

Materials dependence of the spin-transfer torques on DW

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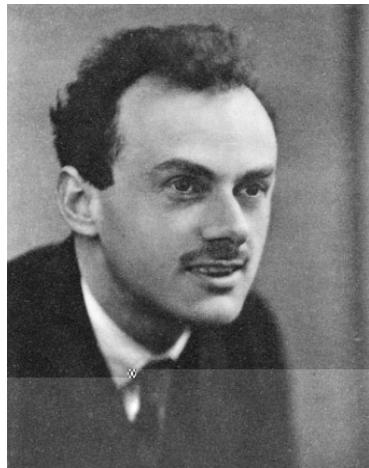
Outline

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

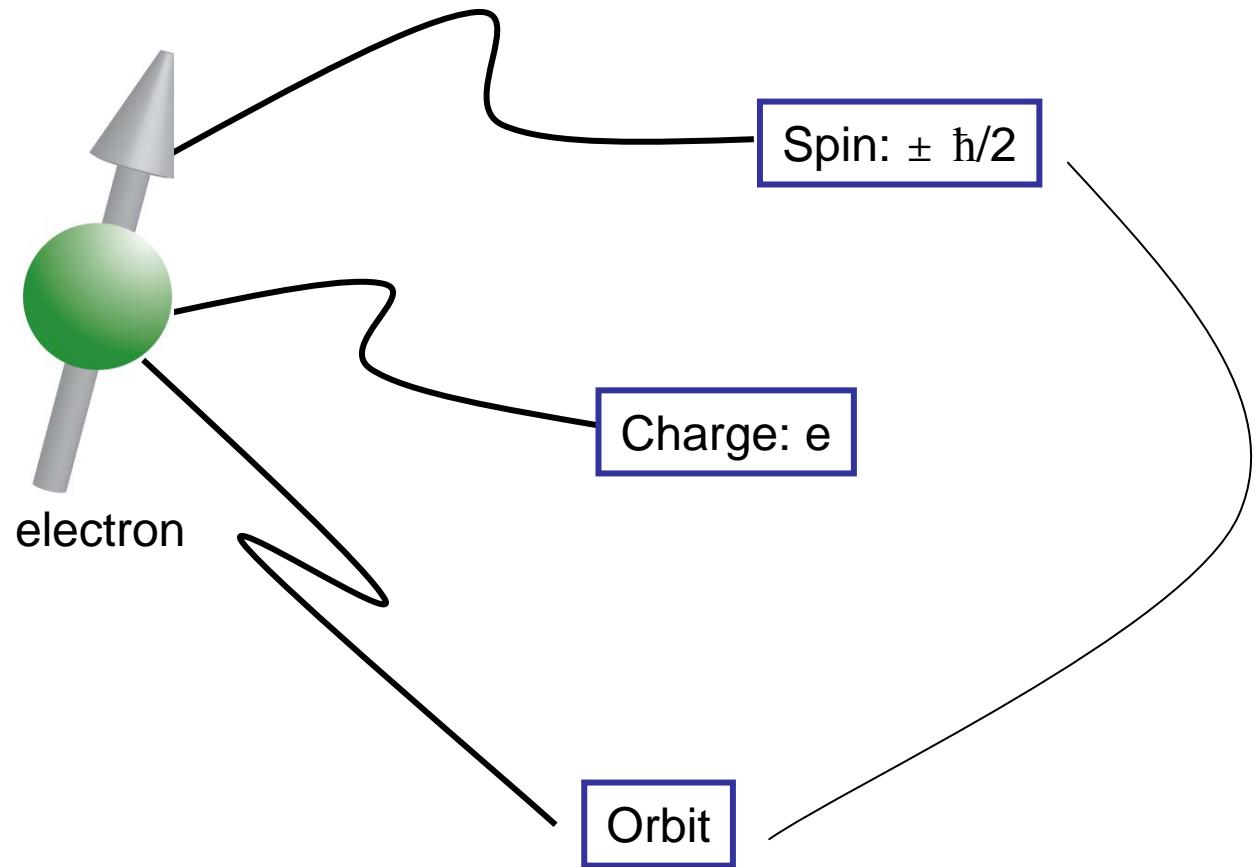
Dirac equation

Electron should have “spin.”

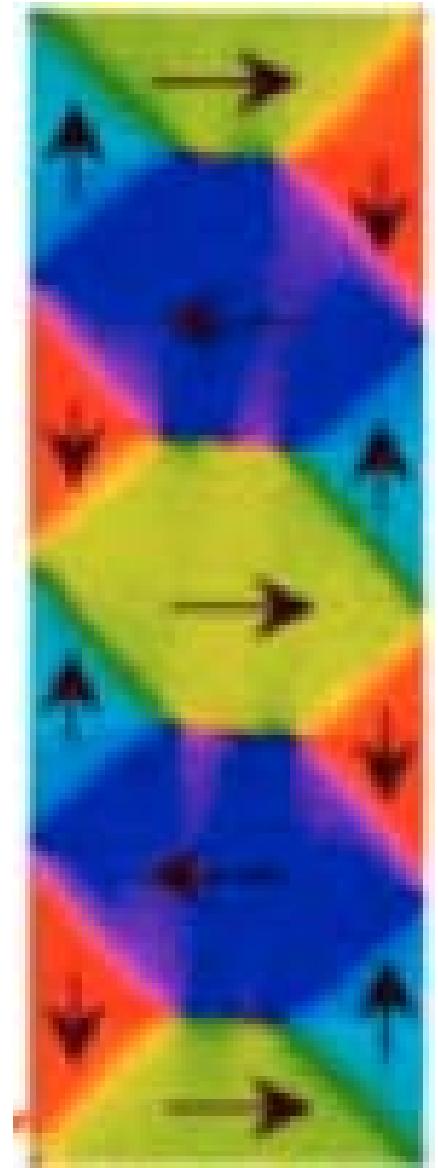
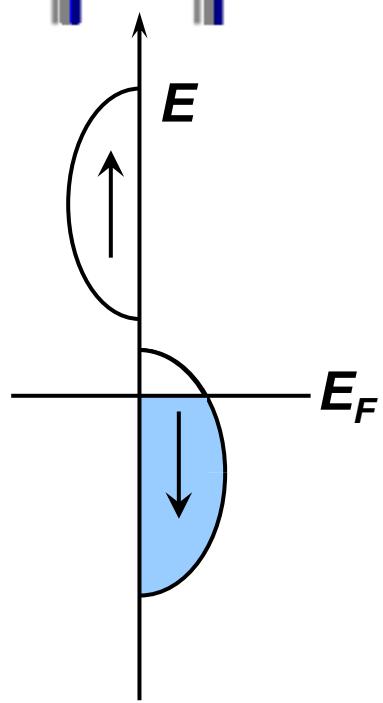
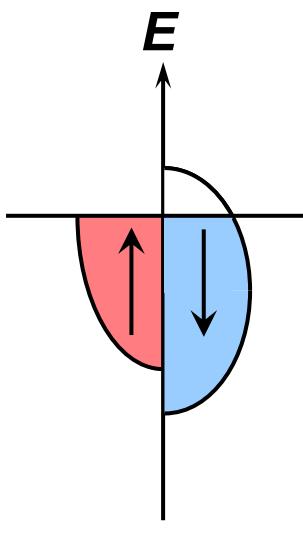
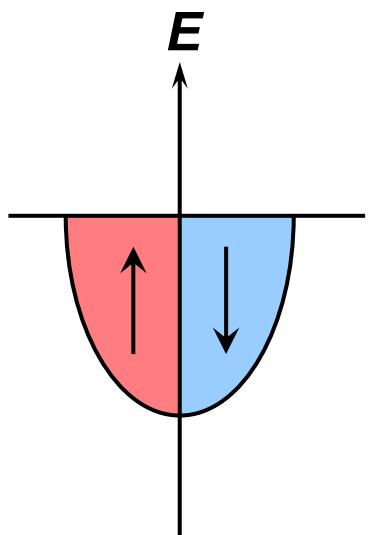
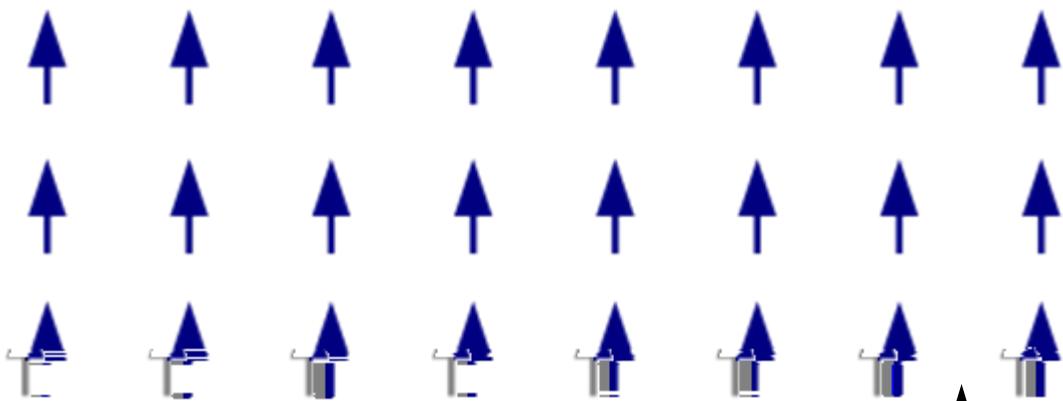
(1928)



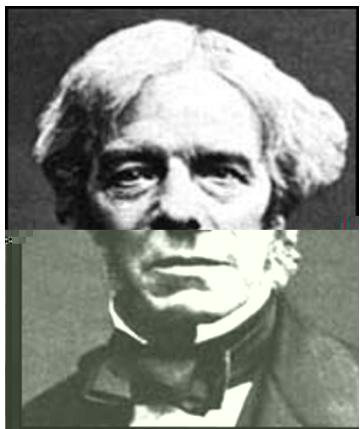
P.A.M. Dirac



Ferromagnetism



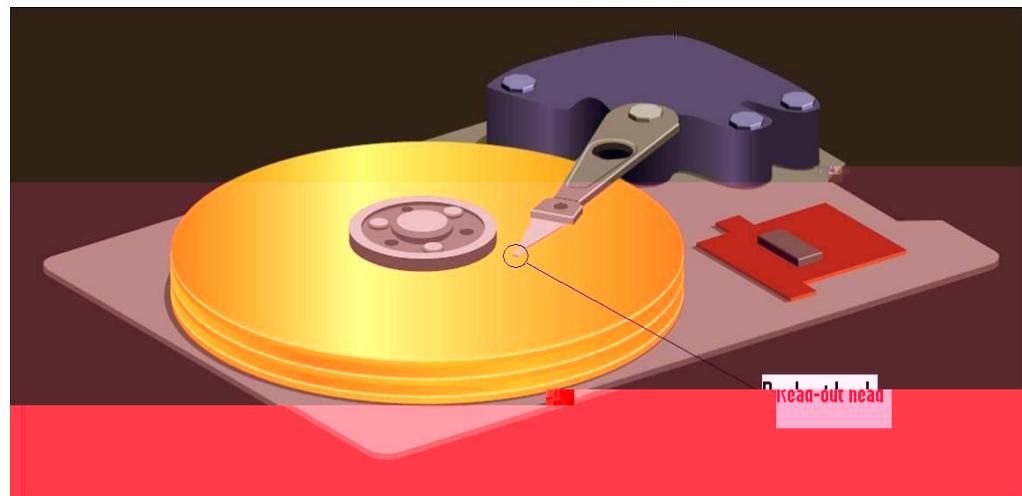
Faraday effect---Maxwell Equation (1865)



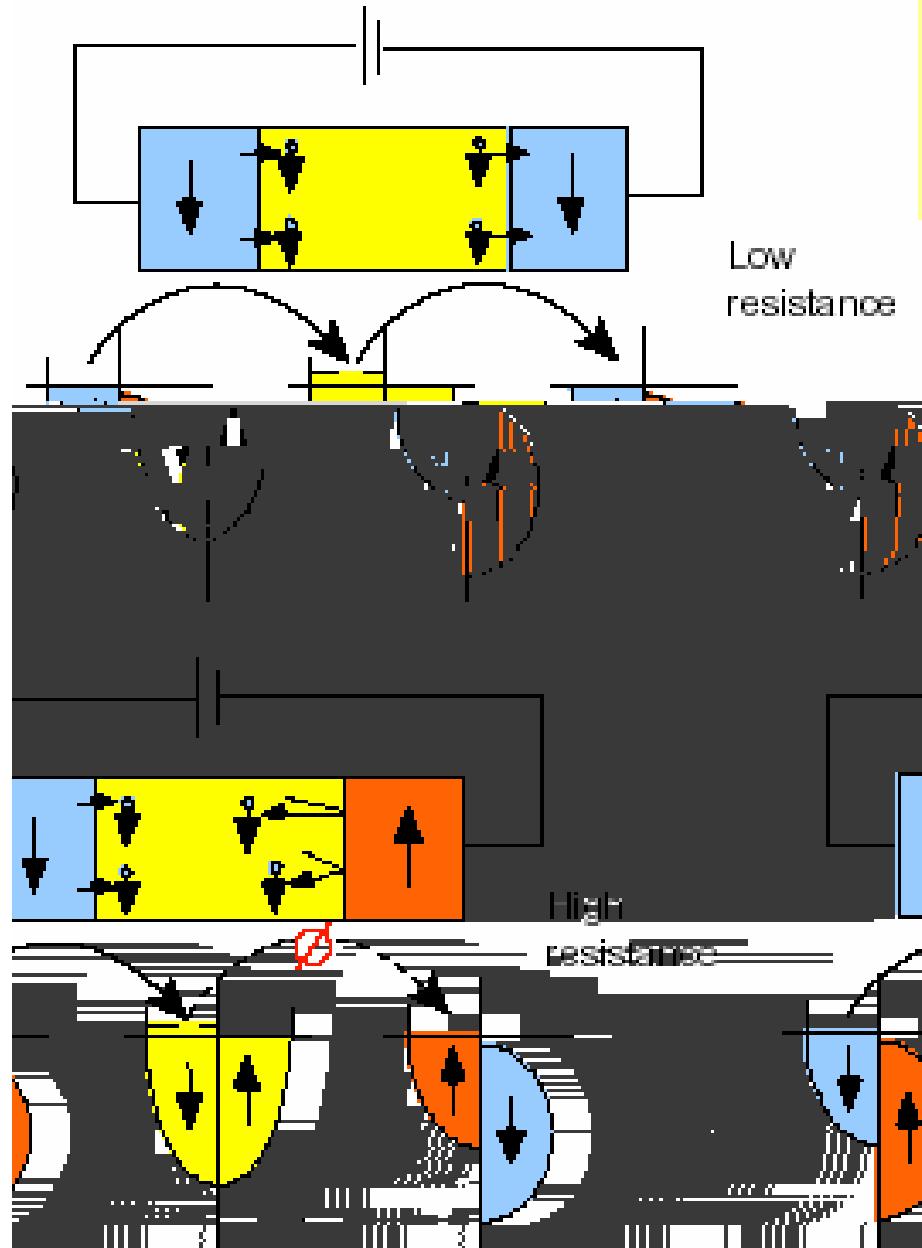
Faraday's law:

