Spin Transport and Spin-Orbit Torque in Metallic Heterostructures

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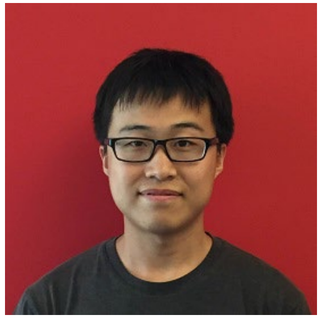
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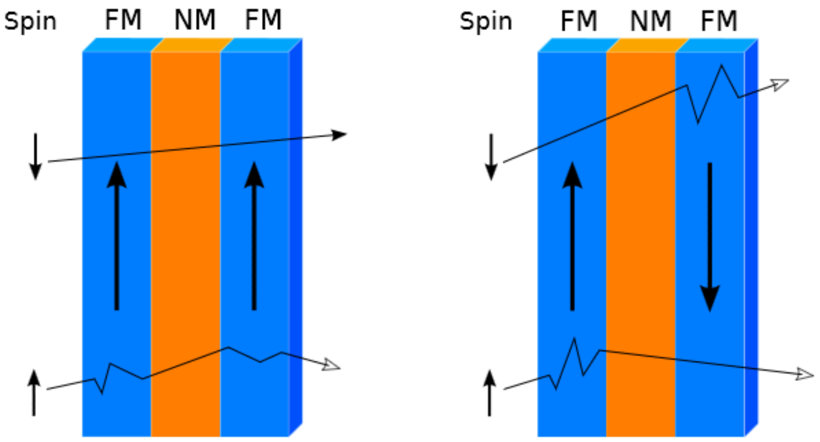
PRB **101**, 020407(R) (2020)
PRB **108**, 144433 (2023)
arXiv:2312.04538
arXiv:2310.13688

Outline

- Introduction
- Spin-orbit torque in F/N bilayers
- Transverse spin transport in a single Pt layer — PRB 108, 144433 (2023)
- Indirect spin current generation and SOT in F/N/F trilayers — arXiv:2312.04538
- Exchange driven spin Hall effect in anisotropic ferromagnets — arXiv:2310.13688

Spintronics and spin-orbitronics

GMR (1988)



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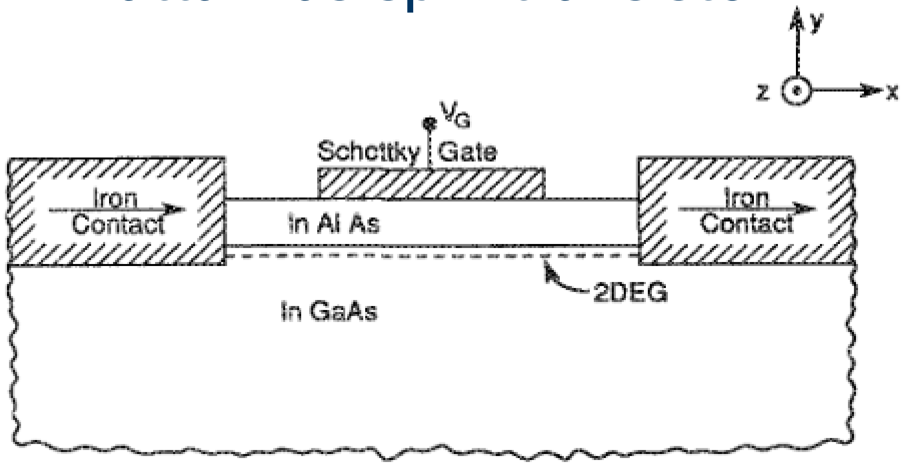
CPP or CIP geometry

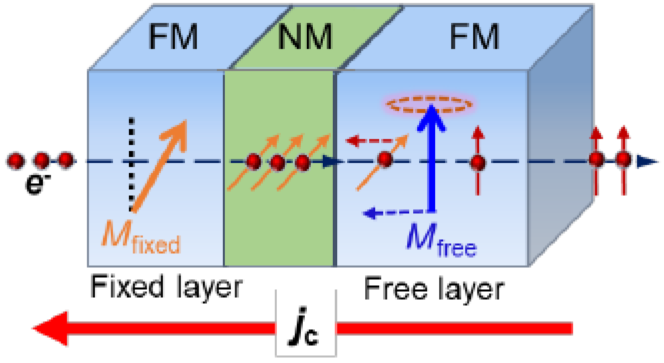
Datta-Das spin transistor



Datta and Das, APL (1990)

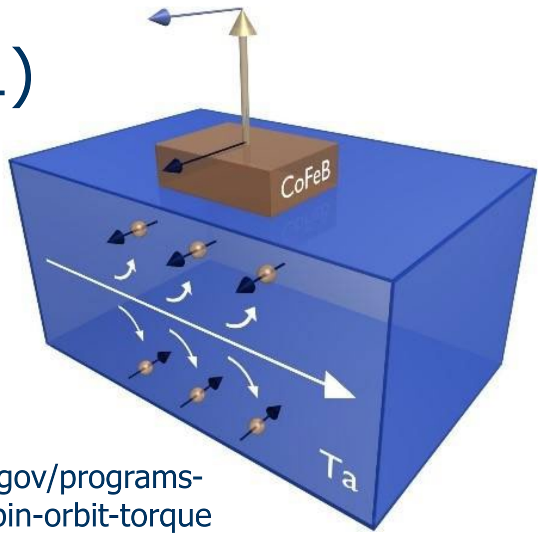
Gate control via spin-orbit coupling

Spin transfer torque (1996)



Sahoo *et al.*, arXiv:2108.10622

Spin-orbit torque (2011)



https://www.nist.gov/programs-projects/theory-spin-orbit-torque

Spin-orbit torque in FM/HM bilayers

Prototypical device structure:

$$\frac{d\boldsymbol{M}}{dt} = LLG + \gamma\boldsymbol{\tau}$$

- Charge-to-spin conversion due to spin-orbit coupling
- 3-terminal device separates read and write currents

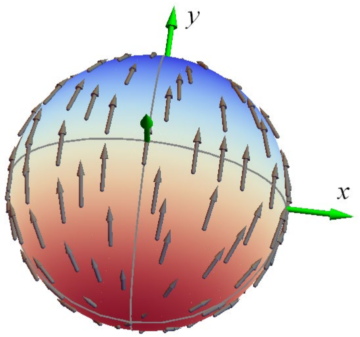
- ❑ Magnetization switching (MRAM)
- ❑ High-frequency nano-oscillators
- ❑ Spin-wave excitation and manipulation
- ❑ Driving force for magnetic textures (domain walls, skyrmions, etc.)

A. Manchon *et al.*, RMP **91**, 035004 (2019)

Basic mechanisms of spin-orbit torque

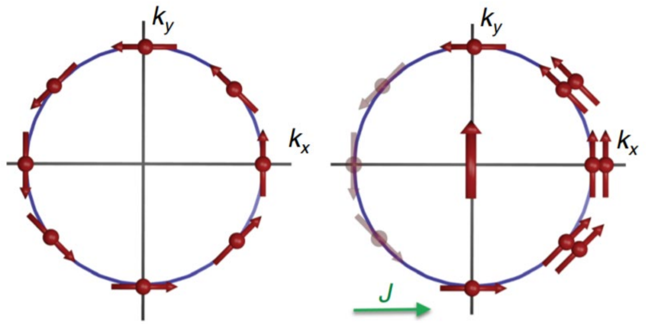
Spin Hall current from HM absorbed by FM

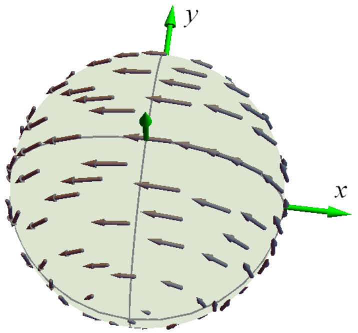
$$\tau_{\mathrm{DL}} \sim \mathbf{m} \times [(\mathbf{z} \times \mathbf{E}) \times \mathbf{m}]$$



Rashba-Edelstein effect

$$\tau_{\mathrm{FL}} \sim (\mathbf{z} \times \mathbf{E}) \times \mathbf{m}$$





Sinova *et al.*, RMP 2015

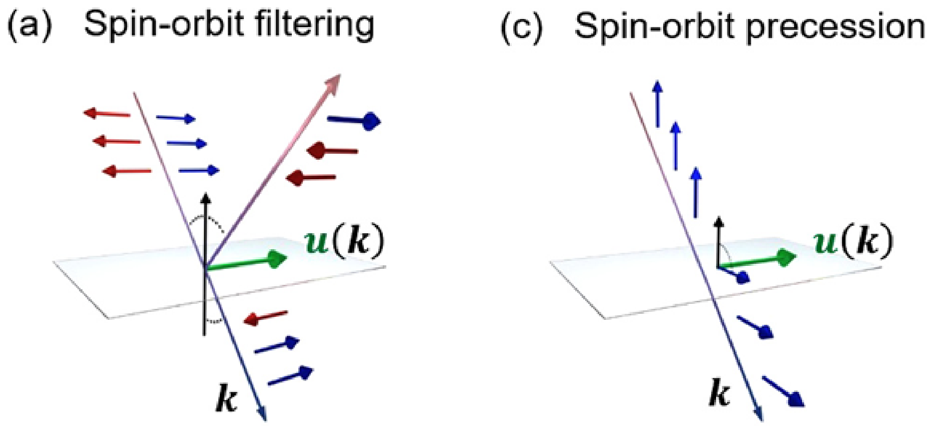
- Current-induced spin accumulation exerts exchange field on the magnetization

Unconventional mechanisms of SOT

- Unconventional sources: SHE in ferromagnets Amin *et al.*, PRB 2019
  Interface-generated spin currents Amin *et al.*, JAP 2020
  Orbital currents Go *et al.*, PRR 2020
- Strong disorder; no clear separation of length scales (thickness; λ_{mfp}; apparent spin-diffusion length)

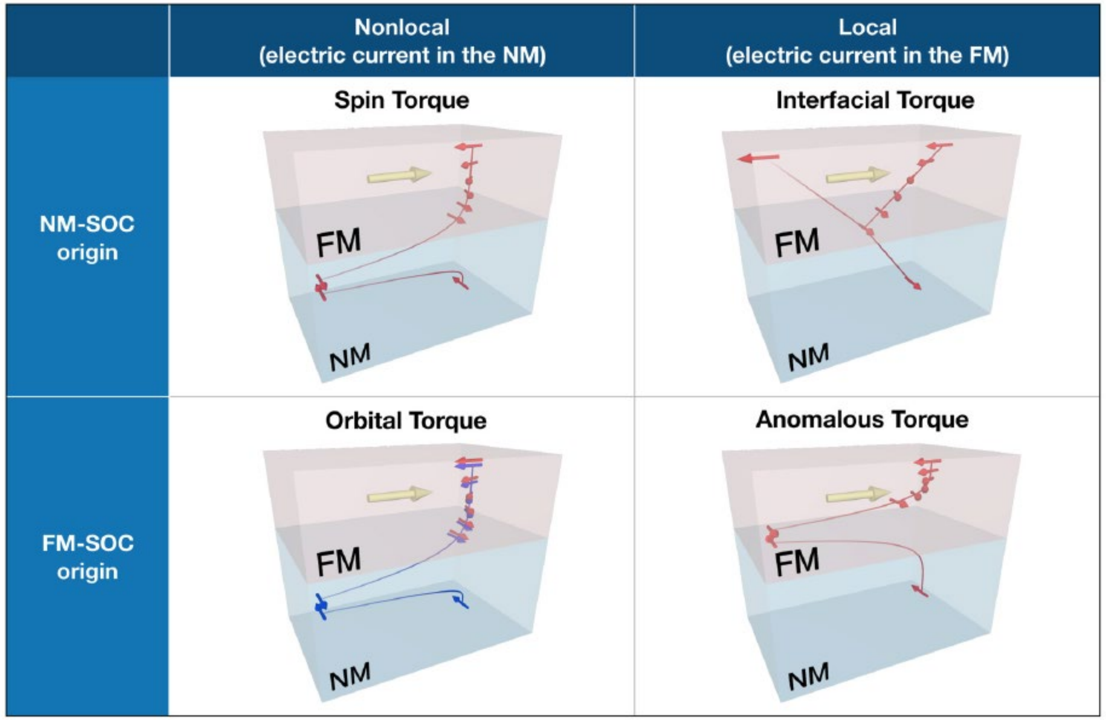
Spin current emission by interfaces

Amin *et al.*, JAP 128, 151101 (2020)



Theory of current-induced angular momentum transfer dynamics in spin-orbit coupled systems

Dongwook Go,[1,2,3,4,*] Frank Freimuth,[1,2] Jan-Philipp Hanke,[1] Fei Xue,[5,6] Olena Gomonay,[2] Kyung-Jin Lee,[7,8] Stefan Blügel,[1] Paul M. Haney,[5,†] Hyun-Woo Lee,[3] and Yuriy Mokrousov[1,2,‡]



PRR 2, 033401 (2020)

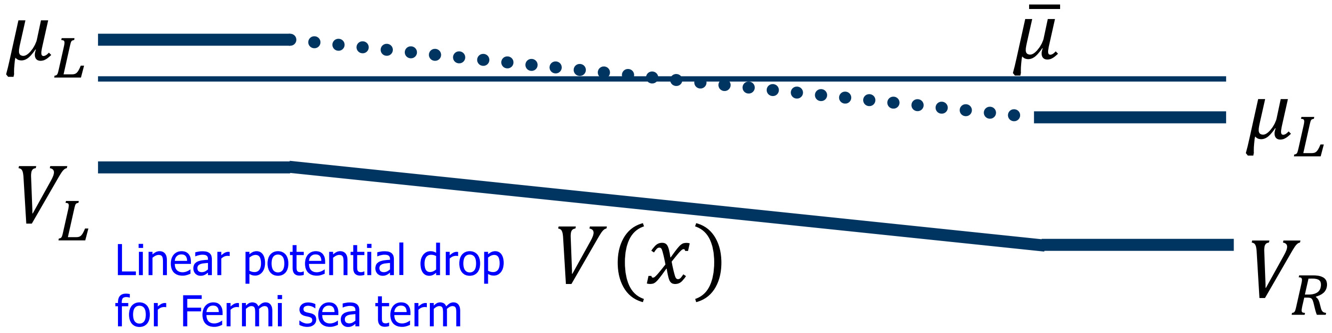
Non-equilibrium Green's function method

$$\mathbf{T} = -\frac{i}{2\pi}\mathrm{Tr}\int_{-\infty}^{\infty}\hat{\mathbf{T}}G^{<}(E)dE$$

$$G^{<} = iG^{R}[f_L(E)\Gamma_L(E) + f_R(E)\Gamma_R(E)]G^{A}$$

$$= \bar{f}(E)\left(G^{A} - G^{R}\right) - i\frac{\partial f}{\partial E}G^{R}(\Gamma_L - \Gamma_R)G^{A}eV$$

Fermi sea — Fermi surface



Torque operator in DFT:

