IEEE Magnetics Summer School 2019

Simulation and theory on magnetism

Part 1

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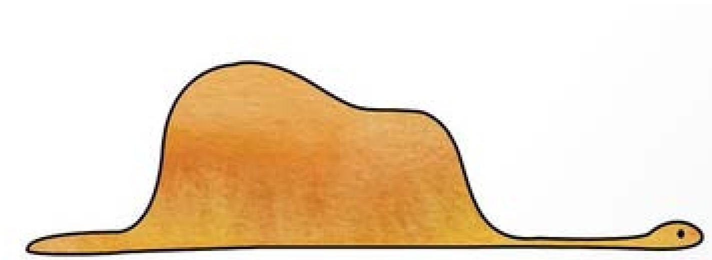
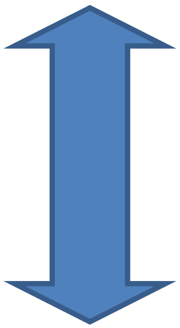
Outline (Part 1)

1. Why simulation and theory?
2. Mean-field theory
3. Monte Carlo simulation
4. Micromagnetics
5. Spin drift-diffusion model (spin-transfer torque)
6. Ab initio + linear response (very brief)

Why simulation and theory?

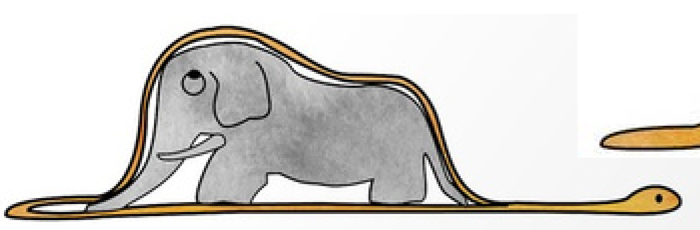


Experiment: many unknowns & do not know what is inside exactly, but always true

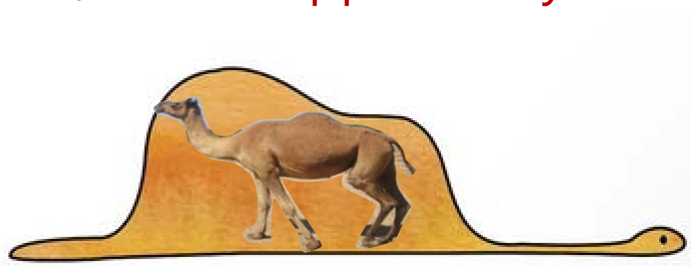


Model: Connecting experiment with theory; Less (more) “black box” than experiment (theory)

Theory: simple & powerful, but its applicability to a specific experiment depend on assumptions



Theory 1: Elephant



Theory 2: Camel

Theory 3: Polar bear

Mean field theory

- Magnetization **M** versus temperature T
- In the classical viewpoint, **M** fluctuates around a preferred direction **e** ➔ The higher T, the more fluctuations ➔ Average <**M**> along **e** decreases with T
- In the quantum mechanical viewpoint, the angular momentum state is quantized (J = 1/2, 3/2, 5/2, …) ➔ Occupation probability of each state varies with T ➔ Average <**J**> along **e** decreases with T
- Mean field approximation: an effective magnetic field acting on a spin $\mathbf{S}_i$ = thermal average <**S**> of neighboring spins

Mean field theory

- Heisenberg exchange Hamiltonian

$$H = -\sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

- With thermal averaged spin $\langle \mathbf{S} \rangle$, fluctuations: $\mathbf{s}_i = \mathbf{S}_i - \langle \mathbf{S} \rangle$

$$\Rightarrow \quad H = -\sum_{i,j} J\left(\mathbf{s}_i + \langle \mathbf{S} \rangle\right)\cdot\left(\mathbf{s}_j + \langle \mathbf{S} \rangle\right)$$

$$= -J\sum_{i,j} \mathbf{s}_i \cdot \mathbf{s}_j - 2ZJ\sum_i \mathbf{S}_i \cdot \langle \mathbf{S} \rangle + ZN\left|\langle \mathbf{S} \rangle\right|^2$$

- Neglecting the first term (fluctuations) and differentiating other terms with $-\vec{S}_i$ give the mean exchange field

$$\mathbf{B}_{ex} = 2ZJ\langle \mathbf{S} \rangle$$

Mean field theory

- Average of angular momentum states gives

$$\langle \mathbf{M}_i \rangle = g\mu_B \langle \mathbf{S}_i \rangle = g\mu_B B_J(x)$$

$$B_S(x) = \frac{2J+1}{2J}\coth\left[\frac{2J+1}{2J}x\right] - \frac{1}{2J}\coth\left[\frac{1}{2J}x\right]$$