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

M. Faraday

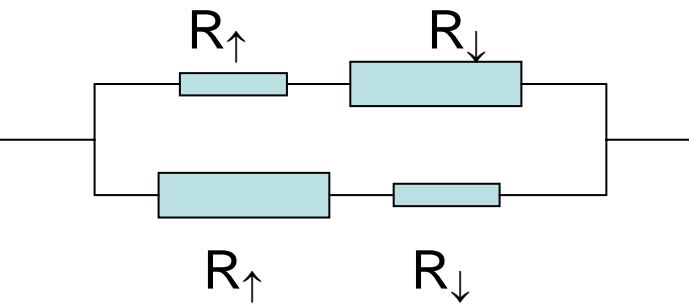
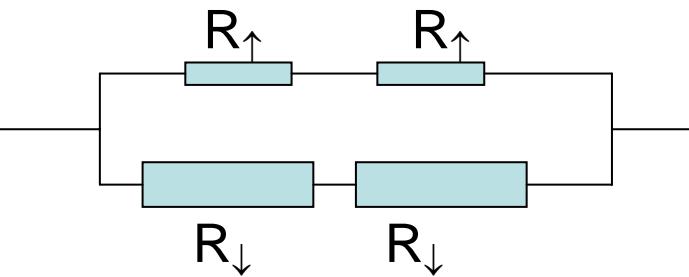


Spin bottleneck magnetoresistance



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

spin

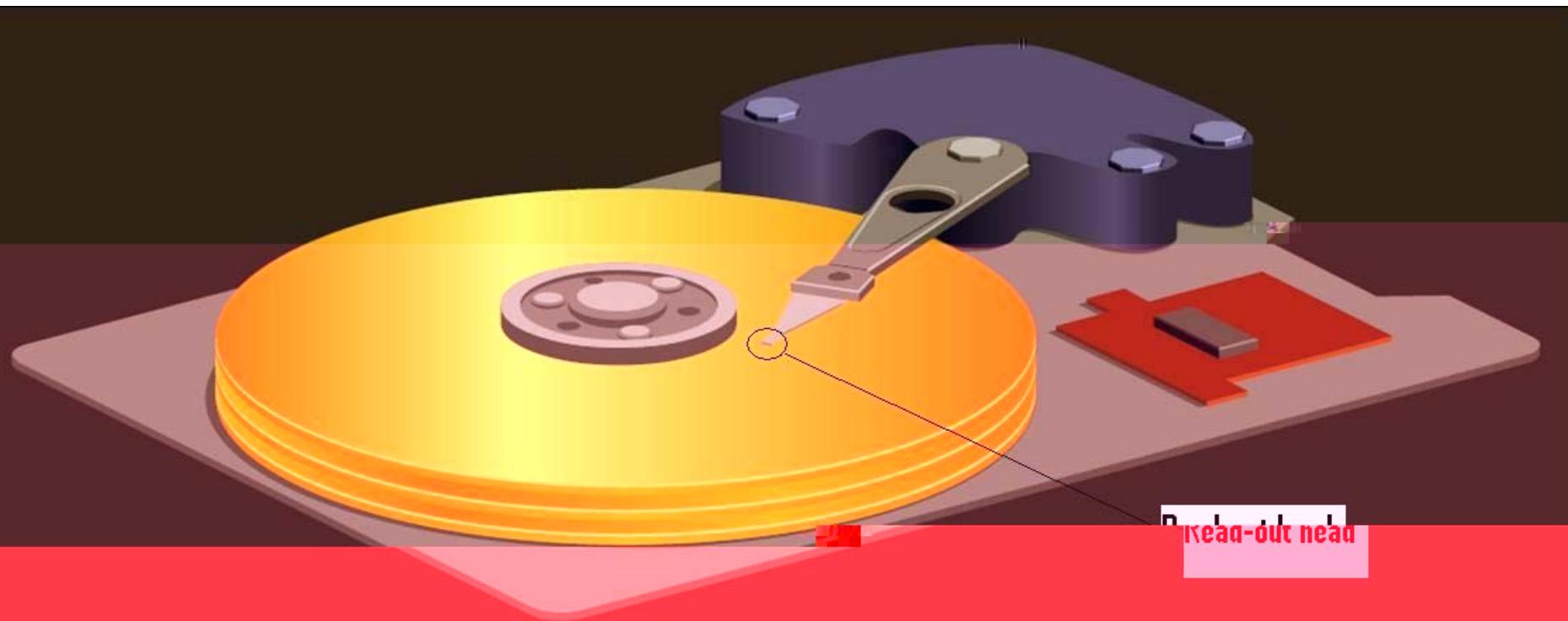
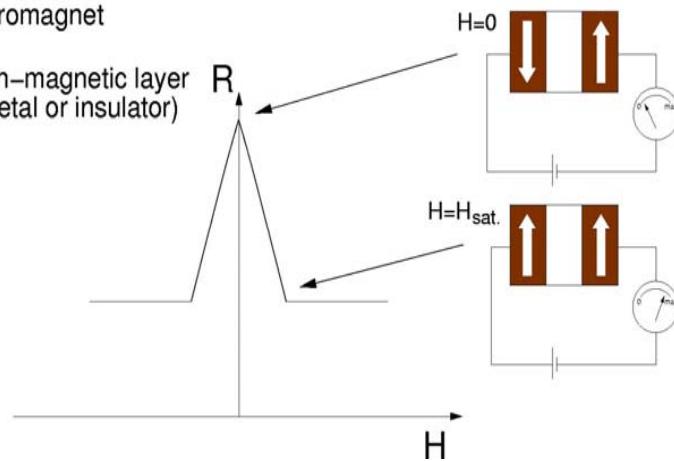


--GMR

-GMR

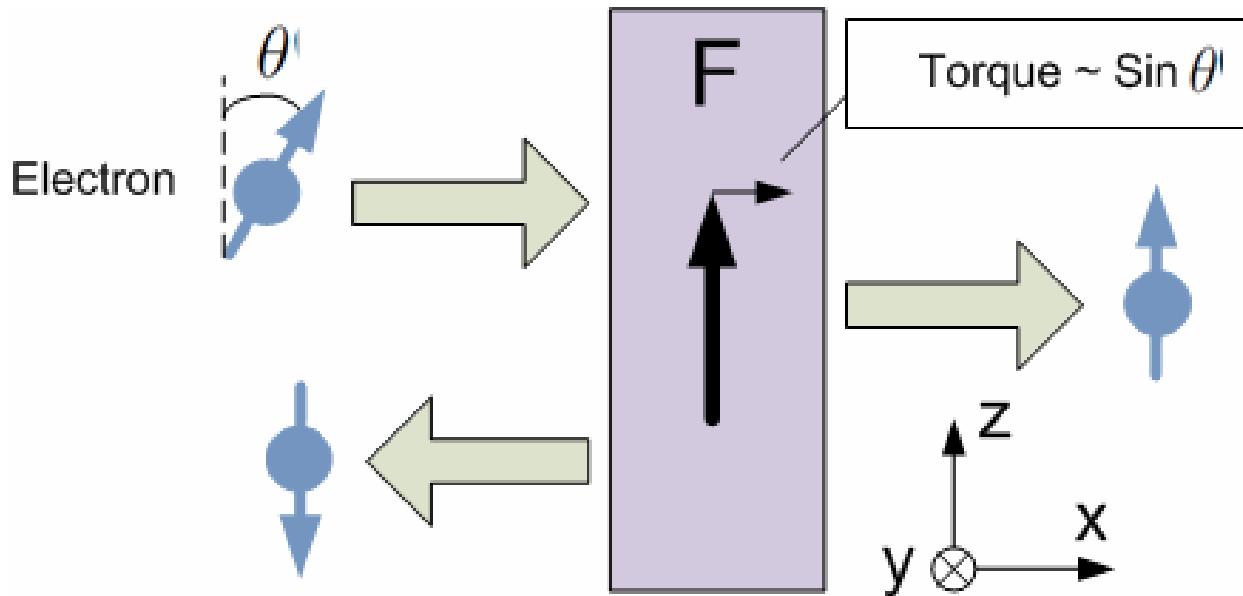
— ferromagnet

— non-magnetic layer
(metal or insulator)



Schematic of exchange torque generated by spin-filtering

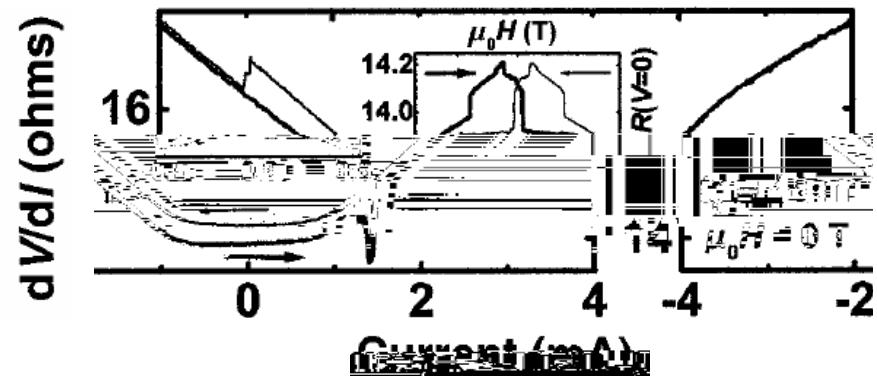
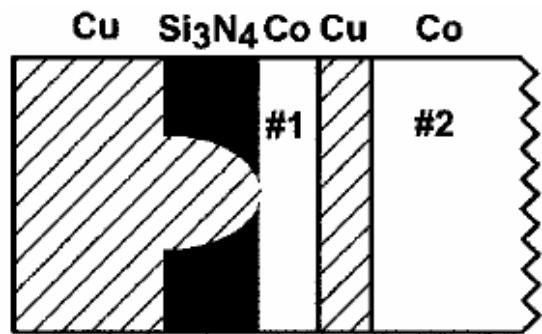
$$|\psi_{in}\rangle = \frac{e^{ik_\uparrow x}}{\sqrt{k_\downarrow}} \cos\left(\frac{\theta}{2}\right) |\uparrow\rangle + \frac{e^{ik_\downarrow x}}{\sqrt{k_\downarrow}} \sin\left(\frac{\theta}{2}\right) |\downarrow\rangle$$



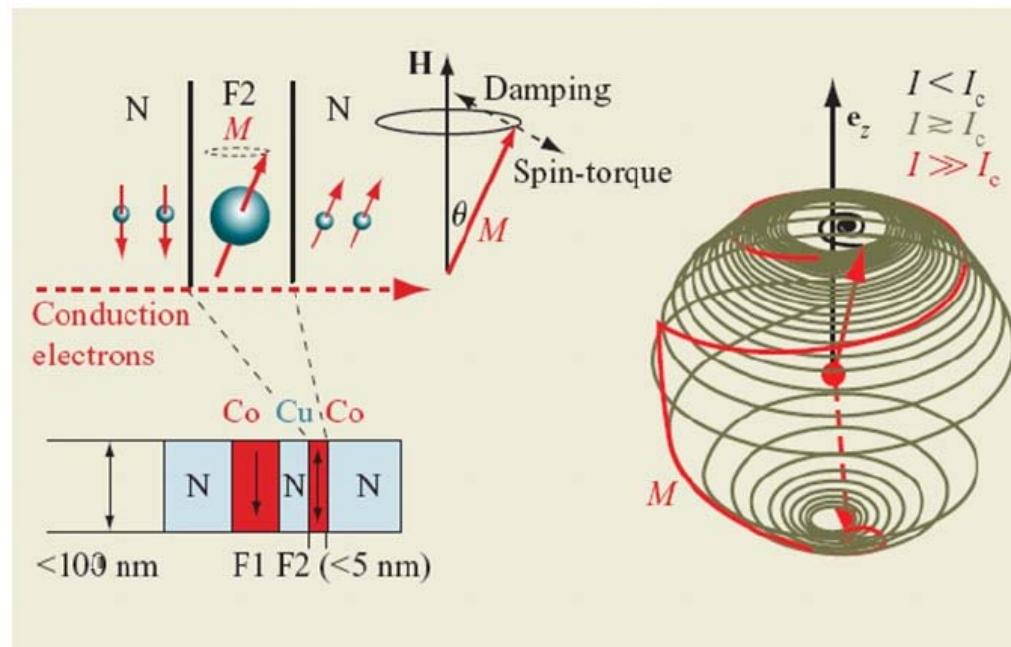
$$\frac{1}{\sqrt{k_\downarrow}} |\psi_{in}\rangle = \frac{e^{-ik_\downarrow x}}{\sqrt{k_\downarrow}} \sin\left(\frac{\theta}{2}\right) |\downarrow\rangle + |\psi_t\rangle$$
$$|\psi_t\rangle = \frac{e^{ik_\uparrow x}}{\sqrt{k_\uparrow}} \cos\left(\frac{\theta}{2}\right) |\uparrow\rangle$$

Slonczewski, J. C. (1996). Berger, L. (1996). L. Berger (1974)

Spin-transfer torques effects (1999)



