

Materials dependence of the spin-transfer torques on DW

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Outline

- Introduction
- Two approaches to STT
- STT in spin valves
- Gilbert Damping
- Summary

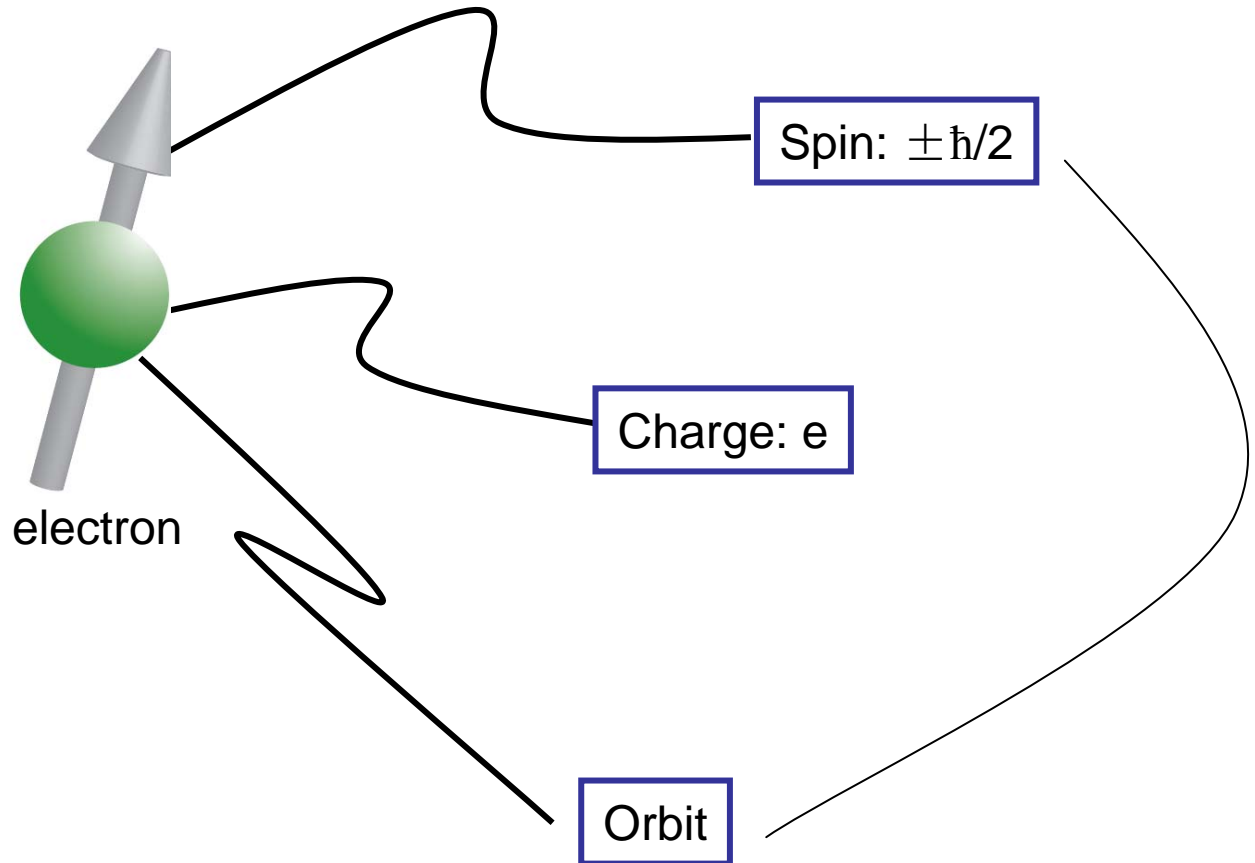
Dirac equation

Electron should have “spin.”

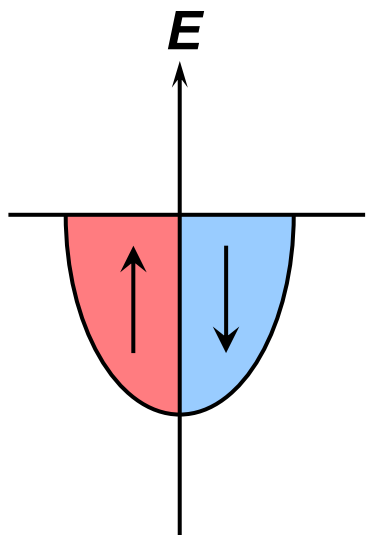
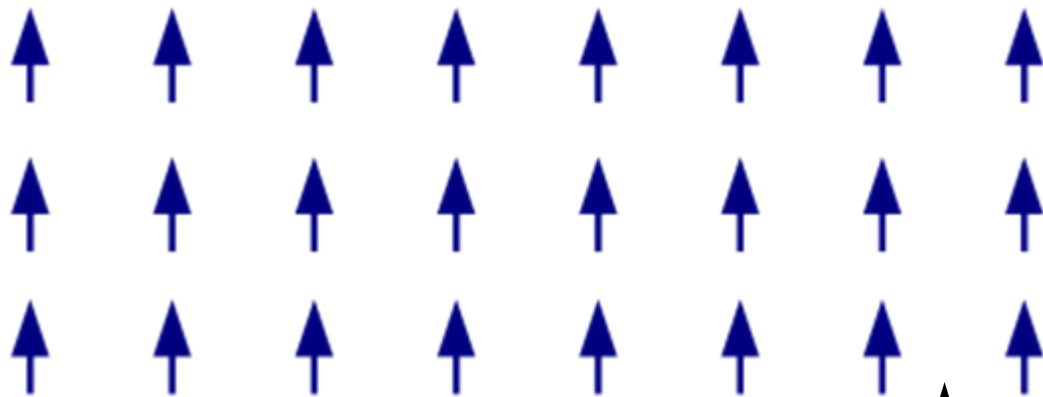
(1928)



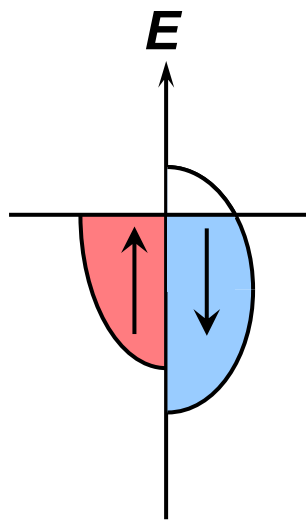
P.A.M. Dirac



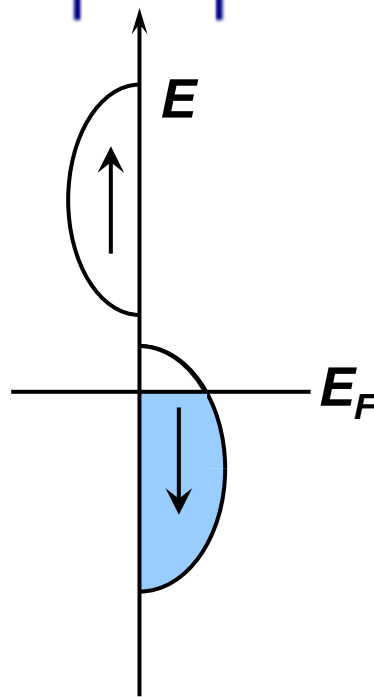
Ferromagnetism



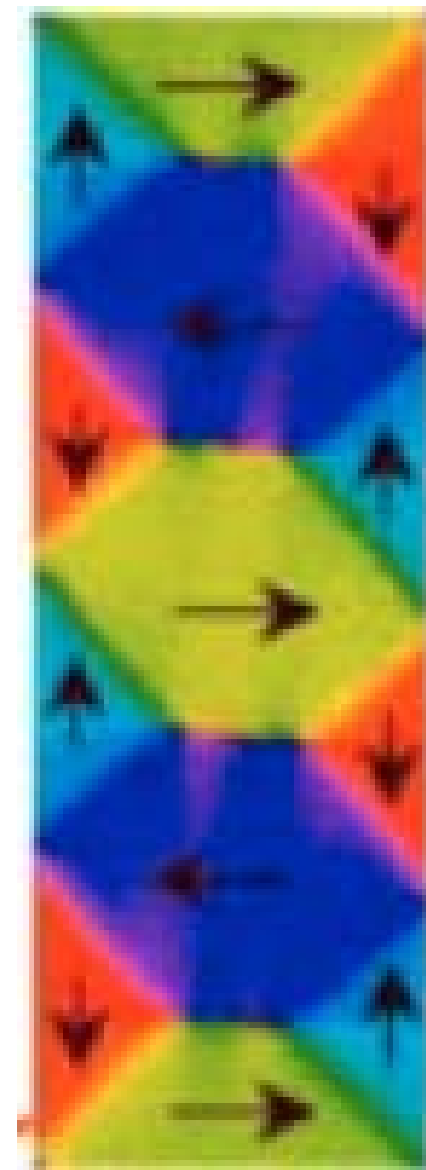
正常金属



铁磁金属



自旋半金属



L. Thomas *et al.*,
(2000).

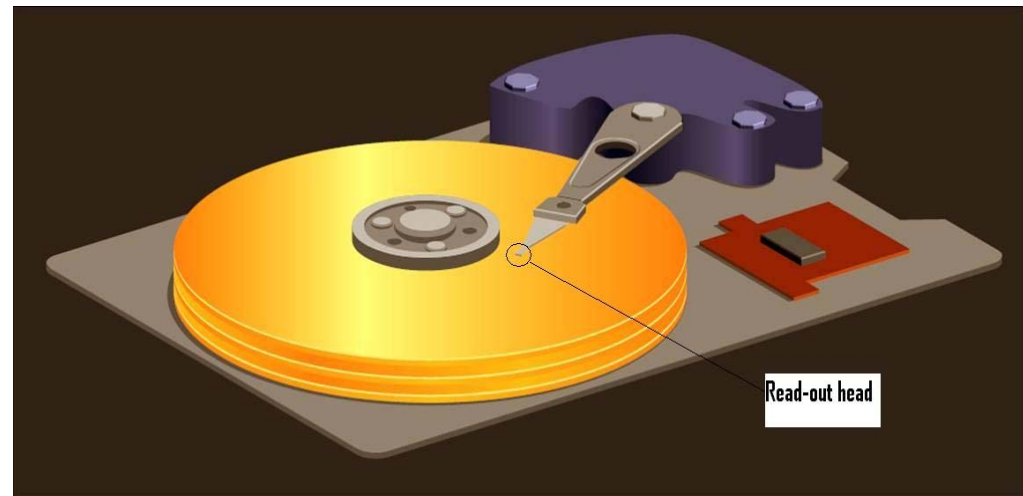
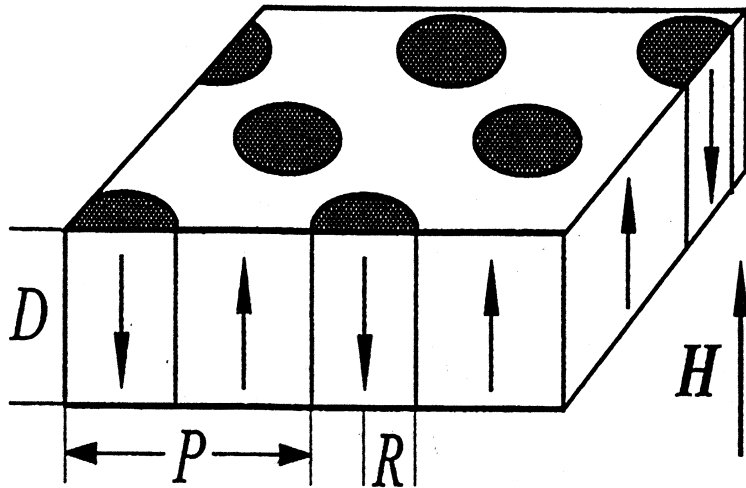
Faraday effect---Maxwell Equation (1865)



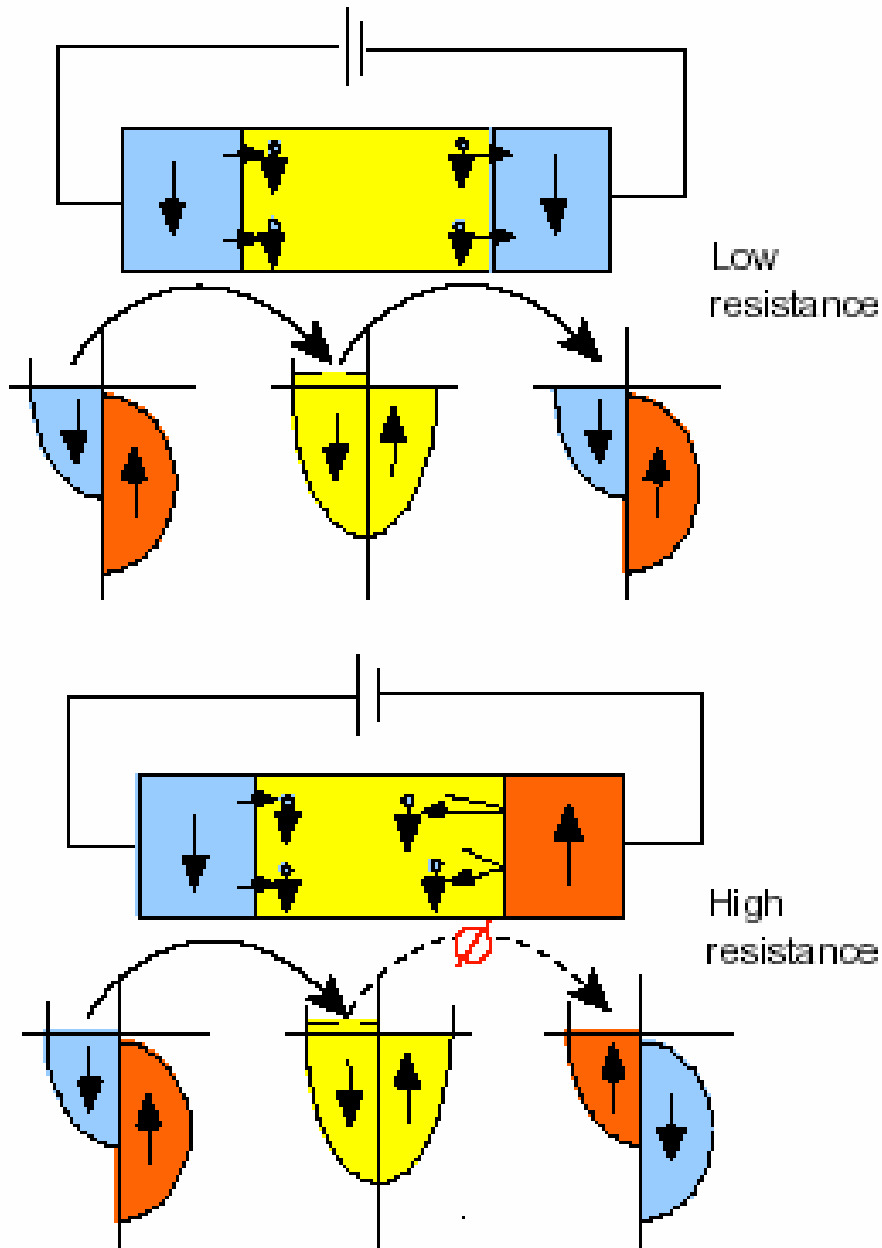
M. Faraday

Faraday's law:

$$\mathcal{E} = -\frac{d\Phi}{dt} \quad (1831)$$

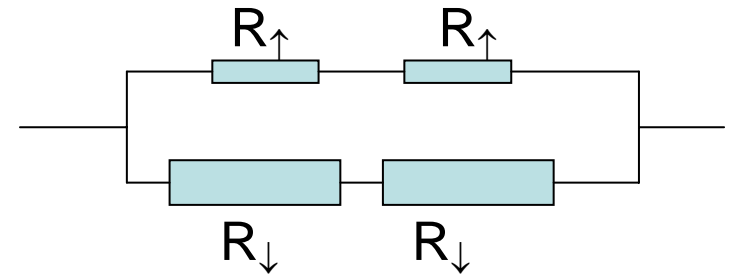


Spin bottleneck magnetoresistance

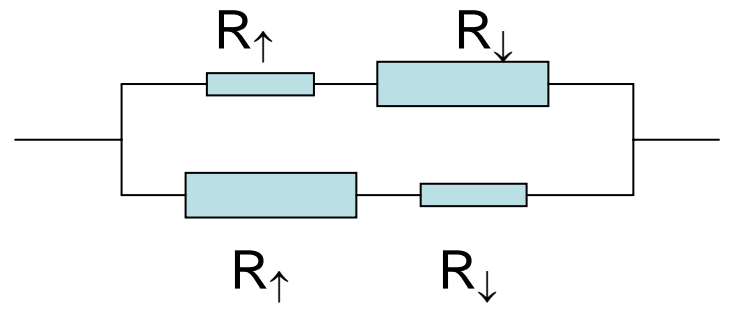


$$MR = \frac{R^{AP} - R^P}{R^P} = \frac{(R_{\uparrow} - R_{\downarrow})^2}{4R_{\uparrow}R_{\downarrow}}$$

