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Microscopic Mechanisms of Gilbert Damping in Transition Metals

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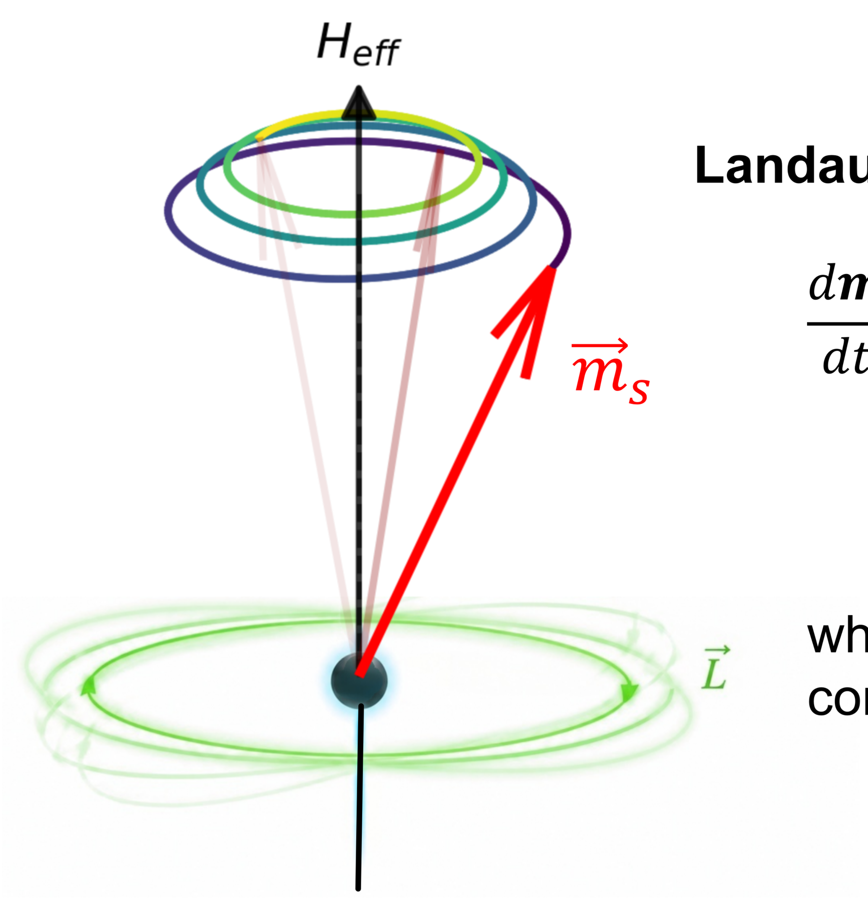
Abstract

Using first-principles calculations, this study systematically elucidates the microscopic physical mechanisms of Gilbert damping in bulk transition metals at low temperatures. The results show that quenching of orbital angular momentum leads to the complete disappearance of the Gilbert damping effect; whereas spin-orbit coupling in degenerate energy bands can partially restore orbital angular momentum, and the degree of restoration at the Fermi surface directly determines the magnitude of the damping coefficient. Furthermore, the degree of orbital angular momentum restoration depends on the orbital components in the wavefunction and the phase differences between orbitals.

Theoretical Framework

Magnetic Moment Precession



Landau-Lifshitz-Gilbert Equation:

$$\frac{dm}{dt} = \gamma \boldsymbol{m} \times \boldsymbol{H}_{eff} + \alpha \boldsymbol{m} \times \frac{dm}{dt}$$