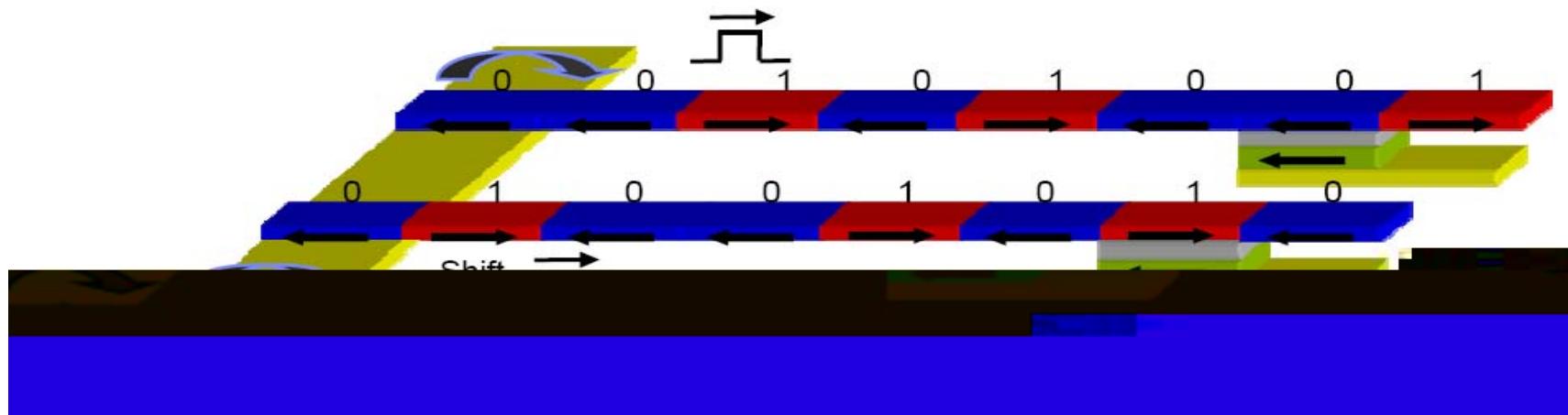
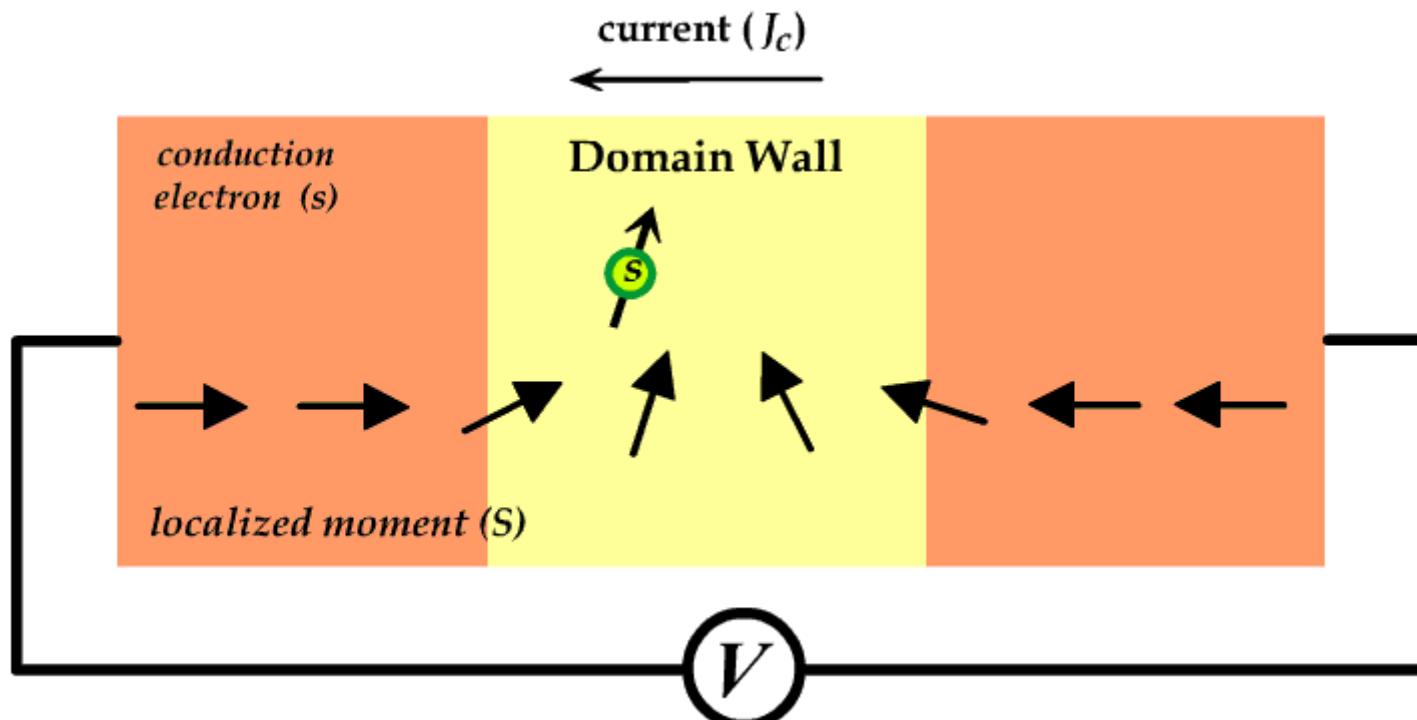
Myers, et al., Science 285, 867 (1999)



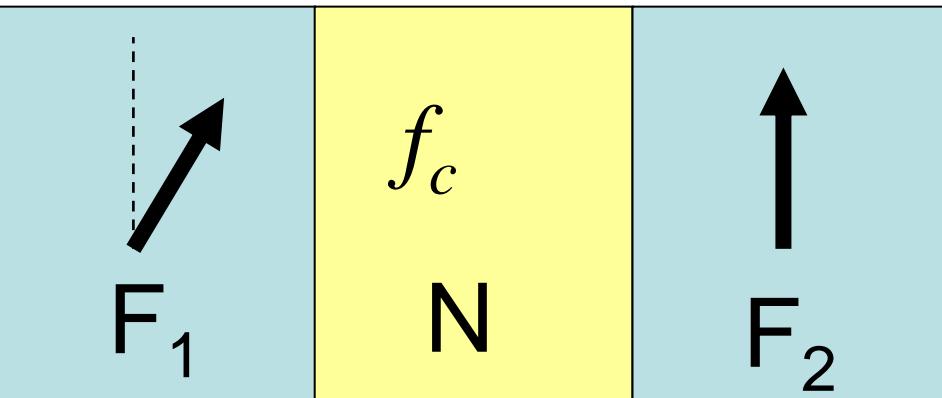
Sun, IBM J. Res. & Dev. 50, 81(2006)

Current-driven domain wall motion:

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



Circuit theory(Batraas2001)



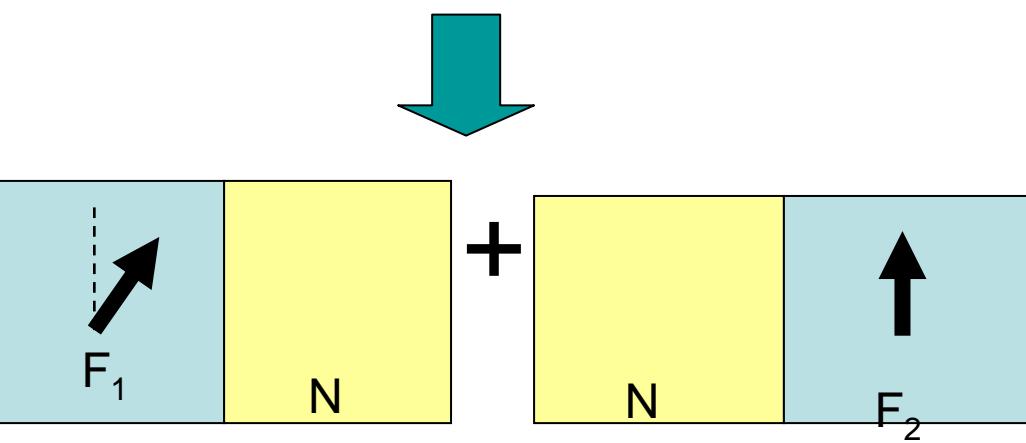
Boundary condition

Charge current

$$I_1 \quad I_2$$

Spin current

$$\mathbf{I}_s \quad \mathbf{I}_s$$



Charge accumulation f_c

Spin accumulation

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

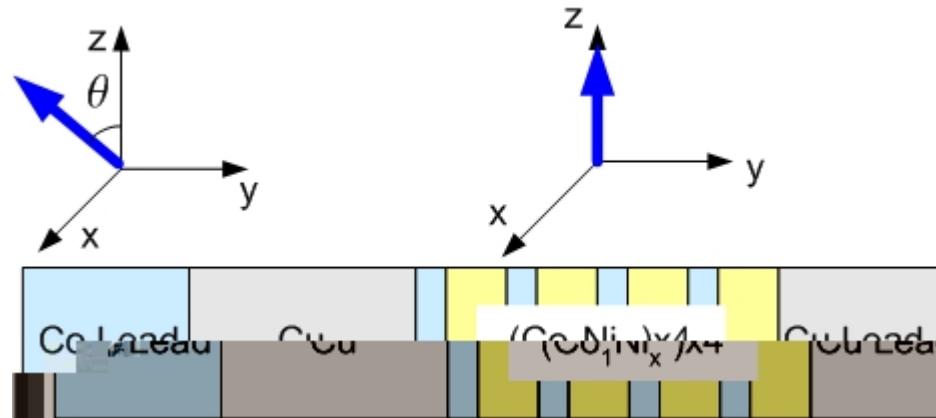
Current and spin current for F_1/N

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

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

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:

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

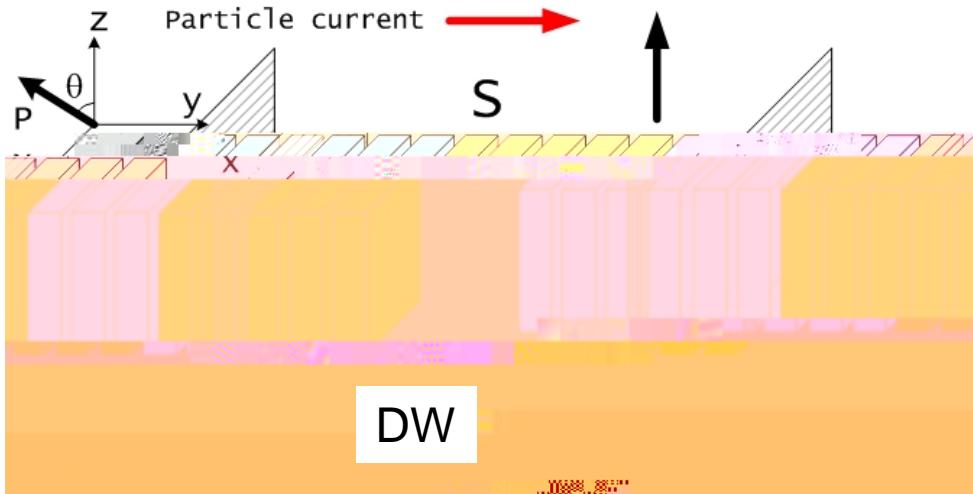
Spin torque from one lead:

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

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

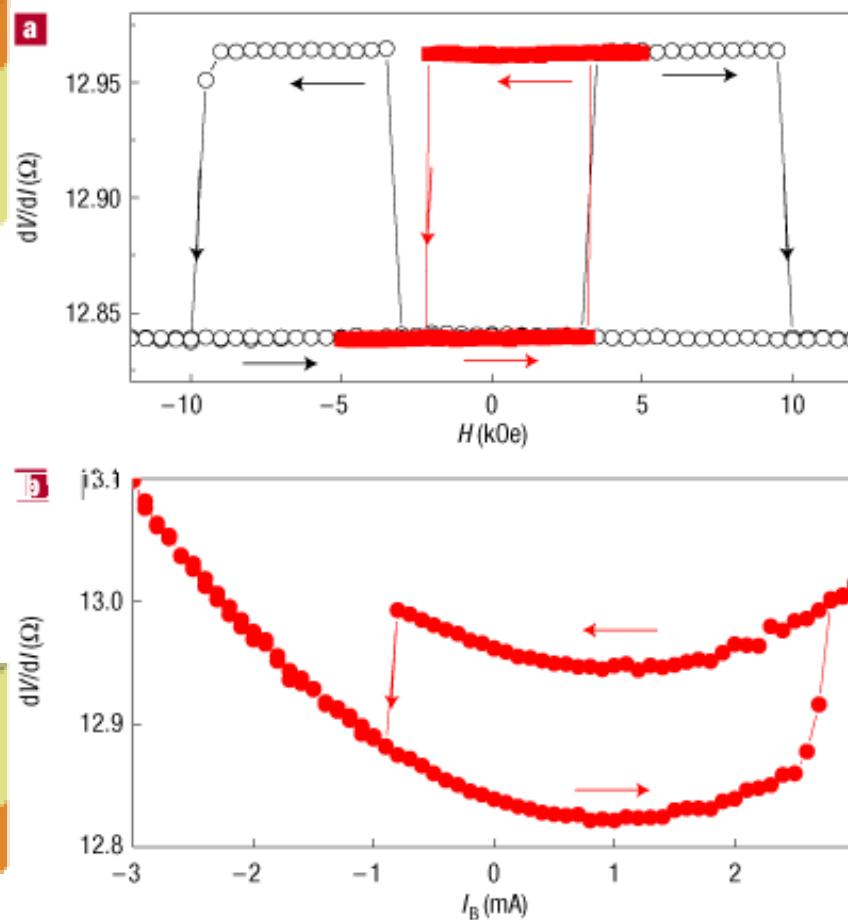
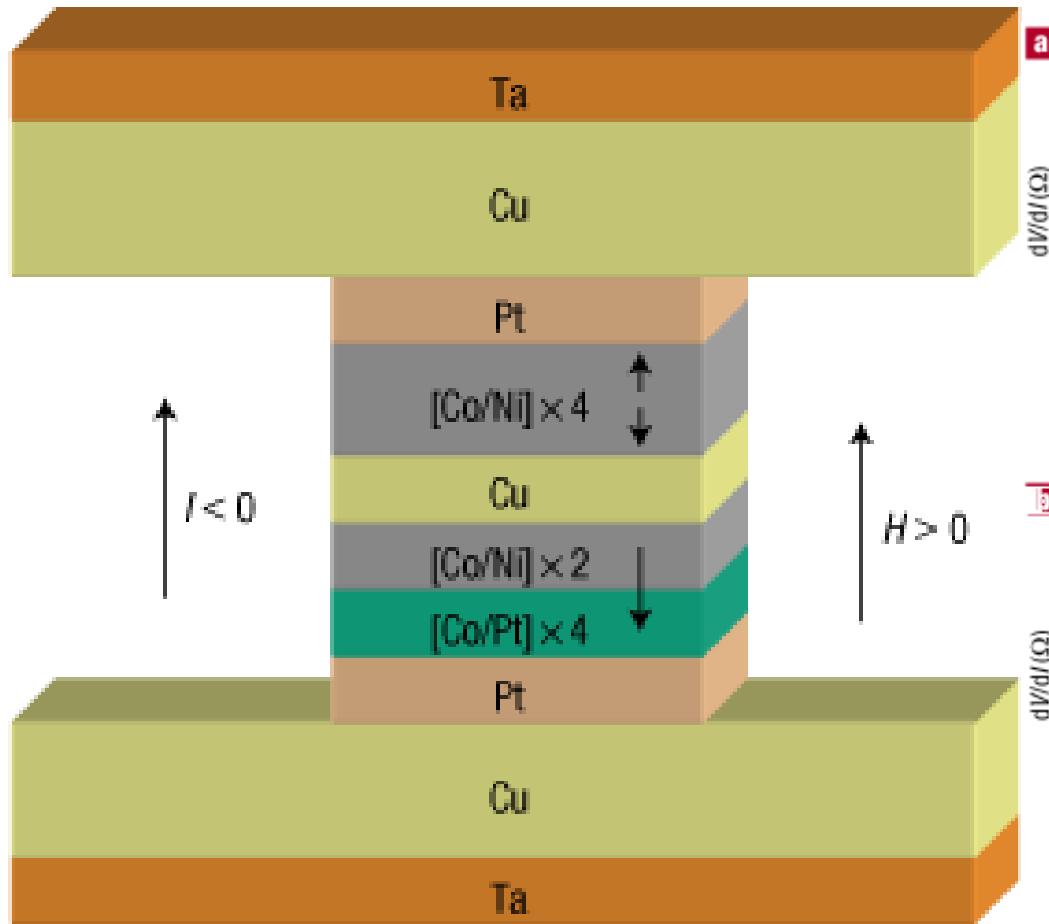