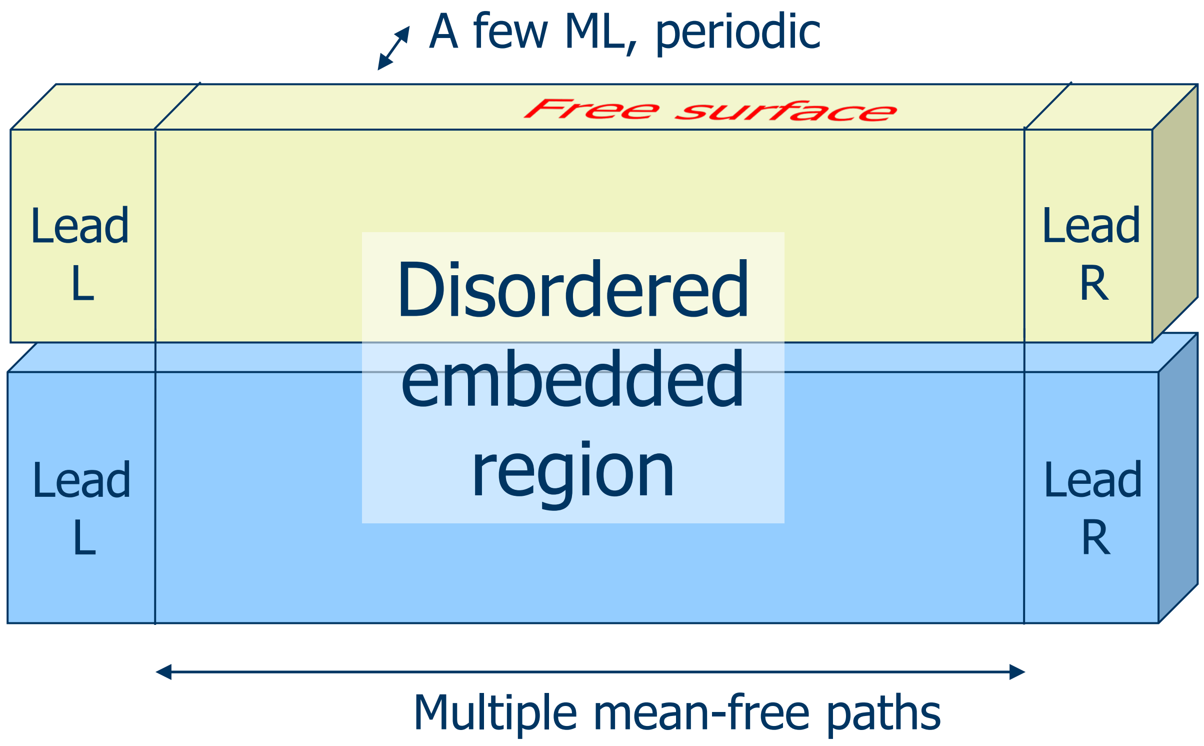
$$\hat{\mathbf{T}} = \gamma\mathbf{B}_{xc,\mathrm{in}} \times \hat{\mathbf{s}}$$

$$\mathbf{T}_i = \int \mathbf{B}_{xc,in}(\mathbf{r}) \times \mathbf{m}_{out}(\mathbf{r})\, d^3r_i$$

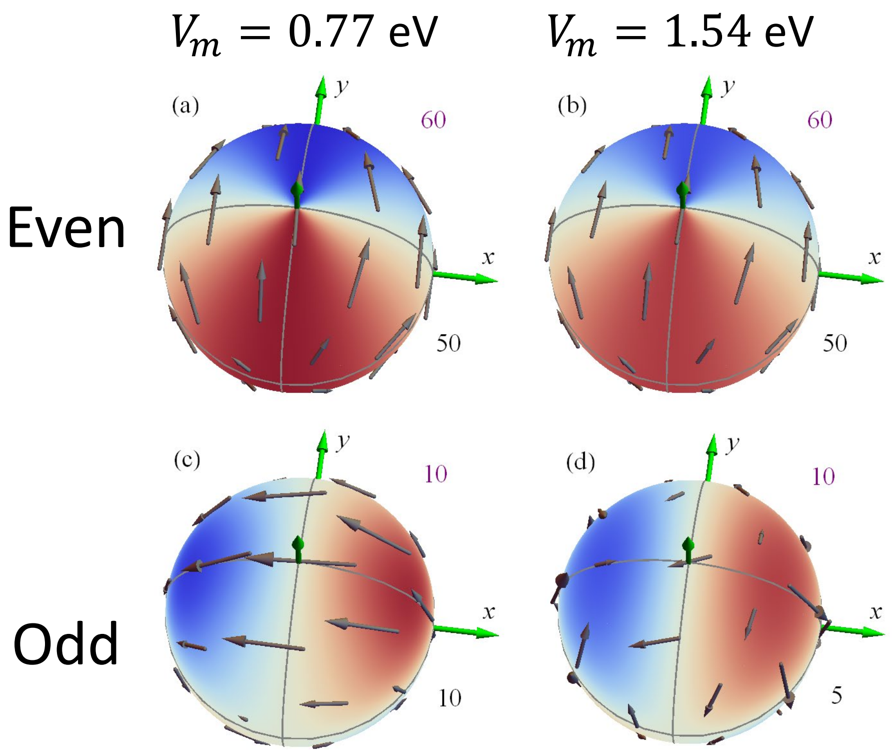
- **Disorder**: Supercell averaging (Anderson or substitutional)
- **All mechanisms on the same footing** (computational experiment), expensive but avoids diagrammatic expansion as in Kubo

❑ ASA-LMTO implementation in Questaal package: Pashov *et al.*, Comput. Phys. Commun. **249**, 107065 (2020)

Typical computational supercell



SOT in Co_6/Pt_6 (Fermi surface contribution)



More disordered (or higher T)

V_m (eV)	0.77	1.09	1.33	1.54
DL SOT	0.31	0.27	0.26	0.25
FL SOT	0.059	0.047	0.013	0.008
PHL SOT	-0.026	-0.031	-0.036	-0.036

Units of ea_0

- DL SOT depends weakly on disorder strength (intrinsic)
- FL SOT declines with increasing disorder (ISGE)
- Appreciable $l = 2$ term (planar-Hall-like), gives damping $\sim m_x m_z$

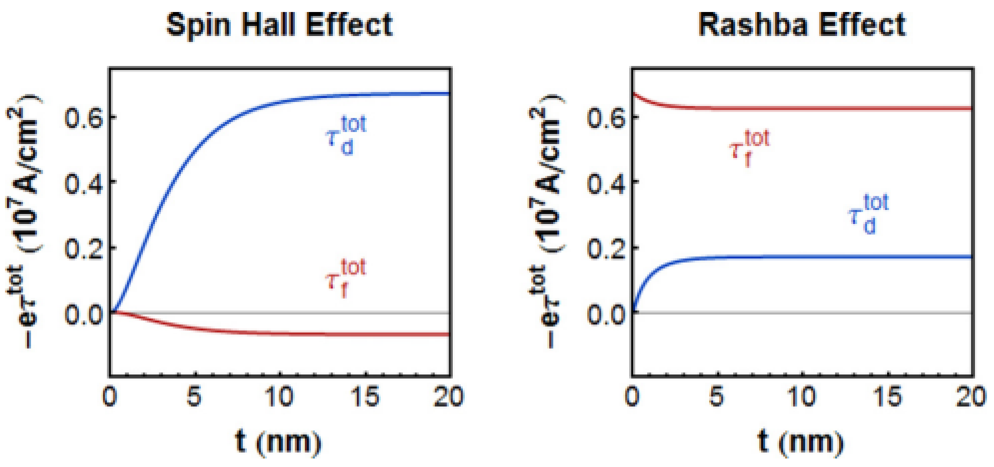
V_m: Anderson disorder amplitude

Color: damping $\Delta\alpha = C\ (E/B)$
$C = \mathbf{m} \cdot \nabla_{\mathbf{m}} \times [\mathbf{m} \times \boldsymbol{\tau}(\mathbf{m})]$

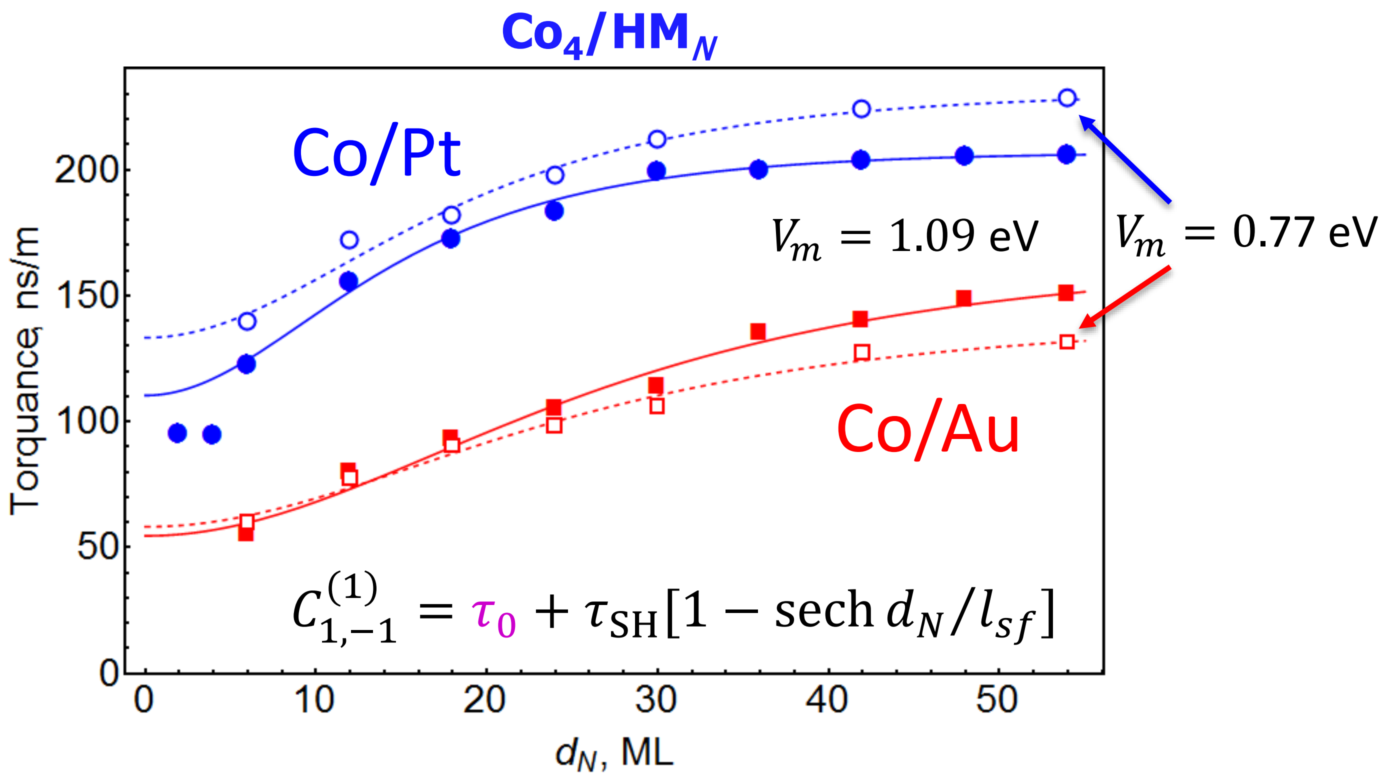
PR Materials **3**, 011401(R) (2019)

Thickness dependence of DL torque

Spin-diffusion model:
Dependence on the thickness of HM



Amin and Stiles, PRB 2016



- **Comparable interfacial and bulk DL SOT**
- **Short $l_{sf} \sim 2$ nm (similar to experiments)**

FM/HM	V_m, eV	$\bar{\rho}$, μΩ cm	τ_0, ns/m	τ_{SH}, ns/m	l_{sf}, nm	θ_{SH}
Co/Pt	1.09	27.2	110.3	96.5	1.94	0.027
	0.77	17.7	133.2	97.5	2.43	0.018
Co/Au	1.09	6.4	54.6	108.9	3.61	0.007
	0.77	4.1	58.2	81.1	3.38	0.003

PRB **101**, 020407(R) (2020)

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Transverse spin transport in a Pt film

Motivation

- Spin-diffusion model is widely used for spin transport and SOT in F/N bilayers
- But is this model applicable to intrinsic spin currents?

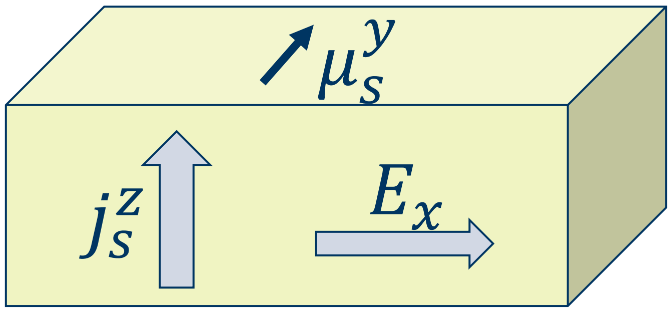
Nair *et al.* [PRB 104, L220411 (2021)]: spin current in a Pt film, fit to spin-diffusion model

- ❑ **Here: Spin current and accumulation in a diffusive Pt film with varied disorder**
- ❑ **Breakdown of spin-diffusion model for spin-Hall transport in Pt**

Spin-Diffusion Model for Nonmagnetic Film

$$j_s^z = \frac{\hbar}{2e}\left(\sigma_{\rm SH} E_x - \underbrace{\sigma_s \frac{d\mu_s^y}{dz}}_{\text{“backflow”}}\right)$$

spin-Hall source plus Einstein relation for backflow (assumes $l_{sf} \gg l_{mfp}$)



Spin accumulation and spin current

$$\frac{dj_s^z}{dz} = -\frac{\hbar}{2}\frac{n_s}{\tau_{sf}}$$

Steady state spin continuity + relaxation

Combine: $$\frac{d^2\mu_s^y}{dz^2} = \frac{\mu_s^y}{l_{sf}^2}$$

Spin diffusion with length l_{sf}

$$\frac{\mu_y(z)}{E} = 2l_{sf}\theta_{\rm eff}\frac{\sinh z/l_{sf}}{\cosh d/(2l_{sf})}$$
$$\frac{j_s(z)}{j} = \theta_{\rm SH} - \theta_{\rm eff}\frac{\cosh z/l_{sf}}{\cosh d/2l_{sf}}$$

$$\theta_{\rm eff} = \frac{\theta_{SH} - \theta_{SSH}}{1 + 2G_{sl} l_{sf}\rho \tanh d/2l_{sf}}$$

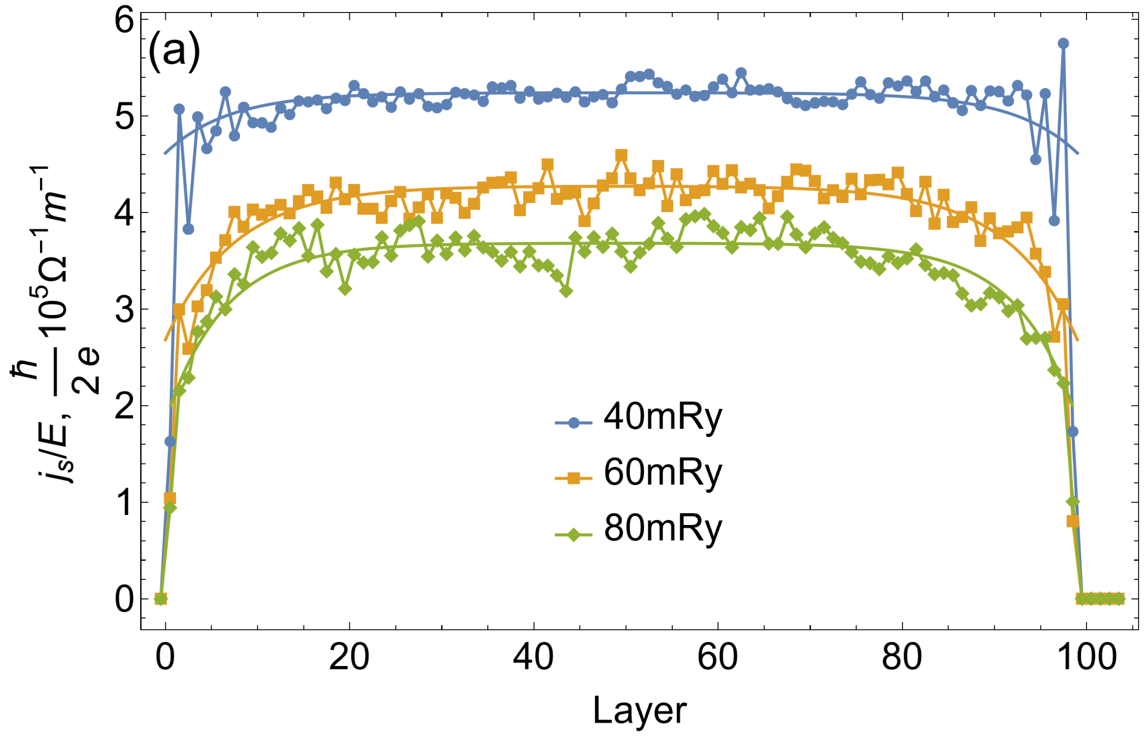
Boundary conditions: $$j_s^z\Big|_0 = G_{sl}\mu_s^y\Big|_0 + \sigma_{\rm SSH}E_x$$