spin
↑
↓

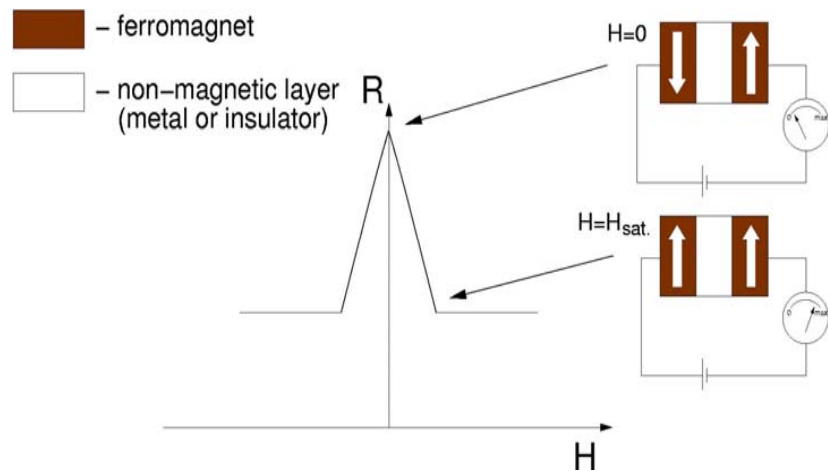


↑
↓

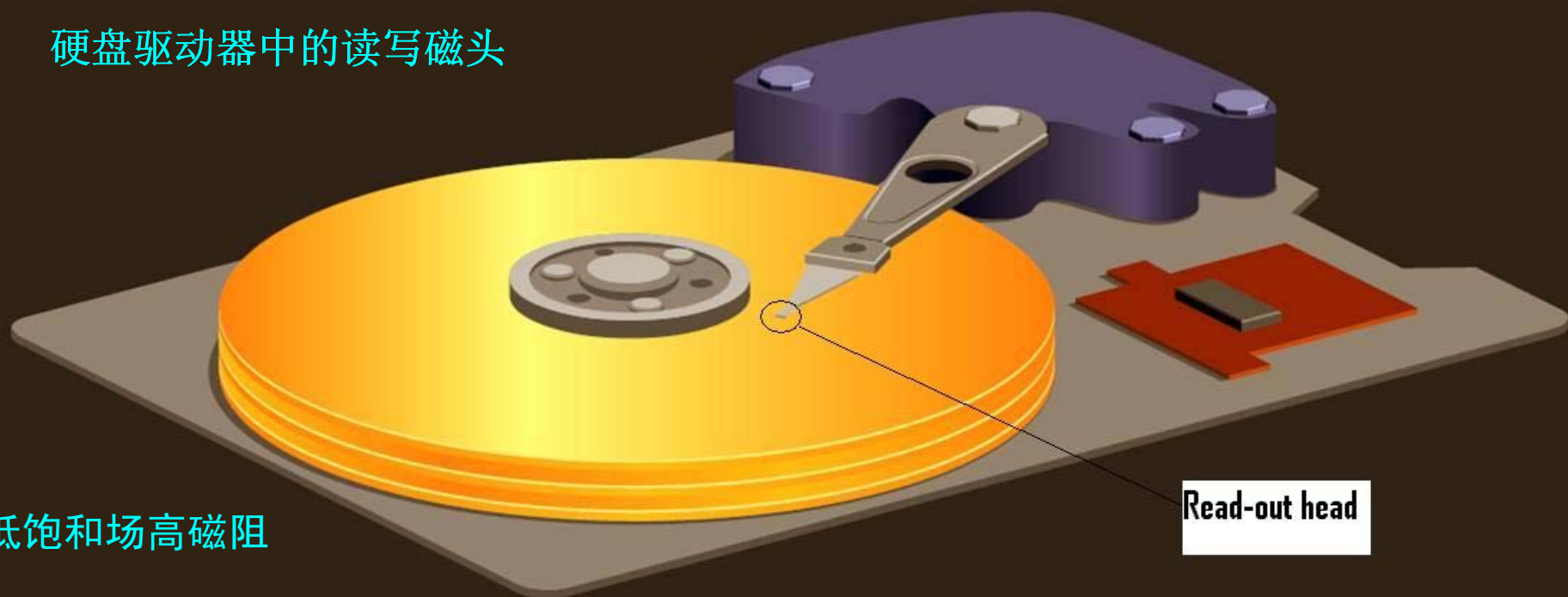


磁矩对电子的散射---GMR

自旋阀-GMR

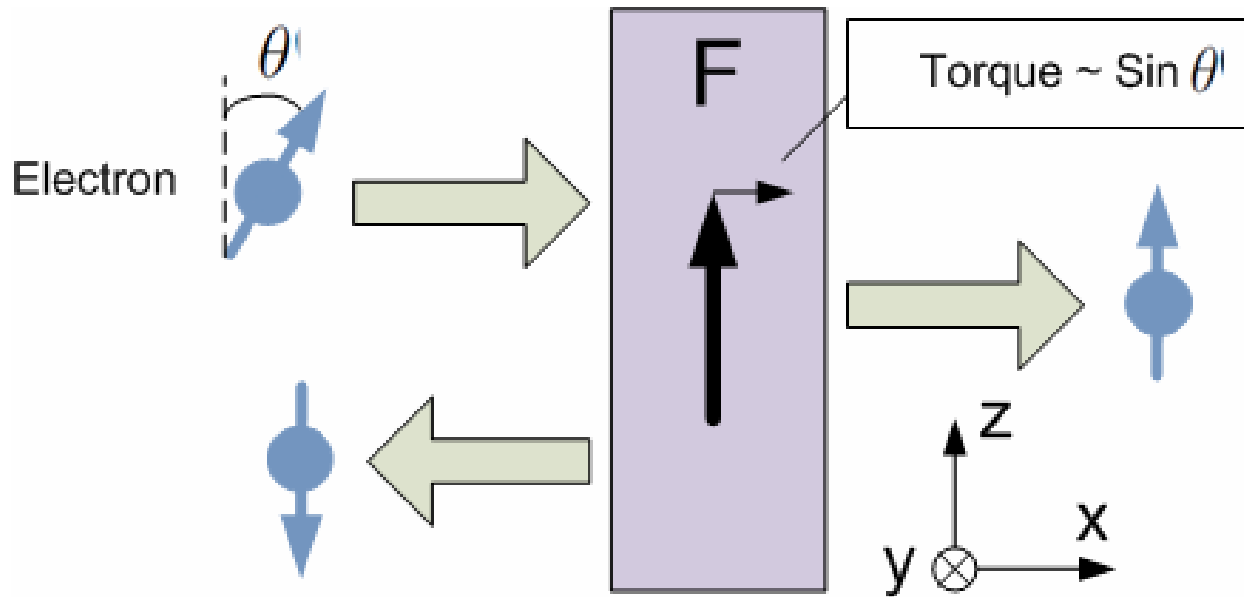


硬盘驱动器中的读写磁头



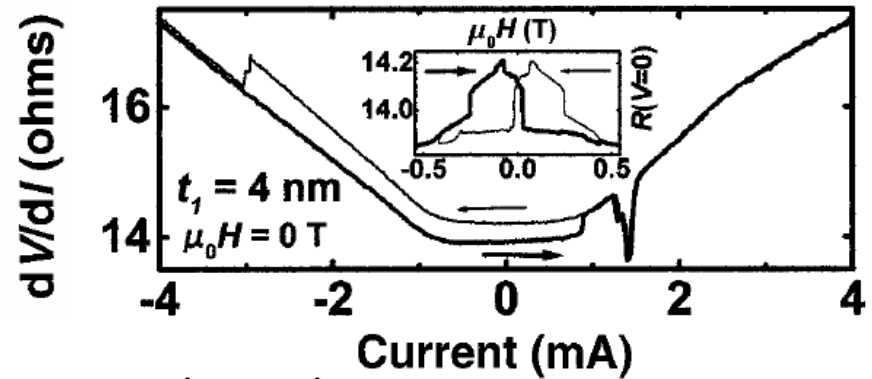
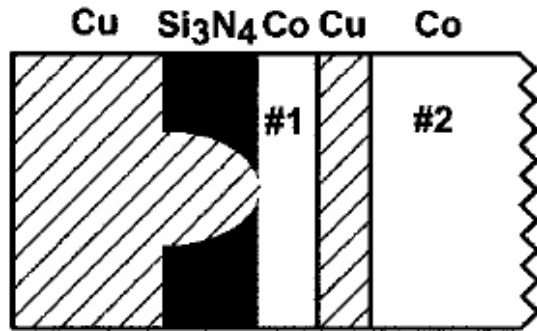
Schematic of exchange torque generated by spin-filtering

$$|\psi_{in}\rangle = \frac{e^{ik_{\uparrow}x}}{\sqrt{k_{\downarrow}}} \cos\left(\frac{\theta}{2}\right) |\uparrow\rangle + \frac{e^{ik_{\downarrow}x}}{\sqrt{k_{\downarrow}}} \sin\left(\frac{\theta}{2}\right) |\downarrow\rangle$$

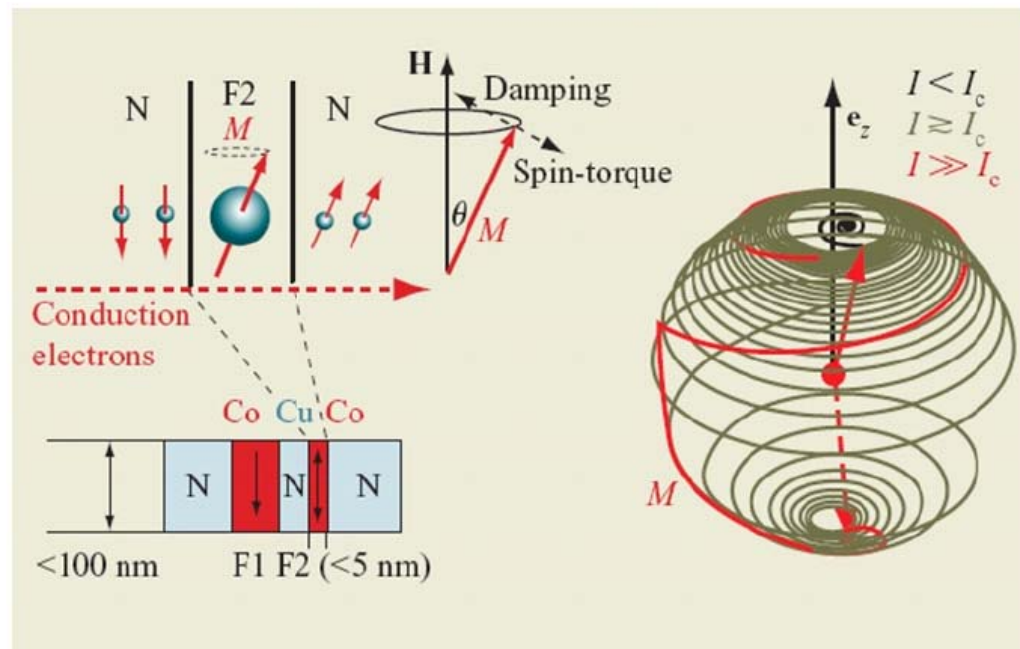


$$|\psi_r\rangle = \frac{e^{-ik_{\downarrow}x}}{\sqrt{k_{\downarrow}}} \sin\left(\frac{\theta}{2}\right) |\downarrow\rangle \quad |\psi_t\rangle = \frac{e^{ik_{\uparrow}x}}{\sqrt{k_{\uparrow}}} \cos\left(\frac{\theta}{2}\right) |\uparrow\rangle$$

Spin-transfer torques effects (1999)



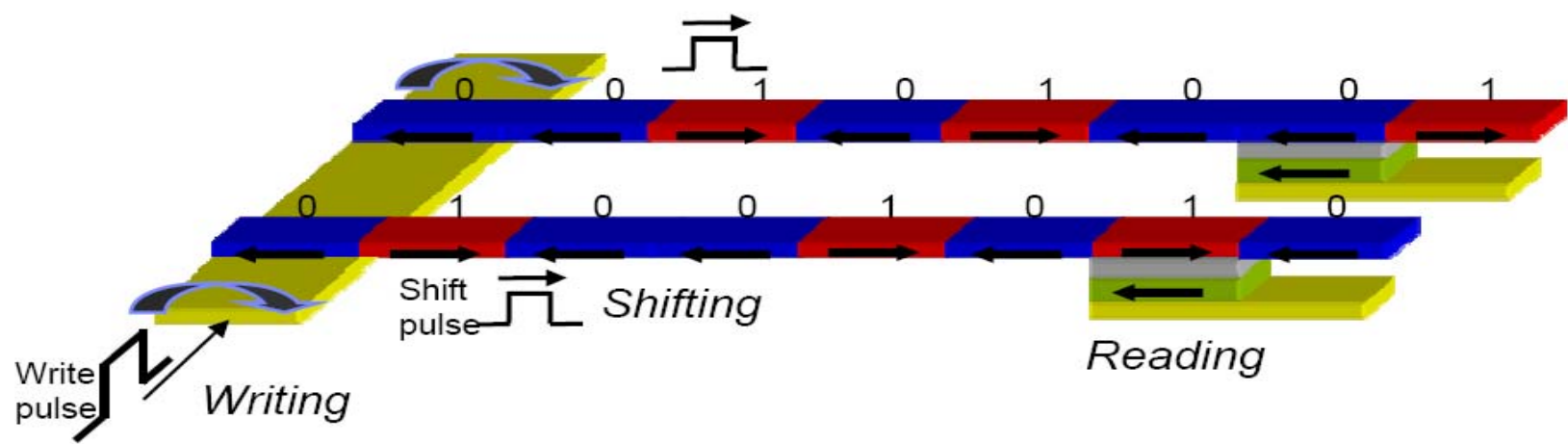
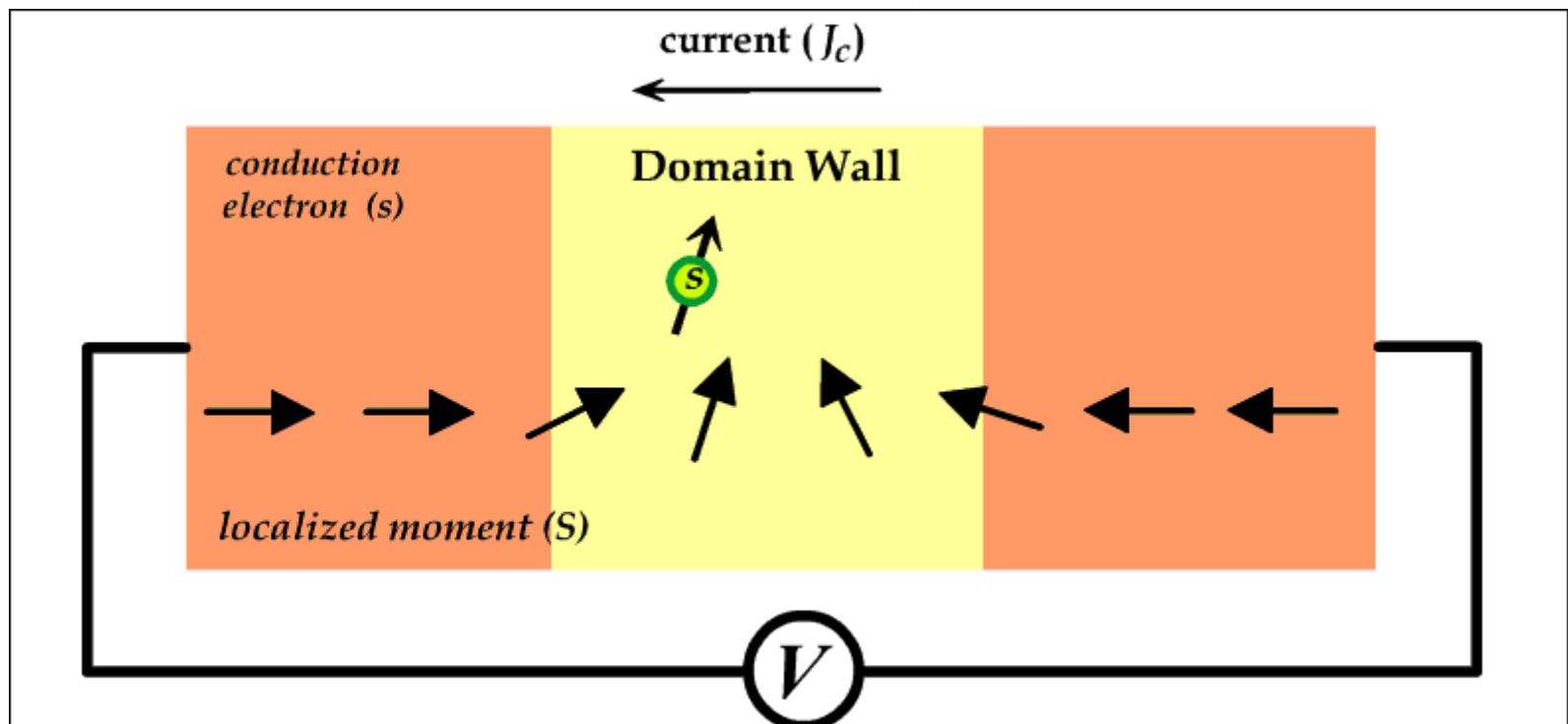
Myers, et al., Science 285,867 (1999)



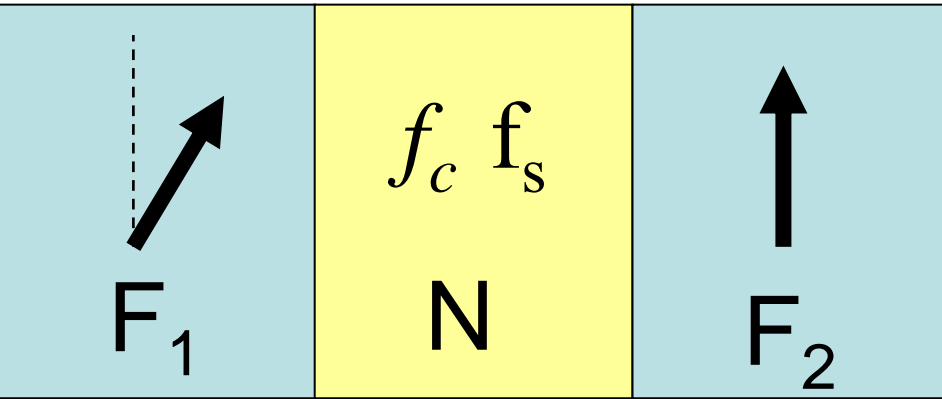
Sun, IBM J. Res. & Dev. 50, 81(2006)

Current-driven domain wall motion:

$$\theta = 2 \cot^{-1} e^{-(z-z_0)/w}$$



Circuit theory (Batraas2001)



Boundary condition

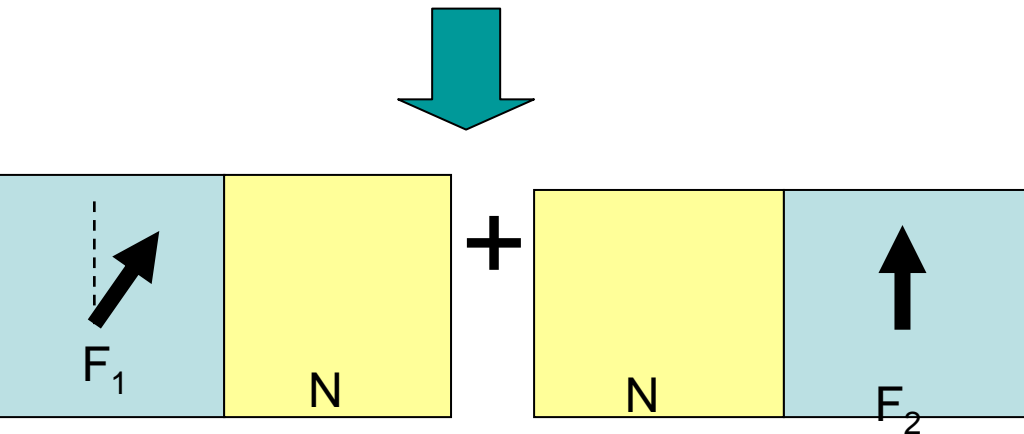
Charge current $I_1 = I_2$

Spin current $\mathbf{I}_{s1} = \mathbf{I}_{s2}$



Charge accumulation f_c
Spin accumulation f_s

In-plane torque $\tau = \frac{\hbar}{2e} (\mathbf{I}_{s1} - \mathbf{I}_{s1} \cdot \mathbf{m}_2)$