$$\tau \propto \langle \vec{S} \rangle \times \dot{\vec{M}}$$

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

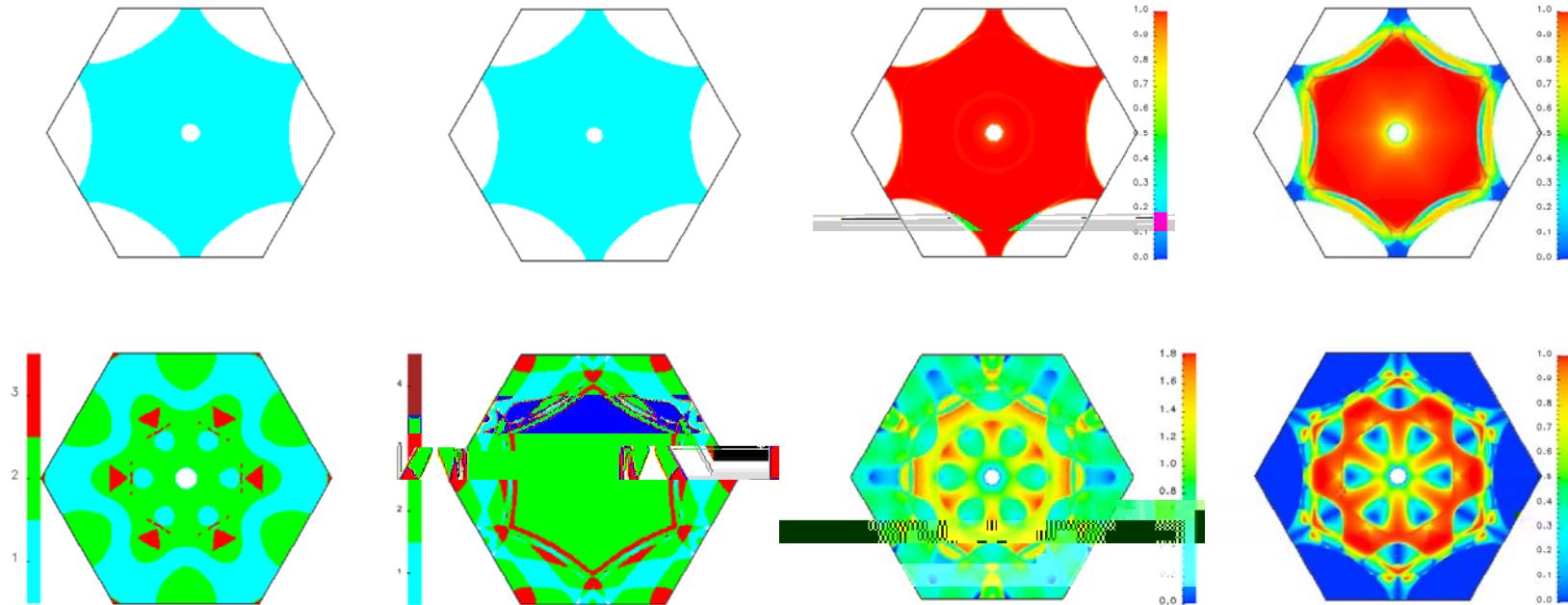
Linear equations of system

$$\begin{pmatrix} \mathbf{C}_0 \\ \mathbf{C}_1 \\ \mathbf{C}_2 \\ \dots \\ \mathbf{C}_N \\ \mathbf{C}_{N+1} \end{pmatrix} = (\mathbf{U}\mathbf{P}\mathbf{U}^+ - \tilde{\mathbf{S}})^{-1} \begin{pmatrix} \mathbf{S}_{0,-1} [\mathbf{F}_L^{-1}(+) - \mathbf{F}_L^{-1}(-)] \mathbf{C}_0(+) \\ 0 \\ 0 \\ \dots \\ 0 \\ 0 \end{pmatrix}$$



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



Interface resistance for Co|Ni(111)

AR unit

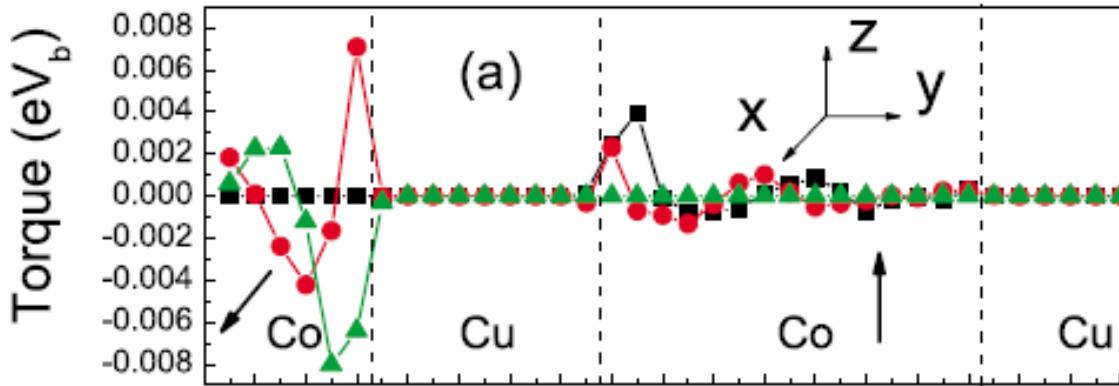
$$\mathbf{f^{-1}\Omega^{-1}m^{-2}}$$

$$AR = \frac{\overline{AR}_{\downarrow} - \overline{AR}_{\uparrow}}{\overline{AR}_{\uparrow} + \overline{AR}_{\downarrow}} \cdot \text{Gamma}$$

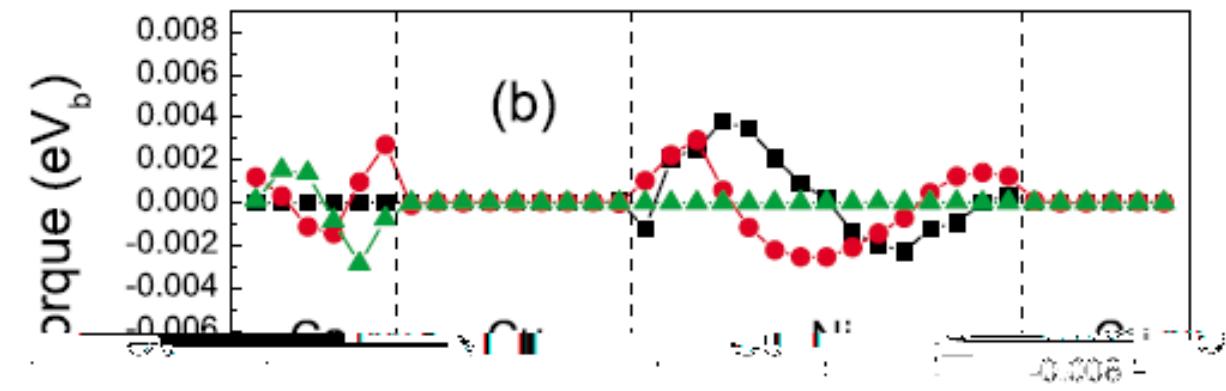
Lattice constant		AR(maj.)	AR(min.)	Gamma
Co	3.54 9	0.014664	0.725067	0.960353
Ni	3.52 4	0.0241504	0.727603	0.935749
$\frac{1}{2}(\text{Co}+\text{Ni})$	3.53 7	0.0186835	0.730984	0.950155

Co_1Ni_3

Co

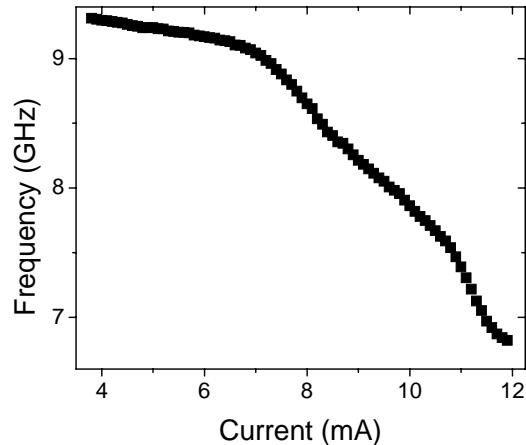


Ni

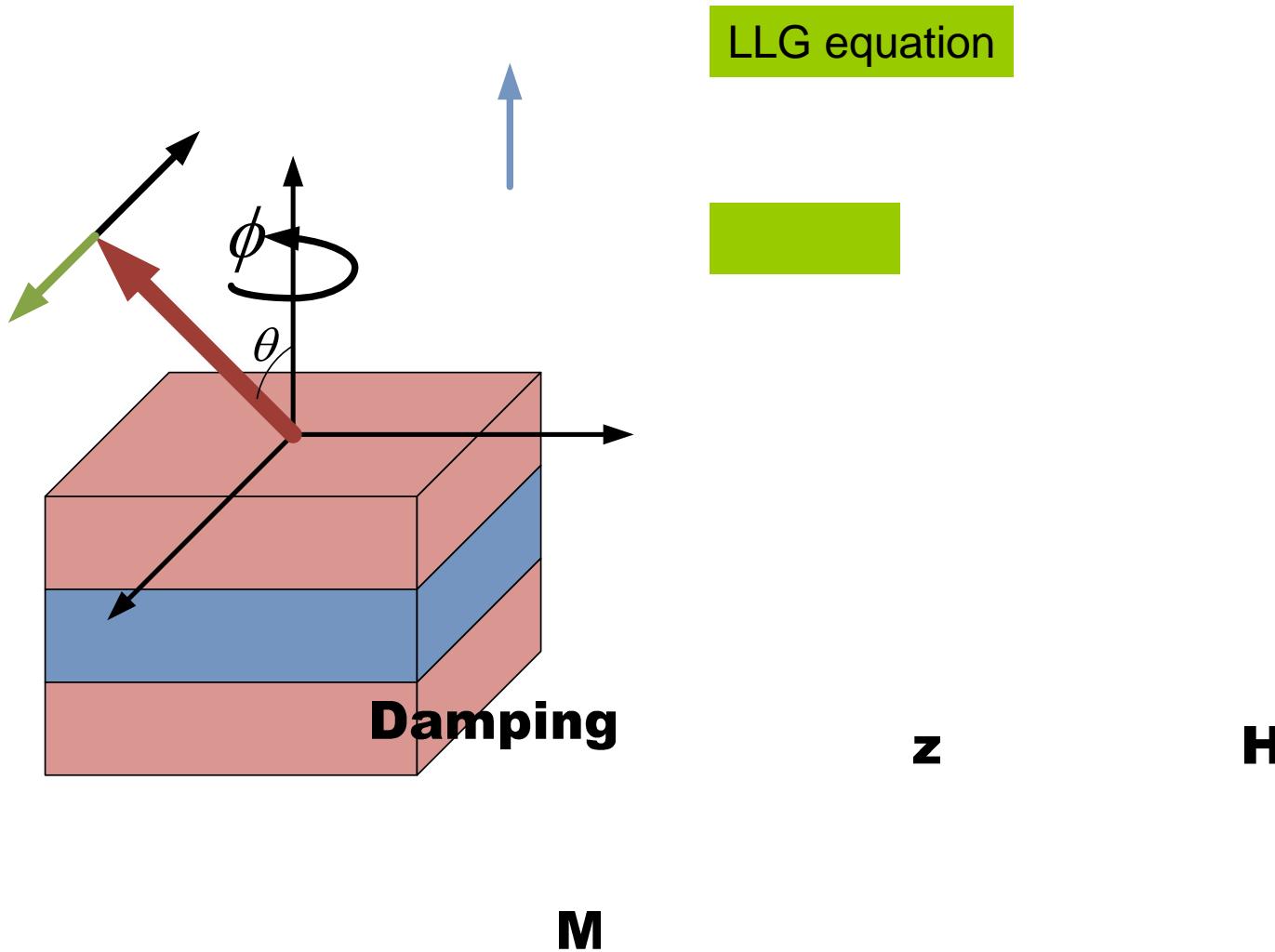


substrate|Ta(3)|Cu(15)|Co₉₀Fe₁₀(20)

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



Spin transfer nanocontact oscillator devices(STNO)



g factor [1]