Spin relaxation at the surface or spin-mixing conductance for F/N

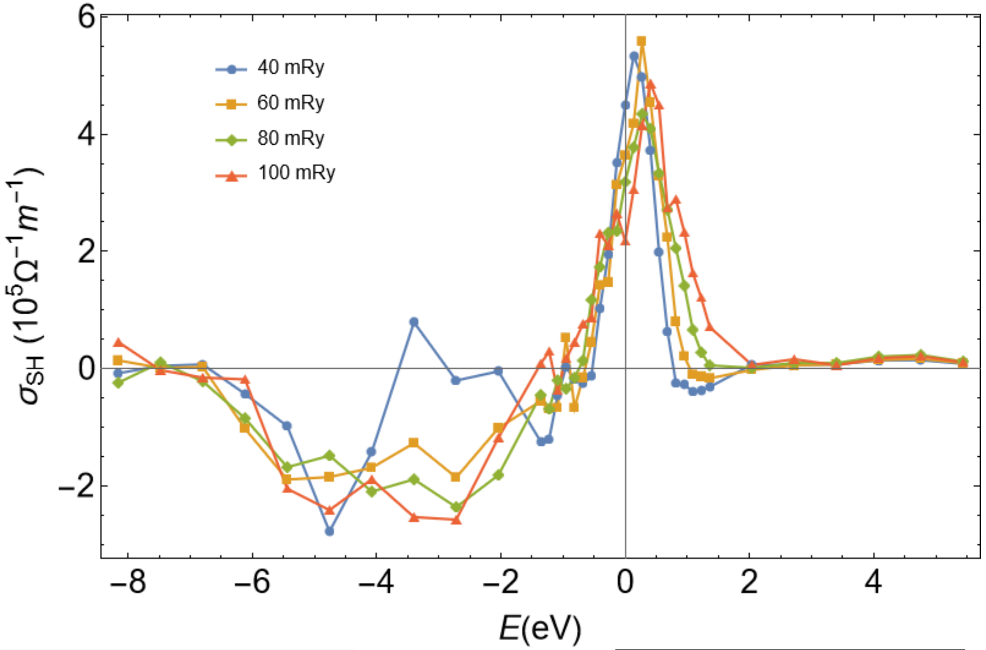
Intrinsic reabsorption into lattice and/or Extrinsic spin current sources Amin et al., PRL 121, 136805 (2018)

Spin Hall current in a 100-ML Pt film

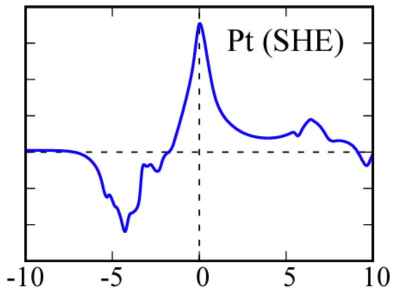
Spin current from SO torque: $\mathbf{J}_s^{i,i+1} = \sum_{j\le i} \mathbf{T}_{SO}^{j}$



Spin-Hall conductivity



V_m (mRy)	ρ ($\mu\Omega$ cm)	λ (nm)
40	15.8	3.0
60	30.4	1.6
80	43.1	1.1

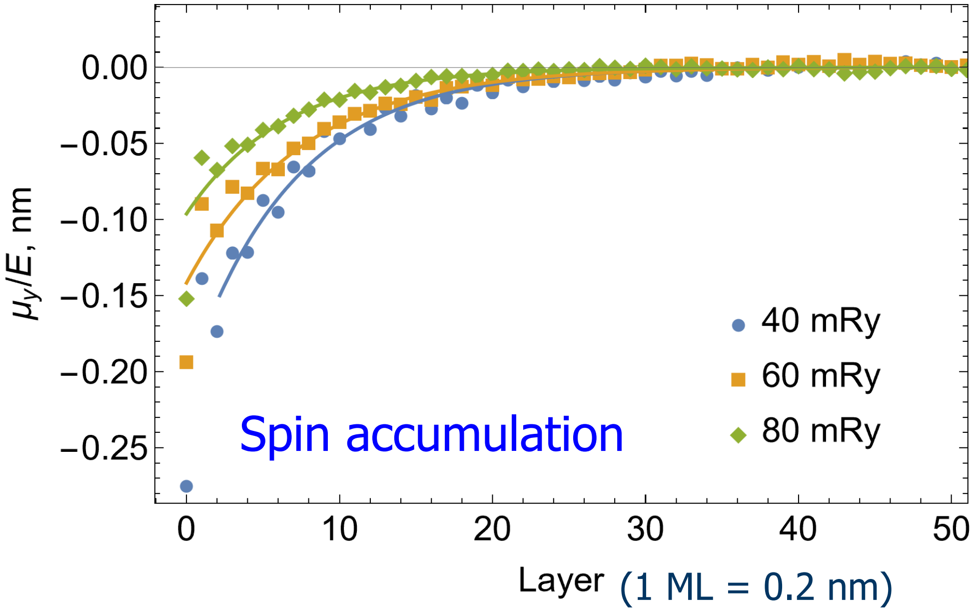


Intrinsic SHE from Kubo
Salemi & Oppeneer, PRM 6, 095001 (2022)

- Weak disorder dependence of SHC in Pt
- Energy dependence agrees well with linear response calculations
- Intrinsic spin current is captured by NEGF

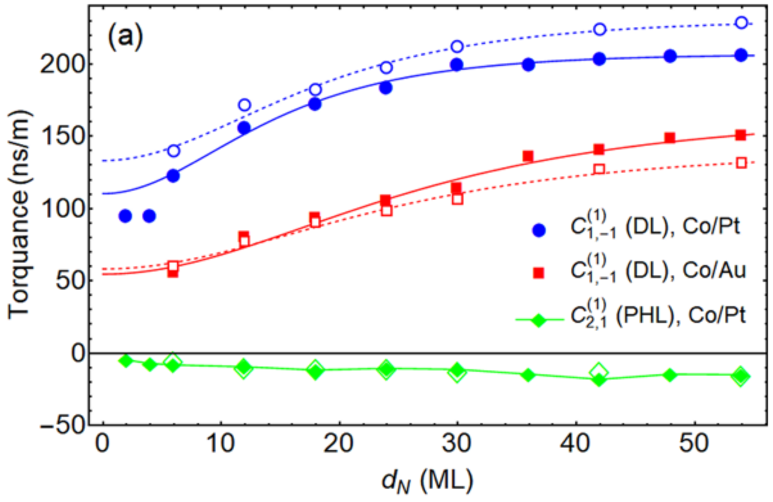
Transverse l_{sf}^T is different from longitudinal l_{sf}^L

Prediction of the spin-diffusion model: $\frac{\mu_y(z)}{E} = 2 l_{sf} \theta_{\text{eff}} \frac{\sinh z/l_{sf}}{\cosh d/(2l_{sf})}$, $l_{sf}\rho \sim \text{const}$ (for Elliott-Yafet)



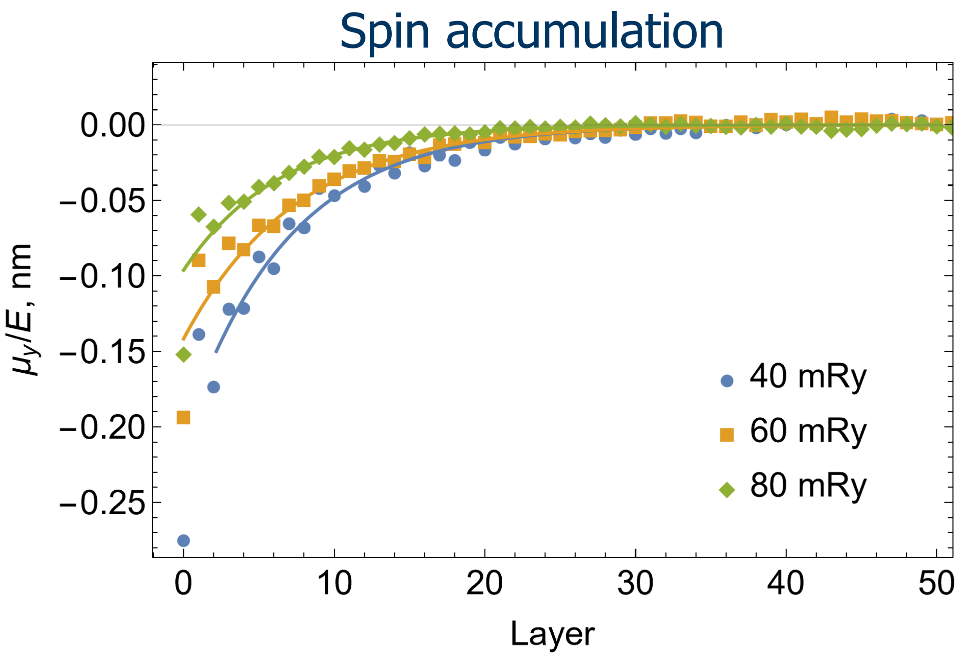
E	V_m (mRy)	ρ (μΩ cm)	λ (nm) (mfp)	l_{sf}^L (nm)	l_{sf}^T (nm)
E_F	40	15.8	3.0	7.7	1.35
E_F	60	30.4	1.6	3.3	1.47
E_F	80	43.1	1.1	2.0	1.26

DL SOT vs thickness of Pt in F/N

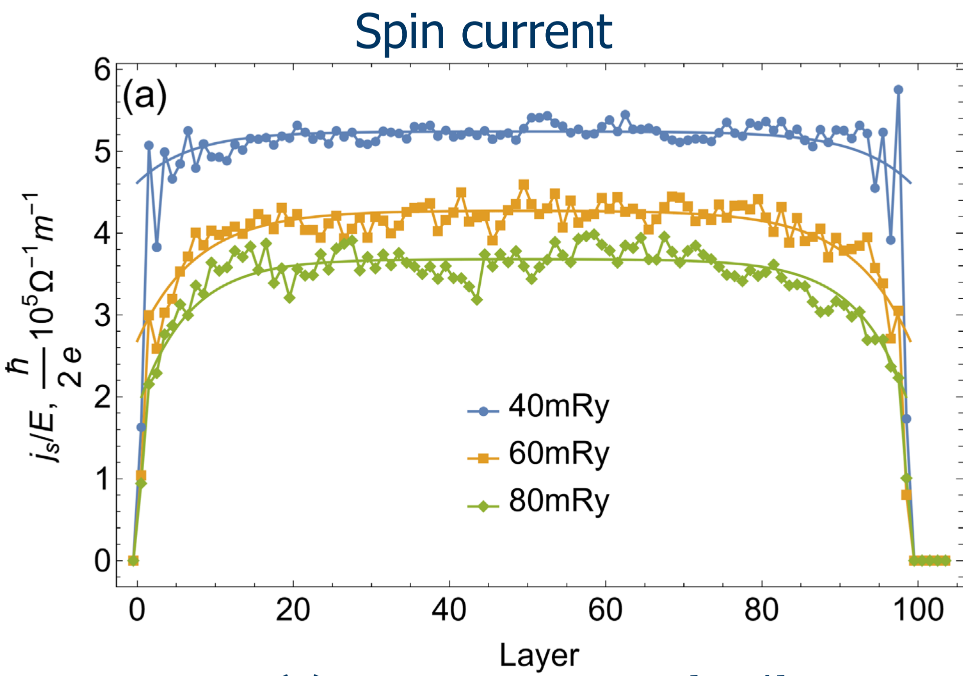


- Short apparent transverse $l_{sf}^T \sim 1.4$ nm, similar to SOT length
- l_{sf}^T is insensitive to disorder strength (not Elliott-Yafet)
- l_{sf}^T shorter than "true" longitudinal l_{sf}^L and even shorter than λ_{mfp}
- Stamm *et al.*, PRL 2017: $l_{sf}^T = 11.4$ nm at $\rho = 20.6$ μΩ·cm (MOKE), but DL SOT (t_N) measurements give $l_{sf}^T \approx 1.5$ nm (Manchon RMP 2019)

Spin backflow relation is not satisfied



$$\frac{\mu_y(z)}{E} = 2l_{sf}\theta_{\text{eff}}\frac{\sinh z/l_{sf}}{\cosh d/(2l_{sf})}$$



$$\frac{j_s(z)}{j} = \theta_{\text{SH}} - \theta_{\text{eff}}\frac{\cosh z/l_{sf}}{\cosh d/2l_{sf}}$$

Disorder	$\theta^{\mu}_{\text{eff}}$	$\theta^{j_s}_{\text{eff}}$
40 mRy	0.076	0.010
60 mRy	0.048	0.048
80 mRy	0.038	0.079

- $\theta^{\mu}_{\text{eff}}$ and θ^{j}_{eff} are different and have opposite trends with disorder
- Backflow relation $j_s = \frac{\hbar}{2e}\left(\sigma_{\text{SH}}E - \sigma_s\frac{d\mu_s}{dz}\right)$ is not satisfied
- Transport is not diffusive at $l^T_{sf} \le l_{\text{mfp}}$; l^T_{sf} is a different length scale

Orbital transport and torques

PHYSICAL REVIEW RESEARCH 2, 013177 (2020)

Orbital torque: Torque generation by orbital current injection

Dongwook Go[1,2,3] and Hyun-Woo Lee[1,*]

Hayashi et al.: "…orbital currents propagate over longer distances than spin currents by more than an order of magnitude in a ferromagnet and nonmagnets"

Orbital relaxation length ~ 50 nm in Ti, ~ 70 nm in α-W

- These findings are surprising because orbital momentum should relax on the scale of the mean-free path along with momentum
- If orbital relaxation length is long, orbital current must be accompanied by orbital accumulation

communications physics

ARTICLE

https://doi.org/10.1038/s42005-023-01139-7 OPEN

Check for

Observation of long-range orbital transport and giant orbital torque

Hiroki Hayashi[1], Daegeun Jo[2], Dongwook Go[3,4], Tenghua Gao[1,5], Satoshi Haku[1], Yuriy Mokrousov[3,4], Hyun-Woo Lee[2] & Kazuya Ando[1,5,6]✉