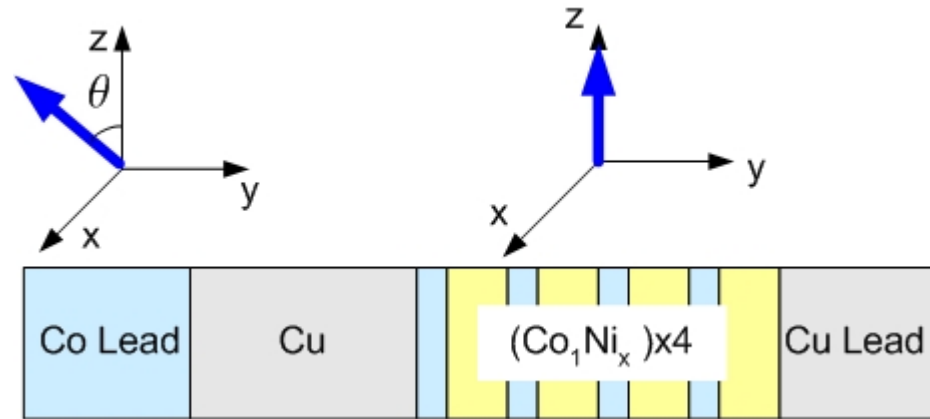
Current and spin current for F_1/N

$$I_1 = (G^\uparrow + G^\downarrow) (f_c^{F1} - f_c^N) + (G^\uparrow - G^\downarrow) (f_s^{F1} - \mathbf{m}_1 \cdot \mathbf{s} f_s^N)$$

$$\mathbf{I}_{s1} = (G^\uparrow + G^\downarrow) (f_c^{F1} - f_c^N) \mathbf{m}_1 + (2\text{Re}G^{\uparrow\downarrow} - G^\uparrow - G^\downarrow) \mathbf{m}_1 \cdot \mathbf{s} f_s^N \mathbf{m}_1 - 2\text{Re}G^{\uparrow\downarrow} \mathbf{s} f_s^N + 2\text{Im}G^{\uparrow\downarrow} f_s^N \mathbf{m}_1 \times \mathbf{s}$$

Methods

First principles approach to spin transfer torques



- First-principles tight-binding LMTO
- Green function method for layered systems.
- Large system with the number of atoms > 1000

Spin current:

$$\hat{\mathcal{J}} \equiv \frac{1}{2} \left[\hat{\sigma} \otimes \hat{\mathbf{V}} + \hat{\mathbf{V}} \otimes \hat{\sigma} \right]$$

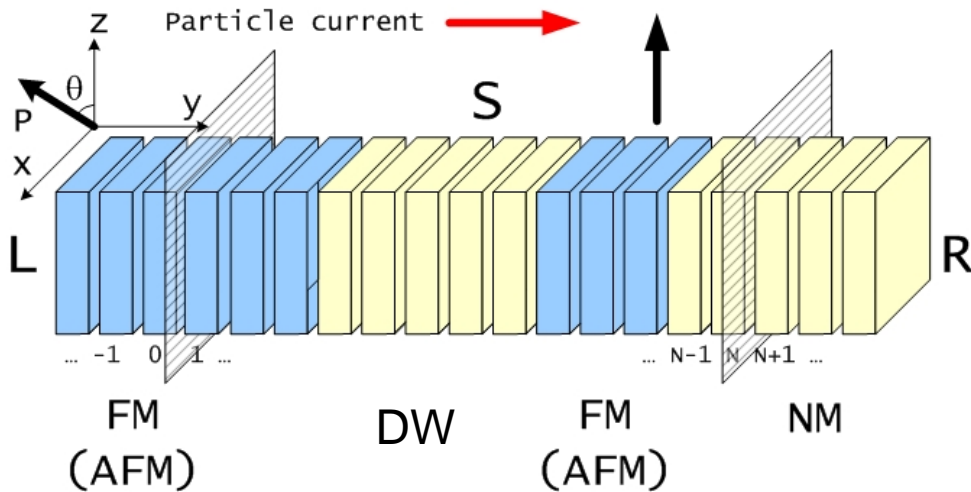
Spin torque from one lead:

$$\langle \hat{\mathbf{T}}_{\mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle = \sum_{\mathbf{R}' \in I-1, I} \langle \hat{\mathcal{J}}_{\mathbf{R}', \mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle - \sum_{\mathbf{R}' \in I, I+1} \langle \hat{\mathcal{J}}_{\mathbf{R}, \mathbf{R}'}^s(\mathbf{k}_{\parallel}) \rangle$$

Spin torque on atom R:

$$\mathbf{T}_{\mathbf{R}} = \left(\frac{\hbar}{2} \right) \frac{e}{2h} \frac{1}{N_{\parallel}} \sum_{s, \mathbf{k}_{\parallel}} \left[\langle \hat{\mathbf{T}}_{\mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle_{\mathcal{L}} - \langle \hat{\mathbf{T}}_{\mathbf{R}}^s(\mathbf{k}_{\parallel}) \rangle_{\mathcal{R}} \right] V_b$$

First principles approach to spin transfer torques



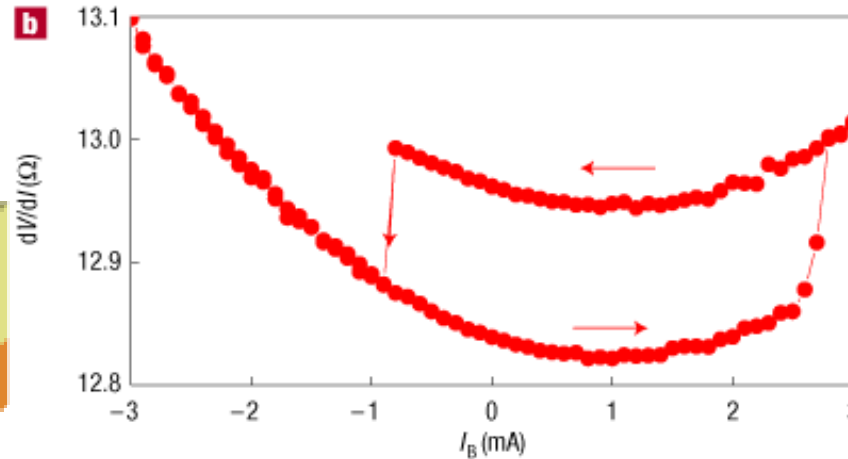
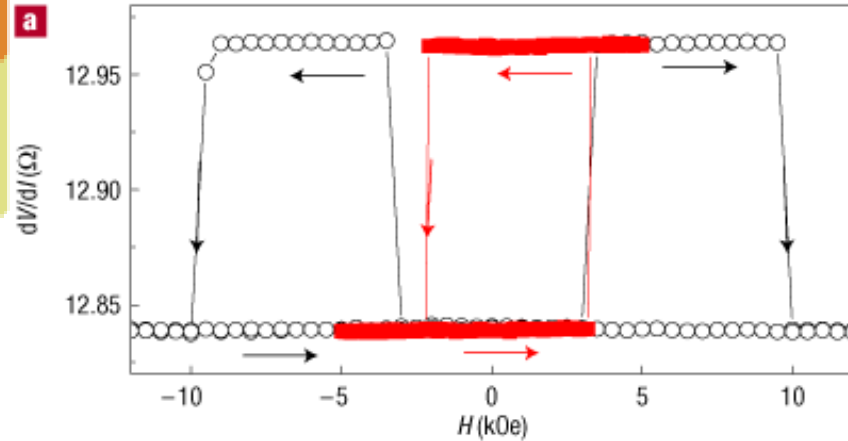
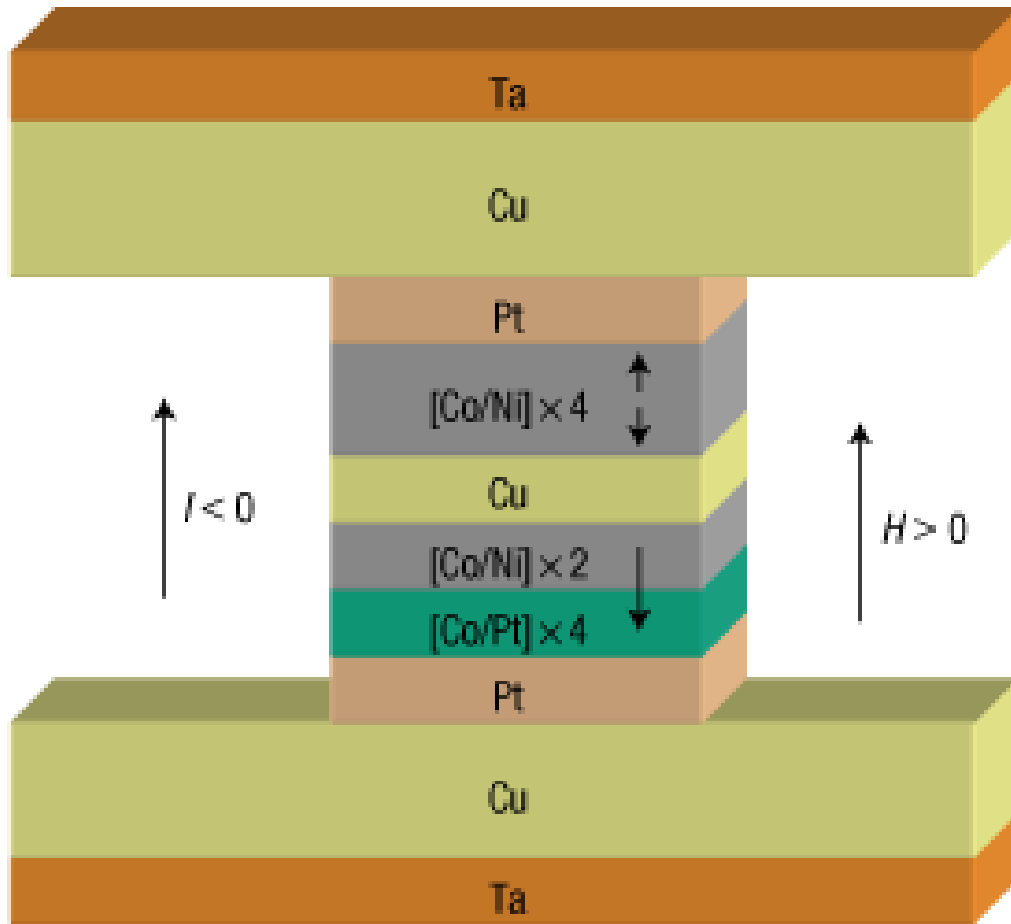
$$\tau \propto \langle \vec{S} \rangle \times \dot{\vec{M}}$$

- TB LMTO
- Green function method
- NEGF if necessary
- Order& disorder

Linear equations of system

$$\begin{pmatrix} C_0 \\ C_1 \\ C_2 \\ \dots \\ C_N \\ C_{N+1} \end{pmatrix} = (\mathbf{U}\mathbf{P}\mathbf{U}^+ - \tilde{\mathbf{S}})^{-1} \begin{pmatrix} S_{0,-1}[\mathbf{F}_L^{-1}(+) - \mathbf{F}_L^{-1}(-)]C_0(+) \\ 0 \\ 0 \\ \dots \\ 0 \\ 0 \end{pmatrix}$$

Perpendicular Magnetized CoNi film



S.MANGIN et.al, Nature materials vol5,210, (2006) , D.Ravelosona, et.al, APL 90,072508 (2007), D.Ravelosona, et.al, PRL 96,186604(2006), D.Ravelosona, et.al, J.Phys.D: Appl.Phys.40,1253(2007)

Co|Ni interface

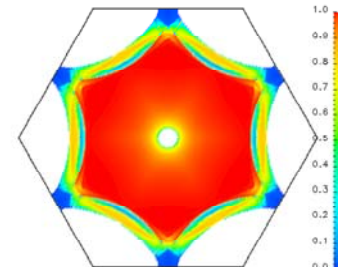
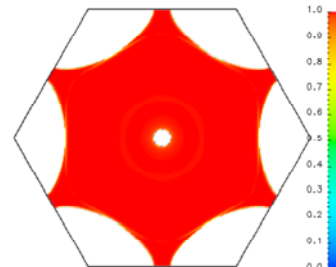
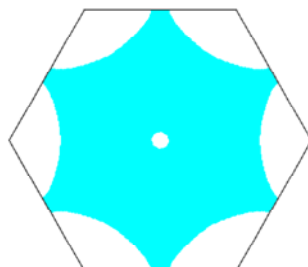
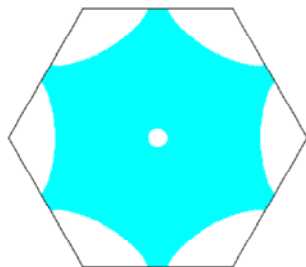
Co

Ni

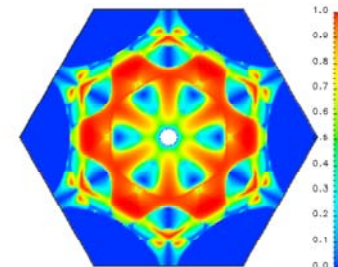
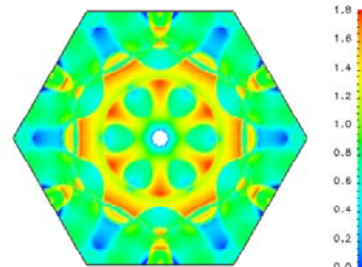
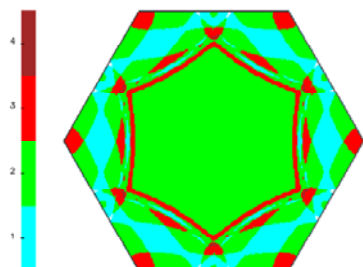
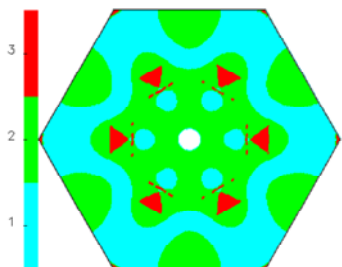
P

AP

Maj.



Min.



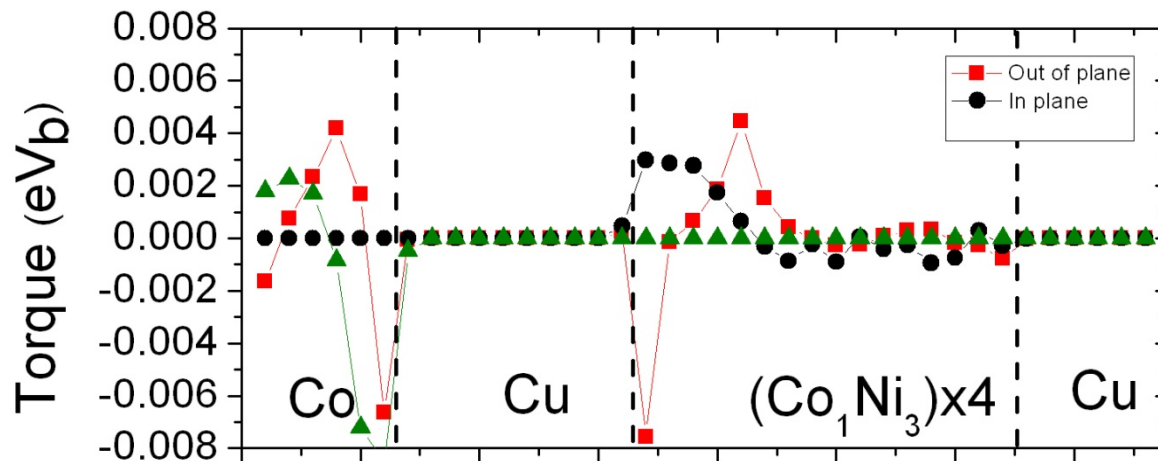
lattice constants	Configuration	AR(maj.)	AR(min.)	Gamma
Co(3.549)	P	0.0147	0.7251	0.9604
	AP	1.1585	2.1302	0.2955
Ni(3.524)	P	0.0242	0.7276	0.9357
	AP	1.1927	2.0679	0.2684
(Co+Ni)/2	P	0.0187	0.7310	0.9502
	AP	1.1567	2.1054	0.2908

Interface resistance for Co|Ni(111)

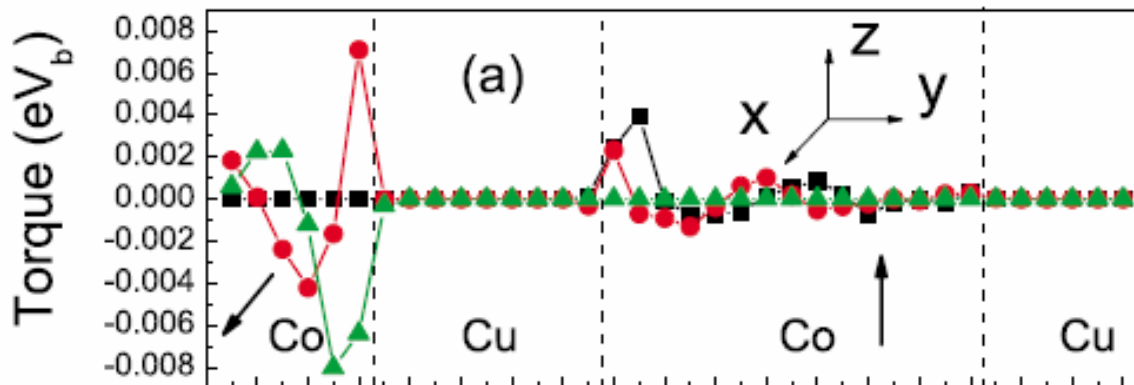
AR unit $\mathbf{f}^{-1}\Omega^{-1}\mathbf{m}^{-2}$ $\mathbf{Gamma} = \frac{AR_{\downarrow} - AR_{\uparrow}}{AR_{\uparrow} + AR_{\downarrow}}$