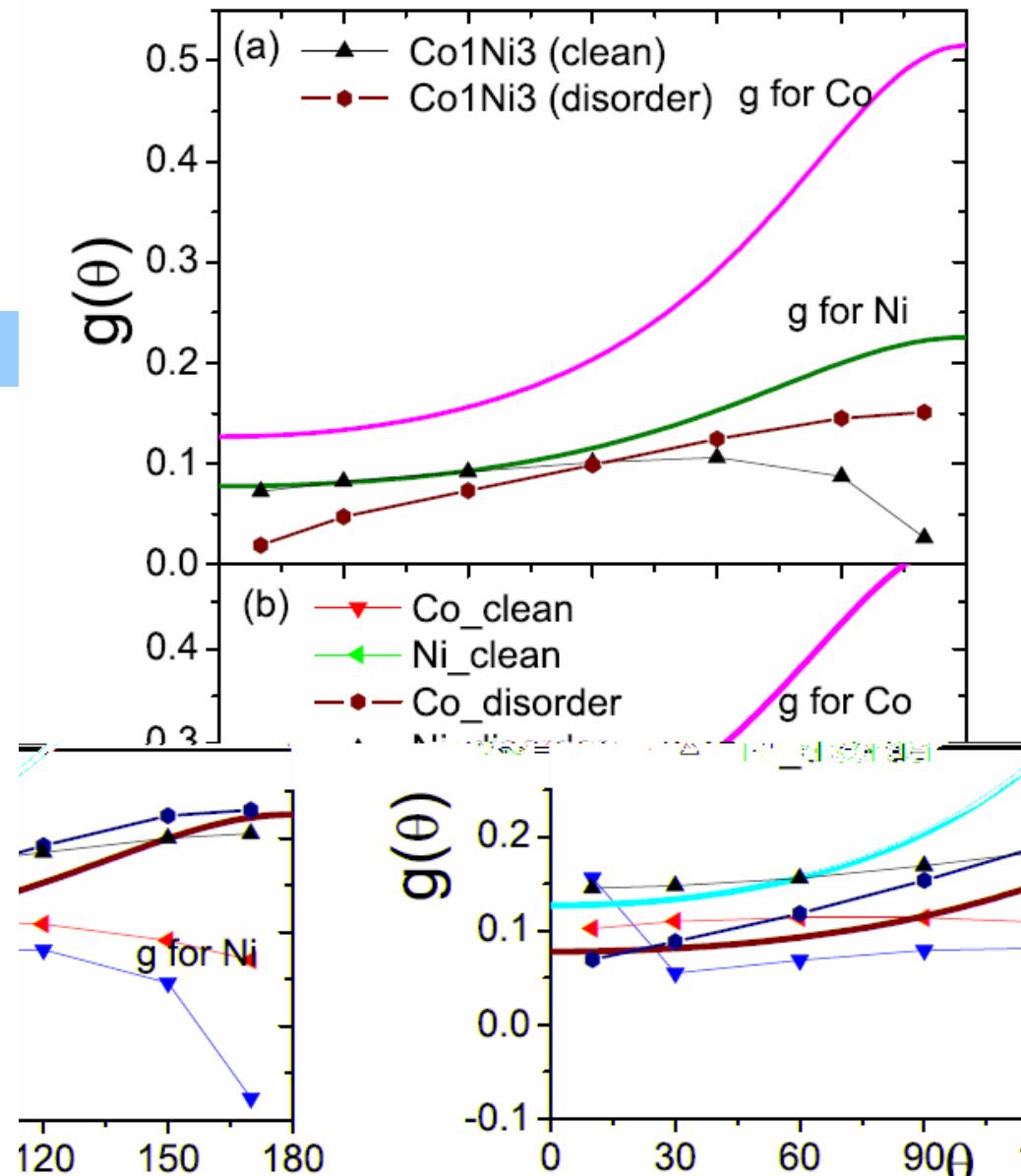
G factor

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

Here Co P=0.35 Ni P=0.23

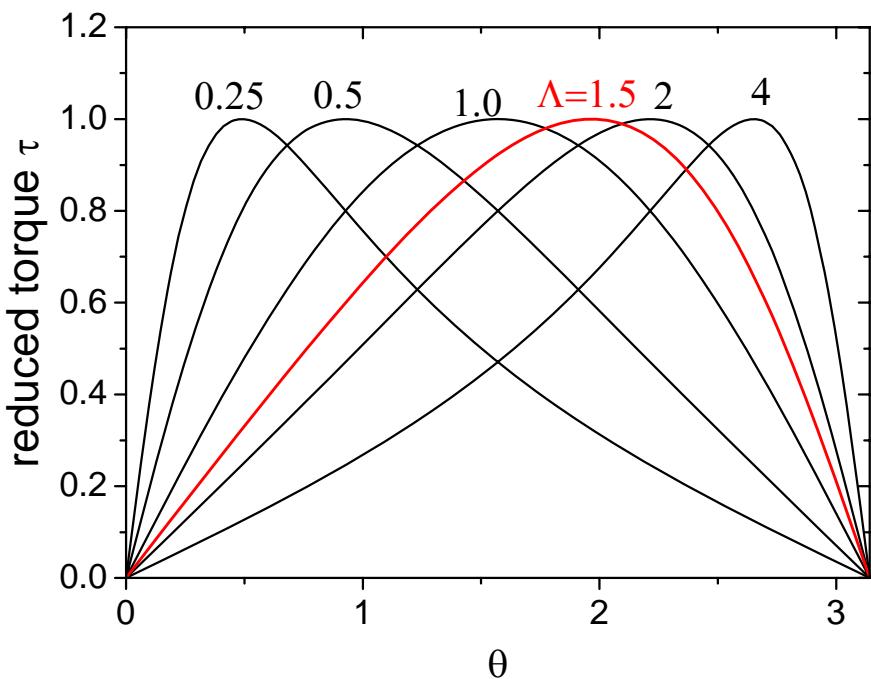
$$g(\theta) = \frac{\text{torque}(\theta)}{\mathbf{I}(\theta) \sin(\theta)}$$

G factor can be enhanced by disorder effect.



Reduced torque

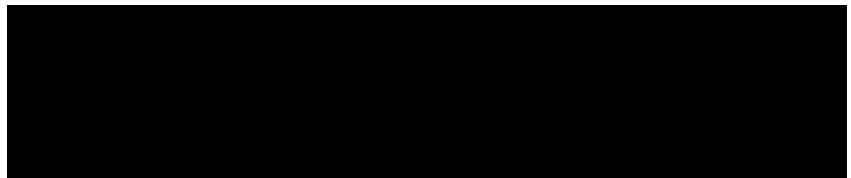
$$\Lambda = 1.5$$

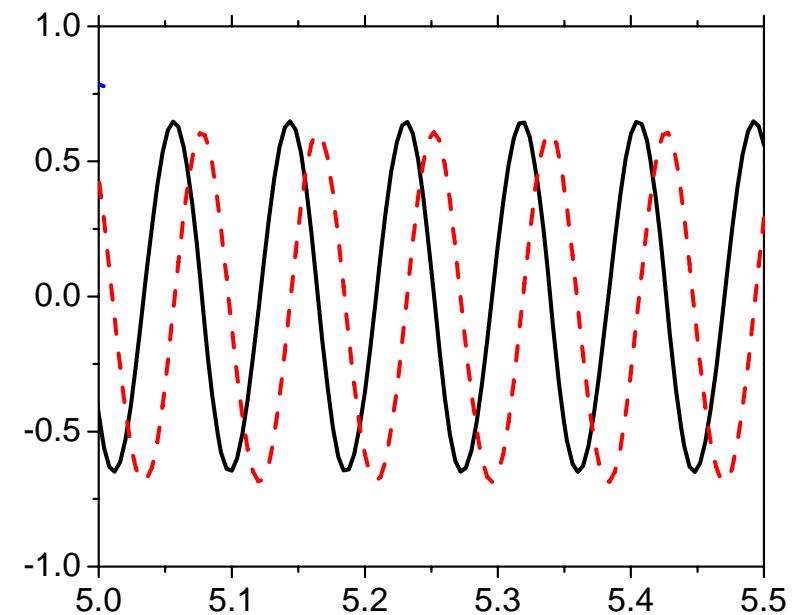


Torques

$$L = \hbar I P_x \Lambda \tau(\theta) / 4 A e$$

Reduced torques

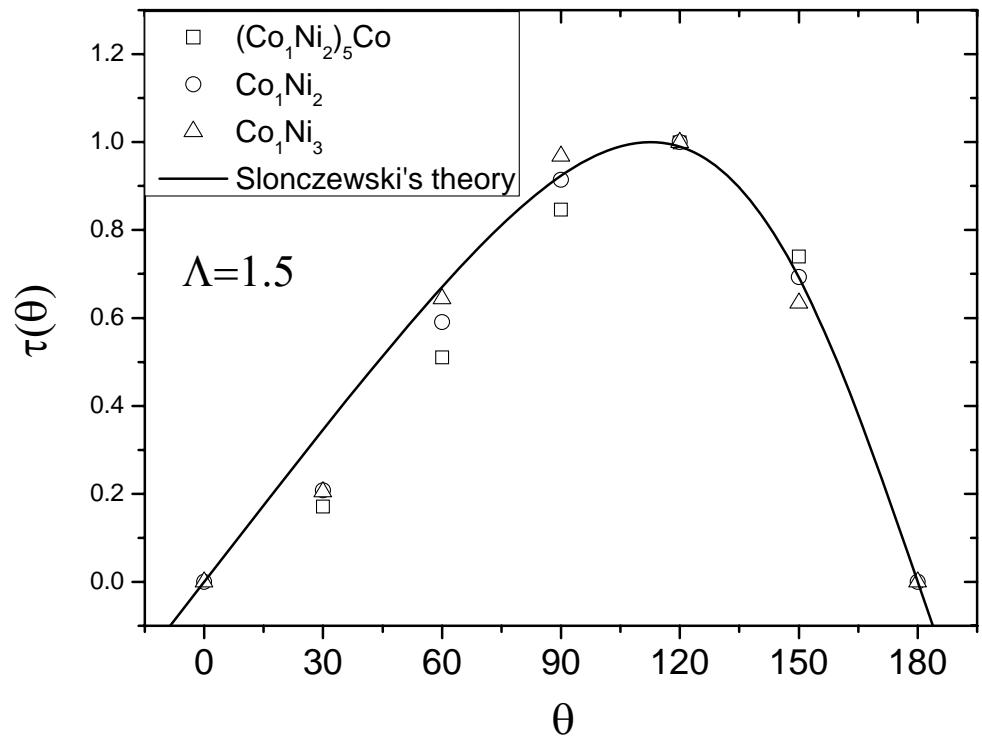




Cu/Co/Cu/(Co₁Ni₂)₅Co/Cu

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

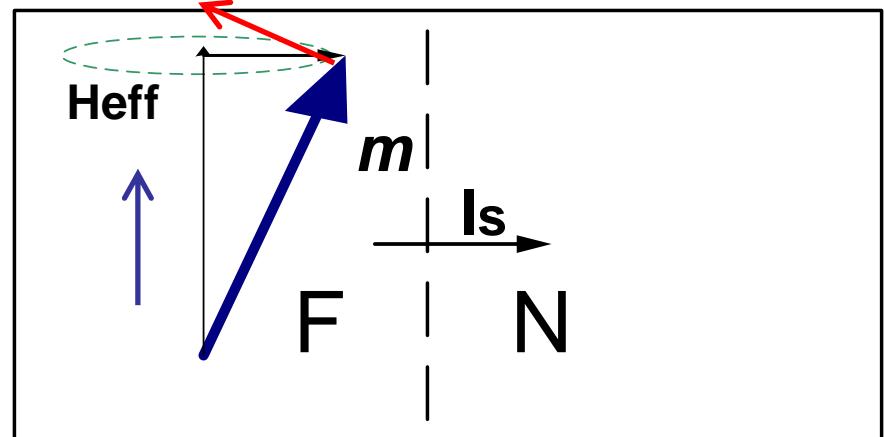
$$\dot{\vec{m}} = \gamma_0 \vec{H}_{eff} \times \vec{m} + \alpha_0 \dot{\vec{m}} \times \vec{m} + \frac{\partial \vec{m}}{\partial t}$$

Precession **Damping** **Spin Transfer Torque
from current I_s**

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

$$A_{eff}^{\uparrow\downarrow}$$

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

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

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

$$I_C = 0.$$

Mixing Conductance (Orbit Function)

$$dI/dV \propto \sin(\omega_m t)$$

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

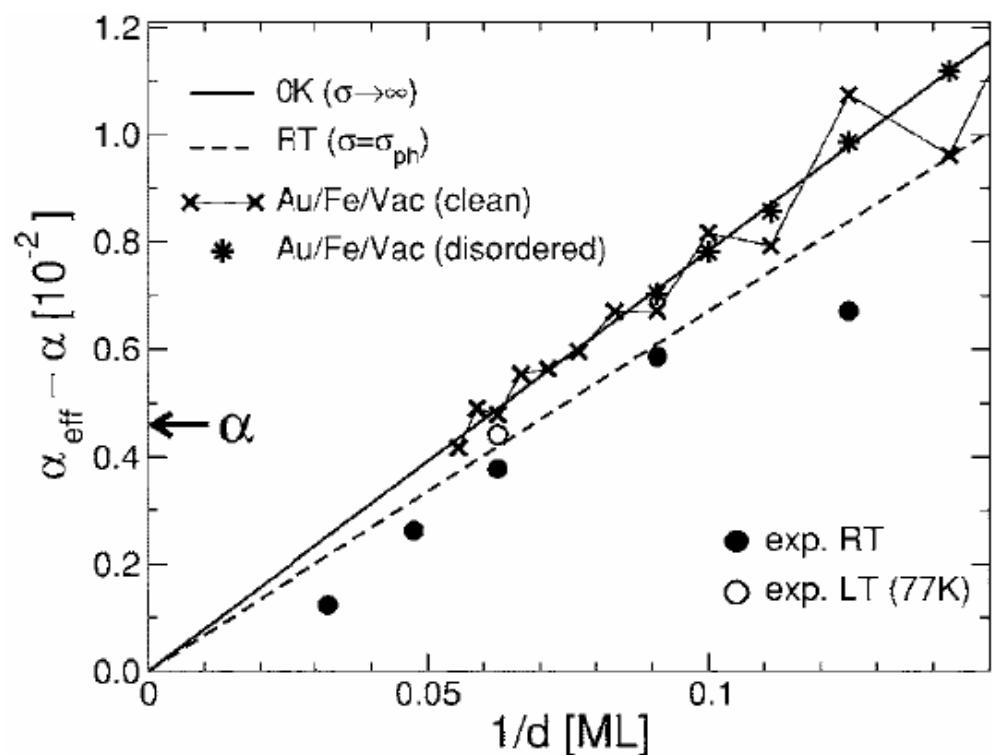
$$\frac{\partial}{\partial t} \vec{m} = -\gamma_{eff} \vec{m} \times \overrightarrow{H_{eff}} + \alpha_{eff} \vec{m} \times \frac{\partial}{\partial t} \vec{m}$$

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

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

Tserkovnyak, Y. et al

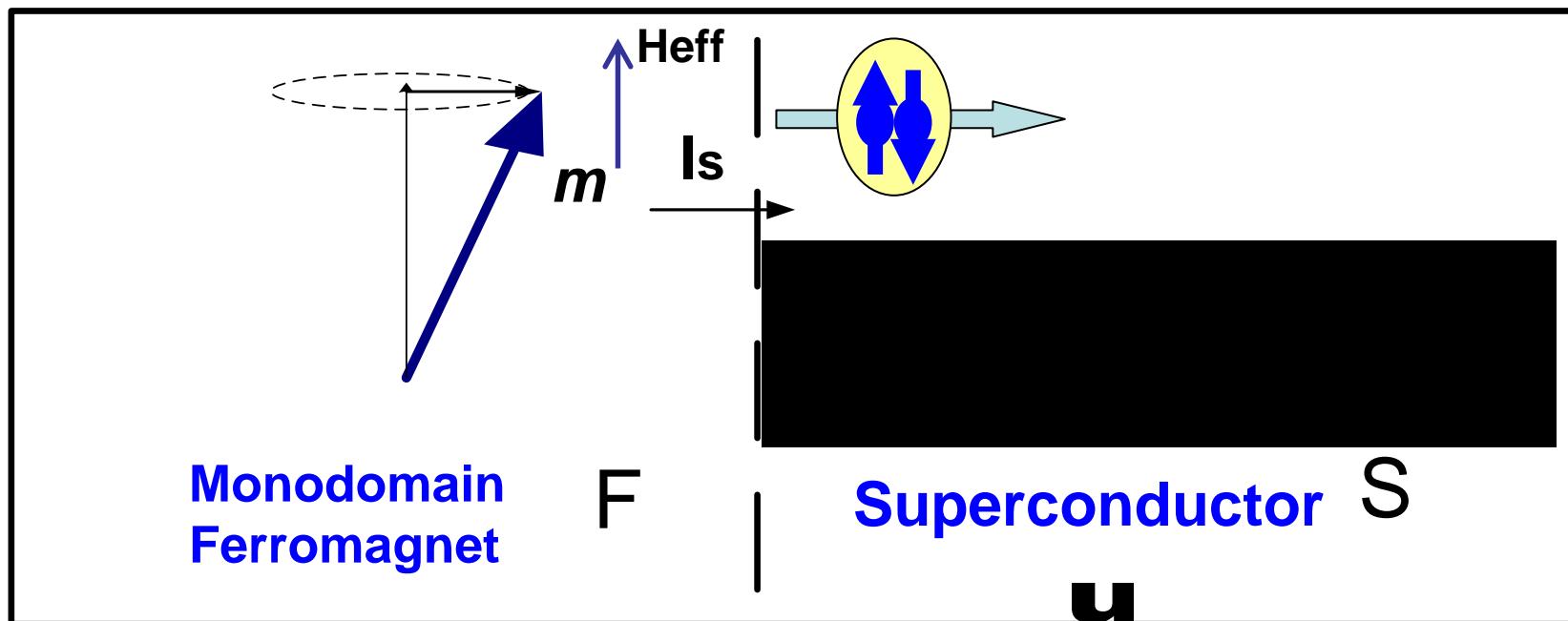
Rev. Mod. Phys. , 77 ,4(2005)