Article

Observation of the orbital Hall effect in a light metal Ti

https://doi.org/10.1038/s41586-023-06101-9

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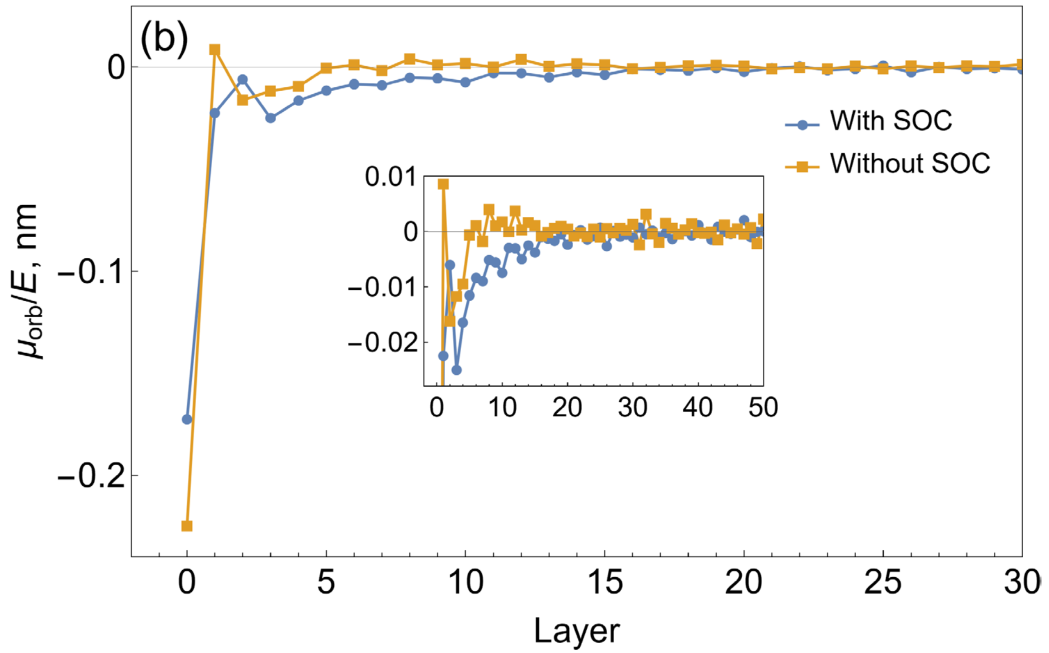
Young-Gwan Choi[1,10], Daegeun Jo[2,10], Kyung-Hun Ko[1,10], Dongwook Go[3,4], Kyung-Han Kim[2], Hee Gyum Park[5], Changyoung Kim[6,7], Byoung-Chul Min[5], Gyung-Min Choi[1,8]✉ & Hyun-Woo Lee[2,9]✉

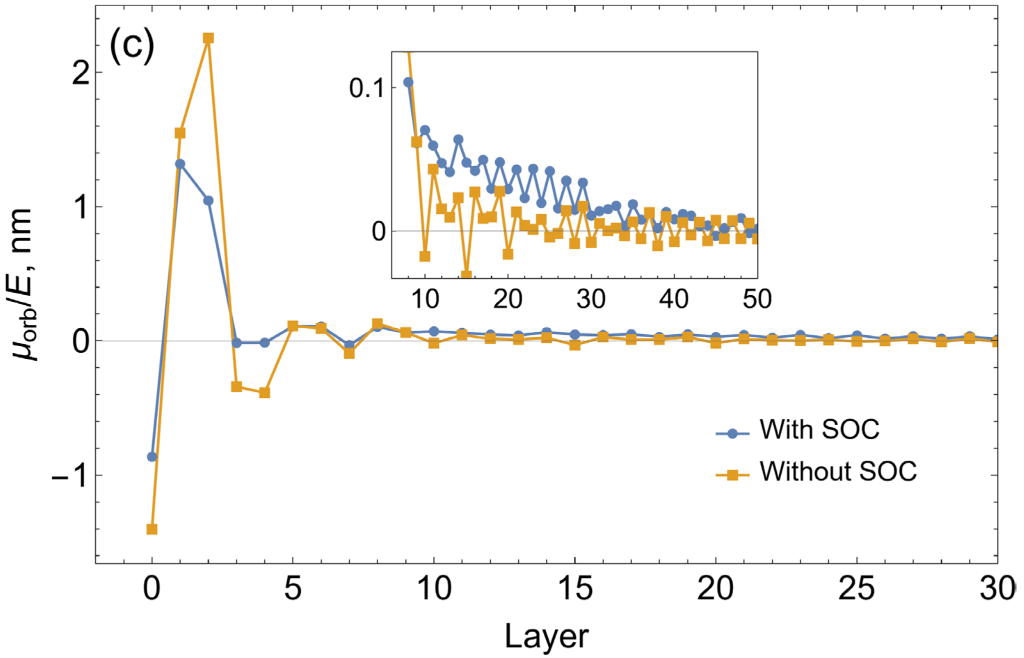
The orbital Hall effect[1] refers to the generation of electron orbital angular momentum flow transverse to an external electric field. Contrary to the common belief that the

Orbital accumulation is a surface effect (no long length scale)

$E = E_F$, 80 mRy disorder



$E = E_F - 0.2$ Ry, 40 mRy disorder



- Orbital accumulation is mostly localized at the surface (within a few ML)
- Weak diffusive "tail" into the bulk, but **only if SOC is included**; similar length to l_{sf}^T
- "Diffusive" orbital accumulation is **induced** by spin accumulation; no long length scale
- Long "orbital relaxation lengths" in light metals could be interpreted as spin-diffusion lengths

Spin transport in a Pt film: Conclusions

- Intrinsic spin current in Pt is captured by the NEGF calculation

- Spin-diffusion equations are not satisfied
- l_{sf}^{T} is much shorter than l_{sf}^{L}, similar to λ_{mfp}
- l_{sf}^{T} is nearly independent of disorder

- Orbital accumulation does not penetrate deep into the bulk except due to spin-orbit coupling

KB, G. Baez Flores, W. Fang, A. Kovalev, M. van Schilfgaarde, P. Haney, M. Stiles, PRB **108**, 144433 (2023)

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Field-free perpendicular switching

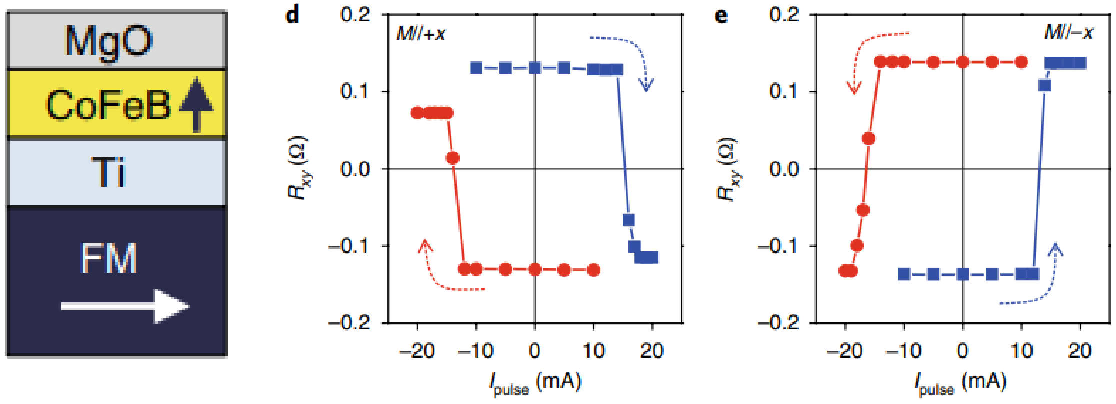
Conventional DL SOT switching of perpendicular M requires H_x (undesirable)

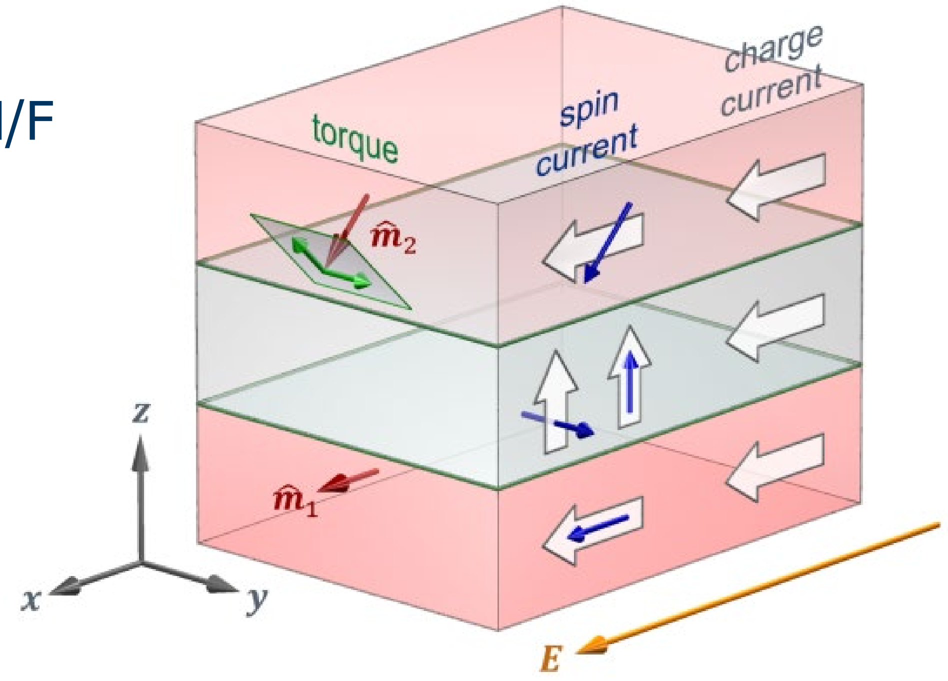
Symmetry breaking enables out-of-plane spin torques

- Yu et al., Nat. Nanotechnol. **9**, 548 (2014) (structural asymmetry)
- MacNeill *et al.*, Nat. Phys. **13**, 300 (2016) (crystal asymmetry)
- Humphries *et al.*, Nat. Commun. **8**, 911 (2017) (ferromagnetic trilayers)

Field-free switching of a perpendicular free layer in F/N/F

Baek *et al.*, Nat. Mater. **17**, 509 (2018)



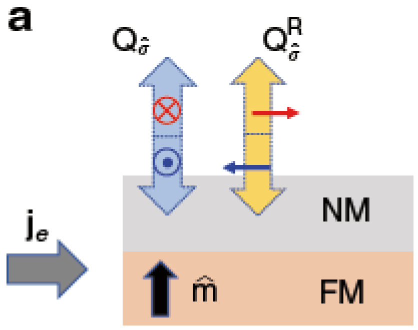


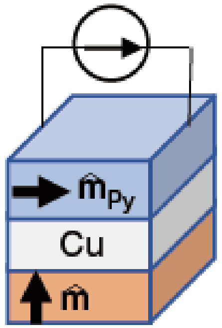
Amin, Haney, Stiles, JAP **128**, 151101 (2020)

Interfaces can emit spin currents with in-plane and out-of-plane spin directions

Amin *et al.*, PRL **121,** 136805 (2018)

“Spin-rotated” torque in trilayers





ARTICLE

DOI: 10.1038/s41467-017-00967-w OPEN

Nat. Commun. **8**, 911 (2017)

Observation of spin-orbit effects with spin rotation symmetry

Alisha M. Humphries[1], Tao Wang[2], Eric R.J. Edwards[3], Shane R. Allen[1], Justin M. Shaw[3], Hans T. Nembach[3], John Q. Xiao[2], T.J. Silva[3] & Xin Fan[1]

$$\mathbf{Q}_{\hat{\boldsymbol{\sigma}}} = \frac{\hbar}{2e}\theta\left(\mathbf{j}_e \times \hat{\boldsymbol{\sigma}}\right)$$

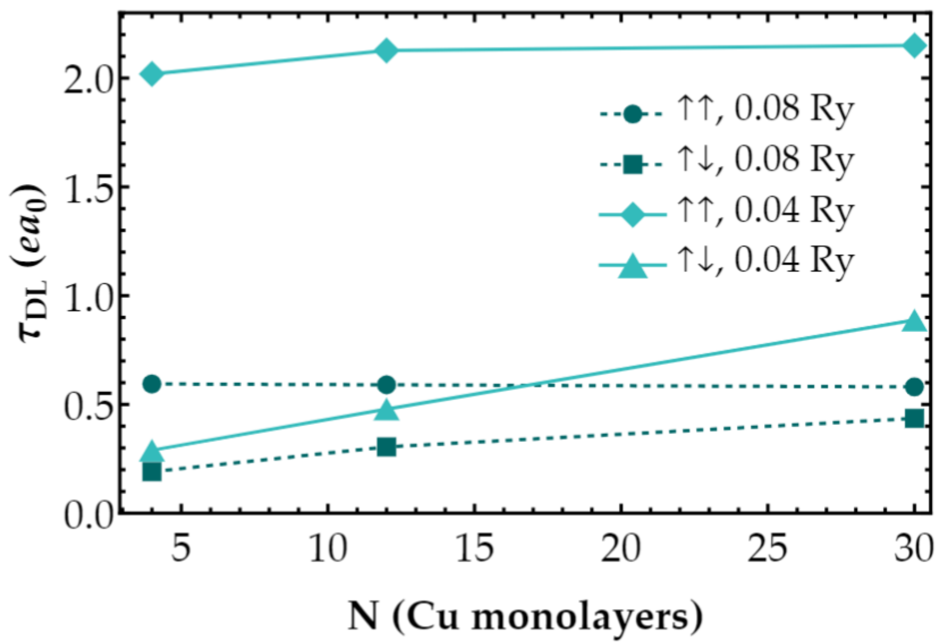
$$\mathbf{Q}^{\mathrm{R}}_{\hat{\boldsymbol{\sigma}}} = \frac{\hbar}{2e}\theta^{\mathrm{R}}\mathbf{j}_e \times \left(\hat{\mathbf{m}} \times \hat{\boldsymbol{\sigma}}\right)$$

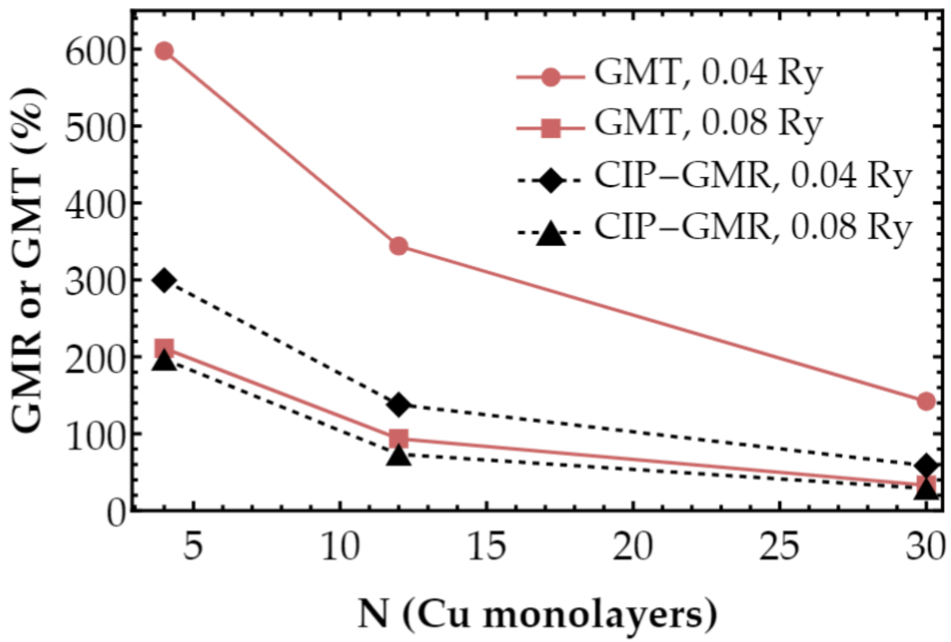
$$h^R_{\mathrm{DL}} = 30 \text{ A/m}$$
$$h^R_{\mathrm{FL}} = 41 \text{ A/m}$$

- ❑ Strong FL torque with polarization along $\mathbf{m} \times \mathbf{y}$
- ❑ **What is its origin?**