Lattice constant		AR(maj.)	AR(min.)	Gamma
Co	3.54 9	0.014664	0.725067	0.960353
Ni	3.52 4	0.0241504	0.727603	0.935749
$\frac{1}{2}(\text{Co}+\text{Ni})$	3.53 7	0.0186835	0.730984	0.950155

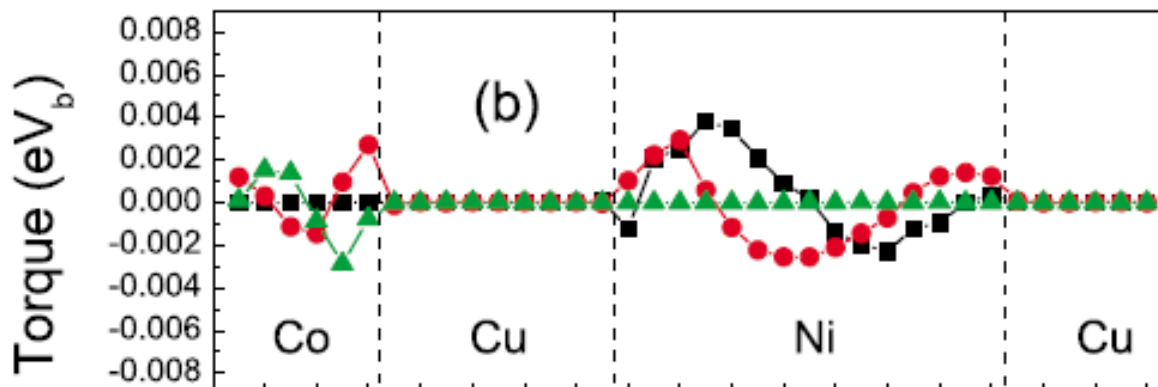
Co_1Ni_3



Co



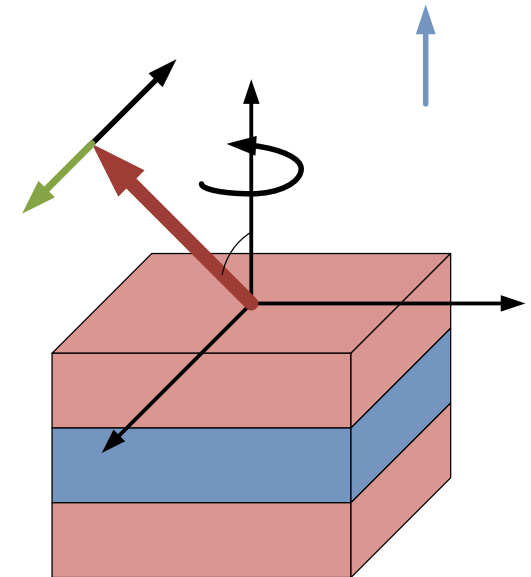
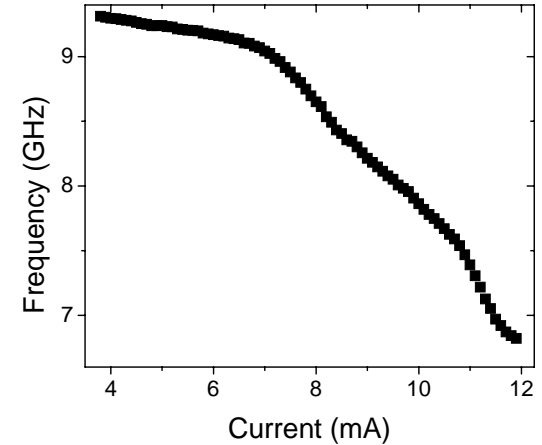
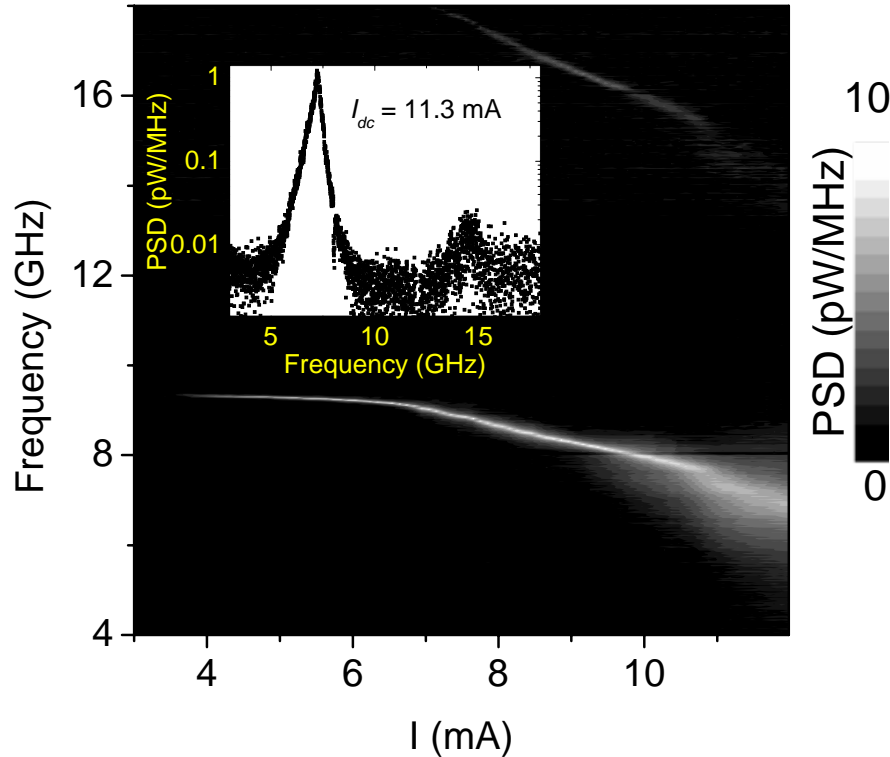
Ni



substrate|Ta(3)|Cu(15)|Co₉₀Fe₁₀(20)

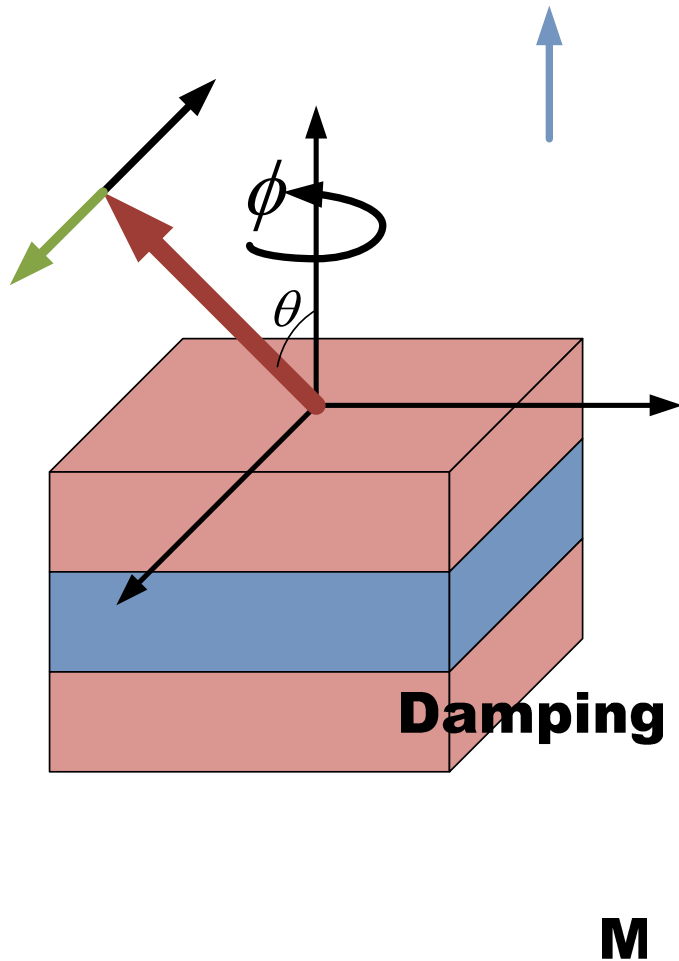
|Cu(4.5)|[Co(0.2)|Ni(0.4)]^{x5}|Co(0.3)|Cu(3)|Ta(3)

$$f = \frac{\gamma\mu_0}{2\pi} (H + (H_k - M_s) \cos(\theta))$$



Two-dimensional plot showing the device oscillation frequency and output power as a function of I_{dc}

Spin transfer nanocontact oscillator devices (STNO)

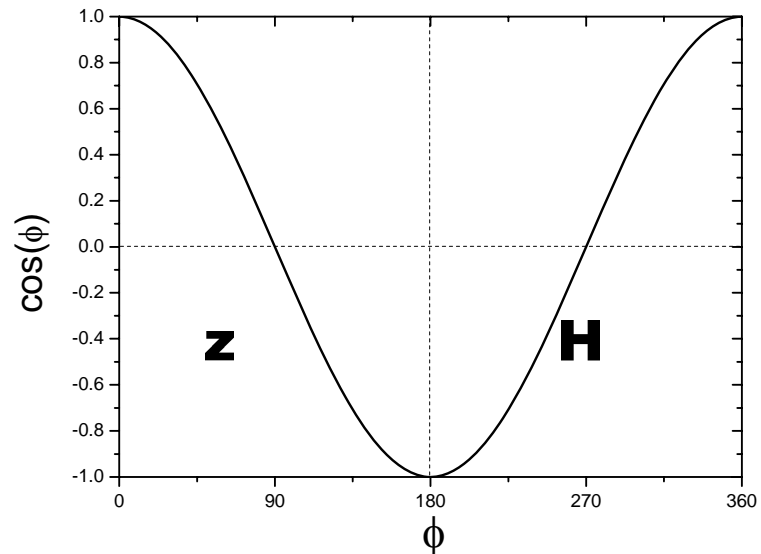


LLG equation

$$\frac{d\hat{m}}{dt} = -\hat{m} \times \vec{H} + \alpha \hat{m} \times \frac{d\hat{m}}{dt} + a(\phi) \hat{m} \times (\hat{m} \times \hat{s})$$

Energy

$$[a(\phi) \hat{m} \times (\hat{m} \times \hat{s})] \cdot \hat{H} = a(\phi) \cos \phi \cos \theta \sin \theta$$



G factor

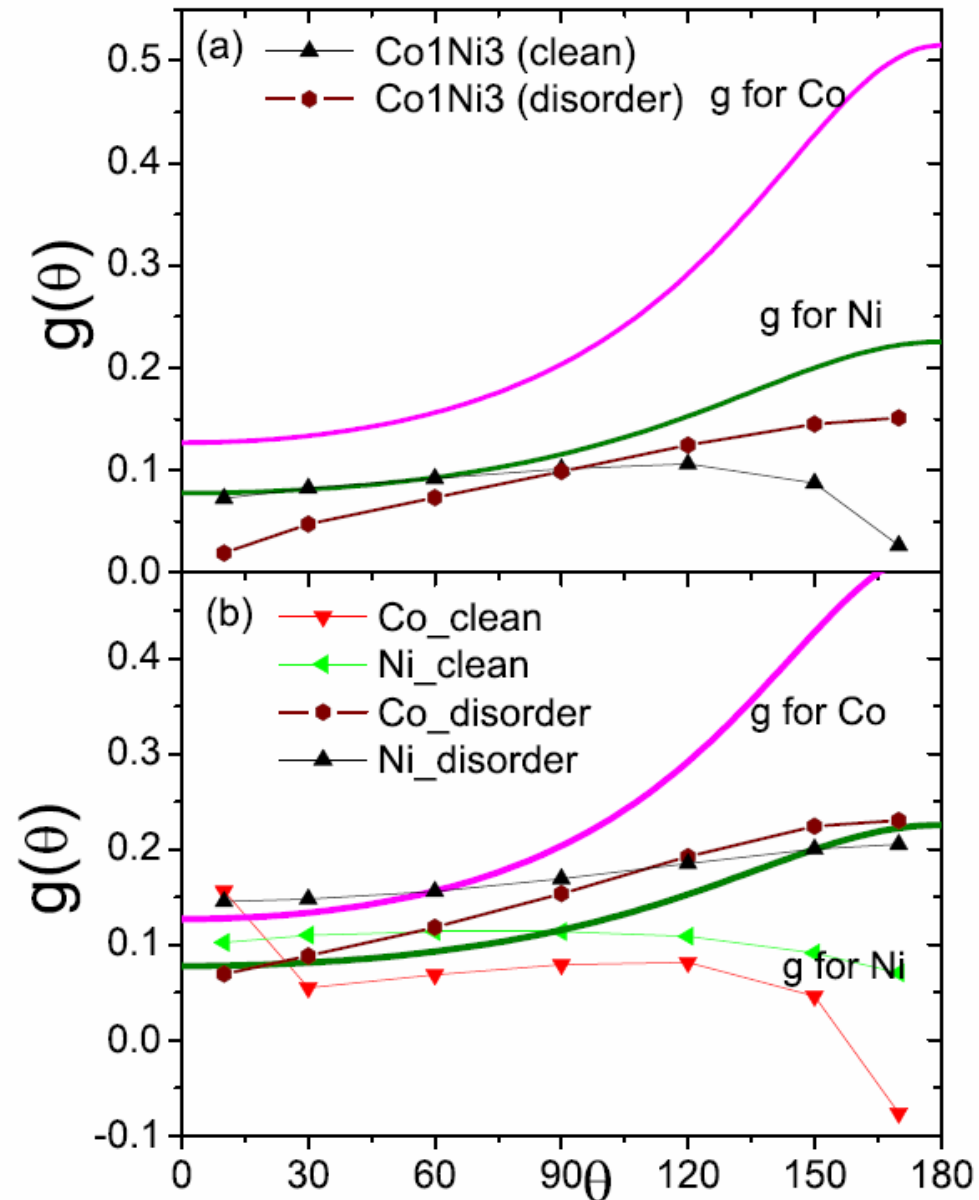
g factor [1]

$$g = \left[-4 + \frac{(1 + P)^3 (3 + \hat{s}_1 \cdot \hat{s}_2)}{4P^{3/2}} \right]^{-1}$$

Here Co P=0.35 Ni P=0.23

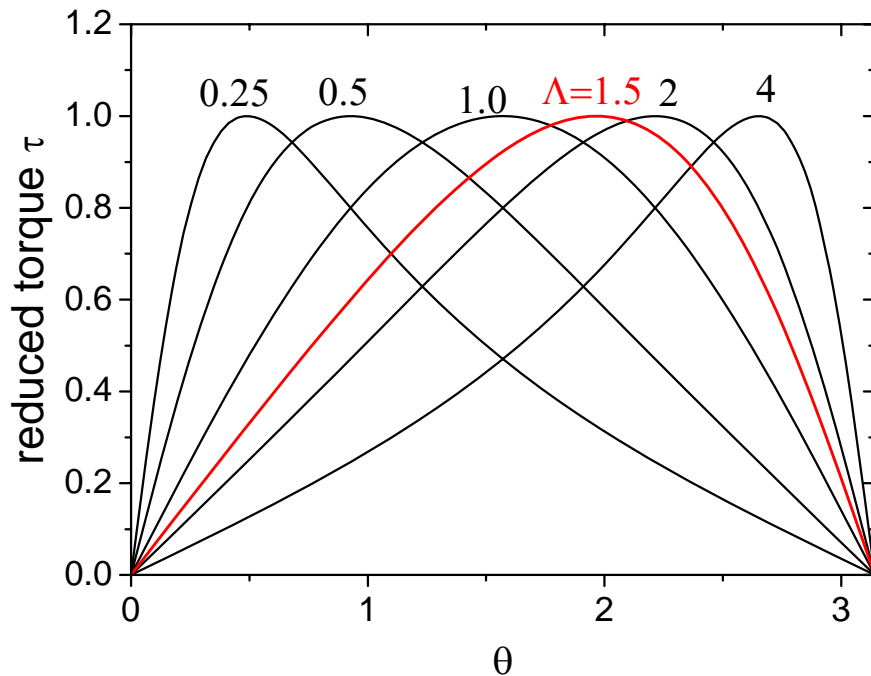
$$g(\theta) = \frac{\text{torque}(\theta)}{\mathbf{I}(\theta) \sin(\theta)}$$

G factor can be enhanced by disorder effect.