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

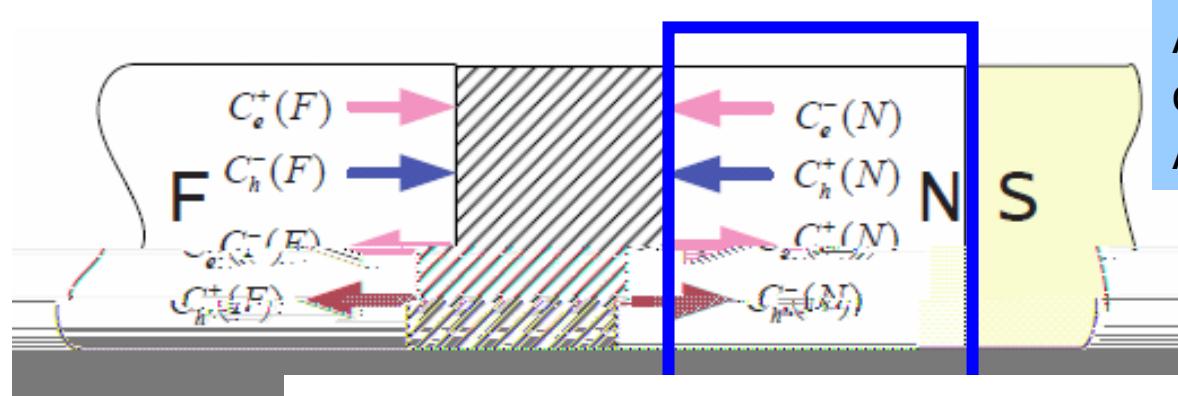
Heinrich, B. et al, J. Appl. Phys. 93, 7545(2003)

Spin Pump at F/S Contacts



z

F/N/S Interface Approach



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

At F/N Interface

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

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

Spin Current in the Presence of Andreev Reflection

Linear Response & Circuit Theory



Spin current and Damping

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

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

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

Mixing Conductance and Andreev Reflection

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

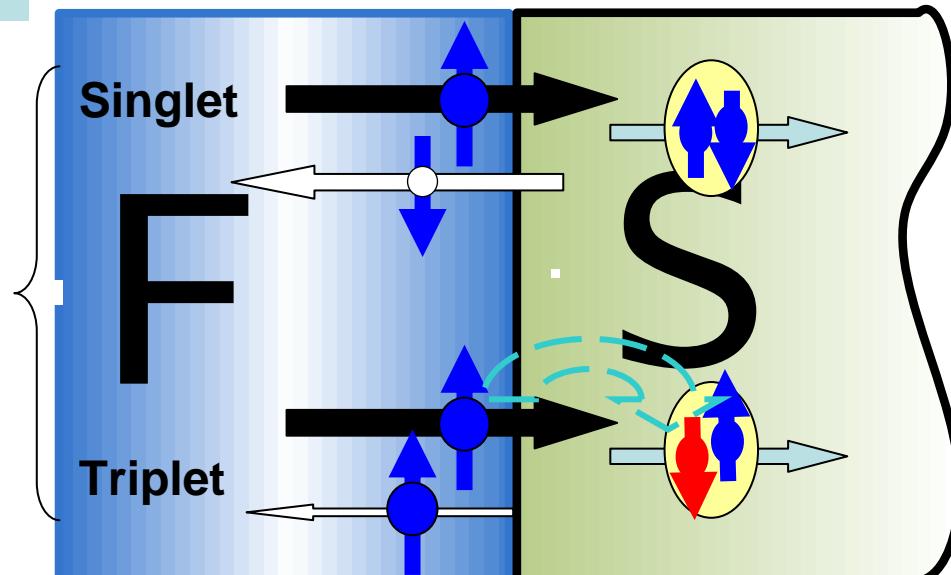
Normal Reflection

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

Singlet

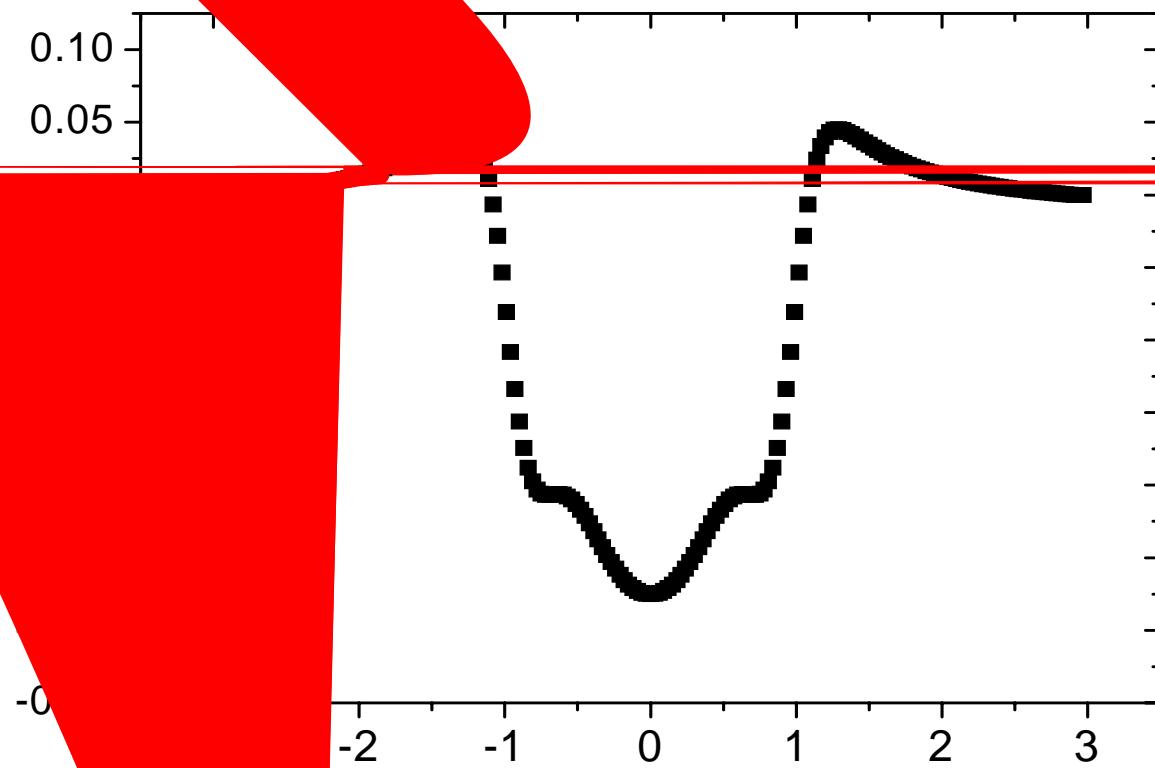
Triplet

Rhe



Andreev Reflection

Charge Conductance Spectrum

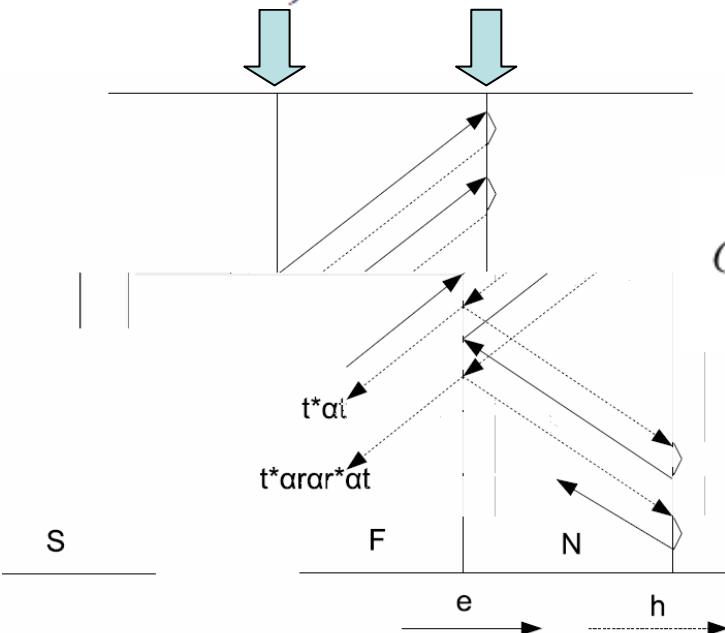


$$r'_{\uparrow(\downarrow)} = |r'_{\uparrow(\downarrow)}| e^{i\phi_{\uparrow}(\phi_{\downarrow})}$$

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

[1]

$$\begin{aligned} r_{he} &= t^* \alpha t + t^* \alpha r \alpha r^* \alpha t + t^* \alpha [r \alpha r^* \alpha]^2 t + \dots \\ &= t^* \alpha [1 - r \alpha r^* \alpha]^{-1} t \end{aligned}$$



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

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

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

F/N

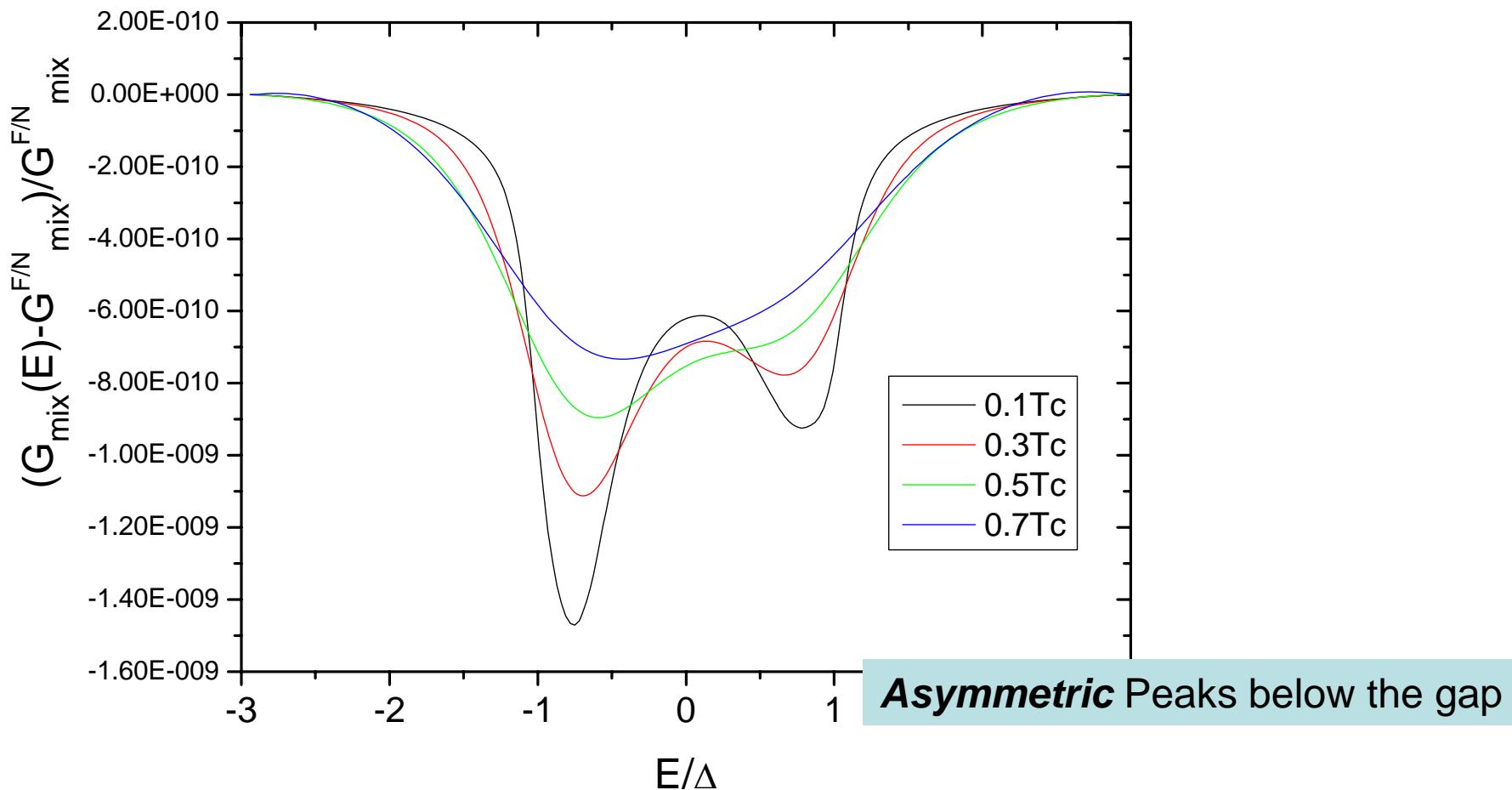
$$\langle G_{FS}(\varepsilon) \rangle = \left| \frac{G_0}{\frac{1}{2\varphi} \int_{-\varphi}^{\varphi} \left(1 - R^2 e^{-i2 \arccos \frac{\varepsilon}{\Delta_0}} e^{i\delta} \right) d\delta} \right|^2$$

$$\delta = \phi_{\uparrow} - \phi_{\downarrow}$$

[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)

