], (b) Co/Pd[111], (c) Co/Pd[011] and (d) Co/Pt[001]. The superlattices are all six Co monolayers deposited on six Pt or Pd monolayers. The dots of two different colors represent the damping eigenvalues in the two transverse directions perpendicular to the spin orientation.

V. ACKNOWLEDGMENTS

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