Reduced torque

$$\Lambda = 1.5$$



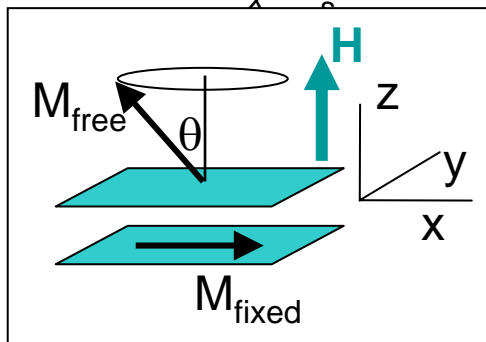
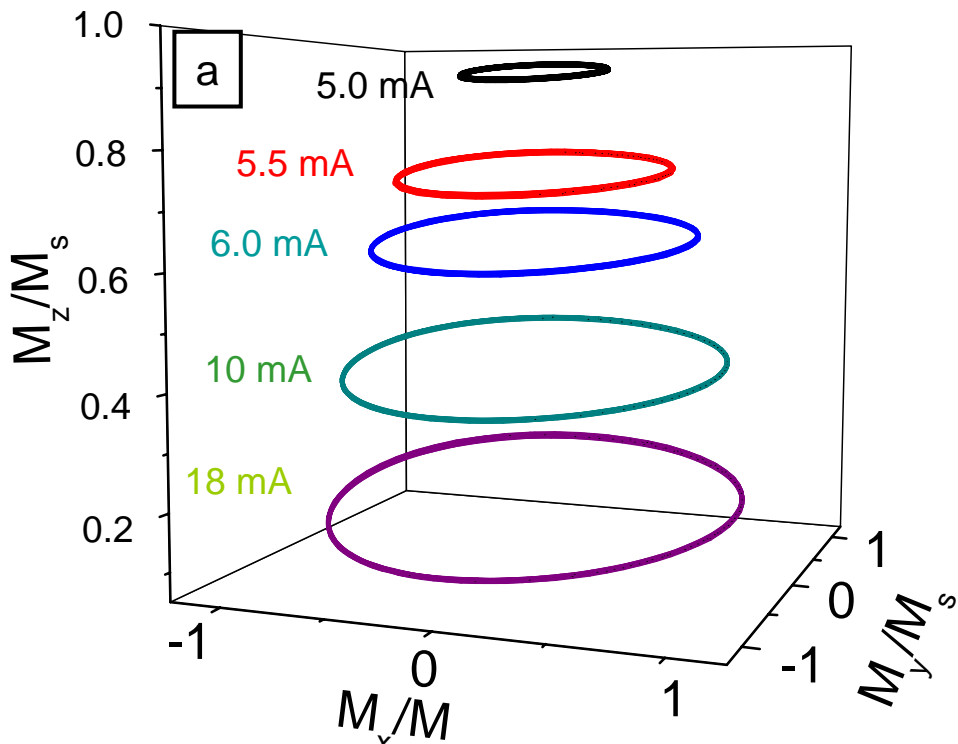
Torques

$$L = \hbar IP_r \Lambda \tau(\theta) / 4Ae$$

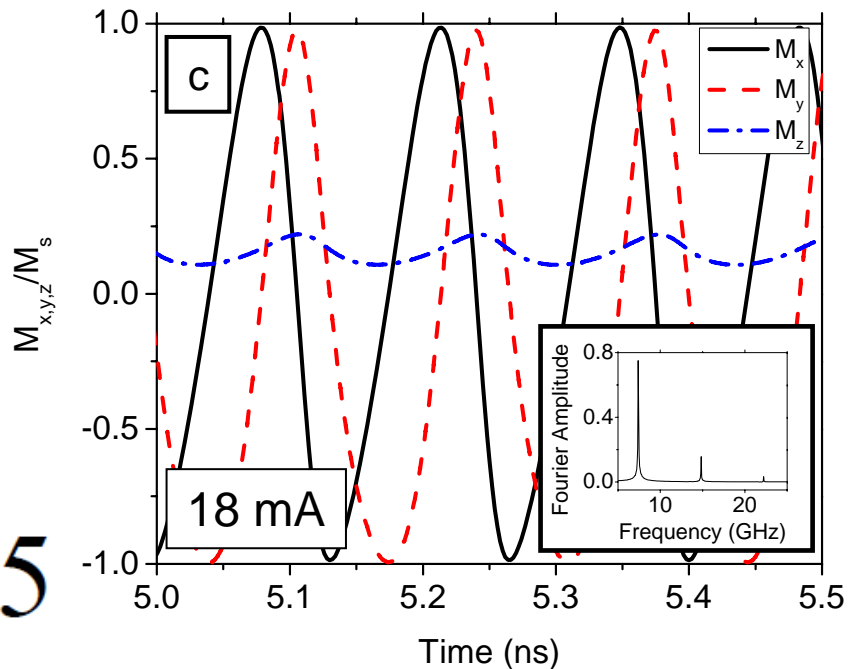
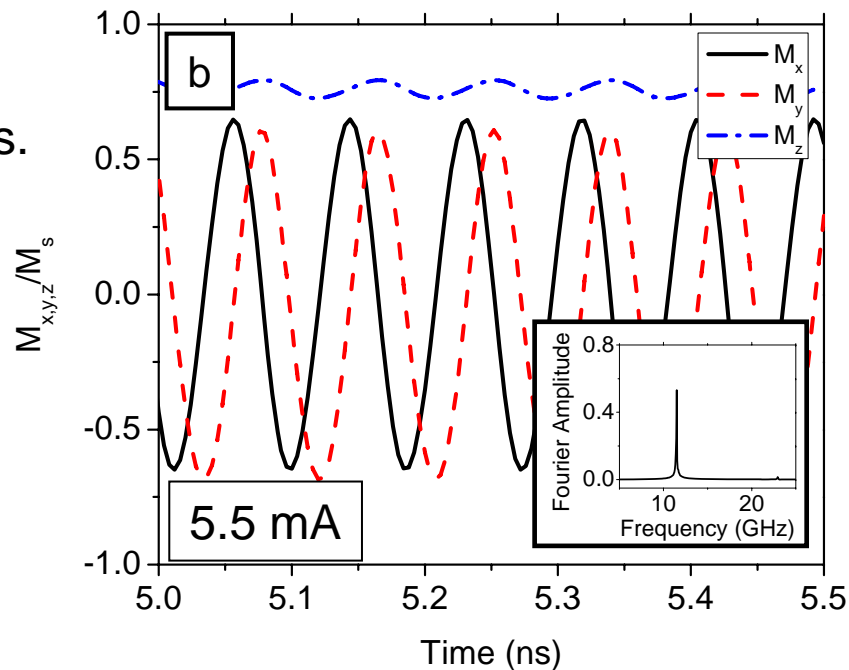
Reduced torques

$$\tau(\theta) = \frac{\sin \theta}{\Lambda \cos^2(\theta/2) + \Lambda^{-1} \sin^2(\theta/2)}$$

Magnetization trajectories from the single domain simulations for several current values.



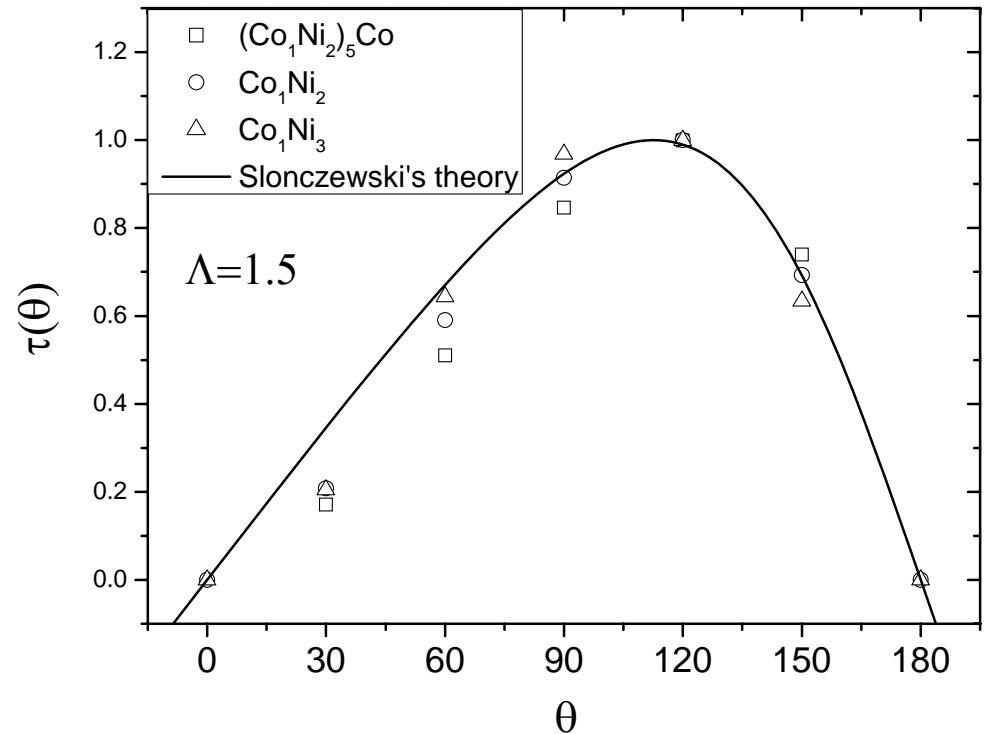
$$\Lambda = 1.5$$



Cu/Co/Cu/(Co₁Ni₂)₅Co/Cu

Reduced torque

$$\tau(\theta) = \frac{t(\theta) / I(\theta)}{(t / I)_{\max}}$$



Experiment $\Lambda = 1.5$

Gilbert Damping In the Presence of Andreev Reflection

Spin Current Induced Dynamics

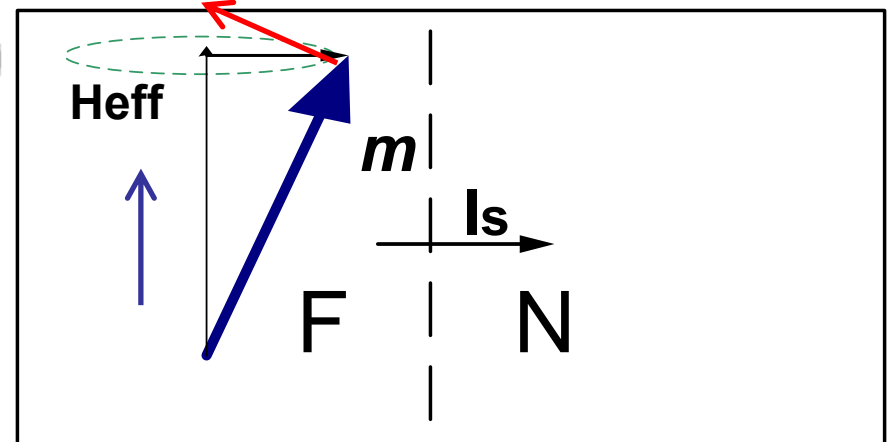
$$\dot{\vec{m}} = \underbrace{\gamma_0 \vec{H}_{eff}}_{\text{Precession}} \times \vec{m} + \underbrace{\alpha_0 \dot{\vec{m}} \times \vec{m}}_{\text{Damping}} + \left. \frac{\partial \vec{m}}{\partial t} \right|_{\text{torque}}$$

Spin Transfer Torque
from current I_s

$$I_s = \frac{\hbar}{4\pi} \left(\text{Re } \mathcal{A}_{eff}^{\uparrow\downarrow} \mathbf{m} \times \frac{d\mathbf{m}}{dt} + \text{Im } \mathcal{A}_{eff}^{\uparrow\downarrow} \frac{d\mathbf{m}}{dt} \right)$$

$\mathcal{A}_{eff}^{\uparrow\downarrow}$ Mixing Conductance
of F/N interface

Ferromagnet/Normal Metal



Spin Dependent Scattering Matrix

$$\hat{S} = S^\uparrow u^\uparrow + S^\downarrow u^\downarrow \quad u^{\uparrow/\downarrow} = \frac{1}{2}(\hat{I}_0 \pm \hat{\sigma} \cdot \vec{m})$$

$$\hat{S} = \frac{S^\uparrow + S^\downarrow}{2} \hat{I}_0 + \frac{S^\uparrow - S^\downarrow}{2} \hat{\sigma} \cdot \vec{m}$$

$$\frac{\partial \hat{S}}{\partial X} = S^\uparrow \frac{\partial u^\uparrow}{\partial X} + S^\downarrow \frac{\partial u^\downarrow}{\partial X} = (S^\uparrow - S^\downarrow) \hat{\sigma} \cdot \frac{\partial \vec{m}}{\partial X}$$

EMISSIVITY

$$\frac{d\hat{n}_l}{dX} = \left(\frac{1}{4\pi i} \sum_{nn'l'} \frac{\partial \hat{S}_{nn',ll'}}{\partial X} \hat{S}_{nn',ll'}^\dagger \right) + \text{H.c.}$$

F/N Spin Pump

$$\text{Current } \hat{I}_{F/N} = e \frac{\partial \hat{N}_{F/N}}{\partial X} \frac{\partial X}{\partial t} = \frac{1}{2} I_C \cdot \hat{i}_0 - \frac{e}{\hbar} \hat{\sigma} \cdot \hat{I}_{F/N}^S$$

$$\text{Precession induced current } \hat{I}_{F/N}^S = \frac{\hbar}{4\pi} \left(\text{Re } A^{\uparrow\downarrow} \vec{m} \times \frac{\partial \vec{m}}{\partial t} + \text{Im } A^{\uparrow\downarrow} \frac{\partial \vec{m}}{\partial t} \right),$$

$$I_C = 0.$$

Mixing Conductance (One Interface)

$$A^{\uparrow\downarrow} = \sum_{nm} \text{Tr}(\delta_{mn} - r_m^\uparrow r_n^{\downarrow\dagger})$$

LLG equation in the presence of spin current pump



$$\frac{\partial \vec{m}}{\partial t} = \gamma_0 \vec{H}_{eff} \times \vec{m} + \alpha_0 \frac{\partial \vec{m}}{\partial t} \times \vec{m} + \frac{\gamma \hbar}{4\pi M_S V} (A_r^{\uparrow\downarrow} \vec{m} \times \frac{\partial \vec{m}}{\partial t} + A_i^{\uparrow\downarrow} \frac{\partial \vec{m}}{\partial t})$$

Effective Damping Enhancement

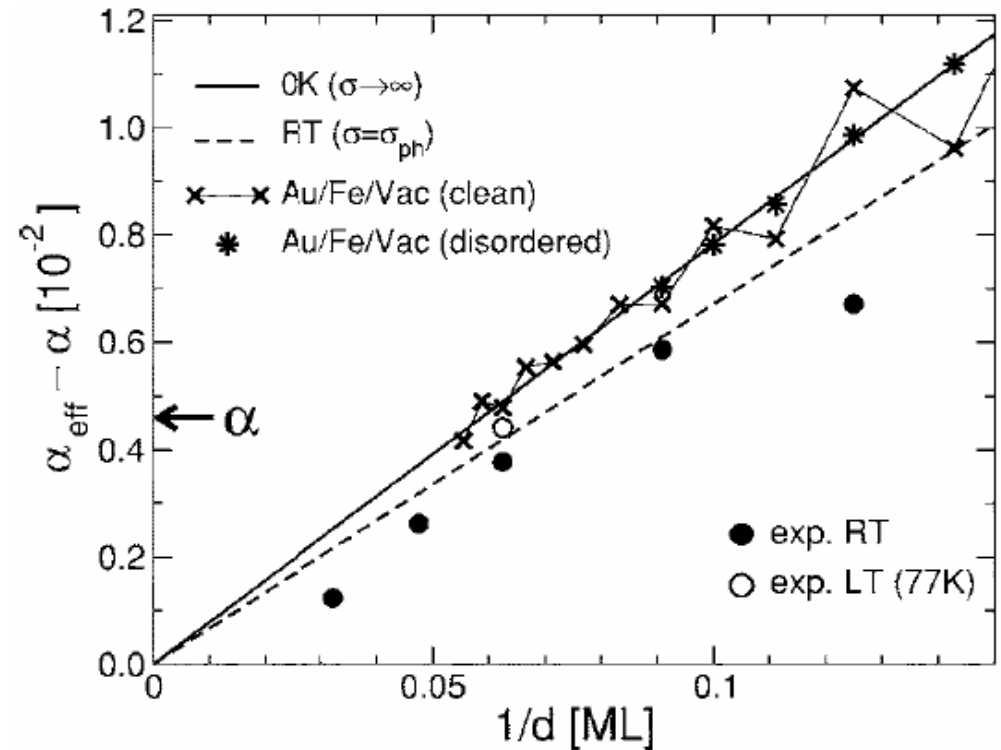
$$\frac{\partial}{\partial t} \vec{m} = -\gamma_{eff} \vec{m} \times \vec{H}_{eff} + \alpha_{eff} \vec{m} \times \frac{\partial}{\partial t} \vec{m}$$

$$\frac{\gamma}{\gamma_{eff}} = 1 - \frac{\gamma \hbar}{4\pi M_s V} A_i^{\uparrow\downarrow}$$

$$\alpha_{eff} = \frac{\alpha + \frac{\gamma \hbar}{4\pi M_s V} A_r^{\uparrow\downarrow}}{1 - \frac{\gamma \hbar}{4\pi M_s V} A_i^{\uparrow\downarrow}}$$

Tserkovnyak, Y. *et al*

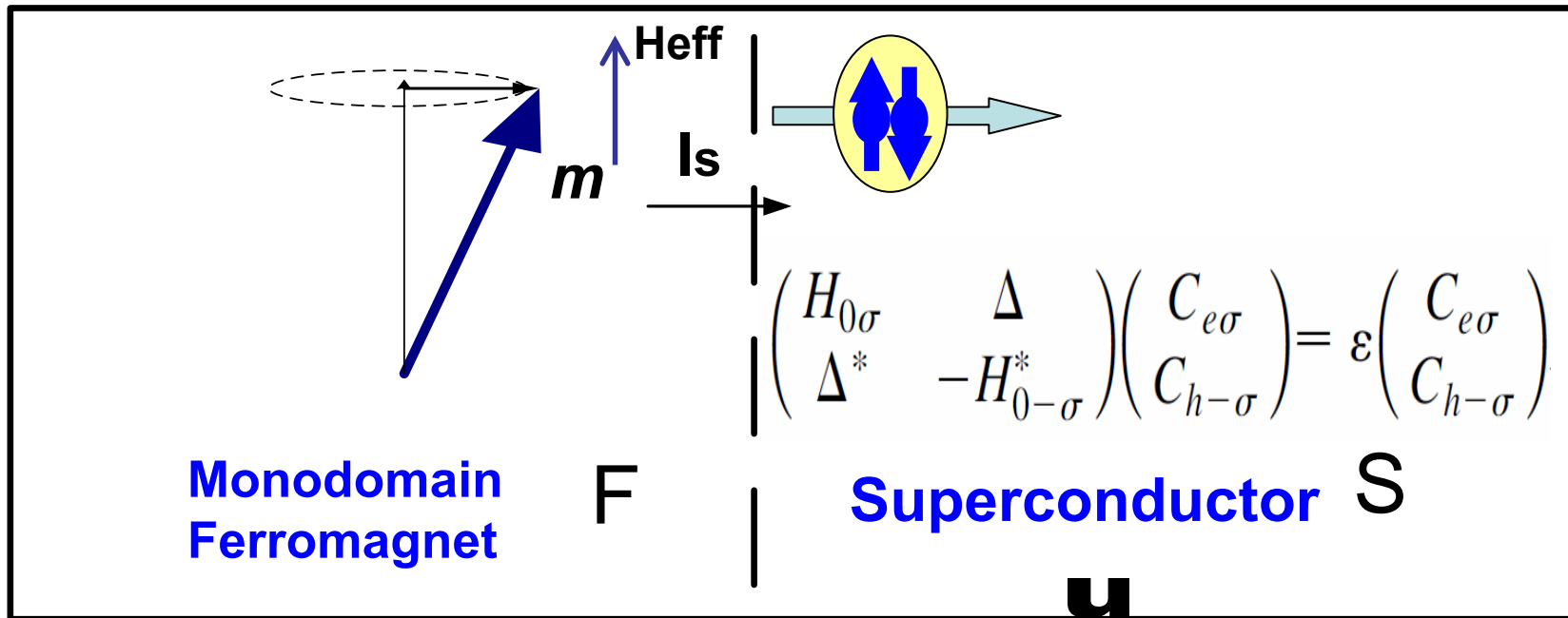
Rev. Mod. Phys., 77, 4(2005)



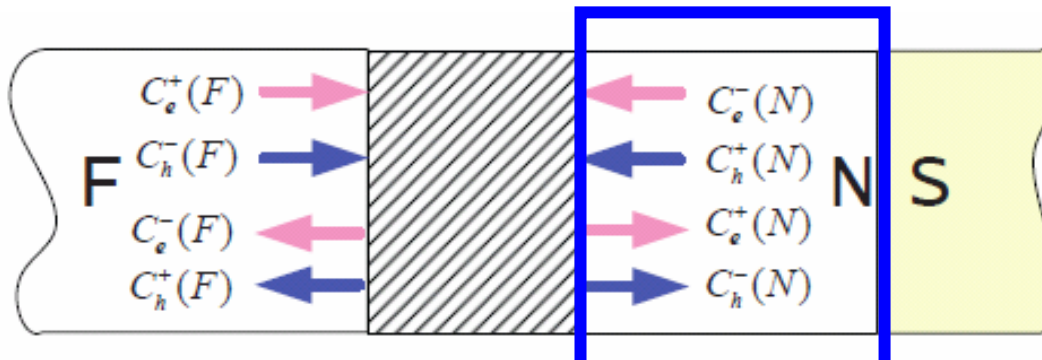
Urban, R *et al Phys. Rev. Lett.* 87, 217204(2001)

Heinrich, B. *et al, J. Appl. Phys.* 93,7545(2003)

Spin Pump at F/S Contacts



F/N/S Interface Approach



At N|S interface we consider there is only Andreev reflection.