$$x = \frac{g\mu_B JB}{k_B T}$$

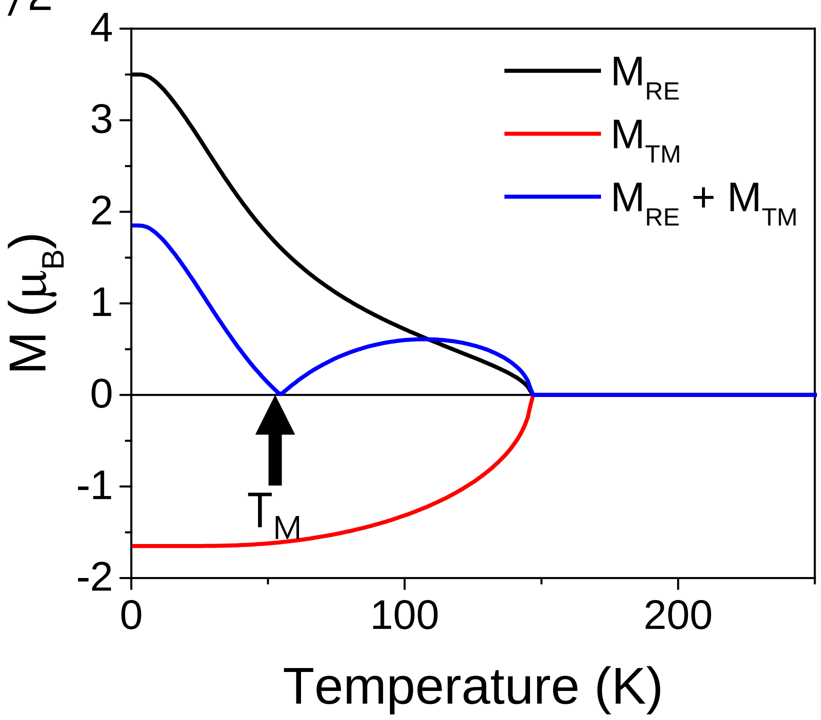
- B also contains <**S**> so that the above equation is solvable iteratively.

Mean field theory: Example

- Rare earth (RE) – transition metal (TM) ferrimagnet (e.g. GdCo)
- Parameters
  - Exchange (T^2/meV): TM-TM = 1200, RE-RE = 30, TM-RE = -120 (antiferro-coupling)
  - Angular momentum: TM = 3/2, RE = 7/2
  - Landé g factor: TM = 2.2, RE = 2.0

T_M = magnetic moment compensation point due to

- Antiferromagnetic coupling
- Different T-dependence (different exchange)

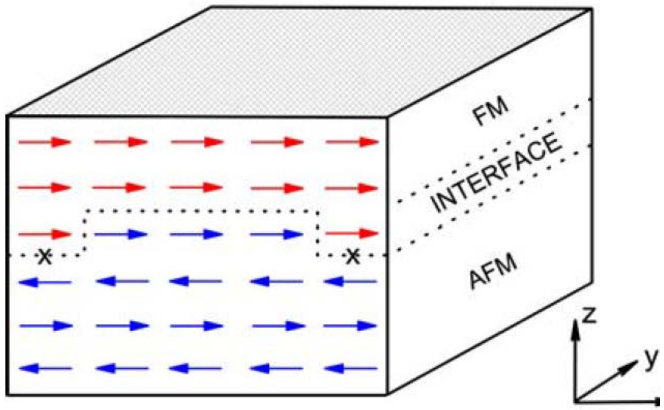


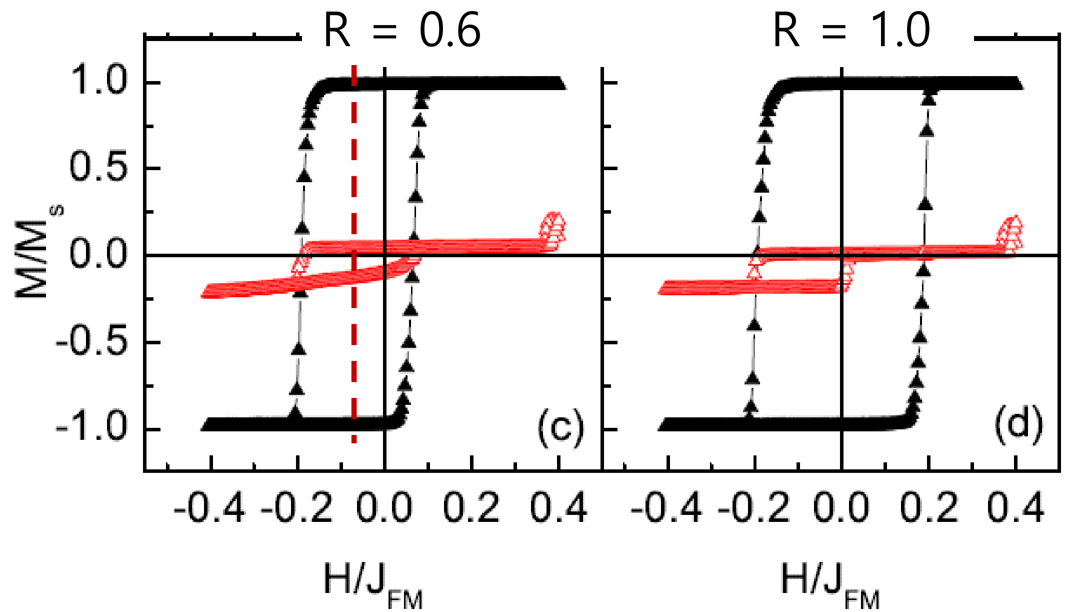
Monte Carlo method

- Flip a spin depending on a probability
- The Metropolis algorithm
  1. From a state (spin configuration) x_0, the next state x_1 is generated with a single spin flip
  2. Calculate $\Delta E = E(x_0) - E(x_1)$ and $P = \exp(-\Delta E/k_B T)$
  3. Generate a random number r within [0, 1]
  4. If $r \le P$, accept x_1
  5. If $r > P$, reject x_1 and instead stay at x_0
  6. Repeat steps 1~5 until a criterion is satisfied

Monte Carlo method: Example

Li, Moon, KJL, J. Magn. **16**, 323 (2011)