Collinear Co|Cu|Co trilayers
Giant magneto-torquance

Torques acting on each layer depend on P or AP orientation





- Giant magneto-torquance: $\boldsymbol{\tau}_{\mathrm{DL}}^{\uparrow\uparrow} > \boldsymbol{\tau}_{\mathrm{DL}}^{\uparrow\downarrow}$ (DL torque on one FM layer)
- Dependence on disorder strength and Cu thickness is similar to CIP-GMR
- Relevant length scale: mean free path in Cu (λ_{Cu})

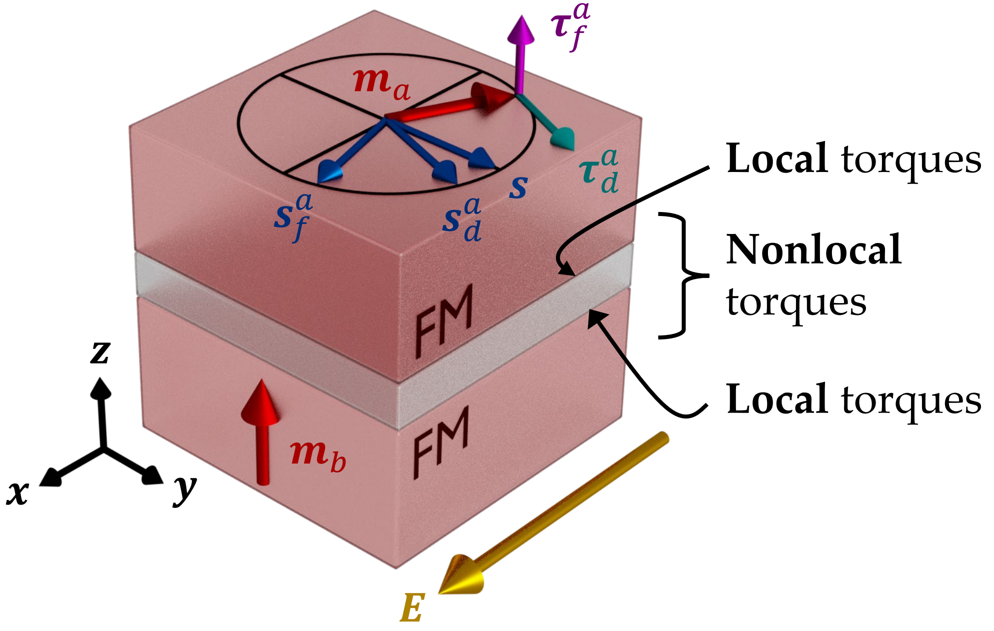
Classification of torques in FNF trilayers

Generically, DL and FL torques on layer a with fixed points $\mathbf{s}_d$ and $\mathbf{s}_f$ depending on the orientation of $\mathbf{m}_b$:

$$\boldsymbol{\tau}_a = \mathbf{m}_a \times (\mathbf{s}_d \times \mathbf{m}_a) + \mathbf{m}_a \times \mathbf{s}_f + \text{higher orders}$$

Fixed points are now functions of $\mathbf{m}_b$ and $\mathbf{s} = \mathbf{z} \times \hat{\boldsymbol{E}}$:

$$\mathbf{s}_d = d_s\mathbf{s} + d_\times \mathbf{m}_b \times \mathbf{s} + (d_m - d_s)\mathbf{m}_b(\mathbf{m}_1 \cdot \mathbf{s})$$
$$\mathbf{s}_f = f_s\mathbf{s} + f_\times \mathbf{m}_b \times \mathbf{s} + (f_m - f_s)\mathbf{m}_b(\mathbf{m}_b \cdot \mathbf{s})$$



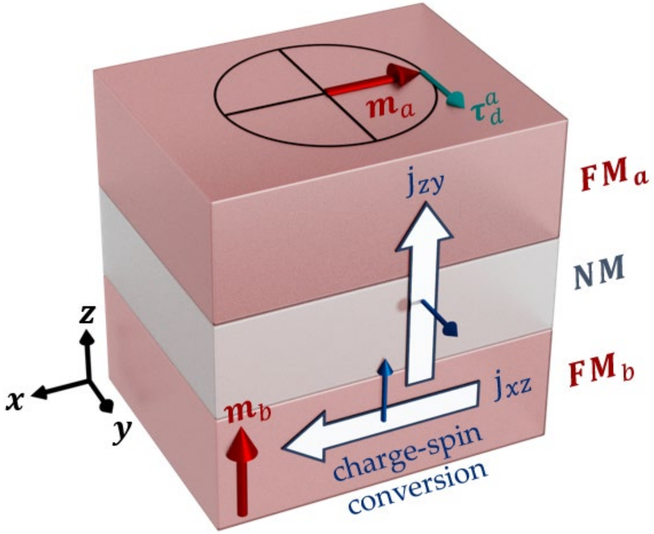
Physical origin:

- d_s: isotropic SHE from layer 1 and its interface
- $d_m - d_s$: spin anomalous Hall effect (SAHE)
- $d_\times$: magnetic SHE and "rotated" spin current
- f_s: nonlocal effective field (nonlocal Edelstein effect)
- $f_\times$, $f_m - f_s$: nonlocal $\mathbf{m}_b$-dependent FL torques on $\mathbf{m}_a$

$f_\times$ is equivalent to h_{FL}^R in Humphries *et al.* (2017)

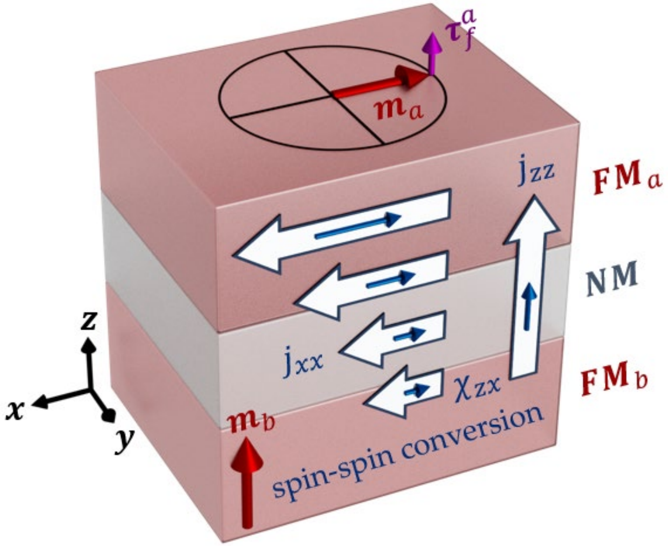
Direct and indirect nonlocal mechanisms

$$\boldsymbol{\tau}_a = \mathbf{m}_a \times (\mathbf{s}_d \times \mathbf{m}_a) + \mathbf{m}_a \times \mathbf{s}_f$$



Direct nonlocal mechanism

1. FM$_b$ emits spin current $j_{z\sigma}$ into spacer
2. FM$_a$ absorbs spin current

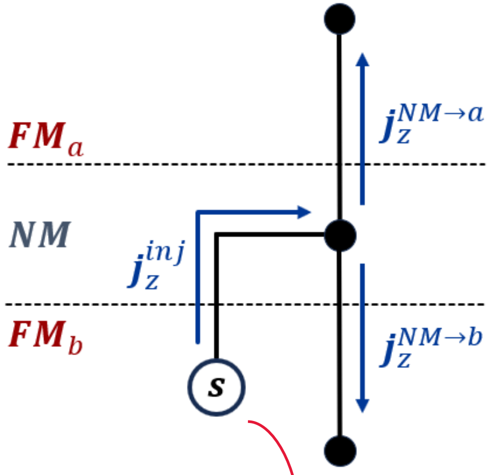


Indirect nonlocal mechanism

1. Longitudinal spin current $j_{x\sigma}$ from FM$_a$ leaks through spacer to FM$_b$/N
2. Scattering at FM$_b$/N interface converts $j_{x\sigma}$ to out-of-plane $j_{z\sigma'}$
3. FM$_a$ absorbs $j_{z\sigma'}$

Circuit theory solution if SOC only in FM_b

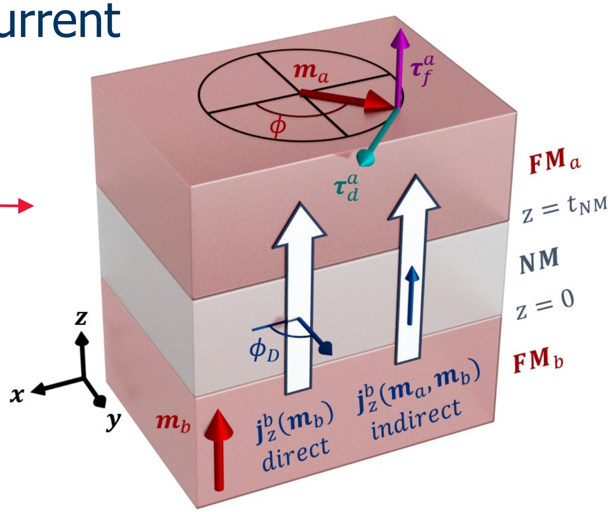
$$\boldsymbol{\tau}_a = \mathbf{m}_a \times (\mathbf{s}_d \times \mathbf{m}_a) + \mathbf{m}_a \times \mathbf{s}_f$$



Backflow currents

$$\mathbf{j}_z^{\mathrm{NM}\to b} = \mathrm{Re}[G^b_{\uparrow\downarrow}]\hat{\mathbf{m}}_b \times (\boldsymbol{\mu}_s \times \hat{\mathbf{m}}_b)$$
$$\mathrm{Im}[G^b_{\uparrow\downarrow}]\hat{\mathbf{m}}_b \times \boldsymbol{\mu}_s$$
$$(G^b_c/2)(\boldsymbol{\mu}_s \cdot \hat{\mathbf{m}}_b)\hat{\mathbf{m}}_b$$

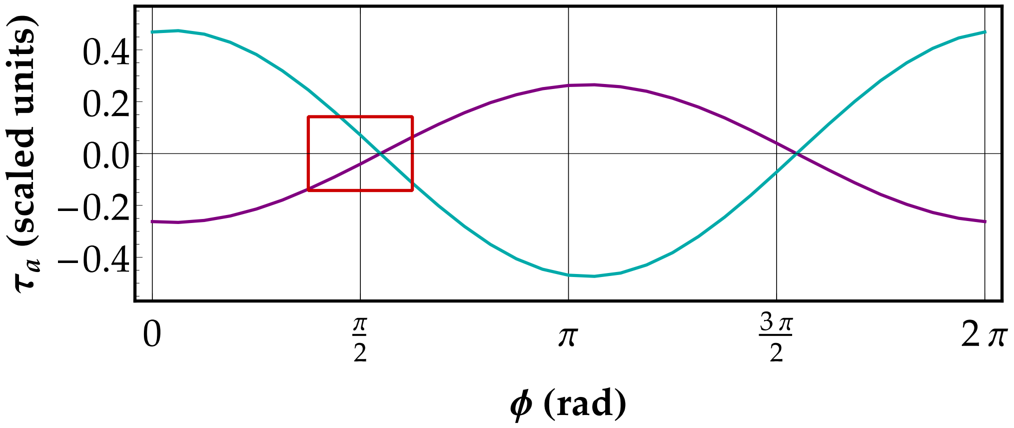
Injected current



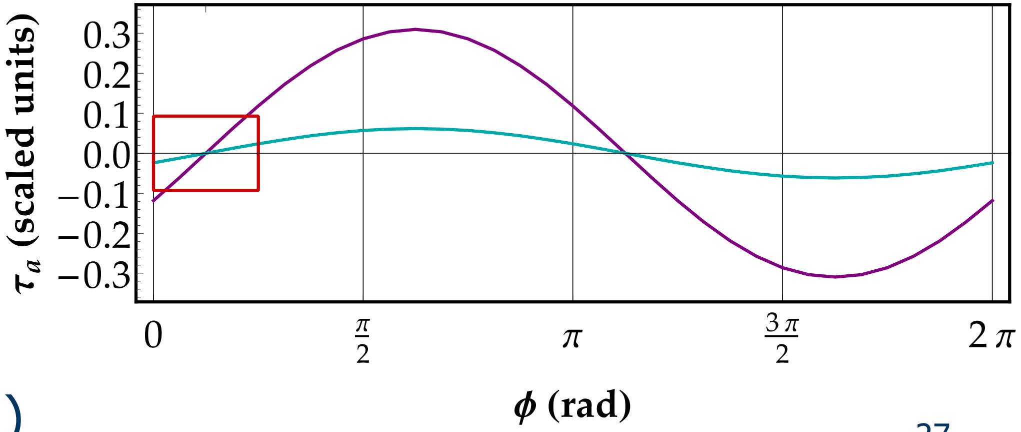
Indirect generation:

$$j_z^{inj} = j_z^b(\hat{\mathbf{m}}_a, \hat{\mathbf{m}}_b) = \mathbf{f}(\hat{\mathbf{m}}_b) \times \hat{\mathbf{m}}_a$$