At F/N Interface

$$\begin{pmatrix} c_e^-(F) \\ c_e^+(N) \\ c_h^+(F) \\ c_h^-(N) \end{pmatrix} = \begin{pmatrix} r_{11}^e & t_{12}^e & 0 & 0 \\ t_{21}^e & r_{22}^e & 0 & 0 \\ 0 & 0 & r_{11}^h & t_{12}^h \\ 0 & 0 & t_{21}^h & r_{22}^h \end{pmatrix} \begin{pmatrix} c_e^+(F) \\ c_e^-(N) \\ c_h^-(F) \\ c_h^+(N) \end{pmatrix}$$

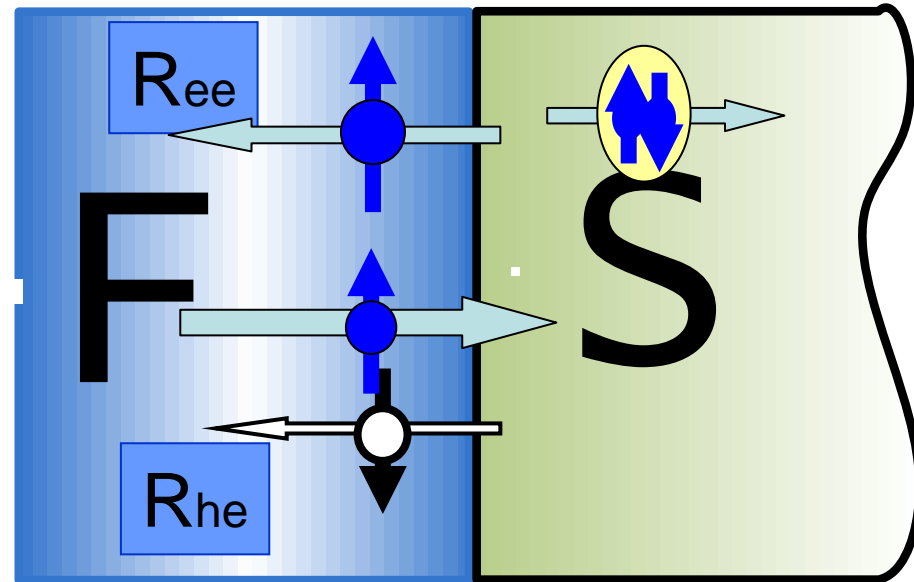
We are interested in wave functions in the *F* layer

Spin Current in the Presence of Andreev Reflection

Linear Response & Circuit Theory

$$I(t) = \frac{dQ(t)}{dt} = q \frac{dN(t)}{dX} \frac{dX}{dt}$$

$$= \left(e \frac{dn_e}{dX} + (-e) \frac{dn_h}{dX} \right) \frac{dX}{dt}$$



$$= e \frac{dX}{dt} \left(\text{Tr} \left(\hat{R}^{ee\dagger} \frac{\partial \hat{R}^{ee}}{\partial X} - \frac{\partial \hat{R}^{ee\dagger}}{\partial X} \hat{R}^{ee} \right) - \text{Tr} \left(\hat{R}^{he\dagger} \frac{\partial \hat{R}^{he}}{\partial X} - \frac{\partial \hat{R}^{he\dagger}}{\partial X} \hat{R}^{he} \right) \right)$$

For Precession Induced Pumping
 $X(t) = \phi(t)$ the precession angle

Spin current and Damping

$$\text{Current } \hat{I}_{F/S} = \frac{1}{2} I_C \cdot \hat{i}_0 - \frac{e}{\hbar} \hat{\sigma} \cdot \hat{I}_{F/S}^S \quad I_C = 0,$$

$$\hat{I}_{F/S}^S = \frac{\hbar}{4\pi} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \left(\text{Re } G^{\uparrow\downarrow}(\varepsilon) \vec{m} \times \frac{\partial \vec{m}}{\partial t} + \text{Im } G^{\uparrow\downarrow}(\varepsilon) \frac{\partial \vec{m}}{\partial t} \right)$$

Effective Damping

$$\alpha_{\text{eff}} = \frac{\alpha_0 + \frac{\gamma \hbar}{4\pi M_s V} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \text{Re } G_{F/S}^{\uparrow\downarrow}(\varepsilon)}{\gamma_0 - \frac{\gamma \hbar}{4\pi M_s V} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \text{Im } G_{F/S}^{\uparrow\downarrow}(\varepsilon)}$$

Mixing Conductance and Andreev Reflection

$$G^{\uparrow\downarrow}(\varepsilon) \equiv \left(N_{\text{Sharvin}} - |R_{he}^{\uparrow\uparrow}(\varepsilon)|^2 - |R_{he}^{\uparrow\downarrow}(\varepsilon)|^2 - |R_{he}^{\downarrow\uparrow}(\varepsilon)|^2 - |R_{he}^{\downarrow\downarrow}(\varepsilon)|^2 \right) - R_{ee}^{\uparrow\uparrow}(\varepsilon)R_{ee}^{\downarrow\downarrow\dagger}(\varepsilon)$$

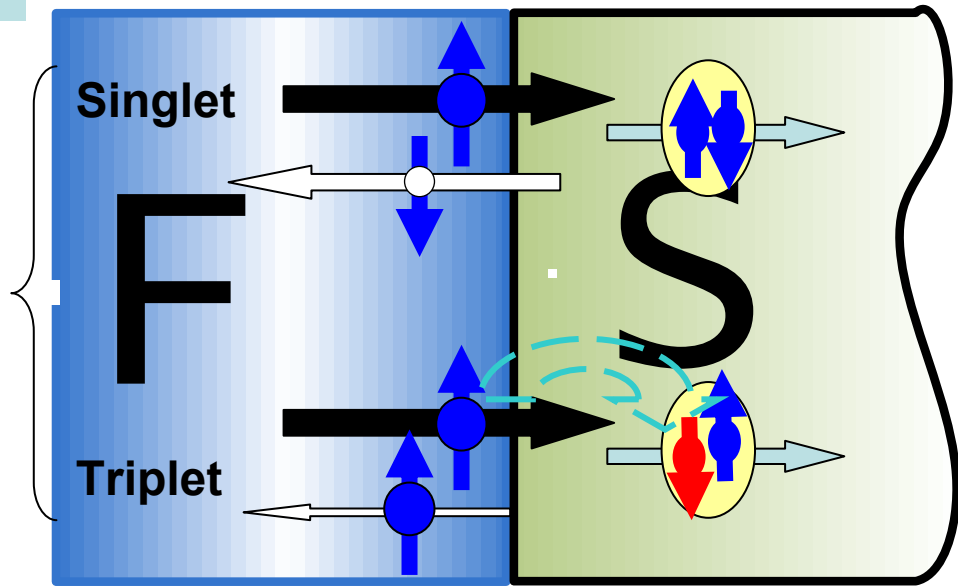
Normal Reflection

$$+ R_{he}^{\downarrow\uparrow}(\varepsilon)R_{he}^{\uparrow\downarrow\dagger}(\varepsilon) + R_{he}^{\uparrow\uparrow}(\varepsilon)R_{he}^{\downarrow\downarrow\dagger}(\varepsilon)$$

Singlet

Triplet

R_{he}



Andreev Reflection

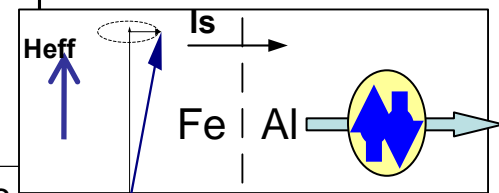
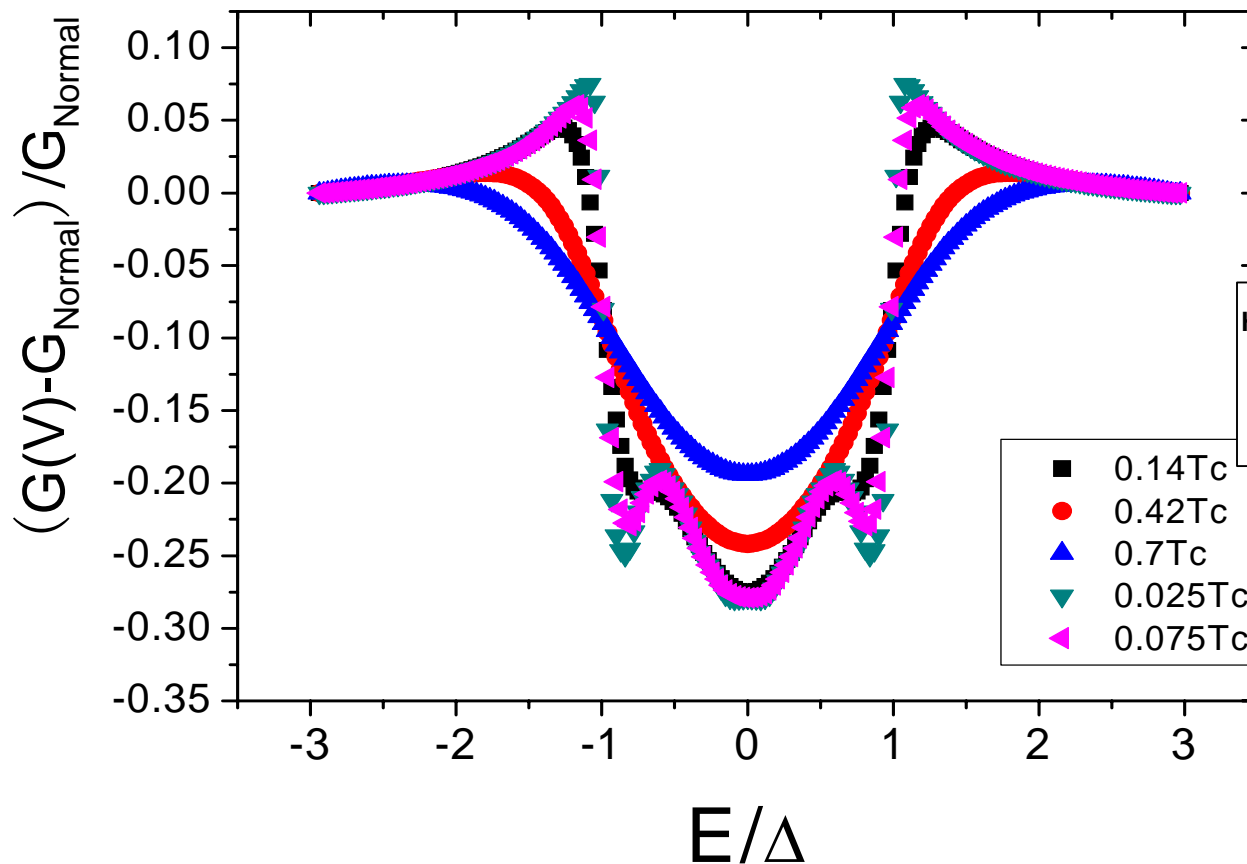
Charge Conductance Spectrum

$$G(\varepsilon) = N_{\text{Sharvin}} \left[-\left| R_{ee}^{\uparrow\uparrow}(\varepsilon) \right|^2 - \left| R_{ee}^{\downarrow\downarrow}(\varepsilon) \right|^2 + \left| R_{he}^{\downarrow\downarrow}(\varepsilon) \right|^2 + \left| R_{he}^{\uparrow\uparrow}(\varepsilon) \right|^2 + \left| R_{he}^{\uparrow\downarrow}(\varepsilon) \right|^2 + \left| R_{he}^{\downarrow\uparrow}(\varepsilon) \right|^2 \right]$$

Normal Reflection

Triplet

Singlet



多重散射公式

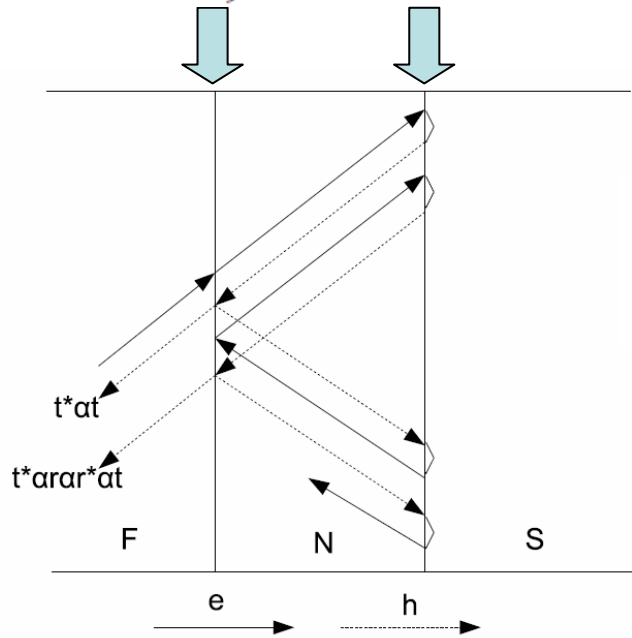
$$r'_{\uparrow(\downarrow)} = |r'_{\uparrow(\downarrow)}| e^{i\phi_{\uparrow}(\phi_{\downarrow})}$$

$$\hat{t}, \hat{r} \alpha = e^{-i \arccos(\varepsilon/\Delta_0)}$$

类比多光束干涉公式[1]

$$r_{he} = t^* \alpha t + t^* \alpha r \alpha r^* \alpha t + t^* \alpha [r \alpha r^* \alpha]^2 t + \dots$$

$$= t^* \alpha [1 - r \alpha r^* \alpha]^{-1} t$$



$$G_0 = \frac{2e^2}{h} |t_{\uparrow}|^2 |t_{\downarrow}|^2, R^2 = |r'_{\uparrow}| |r'_{\downarrow}|$$

考虑自旋极化界面

$$G_{FS}(\varepsilon) = \frac{G_0}{1 + R^4 - 2R^2 \cos\left(-2 \arccos \frac{\varepsilon}{\Delta_0} + \phi_{\uparrow} - \phi_{\downarrow}\right)}$$

$$\varepsilon/\Delta_0 = \cos \frac{\phi_{\uparrow} - \phi_{\downarrow}}{2}$$

出现电导峰

考虑F/N界面无序

$$\langle G_{FS}(\varepsilon) \rangle = \frac{G_0}{\left| \frac{1}{2\varphi} \int_{-\varphi}^{\varphi} \left(1 - R^2 e^{-i2 \arccos \frac{\varepsilon}{\Delta_0}} e^{i\delta}\right) d\delta \right|^2}$$

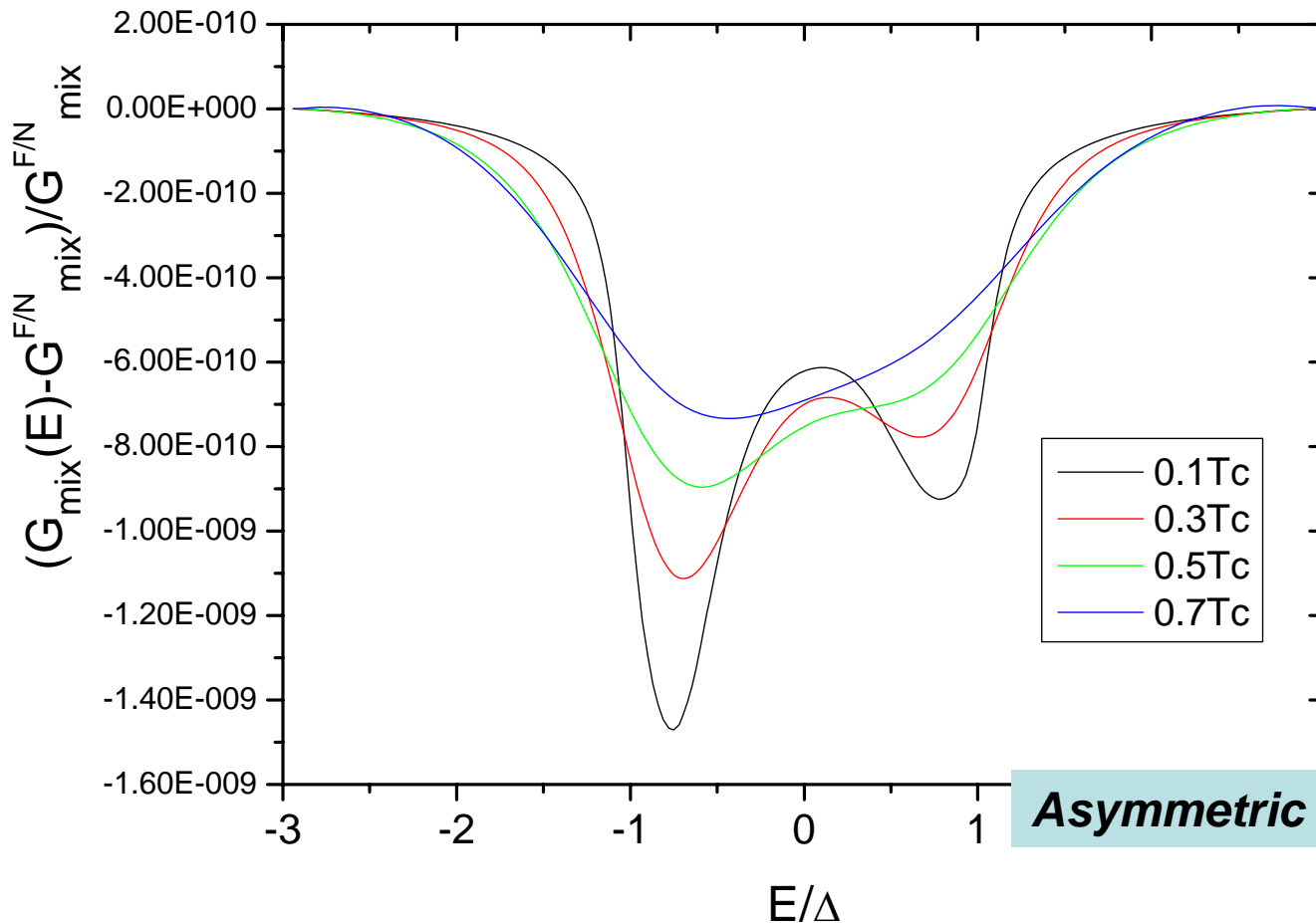
尤电导峰结构

其中 $\delta = \phi_{\uparrow} - \phi_{\downarrow}$ 为随机数

[1] C.W.J. Beenakker, Quantum Mesoscopic Phenomena and Mesoscopic Devices in Microelectronics, edited by I.O. Kulik and R. Ellialtioglu, pp. 51-60, (NATO Science Series, Dordrecht, 2000)