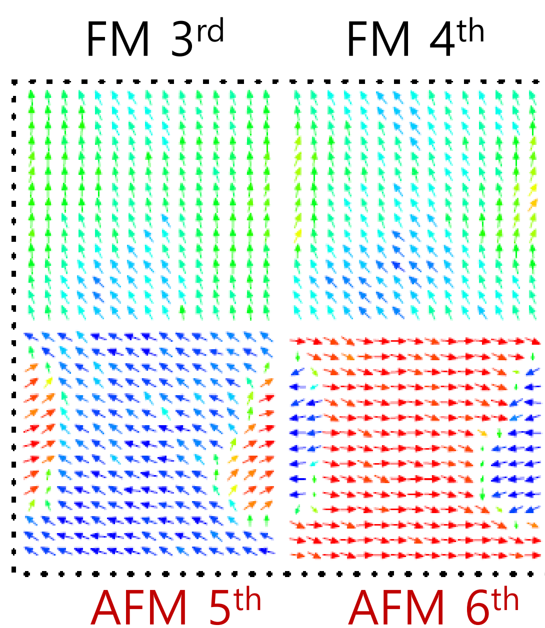


R = (# of FM spins/# of total spins) at the interface layer

R = 0 or 1 ➔ perfect AFM or FM

R = 0.5 ➔ maximally imperfect interface

No exchange bias at R = 1 due to domain wall formation in AFM layers



Micromagnetics

- A standard tool to study magnetization dynamics
- Numerically solve the Landau-Lifshitz-Gilbert (LLG) equation for many interacting magnetic moments

$$\frac{\partial \hat{\mathbf{m}}}{\partial t} = -\gamma\, \hat{\mathbf{m}} \times \mathbf{B}_{eff} + \alpha\, \hat{\mathbf{m}} \times \frac{\partial \hat{\mathbf{m}}}{\partial t} + \boldsymbol{\tau}$$

  - γ = gyromagnetic ratio
  - **m** = unit vector along the magnetization
  - $\mathbf{B}_{\mathrm{eff}}$ = effective magnetic field
  - α = damping constant
  - $\boldsymbol{\tau}$ = torque other than precession (the first term) and damping (the second term) torques (e.g., spin-transfer torque)

Precession torque

$$\frac{\partial \mathbf{s}}{\partial t} = \frac{1}{i\hbar}\left[\mathbf{s}, H\right] \; \& \; H = -\gamma \, \mathbf{s} \cdot \mathbf{B} \; \& \; \left[A, B\right] = AB - BA \; \& \; \mathbf{s} = \frac{\hbar}{2}\boldsymbol{\sigma}$$

$$\boldsymbol{\sigma} = \left(\sigma_x, \sigma_y, \sigma_z\right) \& \; \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Rightarrow \quad \frac{\partial \mathbf{s}}{\partial t} = \gamma \, \mathbf{s} \times \mathbf{B}$$

$$\mathbf{M} = M_S \hat{\mathbf{m}} = -\gamma \, \mathbf{s} \quad \Rightarrow \quad \frac{\partial \hat{\mathbf{m}}}{\partial t} = -\gamma \, \hat{\mathbf{m}} \times \mathbf{B}$$

- The precession torque originates from Zeeman-like coupling between spin and effective magnetic fields

Damping torque

$$\frac{\partial \mathbf{s}}{\partial t} = \frac{1}{i\hbar}[\mathbf{s}, H]$$

$$H = -\gamma\, \mathbf{s} \cdot \mathbf{B} + H_{Spin-Orbit\ Coupling} + H_{electron-electron} + H_{electron-phonon} + \ldots$$

Too complicated to exactly calculate

- Let us take a phenomenological description of damping torque
- What is the direction (or vector form) of the damping torque?
- Damping effect describes energy dissipation

$$\frac{\partial \varepsilon}{\partial t} = -\frac{\partial(\mathbf{M} \cdot \mathbf{B})}{\partial t} = -\frac{\partial \mathbf{M}}{\partial t} \cdot \mathbf{B} < 0$$

$$\Rightarrow \left.\frac{\partial \mathbf{M}}{\partial t}\right|_{damping} \propto \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t}$$

Phenomenological damping constant α is introduced (originating from the red-boxed Hamiltonians)

Effective field B_{eff}

$$\mathbf{B}_i = -\frac{\delta \varepsilon_i}{\delta \mathbf{M}} \Rightarrow \mathbf{B}_{eff} = \mathbf{B}_{exchange} + \mathbf{B}_{anisotropy} + \mathbf{B}_{magnetostatic} + \mathbf{B}_{Zeeman} + \ldots$$

	Energy Density	Origin
Exchange	$\varepsilon_{ex}(\mathbf{r}) = -\frac{A}{M_S^2}[\vec{\nabla}\mathbf{M}(\mathbf{r})]^2$	$V_{ij} = -2J_{ij}\hat{S}_i \cdot \hat{S}_j$ Spin-Spin Coupling
Anisotropy	$\varepsilon_k(\mathbf{r}) = -\frac{K}{M_S^2}[\mathbf{M}(\mathbf{r}) \cdot \hat{\mathbf{k}}(\mathbf{r})]^2$	Spin-Orbital Coupling & Quenching
Magnetostatic	$\varepsilon_d(\mathbf{r}) = -\frac{1}{2}\mathbf{M}(\mathbf{r}) \cdot \mathbf{B}_d(\mathbf{r})$	Coupling among Magnetic Dipoles
Zeeman	$\varepsilon_{Zeeman}(\mathbf{r}) = -\mathbf{M}(\mathbf{r}) \cdot \mathbf{B}_{ext}(\mathbf{r})$	Coupling External Field with Spin

- A = exchange stiffness, K = Magnetic anisotropy constant, **k** = unit vector along the uniaxial anisotropy, $\mathbf{B}_d$ = dipolar field, $\mathbf{B}_{ext}$ = external field