Direct Nonlocal Mechanism

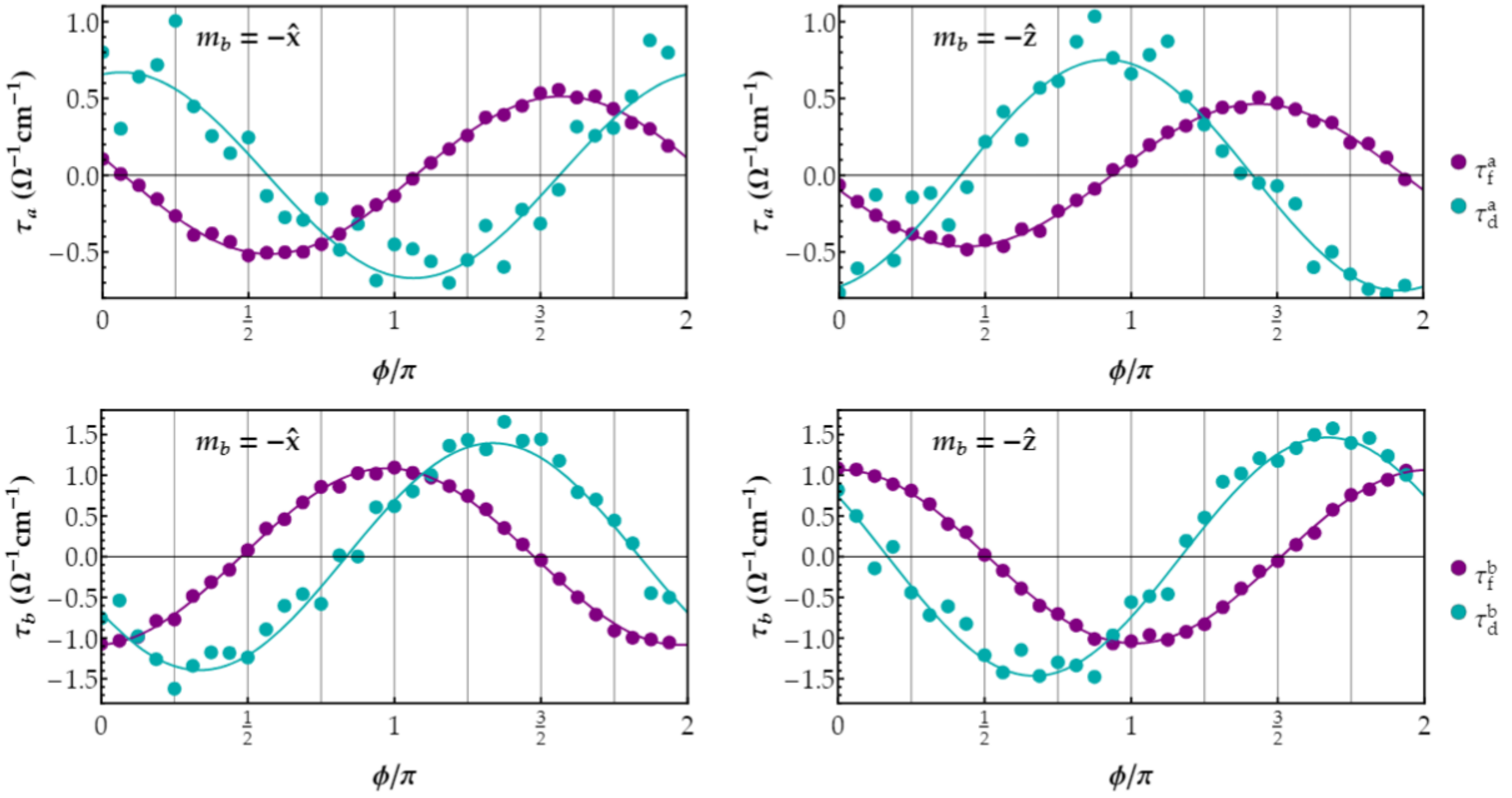


Indirect Nonlocal Mechanism

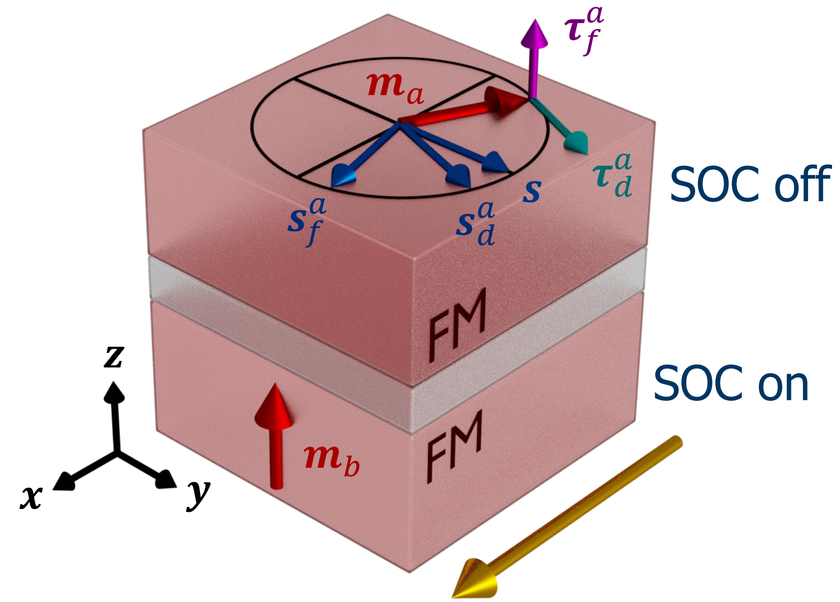


- Direct or indirect mechanism alone leads to $\mathbf{s}_d \parallel \mathbf{s}_f$
- Direct and indirect together lead to $\mathbf{s}_d \nparallel \mathbf{s}_f$ (diagnostic tool)

Ab initio evidence of indirect mechanism

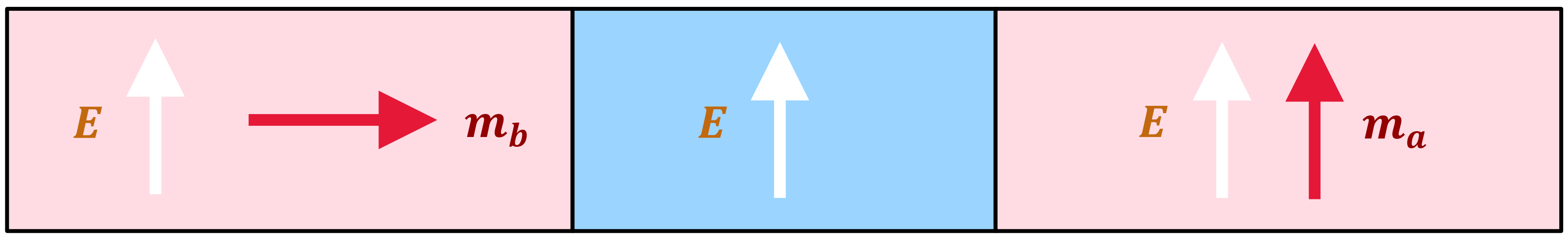


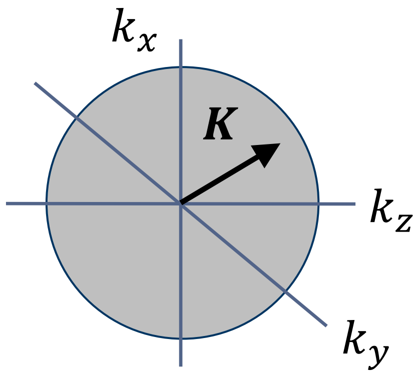
$Co_4Cu_4Co_4$



- ❑ Ab-initio data shows $s_d \nparallel s_f$, relative angle close to $\pi/2$ in $Co_4Cu_4Co_4$
- ❑ Hallmark of an indirect mechanism of spin current generation

Boltzmann simulations of transport with coherent scattering at interfaces





Vivek Amin (IUPUI)

Electron Occupation

$$f_\alpha(\boldsymbol{k}) = f_{eq}(\varepsilon(\boldsymbol{k}))\delta_{0\alpha} + g_\alpha(\boldsymbol{K})\partial f_{eq}/\partial\varepsilon$$

equilibrium nonequilibrium

Components

$\alpha, \beta, \nu \in [0, x, y, z]$

charge spin

Fermi Surface (same for all layers)

*Valet and Fert, PRB **48**, 7099 (1993)*

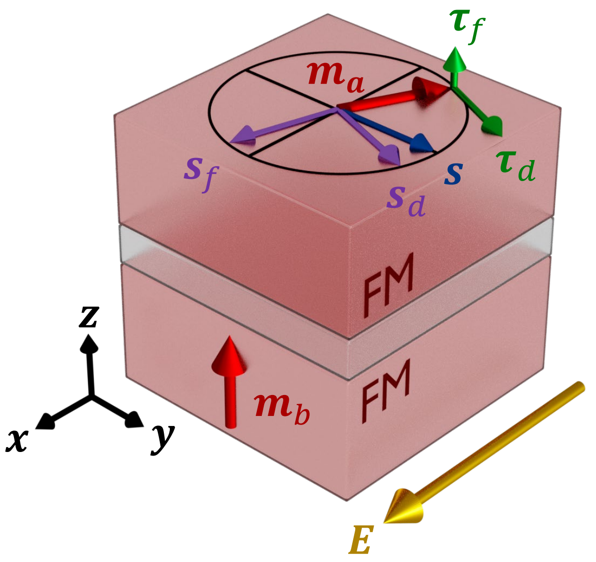
*Penn and Stiles, PRB **72**, 212410 (2005)*

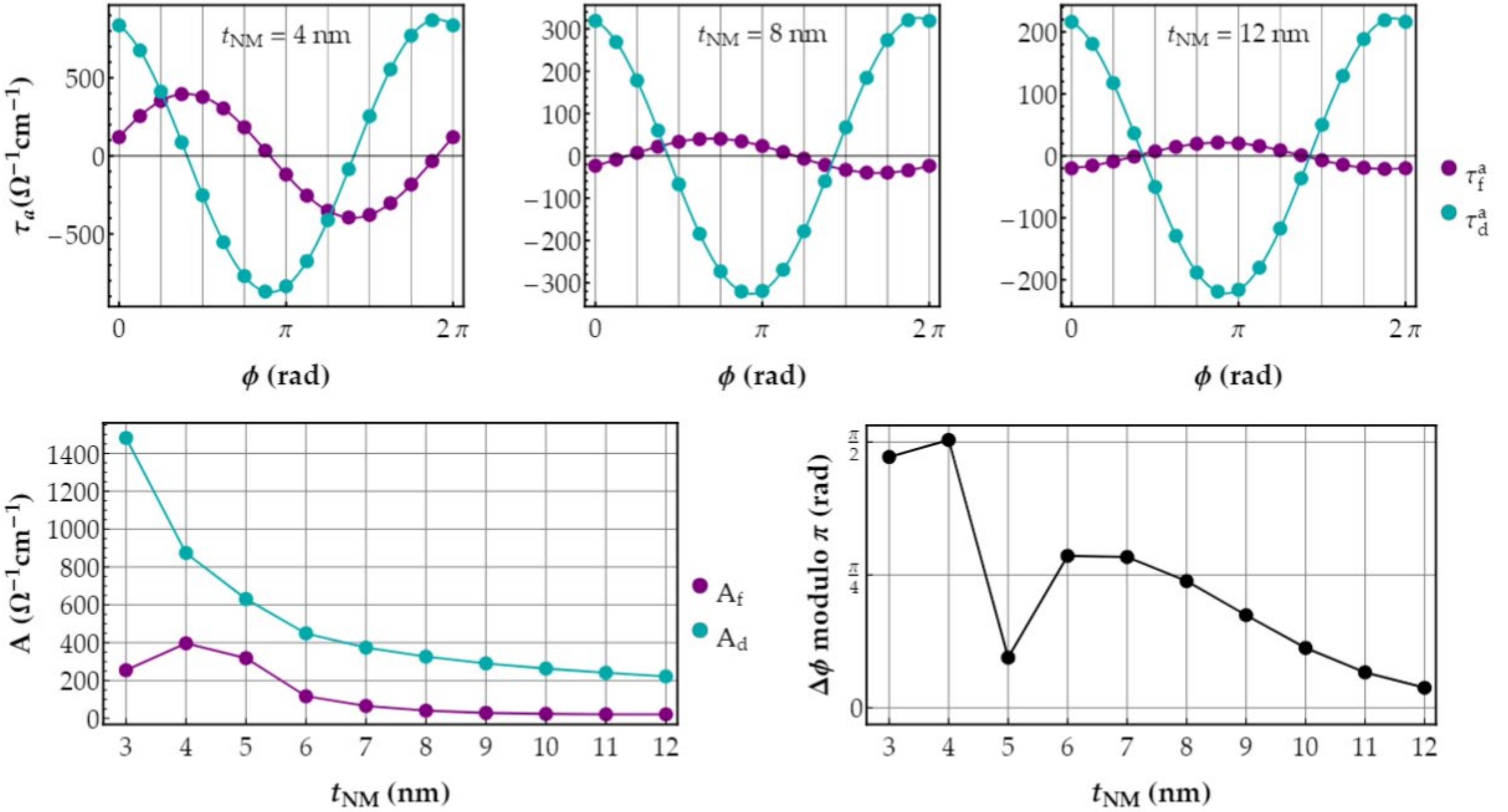
Linearized Boltzmann Equation

$$\boldsymbol{v}(\boldsymbol{K}) \cdot \nabla g_\alpha(\boldsymbol{K}) - e\boldsymbol{E} \cdot \boldsymbol{v}(\boldsymbol{K})\delta_{0\alpha} + \gamma\epsilon_{\alpha\beta\nu} m_\beta g_\nu = -R_{\alpha\beta}(\boldsymbol{K}) g_\beta(\boldsymbol{K}) + \int_{FS} d\boldsymbol{K}' P_{\alpha\beta}(\boldsymbol{K}, \boldsymbol{K}') g_\beta(\boldsymbol{K}')$$

electric field — spin precession, exchange field $\boldsymbol{m}$ — scattering out, scattering in: includes spin-dependent + spin-flip scattering

Evidence of indirect mechanism from Boltzmann calculations





$$\tau_d = A_d \sin(\phi - \Delta\phi_d)\hat{\boldsymbol{m}}_\times$$

$$\tau_f = A_f \sin(\phi - \Delta\phi_f)\hat{\boldsymbol{z}}$$

$$\boldsymbol{m}_\times = \boldsymbol{m}_1 \times \boldsymbol{m}_2$$

$$\Delta\phi = \Delta\phi_d - \Delta\phi_f$$

- Angle between $\boldsymbol{s}_d$ and $\boldsymbol{s}_f$ declines with thickness on the scale of $\lambda_{\mathrm{mfp}} = 3$ nm

SOT in F/N/F trilayers: Conclusions

- New types of spin-orbit torque in F/N/F trilayers with a thin N layer, reminiscent of the CIP-GMR effect
- Direct and indirect spin current generation mechanisms
- Indirect generation leads to “spin-rotated” fieldlike torques of the type observed by Humphries *et al.* [Nat. Commun. **8**, 911 (2017)]

V. Amin, G. Baez Flores, A. Kovalev, KB, arXiv:2312.04538

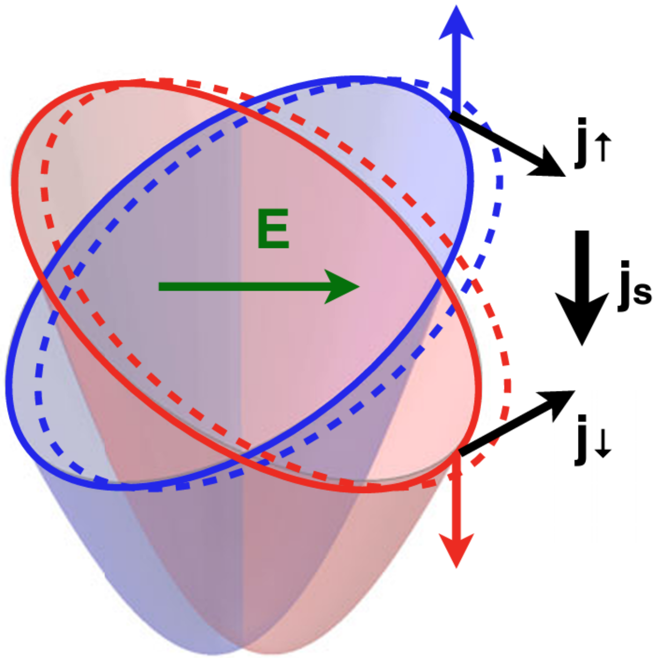
Outline

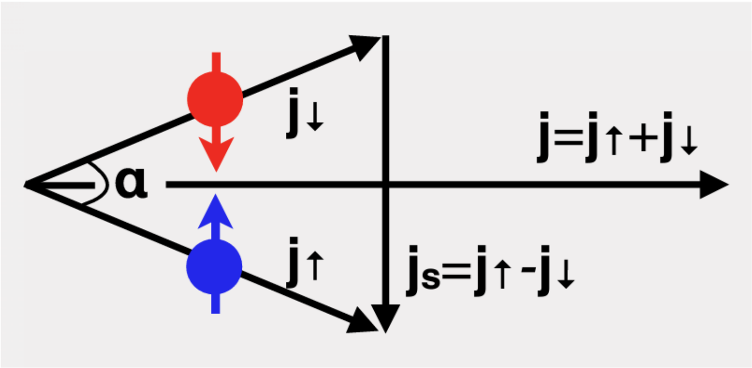
- Introduction
- Spin-orbit torque in F/N bilayers
- Transverse spin transport in a single Pt layer
- Indirect spin current generation and SOT in F/N/F trilayers
- Exchange driven spin Hall effect in anisotropic ferromagnets

Spin-splitting current in altermagnets without spin-orbit coupling

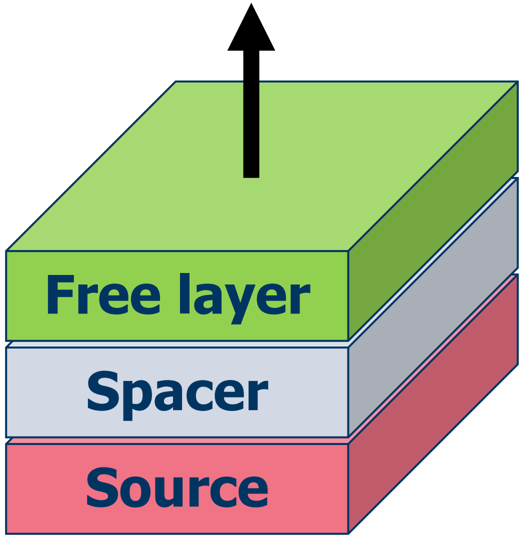
González-Hernández *et al.*, PRL 126, 127701 (2021)