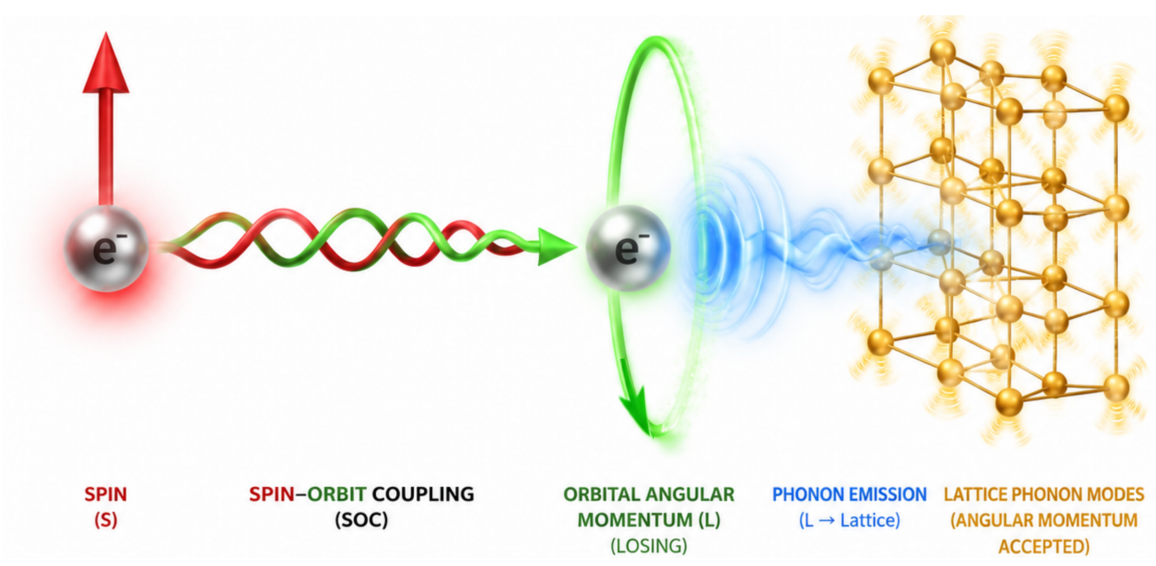
$$\boldsymbol{m} = \vec{m}_s + \vec{m}_L$$

where α is the Gilbert damping constant.

Torque Correlation Model

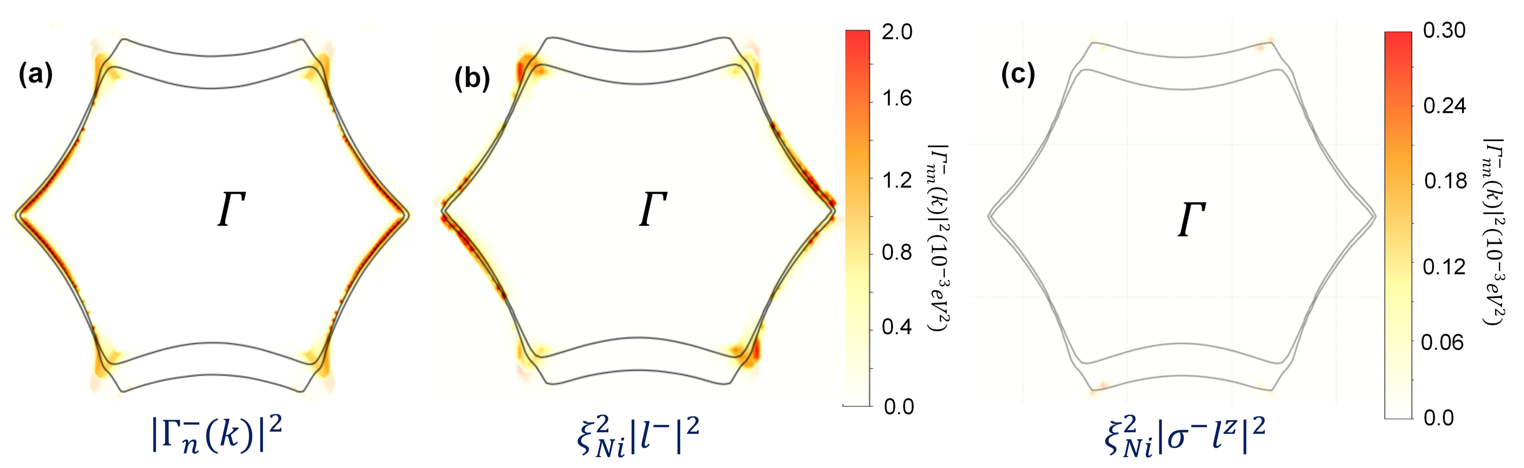
$$\alpha = \pi\hbar \frac{\gamma^2}{\mu_0 M_s} \sum_n \sum_{n\neq m} \frac{d^3k}{(2\pi)^3} \int d\epsilon \eta(\epsilon) g_{nk}(\epsilon) g_{mk}(\epsilon) |\Gamma^-_{mn}(k)|^2$$