Effective field $\mathbf{B}_{eff}$

Exchange　　　　Uniaxial anisotropy

$$\mathbf{B}_{eff}(\mathbf{r}) = \frac{2A}{M_S^2}\vec{\nabla}^2\mathbf{M}(\mathbf{r}) + \frac{2K}{M_S}[\hat{\mathbf{m}}(\mathbf{r})\cdot\hat{\mathbf{k}}(\mathbf{r})]\hat{\mathbf{k}}(\mathbf{r})$$

$$-\int_V d^3\mathbf{r}'\frac{\vec{\nabla}\cdot\mathbf{M}'(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3} + \int_S d^2\mathbf{r}'\frac{\hat{\mathbf{n}}\cdot\mathbf{M}'(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3} + \mathbf{B}_{ext}(\mathbf{r})$$

Dipole: volume charge　　　　surface charge　　　　external

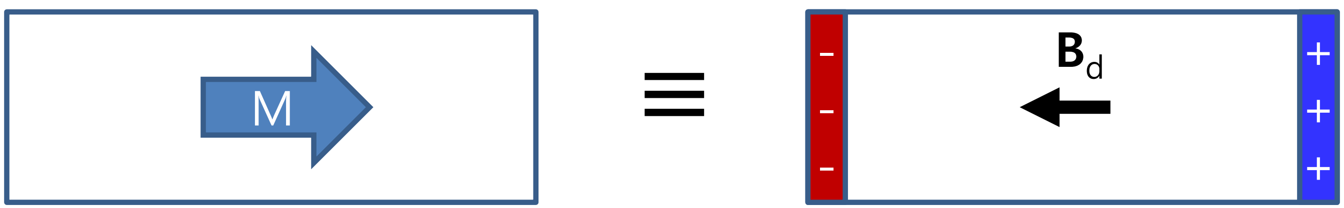
- Exchange: nearest neighbor & prefers uniform **M**
- Anisotropy: local & prefers **M** // **k**
- External: usually uniform & prefers **M** // $\mathbf{B}_{ext}$
- Dipole: nonlocal & prefers zero volume and surface charges

Demagnetization effect due to dipolar field

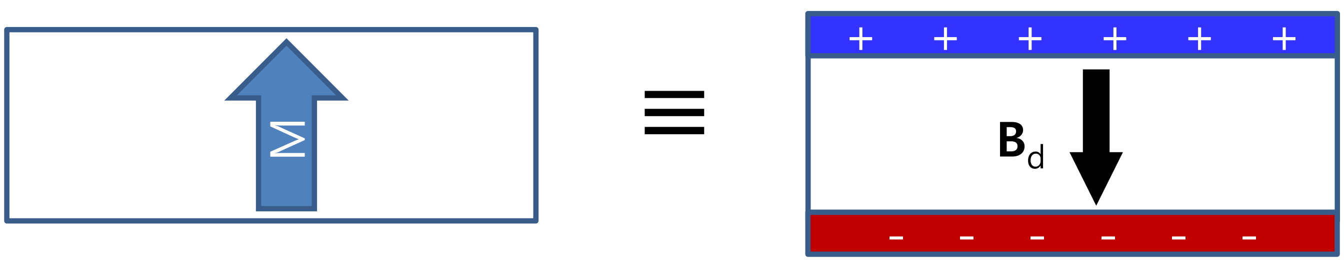
$$\mathbf{B}_d(\mathbf{r}) = -\int_V d^3\mathbf{r}' \frac{\vec{\nabla}\cdot\mathbf{M}'(\mathbf{r}-\mathbf{r}')}{\left|\mathbf{r}-\mathbf{r}'\right|^3} + \int_S d^2\mathbf{r}' \frac{\hat{\mathbf{n}}\cdot\mathbf{M}'(\mathbf{r}-\mathbf{r}')}{\left|\mathbf{r}-\mathbf{r}'\right|^3}$$

Dipole: volume charge surface charge

(A)



(B)



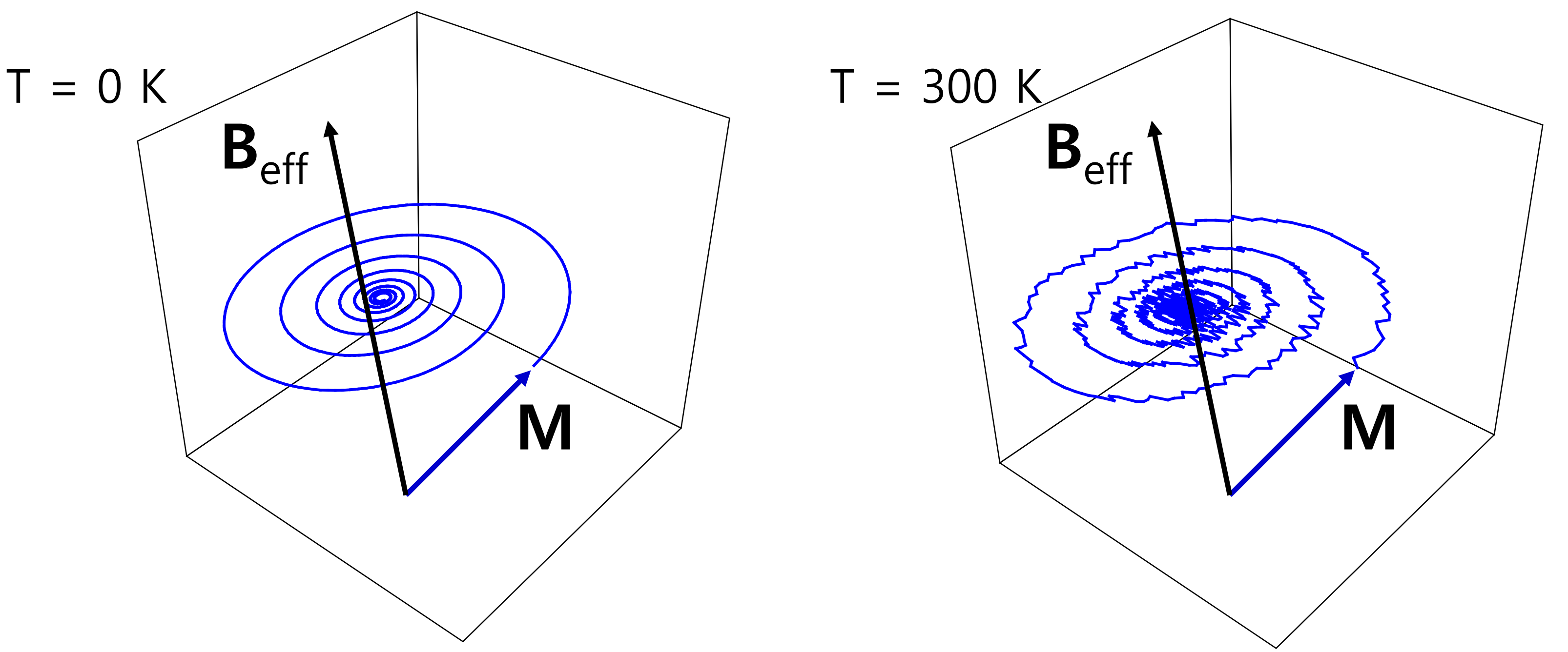
- B_d of (B) >> B_d of (A)
- For thin film, B_d of (A) ~ 0 & B_d of (B) ~ $-4\pi M_S$ (in cgs)