Transverse spin current in a collinear altermagnet (AFM with exchange-split bands)
Requires a single crystal but not spin-orbit coupling



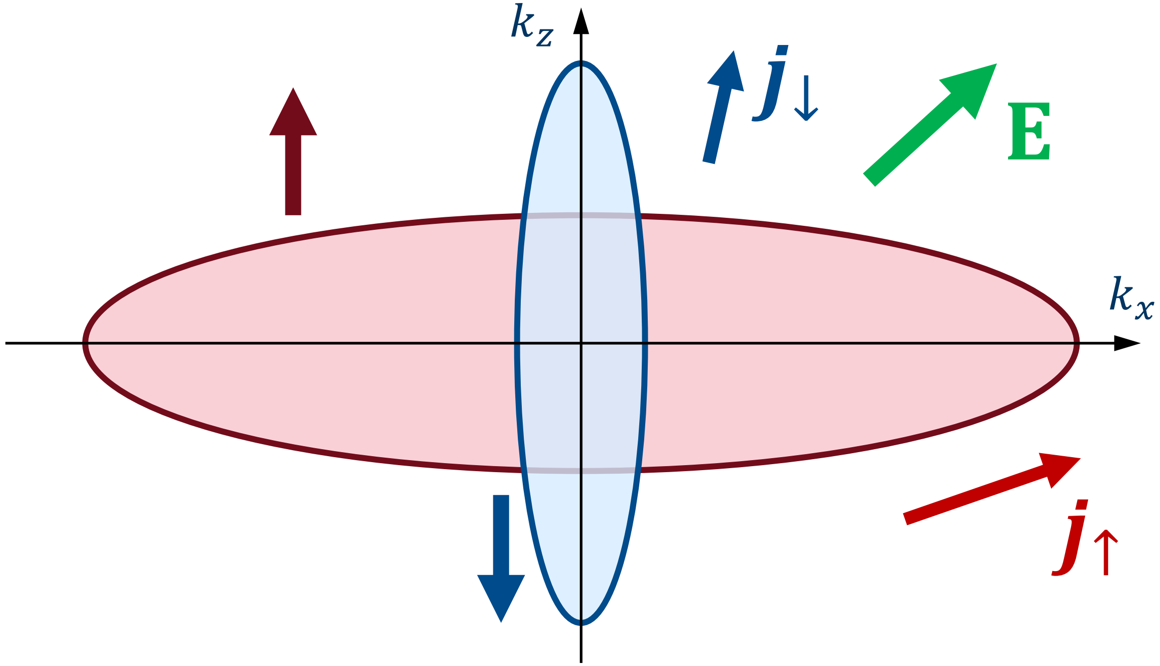


Calculated $\alpha \approx 34^\circ$ in RuO_2

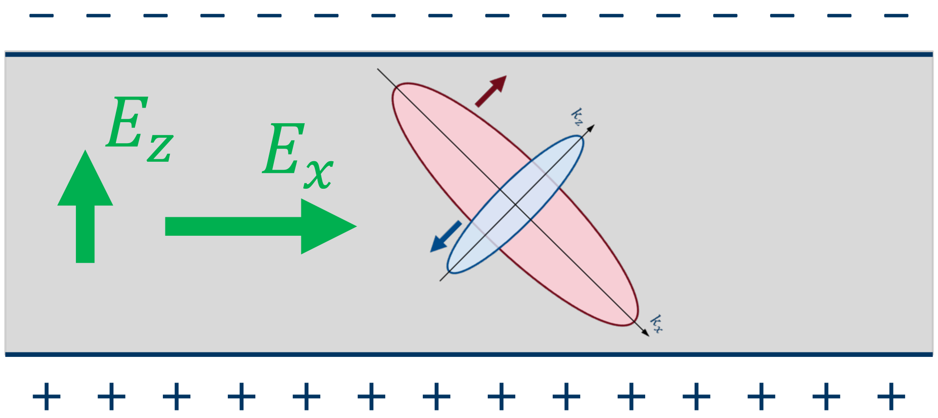


❑ Is this also possible in ferromagnets without spin-orbit coupling?

Transverse spin current in an anisotropic ferromagnet



Film or multilayer geometry: $j_z = 0$

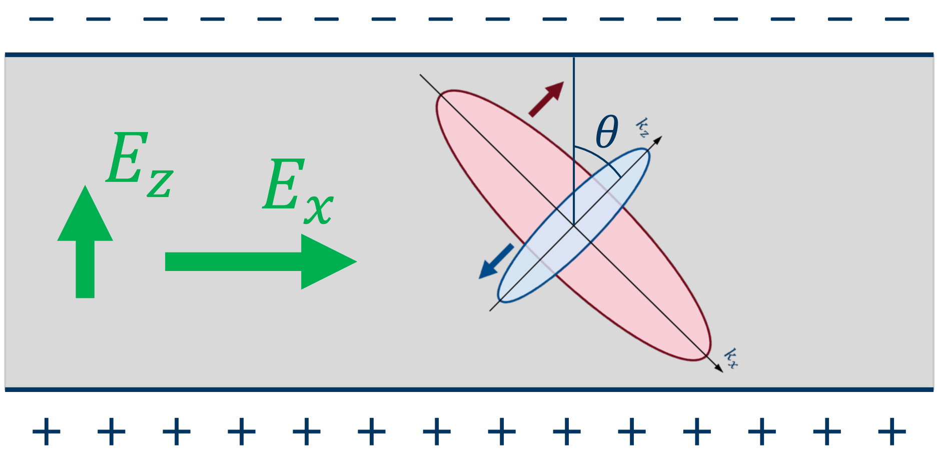


$$j_x^\uparrow = \sigma_{xx}^\uparrow E_x + \sigma_{xz}^\uparrow E_z, \text{ etc.}$$

- Anisotropic bulk ferromagnet: transverse charge and spin currents for a generic orientation of **E**

Impose $j_z = 0$ and find $\theta_{\mathrm{SH}} = j_{sz}/j_x$

Spin Hall angle in a ferromagnetic film with open boundary conditions



Under open boundary conditions:

$$\theta_{\mathrm{SH}} = \frac{1}{2}(\beta_1 - \beta_2)\sin 2\theta$$

$$\beta_i = \frac{\sigma_i^{\uparrow} - \sigma_i^{\downarrow}}{\sigma_i^{\uparrow} + \sigma_i^{\downarrow}}$$

$i = 1,2,3$ (principal axis)

$$|\theta_{\mathrm{SH}}| \leq 1$$

- Source of pure transverse spin current due to anisotropic transport spin polarization
- Warning: $j_z = 0$! This is not a spin-polarized transverse charge current!
- Spin current profile must be determined from spin-diffusion theory for the multilayer

Anisotropy of transport spin polarization

- Response is purely extrinsic without SOC
- Relaxation time approximation (weak to moderate disorder)

$$\sigma_{\alpha\beta}^{\lambda} = e^2 \sum_n \int v_{n\alpha}^{\lambda} v_{n\beta}^{\lambda} \tau_n^{\lambda} \frac{\partial f(E_n^{\lambda})}{\partial \mu} \frac{d^3k}{(2\pi)^3}$$

$$\beta_i = \frac{\sigma_i^{\uparrow} - \sigma_i^{\downarrow}}{\sigma_i^{\uparrow} + \sigma_i^{\downarrow}} \qquad P_\tau = \frac{\tau_{\uparrow} - \tau_{\downarrow}}{\tau_{\uparrow} + \tau_{\downarrow}}$$

Assume τ depends only on spin: $\sigma_{\alpha\beta}^{\lambda} = e^2 \tau_\lambda K_{\alpha\beta}^{\lambda}$

$$P_i = \frac{K_i^{\uparrow} - K_i^{\uparrow}}{K_i^{\uparrow} + K_i^{\uparrow}}$$

$$\beta_1 - \beta_2 = \frac{(1 - P_\tau^2)(\boldsymbol{P_1 - P_2})}{(1 + P_1 P_\tau)(1 + P_2 P_\tau)}$$

$i = 1,2,3$ (principal axis)

- P_τ is usually unknown but is not decisive for $\beta_1 - \beta_2$
- $P_1 - P_2$ is a good descriptor to search for large $\theta_{\mathrm{SH}} \propto \beta_1 - \beta_2$

$$\theta_{\mathrm{SH}} = \frac{1}{2}(\beta_1 - \beta_2) \sin 2\theta$$

Screening pool of ferromagnets

Include (from Materials Project):

- Binary or ternary
- Tetragonal, hexagonal, or orthorhombic
- Has a 3d element (V–Ni)
- Metallic, magnetic DFT ground state

Exclude:

- Actinides or (mostly) rare earths
- No experimental reports of a magnetic phase
- ($\theta_{\mathrm{SH}} \ll 1$) half-metallic; quasi-2D; weak FM
- Very large unit cells

41 FM/FiM compounds

Tetragonal

Formula	T_C (K)
FePt	753
FePd	1193
CoPt	846
MnAl	650
MnGa	629
FeNi	842
Fe_2B	1013
Co_2B	433
$MnAu_4$	385
VAu_4	60
Mn_2Sb	580
Fe_3B	828
Fe_3P	693
Fe_8N	1500
Mn_2Ga_5	450
$Be_{12}Cr$	50
MnAlGe	520
Fe_5B_2P	628

Hexagonal

Formula	T_C (K)
CrTe	340
MnBi	633
Fe_2P	217
Fe_3N	858
YCo_5	980
MnAs	318
MnSb	851
$ZrFe_2$	630
$HfFe_2$	600
Fe_3Ge	670
Fe_3Sn	748
YFe_3	552
Fe_5Si_3	383
Mn_5Ge_3	296

Orthorhombic

Formula	T_C (K)
MnP	293
FeB	598
Mn_3Sn_2	262
Fe_3B	828
Fe_3C	480
Co_3B	747
Co_3C	498
GdNi	78
$AlFe_2B_2$	285

Estimated spin Hall angles (for $P_\tau = 0$)

Compound	P_x	P_z	$\lvert\theta_{SH}\rvert$	Suggested substrate	MCIA (Å²)
MnGa	0.07	0.64	0.29	**$NdGaO_3$(011)/(101)**	49
MnSb	0.91	0.33	0.29	MgF_2(110)/(10-11)	82
MnAl	0.05	0.55	0.25	**$NdGaO_3$(011)/(101)**	49
MnAlGe	0.42	0.88	0.23	**a-TiO_2(101)/(101)**	83
MnAs	0.75	0.29	0.23	GaN(10-11)/(10-11)	116
Mn_2Sb	0.35	-0.09	0.22	MgF_2(101)/(111)	78
MnBi	0.86	0.42	0.22	WTe_2(0001)/(10-11)	89
$Be_{12}Cr$	-0.13	-0.54	0.21		
CrTe	0.30	0.68	0.19	$LiAlO_2$(110)/(10-11)	90
Fe_2B	0.37	0.06	0.16	$LiGaO_2$(010)/(101)	33
Fe_3Ge	0.16	0.46	0.15	Cu(100)/(10-11)	
YFe_3	-0.08	0.21	0.15		
Fe_5Si_3	0.51	0.20	0.15	GaAs(100)/(11-21)	67
Co_2B	0.34	0.63	0.14	$LiGaO_2$(010)/(101)	32
Mn_2Ga_5	0.47	0.20	0.14	TiO_2(100)/(101)	83
Fe_3B	0.47	0.70	0.12		
Fe_8N	0.03	0.26	0.12	$BaTiO_3$(110)/(101)	48
$HfFe_2$	-0.26	-0.05	0.10	MgO(100)/(11-21)	72
Fe_3Sn	0.72	0.52	0.10	$LaAlO_3$(100)/(10-11)	70
CoPt	0.23	0.07	0.08	**$YAlO_3$(011)/(101)**	51
Fe_2P	0.28	0.43	0.07	LiF(110)/(10-11)	71
Fe_3N	-0.14	-0.01	0.07	C(0001)/(11-21)	79
YCo_5	0.51	0.63	0.06	GaN(10-11)/(10-11)	57
Mn_5Ge_3	0.54	0.66	0.06	BaF_2(100)/(11-21)	76
FePt	0.34	0.24	0.05	**$NdGaO_3$(011)/(101)**	51
FeNi	0.27	0.36	0.04	BN(0001)/(101)	11
FePd	0.37	0.31	0.03	**$NdGaO_3$(011)/(101)**	51
Fe_3P	0.70	0.77	0.03	Fe_2O_3(0001)/(101)	91
Fe_5B_2P	0.23	0.17	0.03	$GdScO_3$(001)/(101)	64
$MnAu_4$	0.45	0.49	0.02	GaSe(0001)/(101)	51
VAu_4	-0.54	-0.58	0.02		
$ZrFe_2$	-0.38	-0.41	0.02		

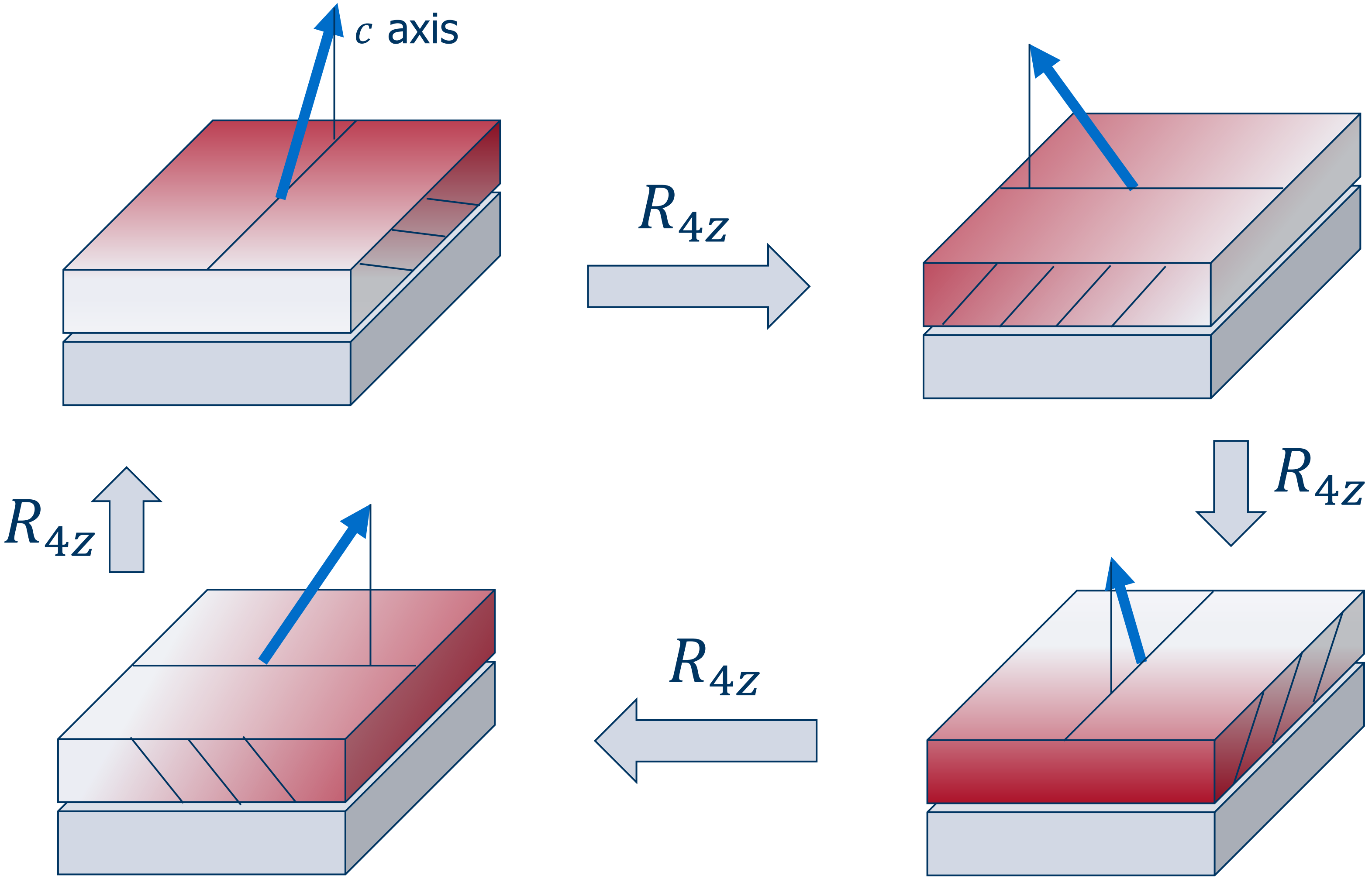
63%: $\tilde{\theta}_{SH} > 0.1$
29%: $\tilde{\theta}_{SH} > 0.2$
Comparable to the best heavy-metal sources (Pt, W)