$\Gamma^- = \xi \ (l^z\sigma^- - l^-\sigma^z)$ ξ is the spin-orbit coupling constant



For pure spin bands,

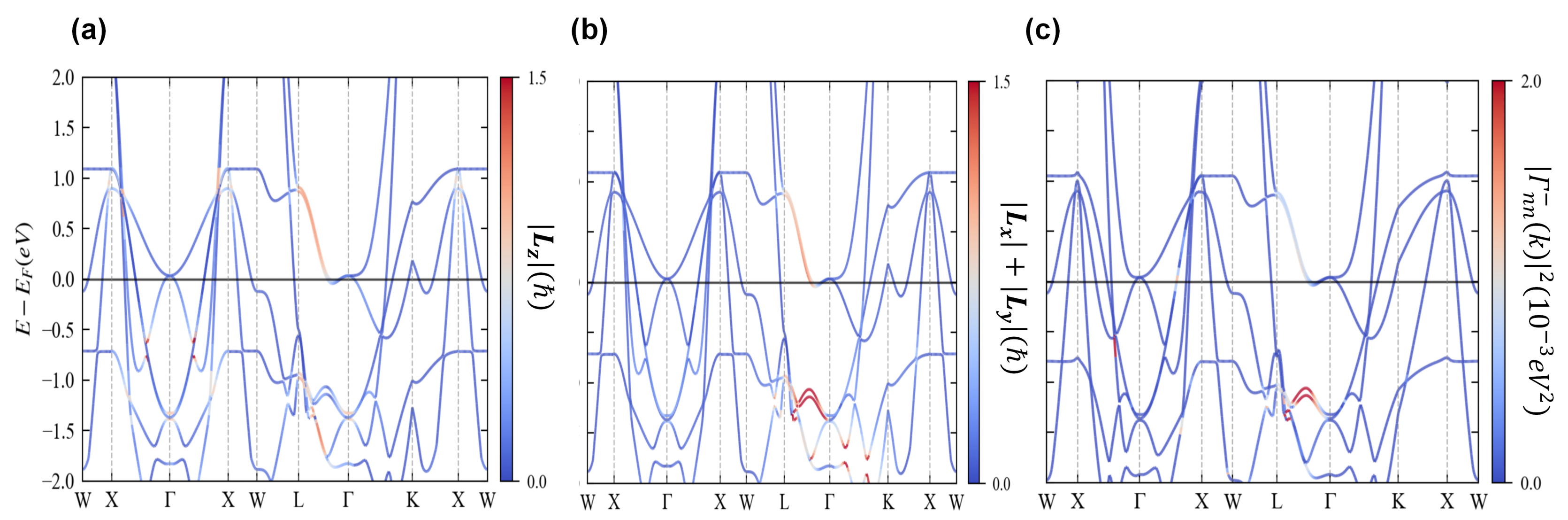
$$\langle\sigma^-\rangle = 0, |\Gamma^-_n(k)|^2 = \xi^2|l^-|^2 = \xi^2(|l^x|^2 + |l^x|^2)$$



(a), (b), and (c) correspond to $|\Gamma^-_n(k)|^2$, $\xi^2_{Ni}|l^-|^2$, and $\xi^2_{Ni}|\sigma^- l^z|^2$on the Ni Brillouin zone's $k_x = k_y$ surface, respectively.

Theoretical Calculations

Electronic Structure



The energy bands and physical quantities of Co. (a) and (b) correspond to$|L_z|$ and $|L_x| + |L_y|$, which is only positive in degenerate bands after considering SOC effects. (c) Plot of $|\Gamma^-_{nn}(k)|^2$ for the Co bands in units of $10^{-3}eV^2$.

Key Findings: Quenching of orbital angular momentum leads to the disappearance of damping; orbital angular momentum can only be restored in degenerate bands.