➔ demag energy = $-1/2(\mathbf{M}.\mathbf{B}_d) = 2\pi M_S^2$

Thermal fluctuation

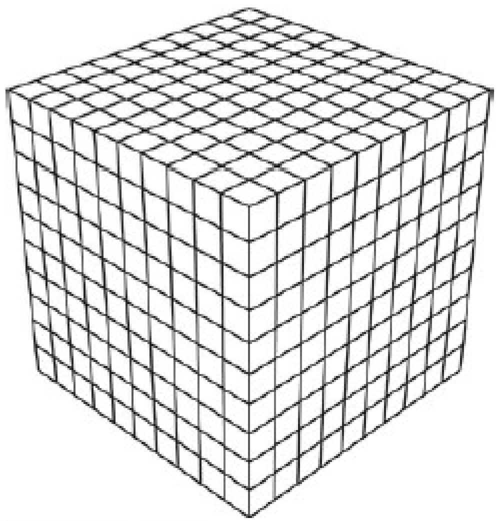
- Effect of temperature ➔ thermal fluctuations of **M**
- Add a thermal fluctuation field $\mathbf{B}_{th}$ to $\mathbf{B}_{eff}$
- From the Fluctuation-Dissipation theorem, $\mathbf{B}_{th}$ (= h) must have the following statistical properties

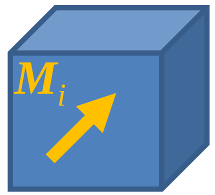
$$\langle h_i(t)\rangle = 0, \quad \langle h_i(0)h_j(t)\rangle = \delta(t)\delta_{ij}\, 2\alpha\, k_B T / \gamma M_S V \Delta t$$



How to numerically solve?

- The system is discretized by uniform cells (finite difference method)





$$\frac{\partial \hat{\mathbf{m}}}{\partial t} = -\gamma\, \hat{\mathbf{m}} \times \mathbf{B}_{eff} + \alpha\, \hat{\mathbf{m}} \times \frac{\partial \hat{\mathbf{m}}}{\partial t} + \boldsymbol{\tau}$$

- $|\mathbf{M}_i|$ = M_S and is uniform within a cell: $\mathbf{M}_i = M_S \hat{\mathbf{m}}_i$
- For each $\hat{\mathbf{m}}_i$, the LLG equation is numerically solved using the continuum approximation (d = unit cell size);

$$\mathbf{B}_{ex,i} = \frac{2A}{M_S} \vec{\nabla}^2 \hat{\mathbf{m}}_i \approx \frac{2A}{M_S} \frac{\hat{\mathbf{m}}_{i+1} + \hat{\mathbf{m}}_{i-1} - 2\hat{\mathbf{m}}_i}{d^2}$$

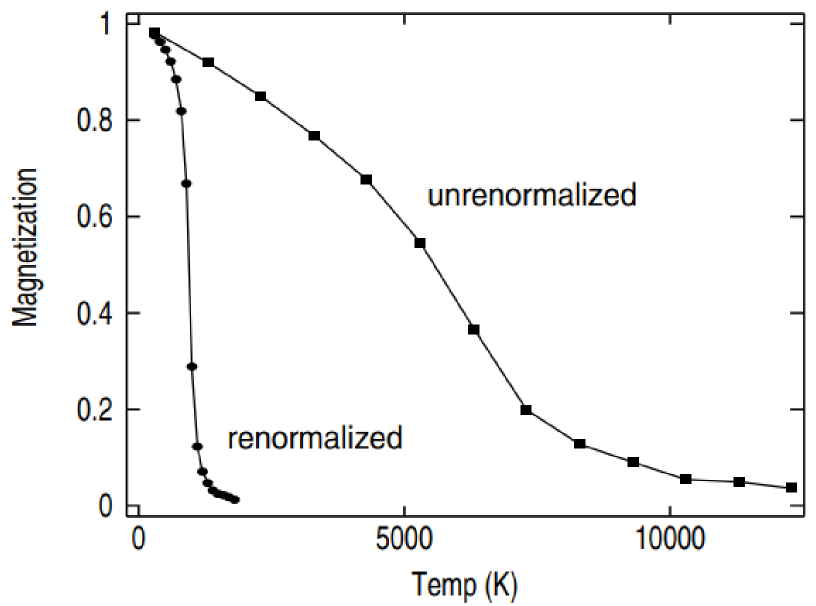
Two main assumptions

(1) $\mathbf{M}_i$ is uniform within a cell: $\mathbf{M}_i = M_S \hat{\mathbf{m}}_i$