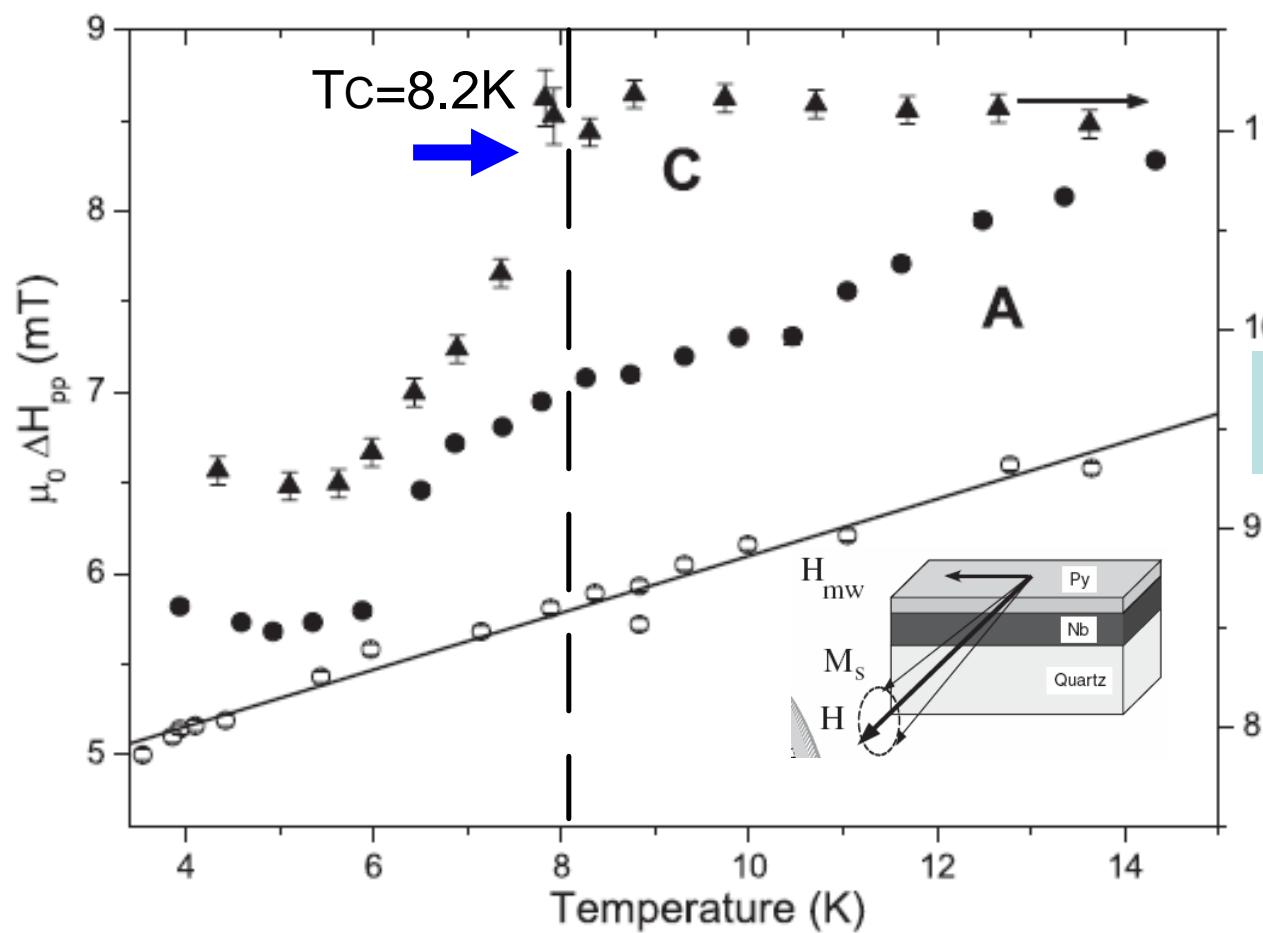
Mixing Conductance Spectrum

$$G_{ee}^{\uparrow\downarrow} = G_{ne}^{\uparrow\downarrow} + G_{,ne}^{\uparrow\downarrow \text{singlet}} + G_{,ne}^{\uparrow\downarrow \text{triplet}}$$

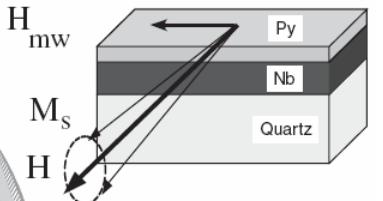


Temperature Dependence of Gilbert Damping Enhancement

Experiment: FMR linewidth



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



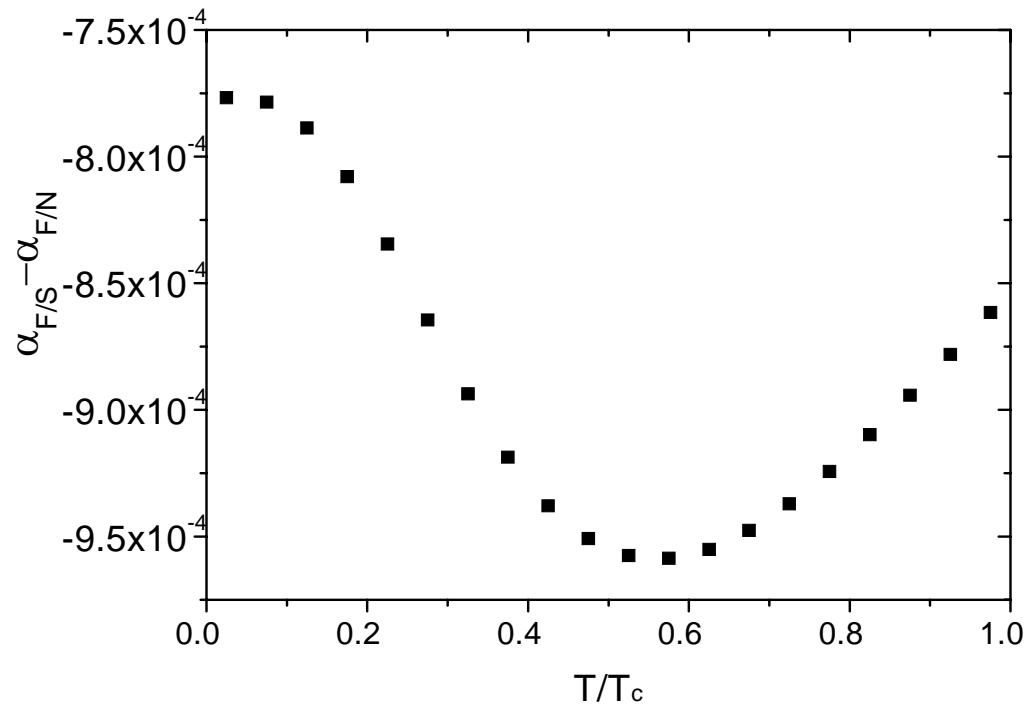
Temperature Dependence of Gilbert Damping Enhancement

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

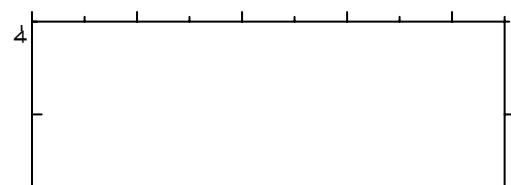
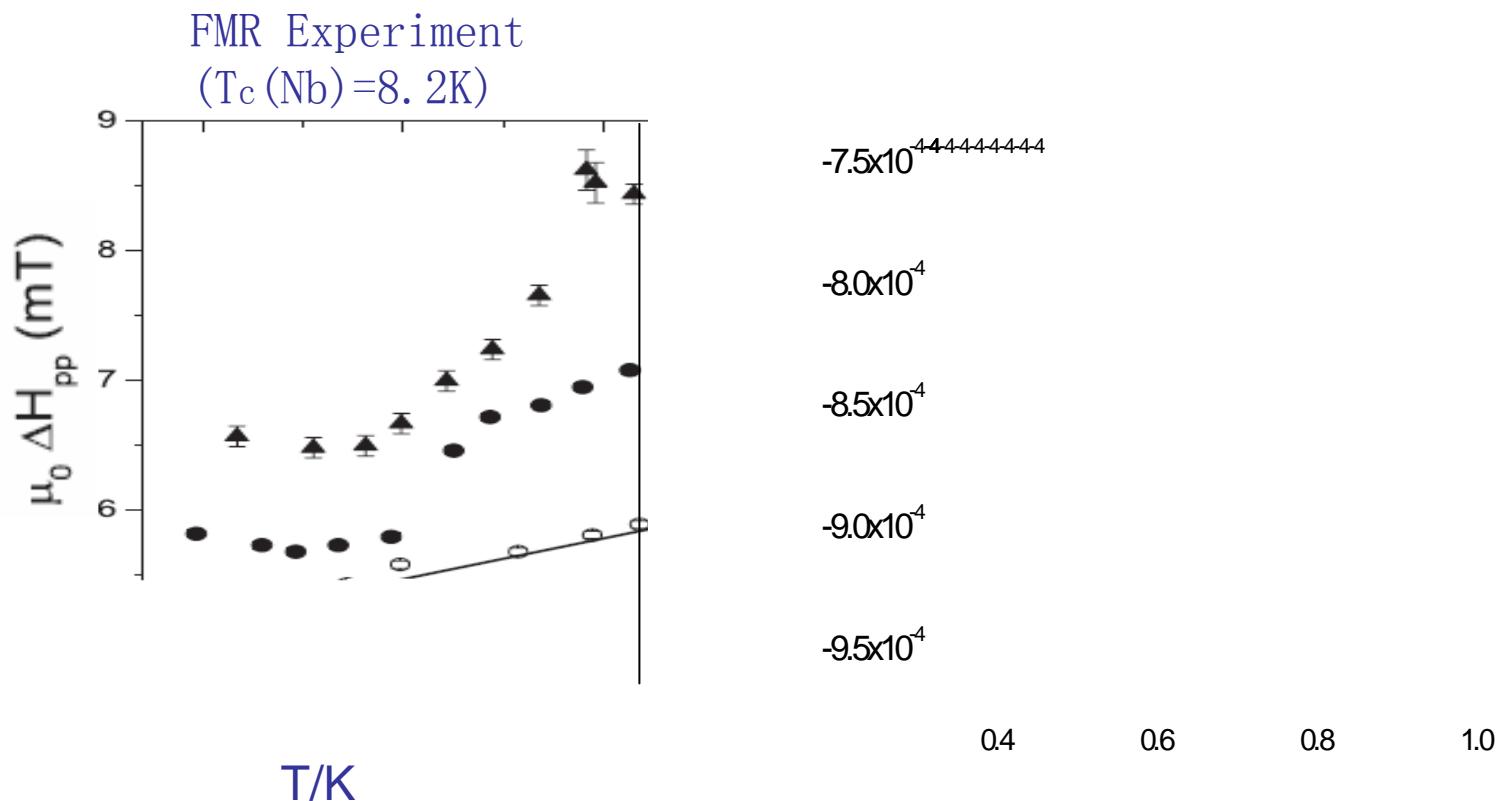
$$\frac{\delta\alpha_{F/S}}{\partial\epsilon} = N_{eff} - Tr(R^{\uparrow\uparrow}R^{\downarrow\downarrow\dagger})$$
$$= \frac{v\hbar}{4\pi M_s V} \frac{\partial f}{\partial E}$$

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

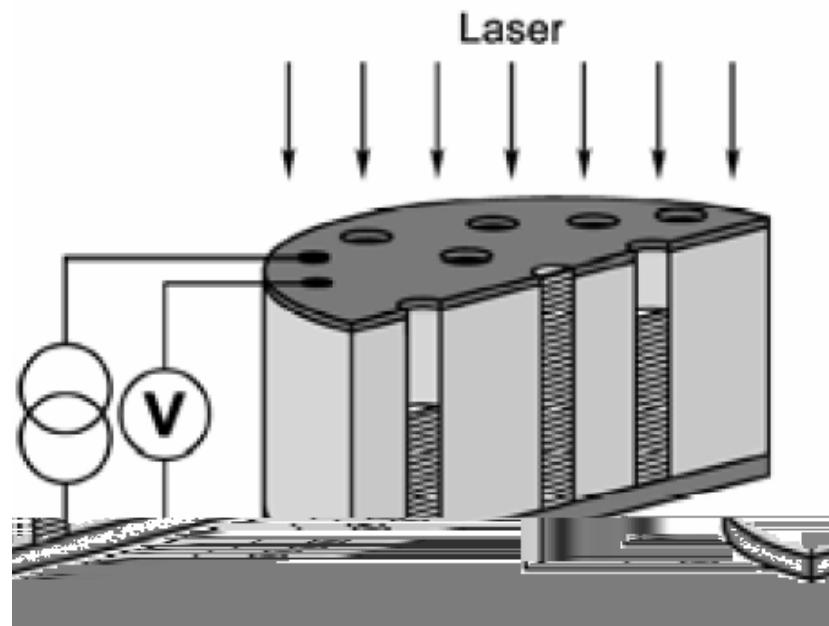
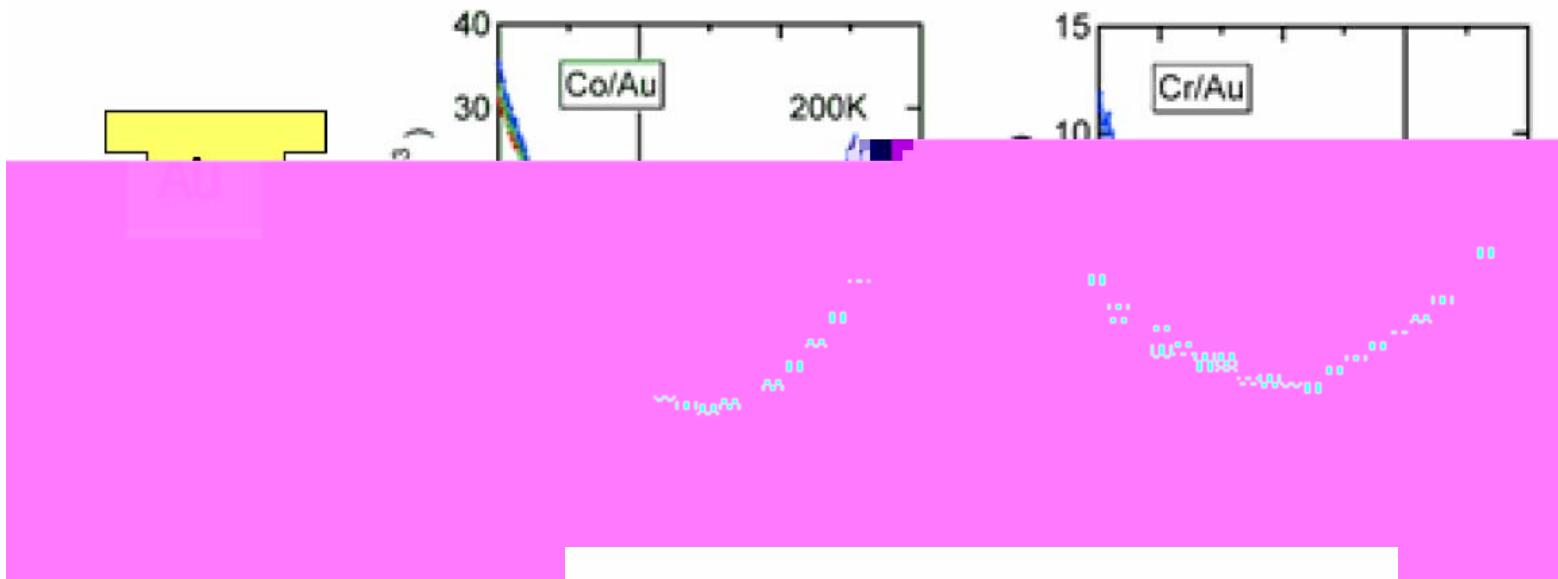
(Thickness of F layer is 10ML)