Probability Flow & OAM

define $\Psi = \psi + e^{i\beta}\phi$,$\psi, \phi$ all are real functions, probability flow

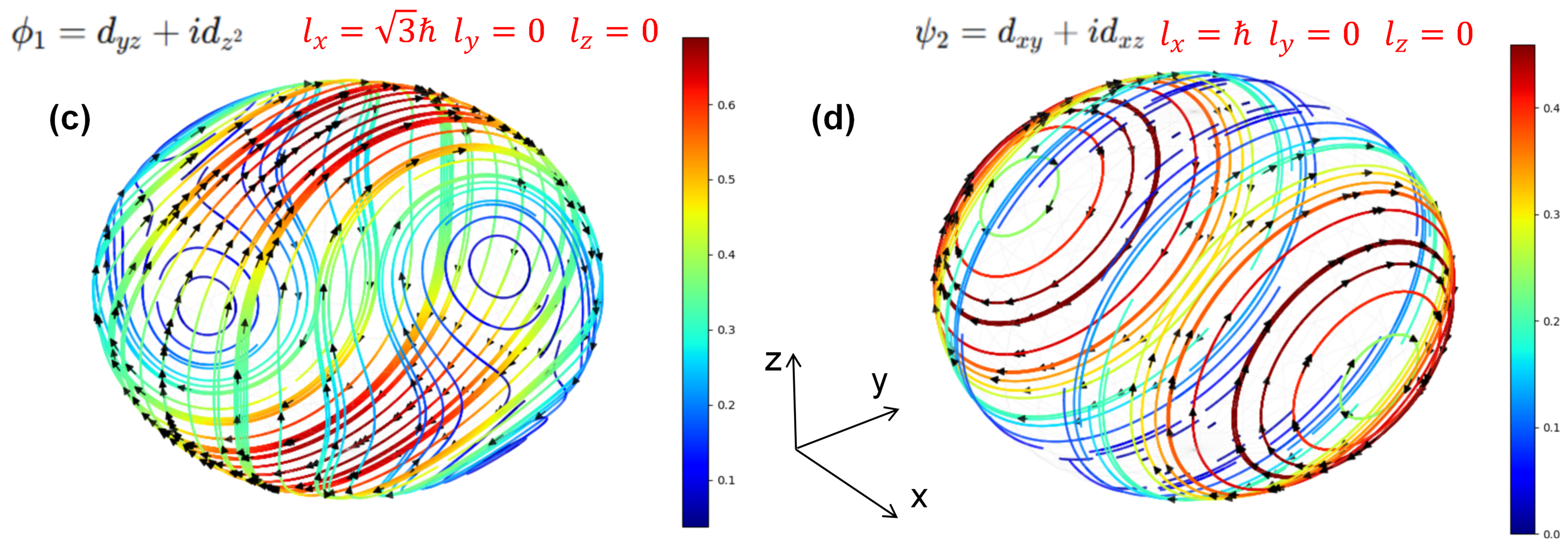
$$J = -\frac{i\hbar}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi) = \frac{\hbar}{m} sin\beta(\phi\nabla\psi - \psi\nabla\phi)$$

(a)

l^x	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$
d_{xy}	0	0	0	$-i$	0
d_{yz}	0	0	$-i\sqrt{3}$	0	$-i$
d_{z^2}	0	$i\sqrt{3}$	0	0	0
d_{xz}	i	0	0	0	0
$d_{x^2-y^2}$	0	i	0	0	0

(b)

l^y	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$
d_{xy}	0	i	0	0	0
d_{yz}	$-i$	0	0	0	0
d_{z^2}	0	0	0	$-i\sqrt{3}$	0
d_{xz}	0	0	$i\sqrt{3}$	0	$-i$
$d_{x^2-y^2}$	0	0	0	i	0



(a) and (b) are the matrix representations of l_x and l_y in the real spherical harmonic basis, while (c) and (d) show the probability current distributions of the $d_{yz} + id_{z^2}$ and $d_{xy} + id_{xz}$ wave functions on the unit sphere, respectively.