(2) Continuum approximation ($d\nabla\hat{\mathbf{m}}_i$ is a small parameter)

- Assumption (1) ➔ micromagnetic simulation is invalid near T_C (Curie Temperature) because it ignores short wavelength magnons (λ < d)

- Grinstein and Koch, PRL **90**, 207201 (2003) [right figure]
- Conventional micromagnetics overestimates T_C substantially
- Proper T-dependent renormalization is required



Two main assumptions

(1) $\mathbf{M}_i$ is uniform within a cell: $\mathbf{M}_i = M_S \hat{\mathbf{m}}_i$

(2) Continuum approximation ($d\nabla\hat{\mathbf{m}}_i$ is a small parameter)

- Assumption (2) ➔ micromagnetic simulation is invalid for $d\nabla\hat{\mathbf{m}}_i >> 1$
- For ferromagnets: Criterion of "d"

$$d < \sqrt{\frac{\varepsilon_{ex}}{\varepsilon_{an}}} \approx \text{ a few nm}$$

- Antiferromagnets or antiferromagnetically coupled ferrimagnets: continuum approximation does not work ➔ Atomistic LLG

What to do with micromagnetics

- When two assumptions are fine, micromagnetic simulation has been successful to describe various types of magnetization dynamics
- Several examples

(1) Current-induced magnetization precession in spin valve structures

(2) Current-controlled spin-wave attenuation

(3) Spin-wave propagation in the presence of Dzyaloshinskii-Moriya interaction (DMI)

(4) Magnetic droplet nucleation in the presence of DMI

Current-induced magnetization precession

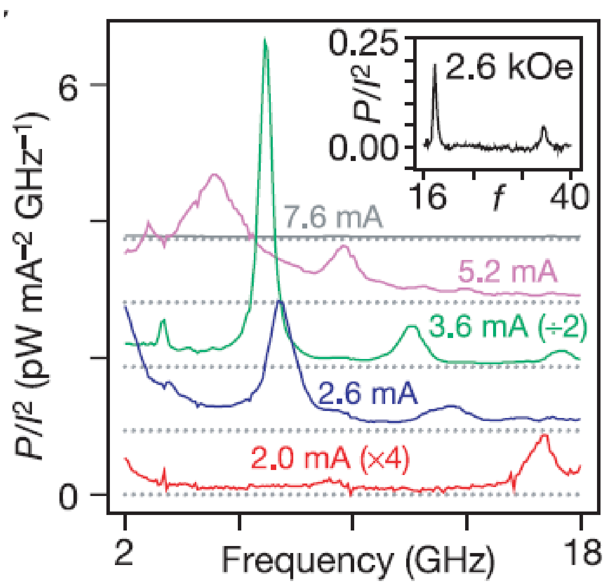
- Current injection into a spin valve FM1/NM/FM2 generates a spin-transfer torque (STT), resulting in magnetization dynamics

$$\frac{\partial \hat{\mathbf{m}}}{\partial t} = -\gamma\, \hat{\mathbf{m}} \times \mathbf{B}_{eff} + \alpha\, \hat{\mathbf{m}} \times \frac{\partial \hat{\mathbf{m}}}{\partial t} \boxed{+ \gamma\, a_J\, \hat{\mathbf{m}} \times (\hat{\mathbf{m}} \times \hat{\mathbf{s}})}$$

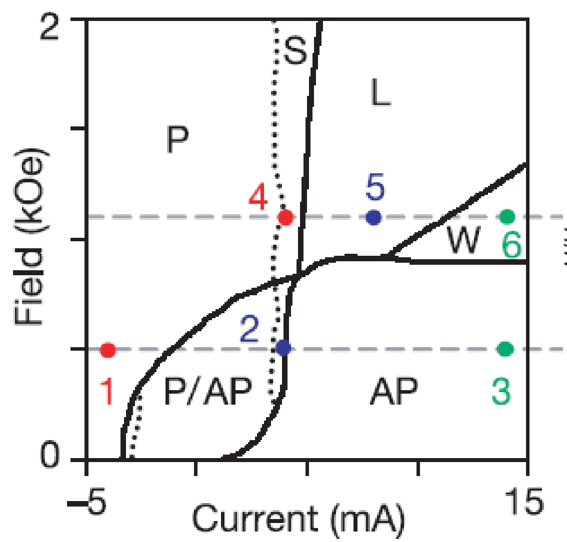
STT

- Experiment: Kiselev et al. Nature **425**, 381 (2003)