Temperature Dependence of Gilbert Damping Enhancement

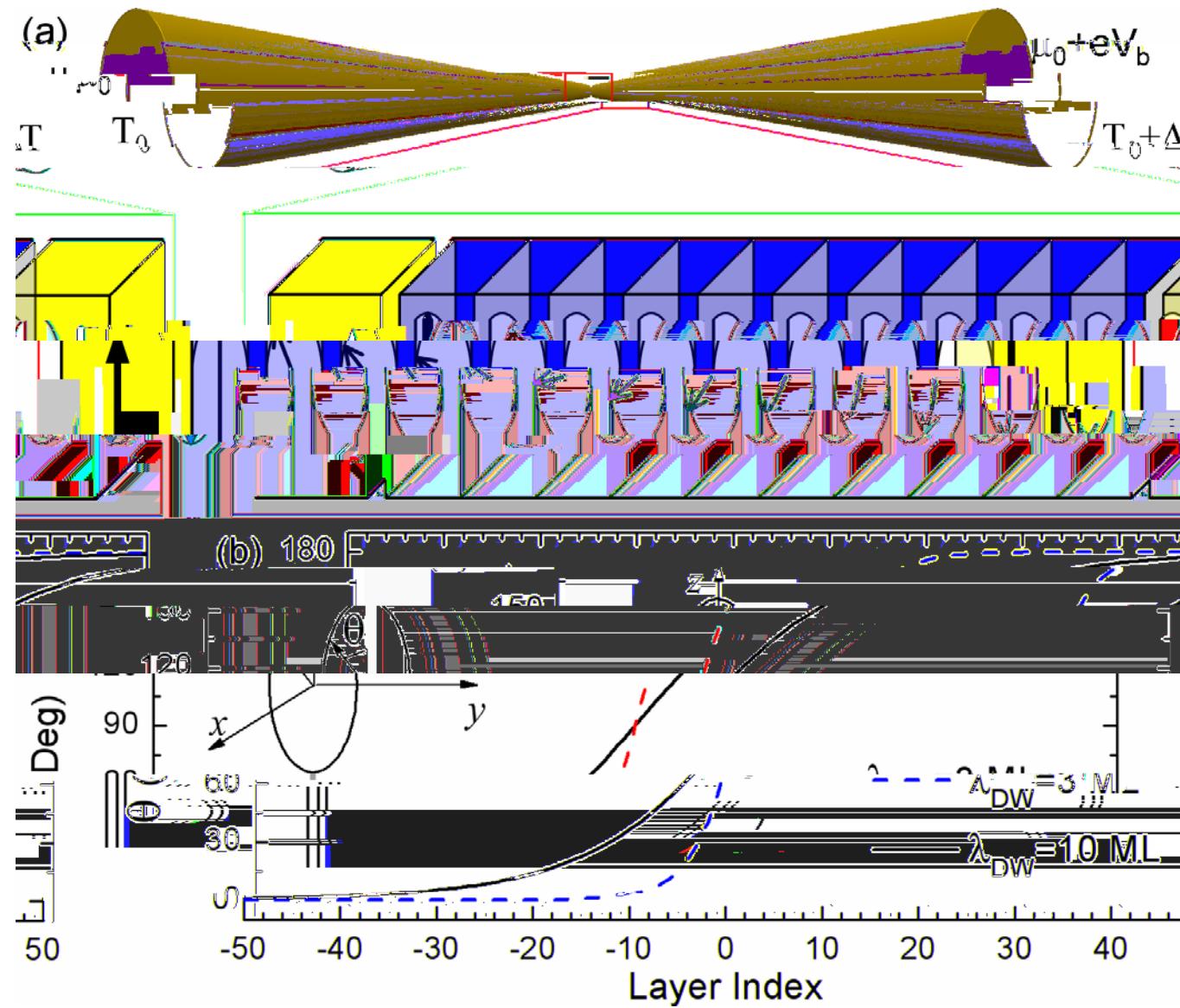


Metallic nanopillars (Fukushima et al., 2005)



L. Gravier et al. (2005).

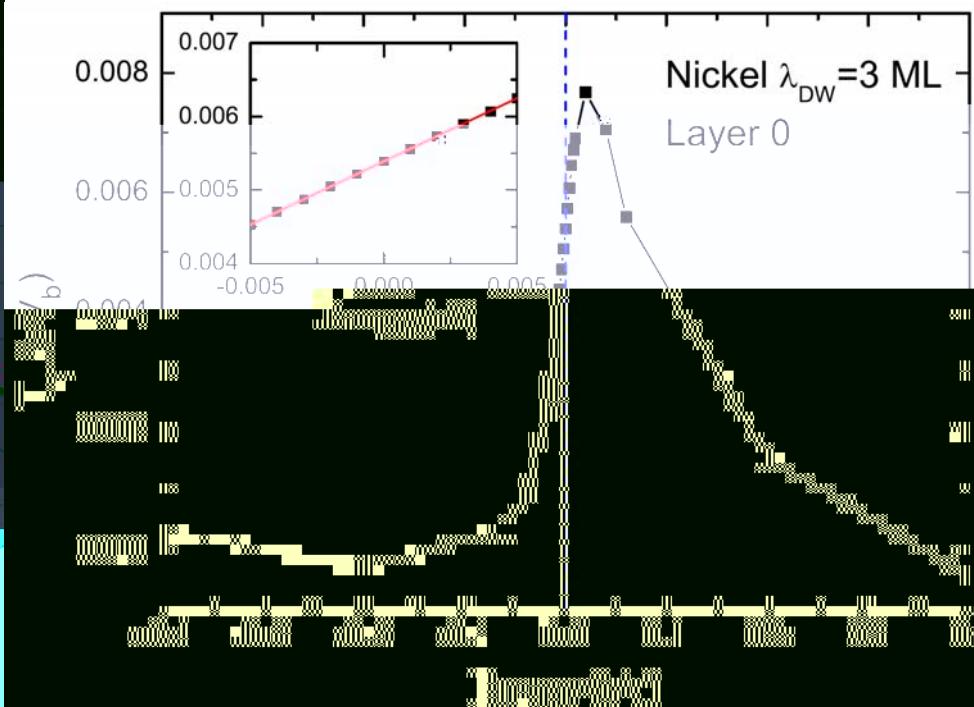
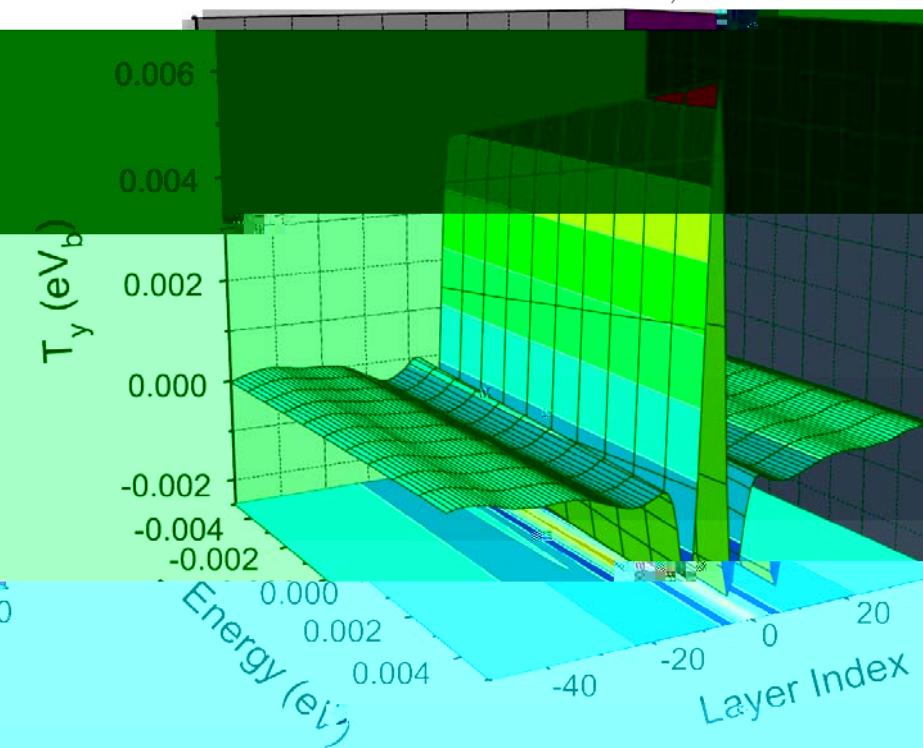
Model



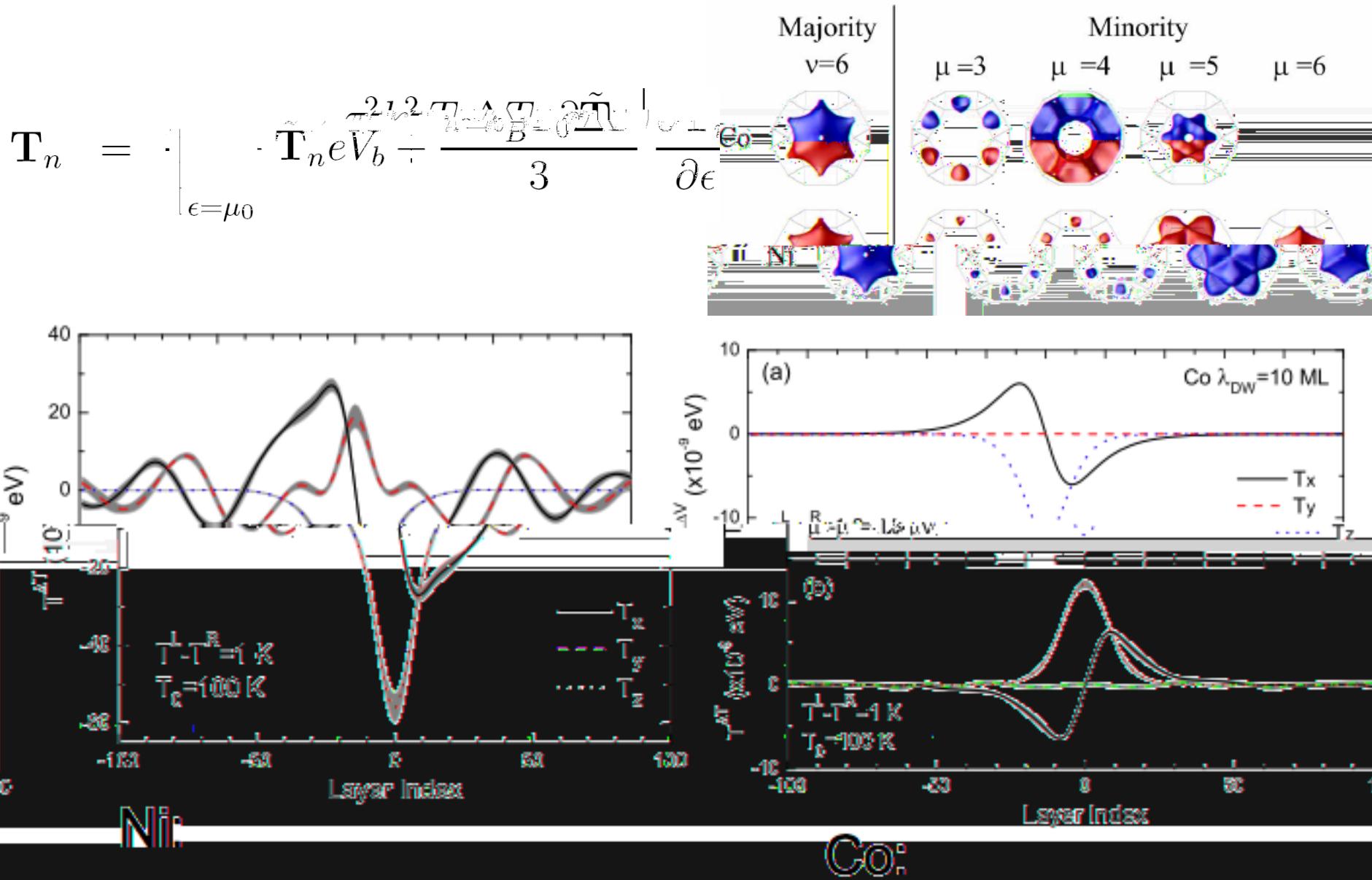
First-principles spin-transfer torque

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

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



Bias- and temperature-STT

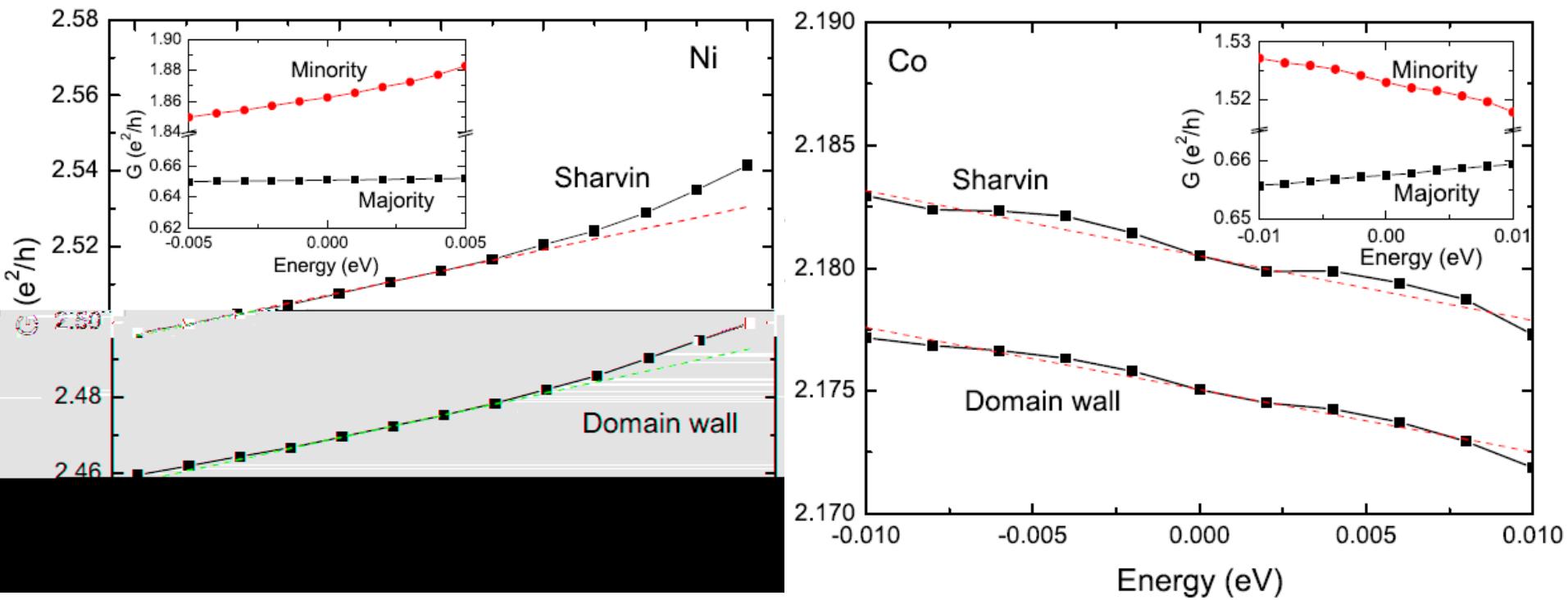


Peltier and Seebeck coefficients

	$G' (e/hV)$	$G (e^2/h)$	$\partial_e \ln G _{e_F}$ (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	—	—	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	—	—	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 Material Science
The End