Mixing Conductance Spectrum

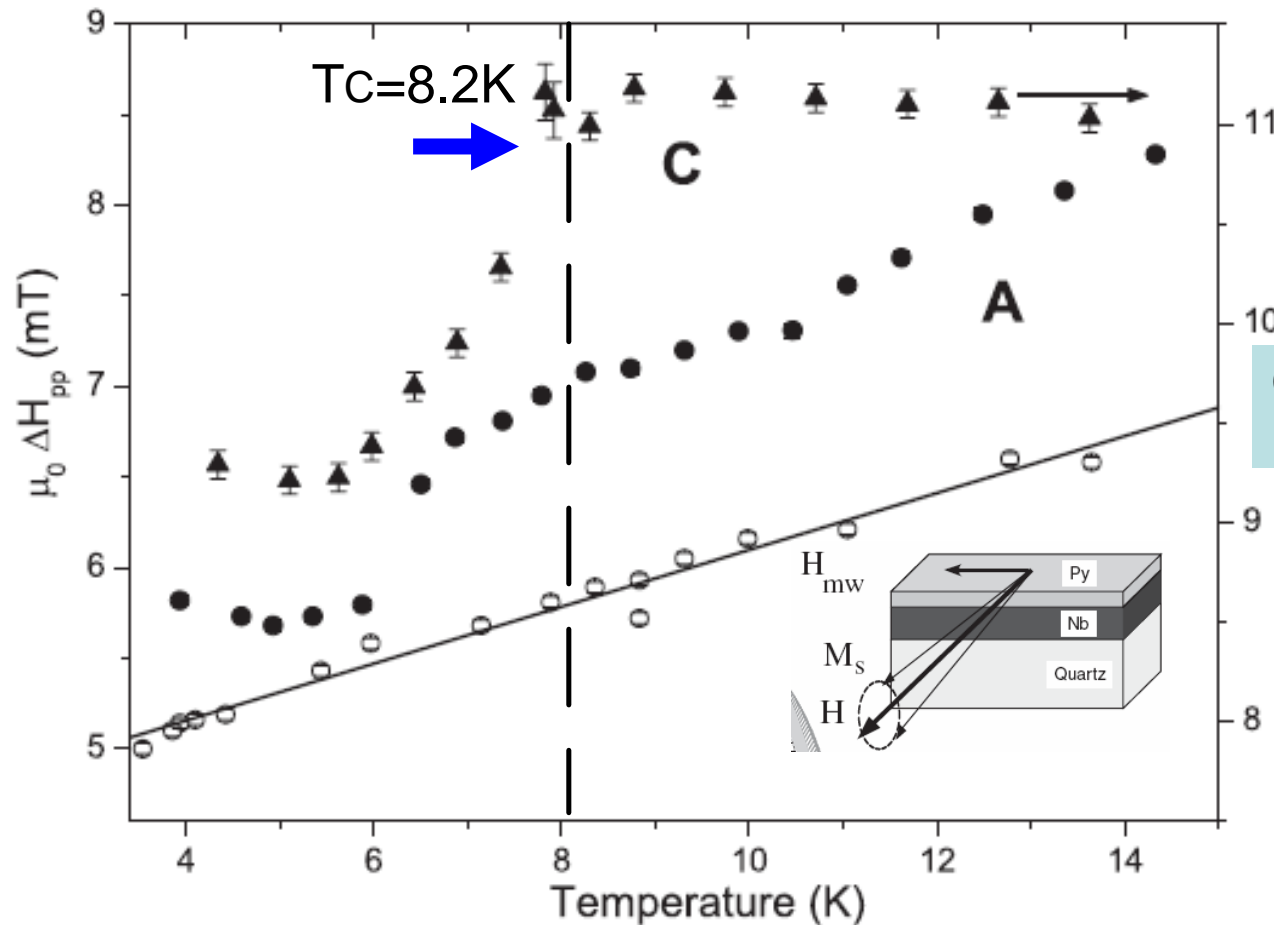
$$G^{\uparrow\downarrow} = G_{ee}^{\uparrow\downarrow} + G_{he}^{\uparrow\downarrow \text{singlet}} + G_{he}^{\uparrow\downarrow \text{triplet}}$$



Asymmetric Peaks below the gap

Temperature Dependence of Gilbert Damping Enhancement

Experiment: FMR linewidth



Sample A,C
Superconductor

Sample B

Non-superconductor

C. Bell J. Aarts *et al*
Phys.Rev.Lett.100,047002(2008)

Temperature Dependence of Gilbert Damping Enhancement

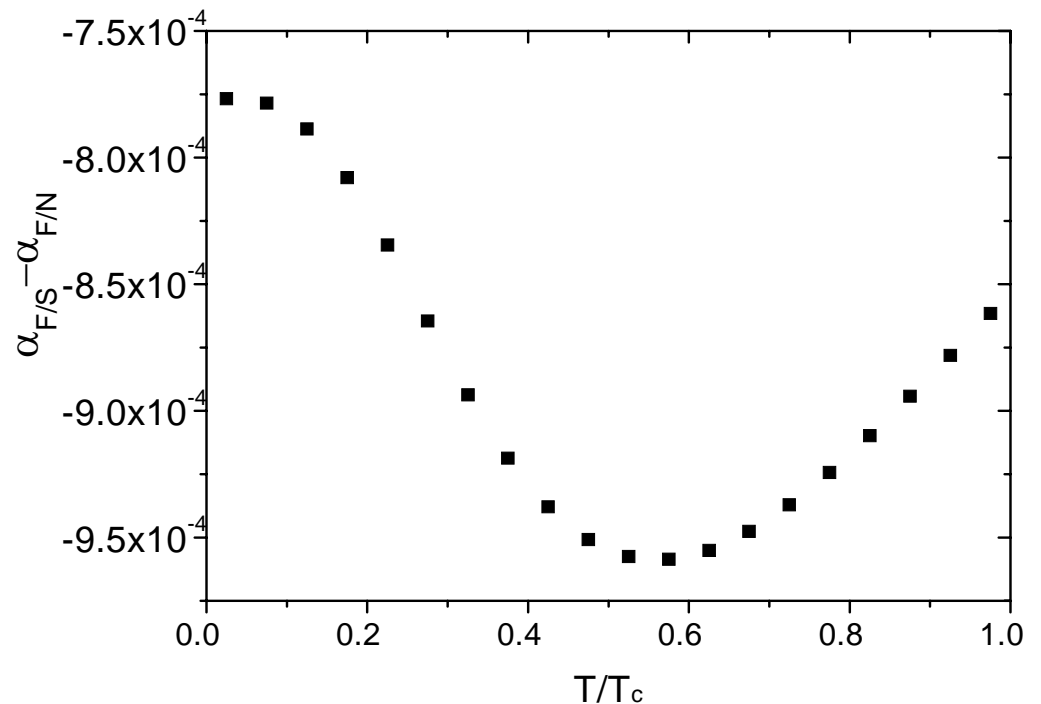
$T \rightarrow T_c, \Delta(T) \rightarrow 0, R_{he} \rightarrow 0, \delta\alpha_{F/S}(T)$ reduces to

$$\delta\alpha_{F/N} = N_{Sharvin} - Tr \left(R_{ee}^{\uparrow\uparrow} R_{ee}^{\downarrow\downarrow\dagger} \right)$$

$$\delta\alpha(T) = \alpha_{eff} - \alpha_0 \approx \frac{\gamma\hbar}{4\pi M_s V} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \text{Re} G^{\uparrow\downarrow}(\varepsilon),$$

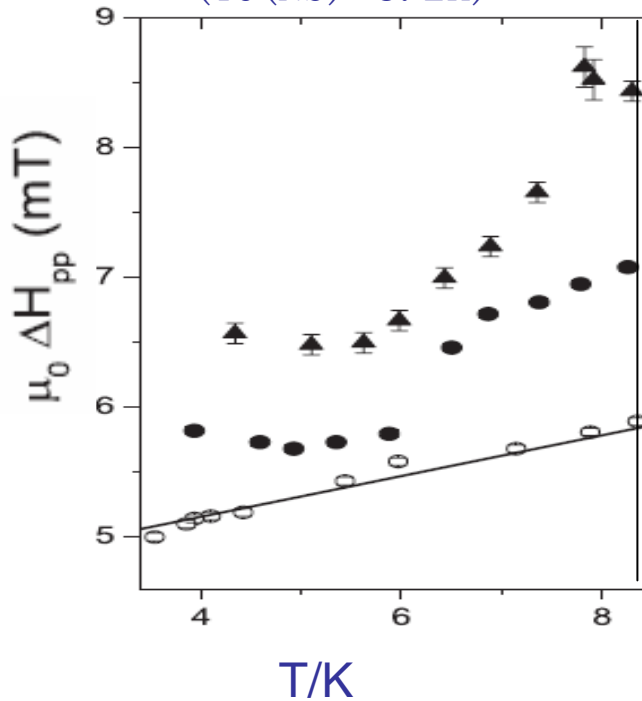
For $\mu_{Fe} = 2.2\mu_B$

(Thickness of F layer is 10ML)

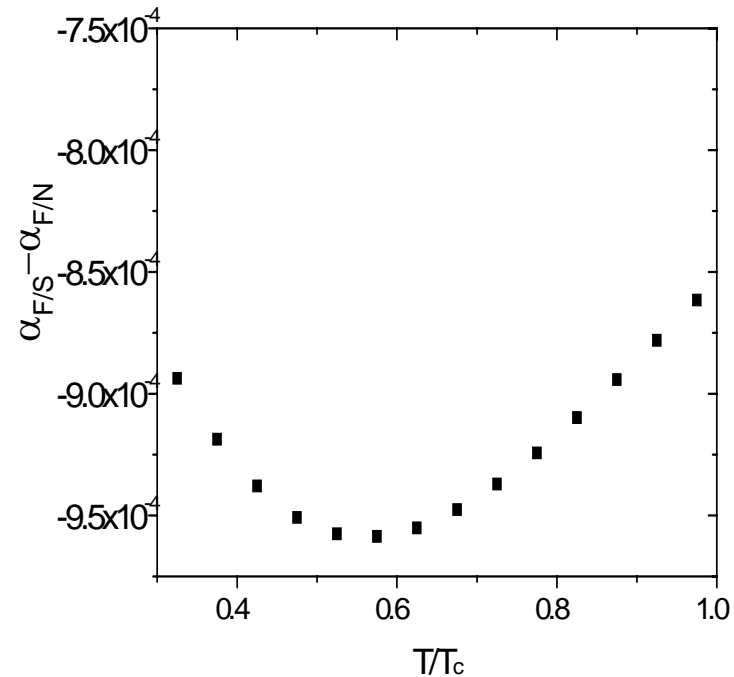


Temperature Dependence of Gilbert Damping Enhancement

FMR Experiment
($T_c(\text{Nb})=8.2\text{K}$)

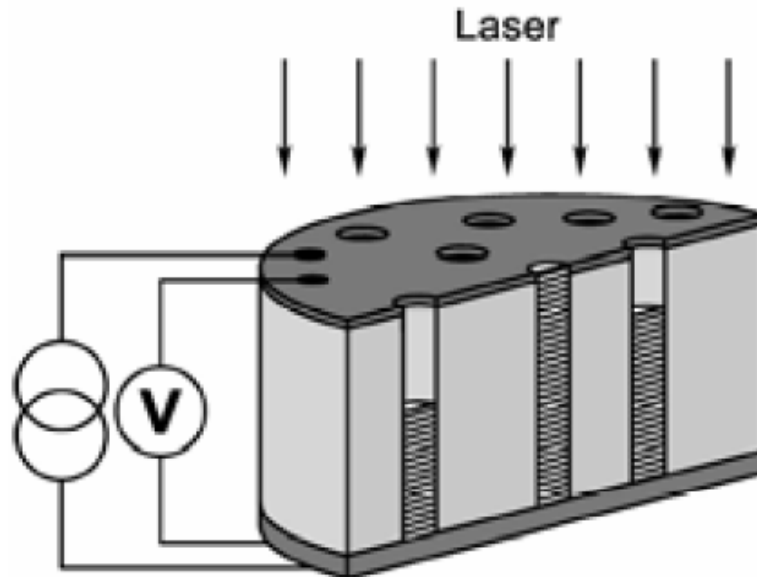
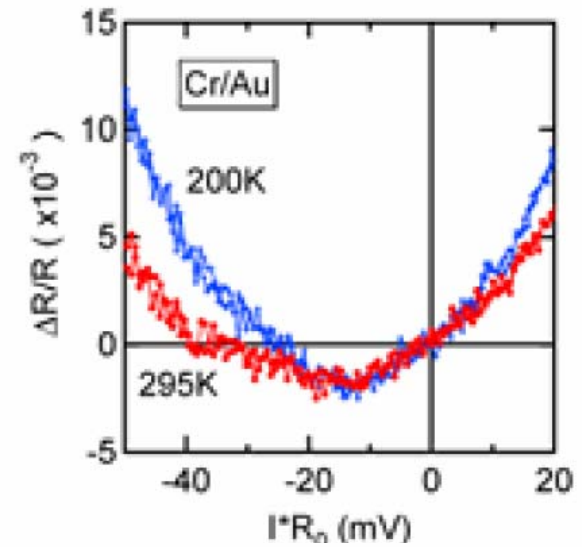
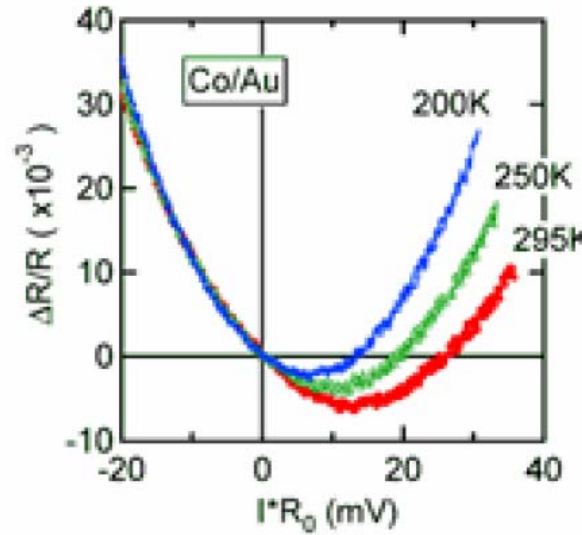
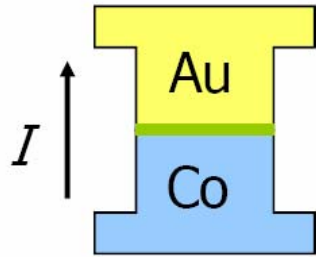


Calculated $\Delta \alpha$
($T_c(\text{Al})=1.14\text{K}$)



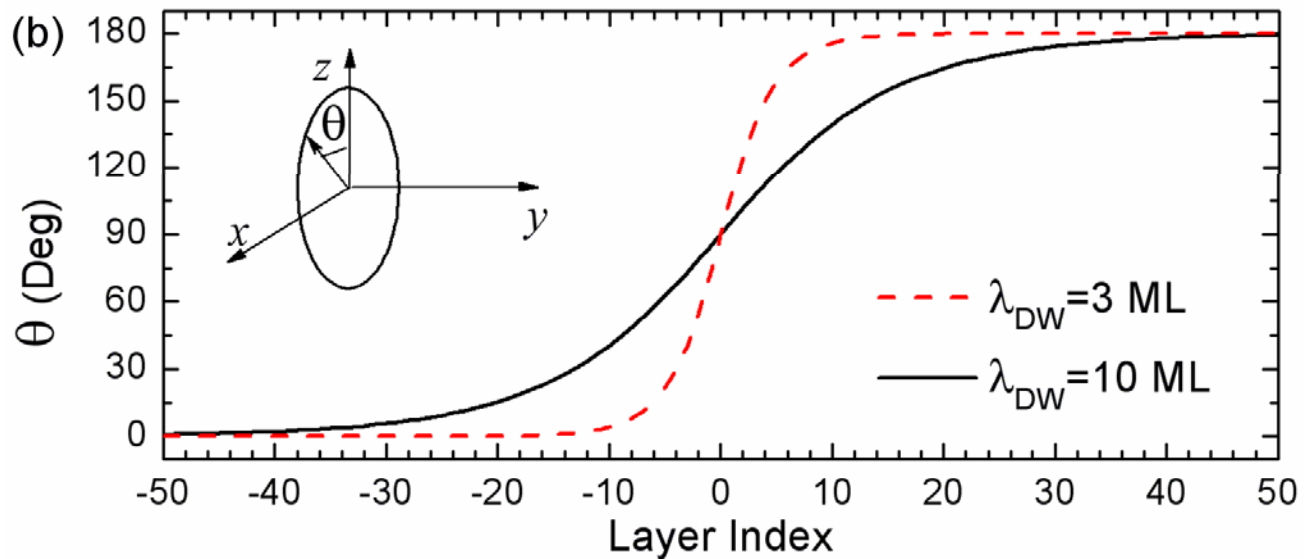
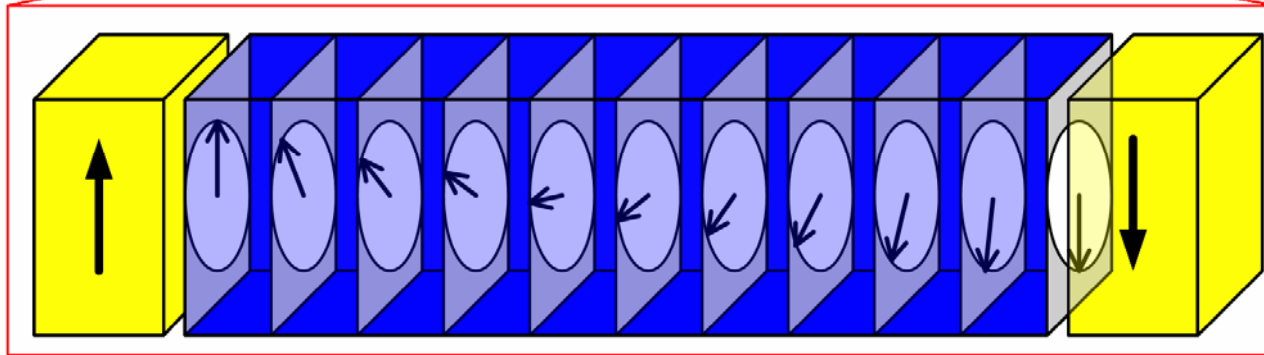
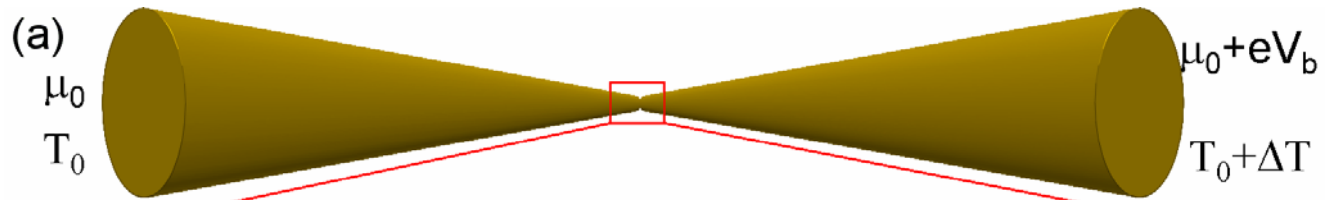
When Normal metal in F/N interface becomes superconducting, spin pump induced damping decreases, i.e. $\Delta \alpha < 0$