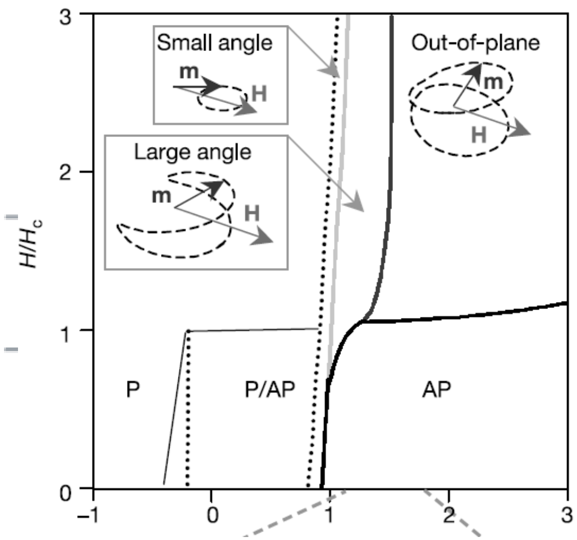
Power spectra



Experiment



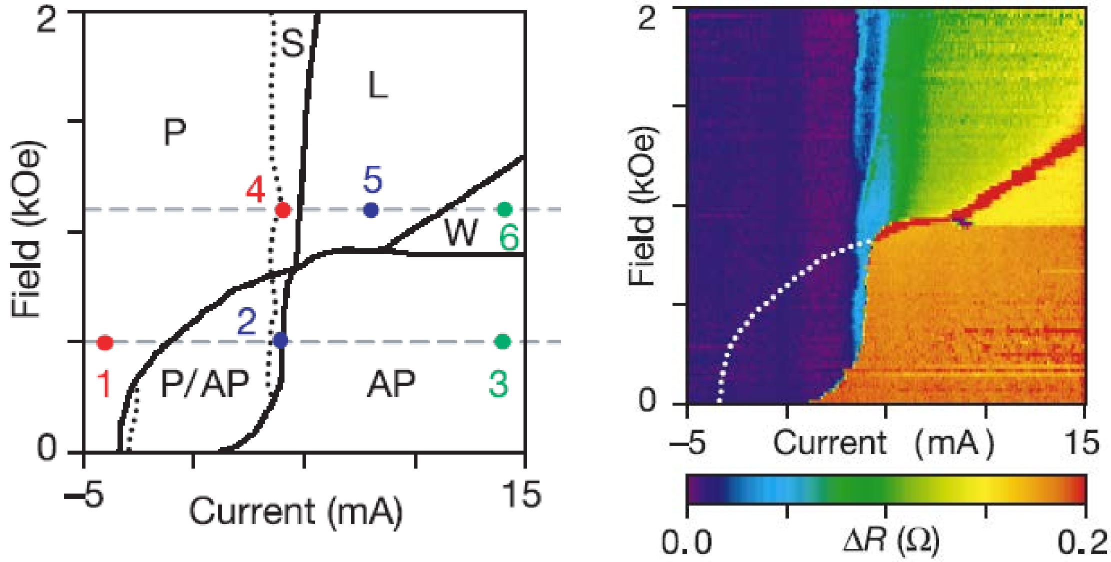
Theory



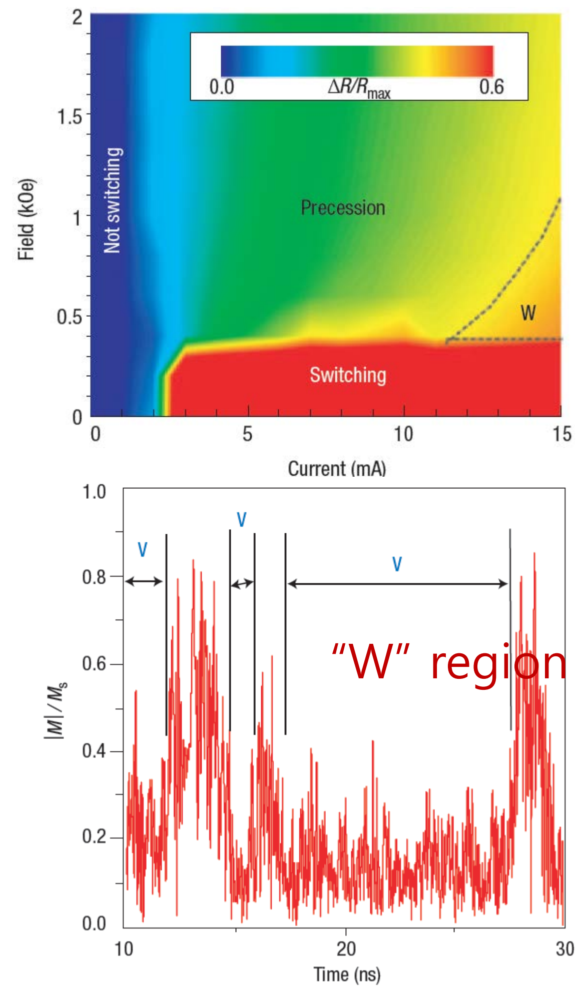
Current-induced magnetization precession

- Micromagnetic simulation: KJL et al. Nat. Mater. **3**, 877 (2004)