- Substrate is needed to support misaligned growth
- Many such substrates allow orientation domains
- Highlighted: macroscopic SHE for a uniformly magnetized film (finite average over orientation domains)

MCIA: minimal coincident area

Orientation domains on a substrate

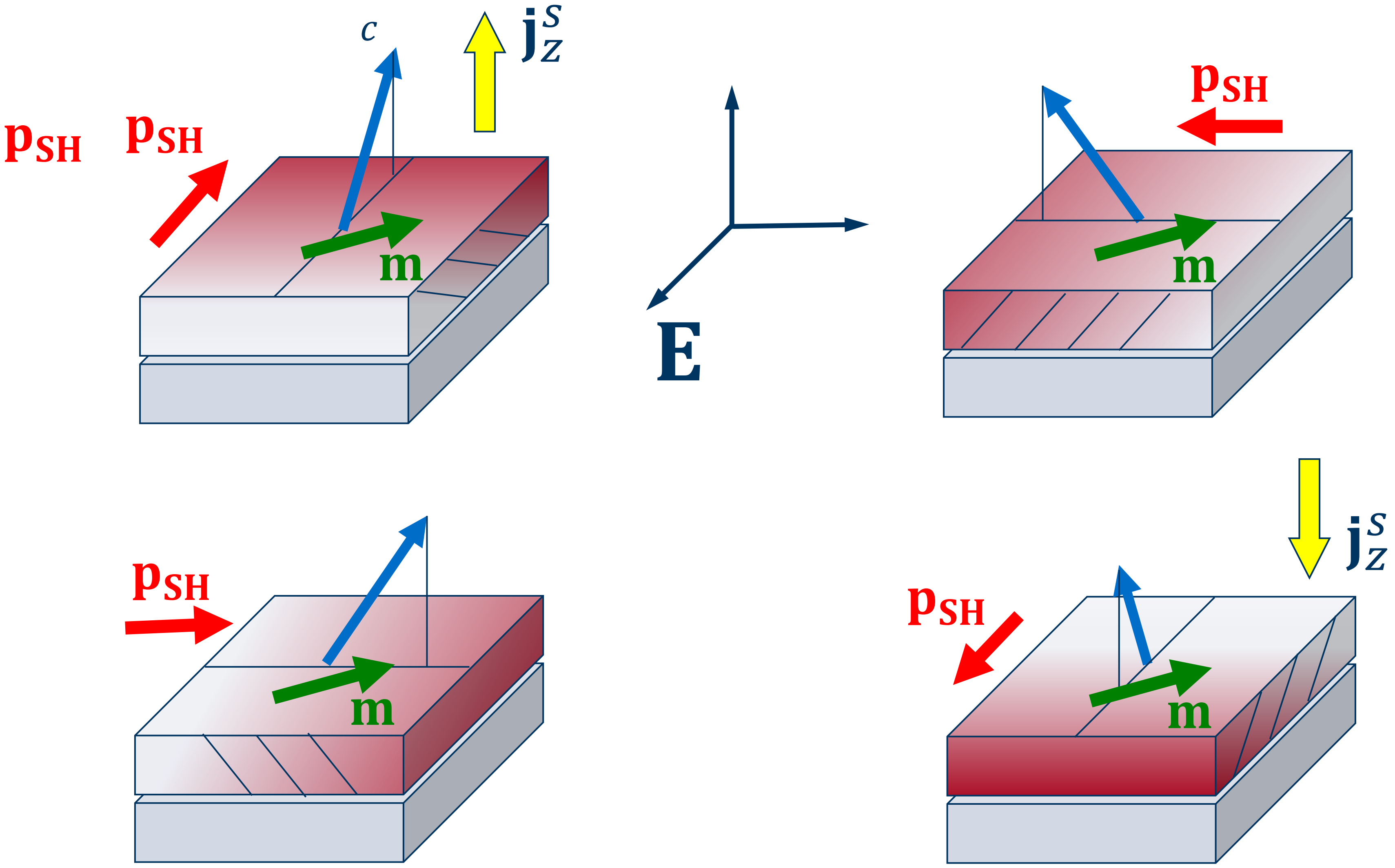
<u>Example</u>: C_{1v} ferromagnet on a C_{4v} substrate with a coincident mirror plane



Four orientation domains are generated by the elements of the point group of the substrate (C_{4v})

Spin Hall domains (uniform magnetization)

$\sigma^i_{jk} = m_i \tilde{\sigma}_{jk}$, $\tilde{\sigma}_{jk} \rightarrow \mathbf{p}_{\mathrm{SH}}$ (response of $\mathbf{j}^s_z$ to in-plane $\mathbf{E}$ if no SOC)



Spin current ⊥ film plane:

$$\mathbf{j}^s_z = \mathbf{m}\left(\mathbf{p}^{(i)}_{\mathrm{SH}}\mathbf{E}\right)$$

In this example $\left\langle \mathbf{p}^{(i)}_{\mathrm{SH}} \right\rangle = 0$,

no macroscopic SHE

But macroscopic SHE is possible for low symmetry groups

Examples:

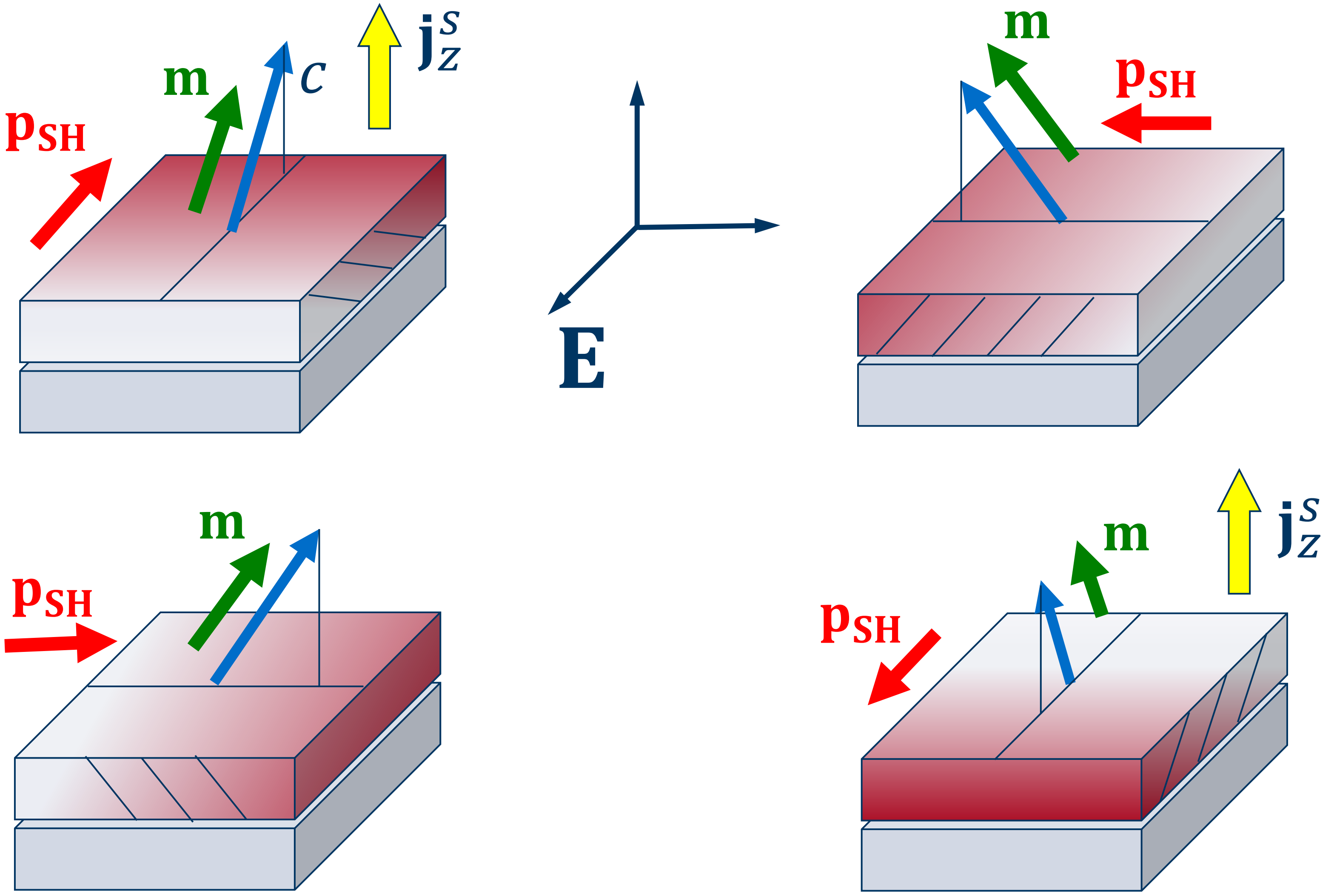
FePt(101)/$NdGaO_3$(011)

MnAlGe(101)/anatase-TiO_2(101)

FeB(110)/$LiGaO_2$(001)

Spin Hall domains (strong anisotropy)

Assume **m** is parallel to the c axis (strong anisotropy) and magnetized "up"



Spin current ⊥ film plane:

$$\mathbf{j}_z^s = \mathbf{m}\left(\mathbf{p}_{\mathrm{SH}}^{(i)}\mathbf{E}\right)$$

$\left\langle \mathbf{m}^{(i)} \otimes \mathbf{p}_{\mathrm{SH}}^{(i)} \right\rangle \neq 0$

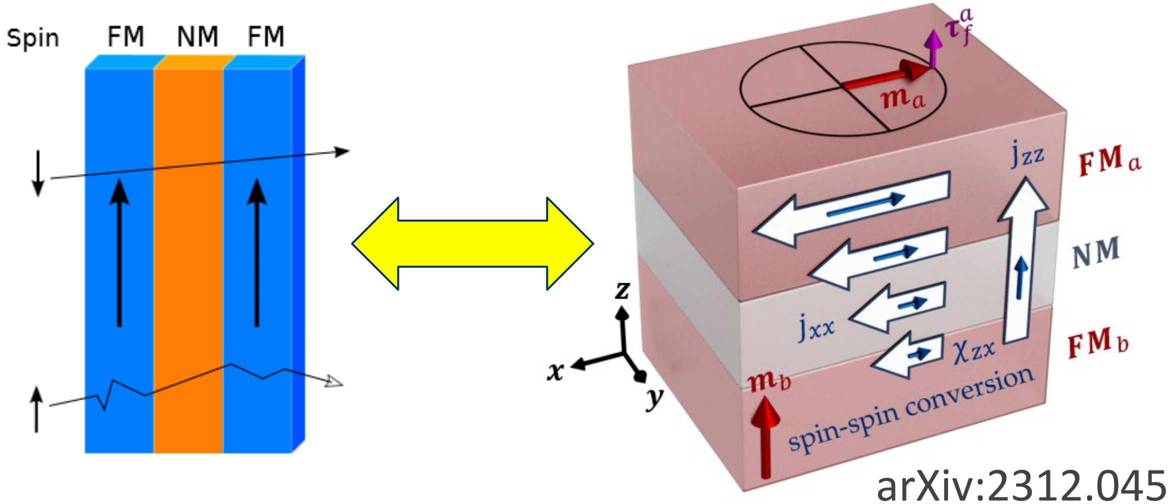
for any substrate,
finite macroscopic SHE

Exchange-driven SHE in FM: Conclusions

- Crystalline FM layer with tilted axes generates pure transverse spin current without SOC (similar to spin-splitting effect in altermagnets)
- Typical spin Hall angles: 0.1-0.2
- Orientation domains are a practical concern, but sufficiently low substrate/magnet symmetries allow macroscopic spin Hall effect for a uniformly magnetized film
- Strong magnetocrystalline anisotropy: macroscopic SHE for any substrate
- SOT-like 3-terminal device configuration without SOC

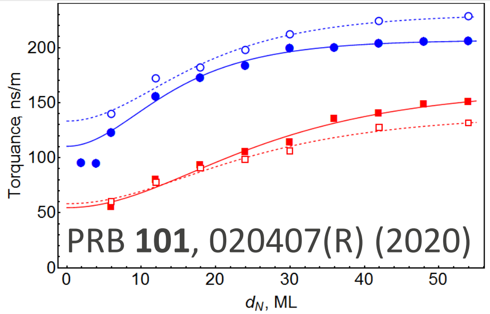
arXiv:2310.13688

Summary



arXiv:2312.04538

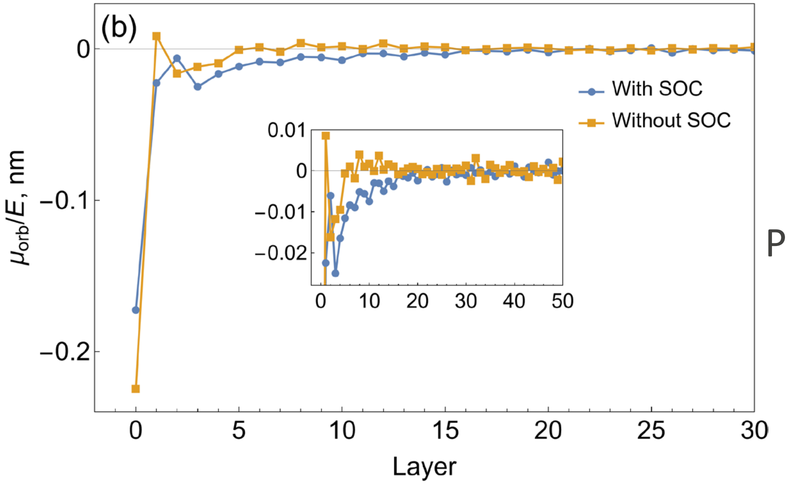
Indirect spin current generation in F/N/F
at $t_N \sim \lambda_{\mathrm{mfp}}$ results in spin-rotated FL SOT



PRB **108**, 144433 (2023)

E	V_m (mRy)	ρ (μΩ cm)	λ (nm)	l_{sf}^L (nm)	l_{sf}^T (nm)
E_F	40	15.8	3.0	7.7	1.35
E_F	60	30.4	1.6	3.3	1.47
E_F	80	43.1	1.1	2.0	1.26

Breakdown of spin-diffusion model near
Pt surface; non-diffusive length scale l_{sf}^T



PRB **108**, 144433 (2023)

No long-range orbital accumulation w/o SOC

arXiv:2310.13688

3-terminal SOT-like device with
exchange-driven transverse
spin current from crystalline FM
layer, possibly PMA switching