Metallic nanopillars (Fukushima et al., 2005)



L. Gravier et al. (2005).

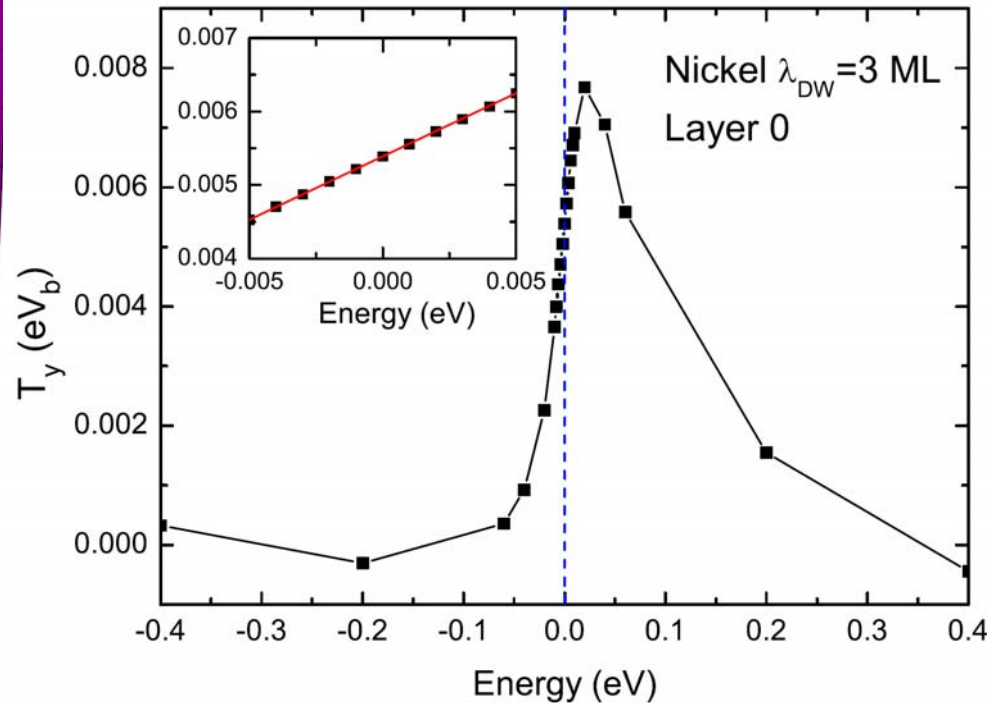
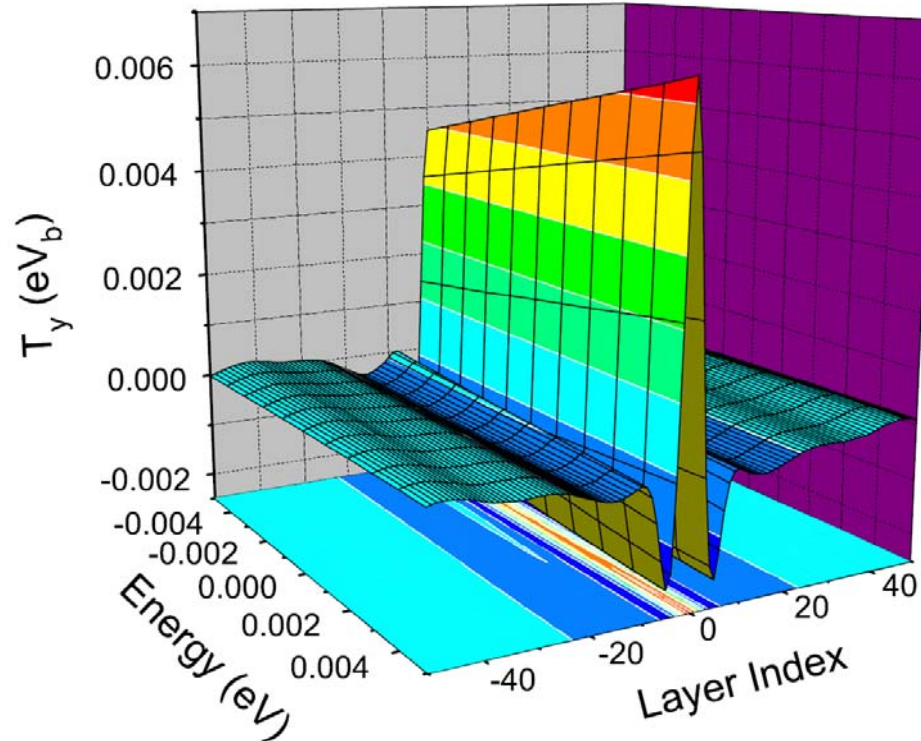
Model



First-principles spin-transfer torque

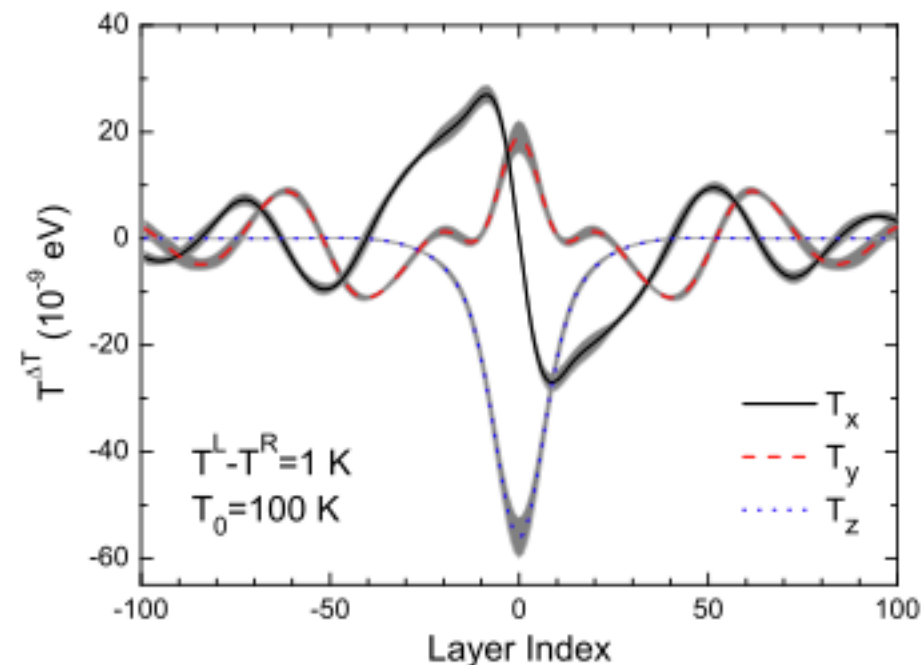
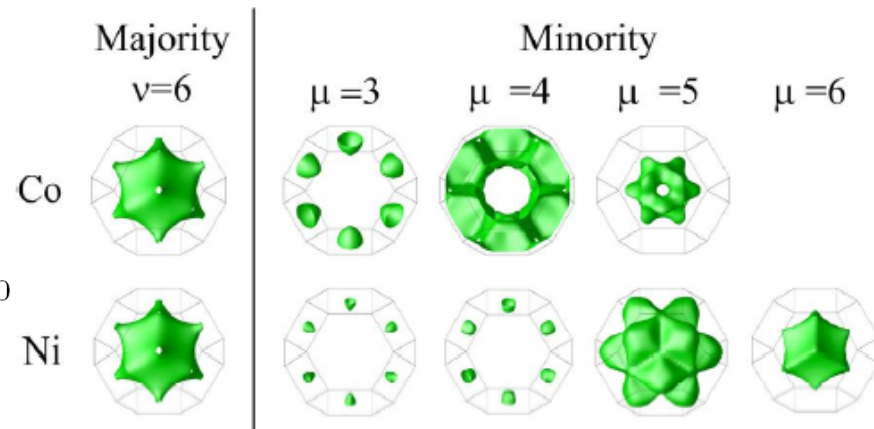
$$\hat{\mathcal{J}} \equiv \frac{1}{2} \left[\hat{\sigma} \otimes \hat{\mathbf{V}} + \hat{\mathbf{V}} \otimes \hat{\sigma} \right]$$

$$\mathbf{T}_{\mathbf{R}}(\mathbf{k}_{\parallel}, \epsilon) = \sum_{\mathbf{R}' \in I-1, I} \mathcal{J}_{\mathbf{R}', \mathbf{R}}(\mathbf{k}_{\parallel}, \epsilon) - \sum_{\mathbf{R}' \in I, I+1} \mathcal{J}_{\mathbf{R}, \mathbf{R}'}(\mathbf{k}_{\parallel}, \epsilon)$$

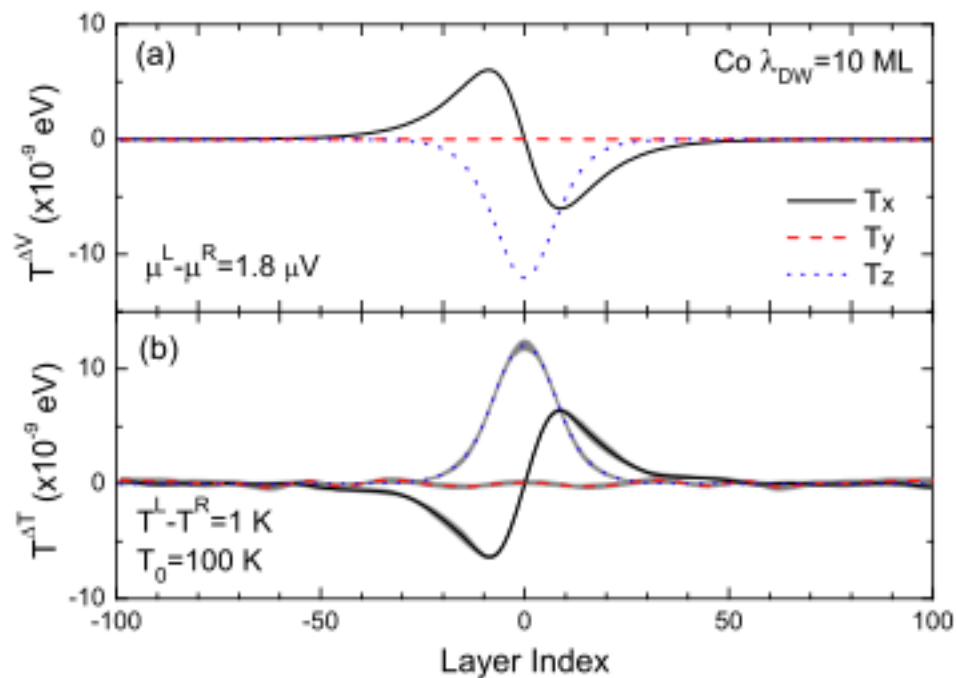


Bias- and temperature-SIT

$$\mathbf{T}_n = \tilde{\mathbf{T}}_n e V_b + \frac{\pi^2 k_B^2 T_0 \Delta T}{3} \left. \frac{\partial \tilde{\mathbf{T}}_n}{\partial \epsilon} \right|_{\epsilon = \mu_0}$$



Ni:



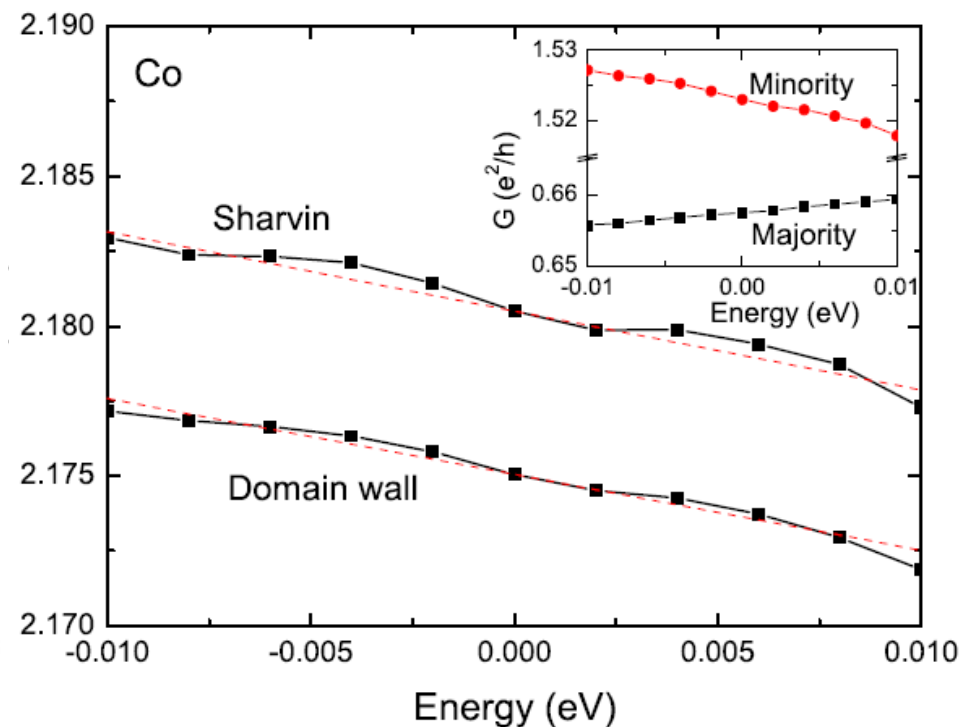
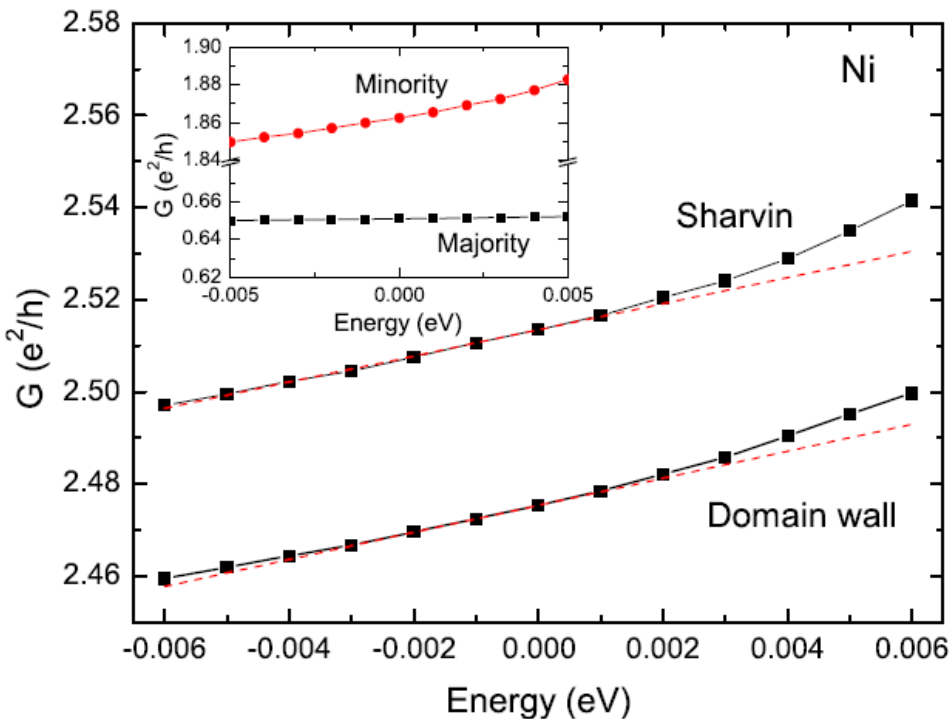
Co:

Peltier and Seebeck coefficients

	G' (e/hV)	G (e^2/h)	$\partial_\epsilon \ln G _{\epsilon_F}$ (eV^{-1})	S/T (nV/K^2)
Ni domain wall	2.94	2.48	1.19	-28.9
Ni Sharvin	2.84	2.51	1.13	-27.5
Polarized Sharvin $P=0.23$	-	-	0.57	-13.9
Co domain wall	-0.253	2.175	-0.116	2.83
Co Sharvin	-0.264	2.181	-0.121	2.95
Polarized Sharvin $P=0.35$	-	-	0.184	-4.50

$$P \equiv \frac{w_\uparrow G_\uparrow - w_\downarrow G_\downarrow}{w_\uparrow G_\uparrow + w_\downarrow G_\downarrow}$$

$$\bar{S} = w_\uparrow S_\uparrow + w_\downarrow S_\downarrow$$



Messages

- Spin-dependent transport properties of interfaces govern many magnetoelectronic phenomena.
- Agreement between interface-dominated transport properties calculated by first principles and the isotropy assumption with experimental values is (semi)-quantitative for itinerant systems like transition metals.
- Mixing conductance and spin-torque can be calculated and measured accurately.

Computational Materials Science

The End