Experiment



Micromagnetics



Highly nonlinear magnetization dynamics induced by STT

Current-controlled spin-wave attenuation

- STT acting on continuously varying magnetizations

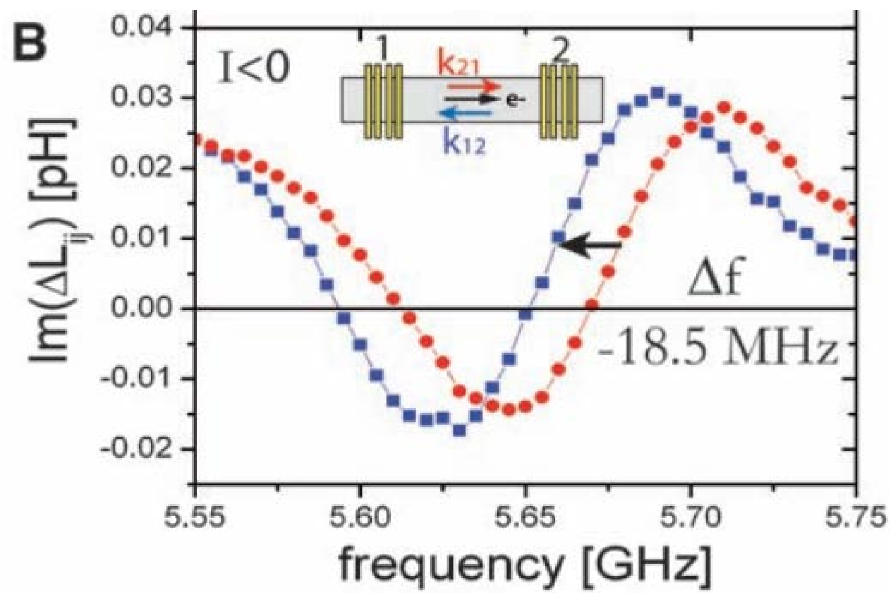
$$\frac{\partial \hat{\mathbf{m}}}{\partial t} = -\gamma\, \hat{\mathbf{m}} \times \mathbf{B}_{eff} + \alpha\, \hat{\mathbf{m}} \times \frac{\partial \hat{\mathbf{m}}}{\partial t} - b_J \frac{\partial \hat{\mathbf{m}}}{\partial x} + \beta b_J \left(\hat{\mathbf{m}} \times \frac{\partial \hat{\mathbf{m}}}{\partial x} \right)$$

Adiabatic STT   Non-adiabatic STT

- Adiabatic STT = spin-current flow
- Spin waves on spin-current flow = A walking person on moving walk

➔ Spin wave Doppler shift

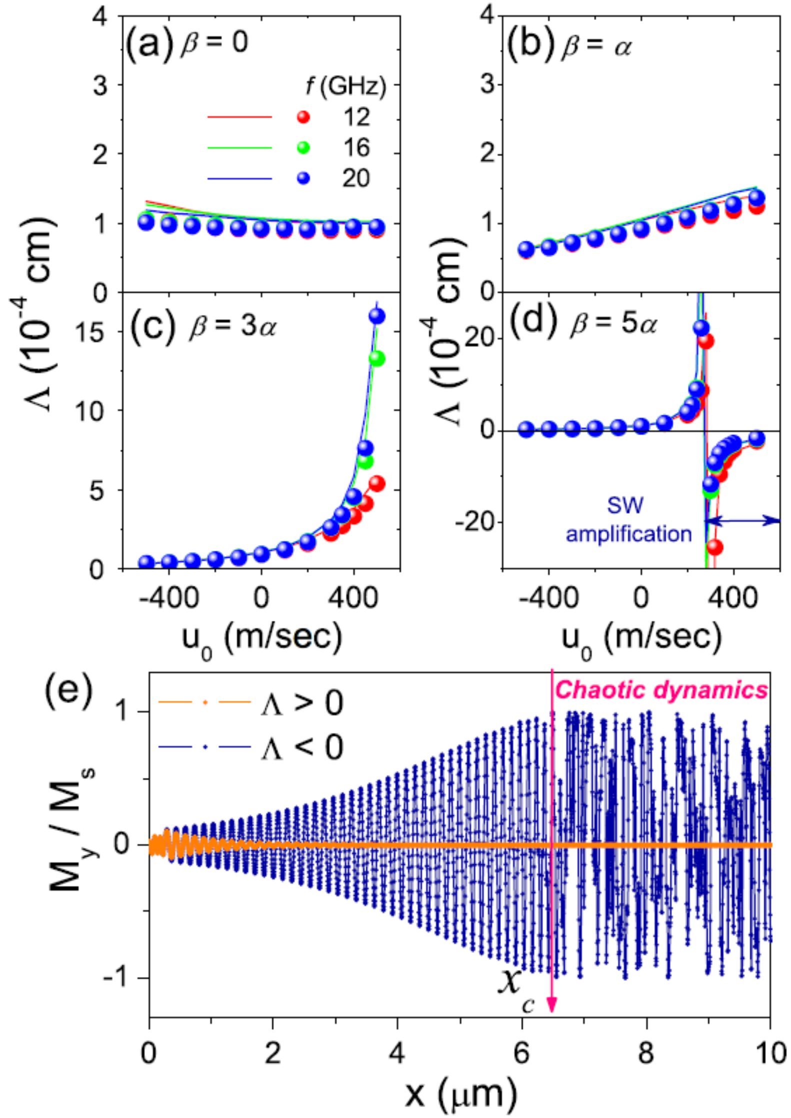
- Prediction: Lederer & Mills, Phys. Rev. **148**, 542 (1966)
- Experiment; Vlaminck & Bailleul, Science **322**, 410 (2008)



Current-controlled spin-wave attenuation

- What is the role of non-adiabatic STT in spin-wave propagation?
- Seo, KJL, et al., PRL **102**, 147202 (2009): Non-adiabatic STT competes with damping torque and thus controls spin-wave attenuation
- Spin-wave attenuation length

$$\Lambda = \frac{2\gamma D k}{\alpha\omega_f - \beta u_0 k}.$$



Spin-wave propagation in the presence of DMI

- DMI is the antisymmetric exchange interaction between neighboring spins

$$\mathcal{H}_{\mathrm{DMI}} = -\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j),$$

- DMI prefers a chiral spin textures (rotating around the DMI vector **D**)
- Spin-wave dispersion [Moon, KJL, et al., PRB **88**, 184404 (2013)]

$$\frac{\omega}{\gamma \mu_0} = \sqrt{(H + M_s/4 + Jk^2)(H + 3M_s/4 + Jk^2) - \frac{e^{-4|k|d} M_s^2}{16}(1 + 2e^{2|k|d})} + \boxed{pD^*k}$$

DMI contribution

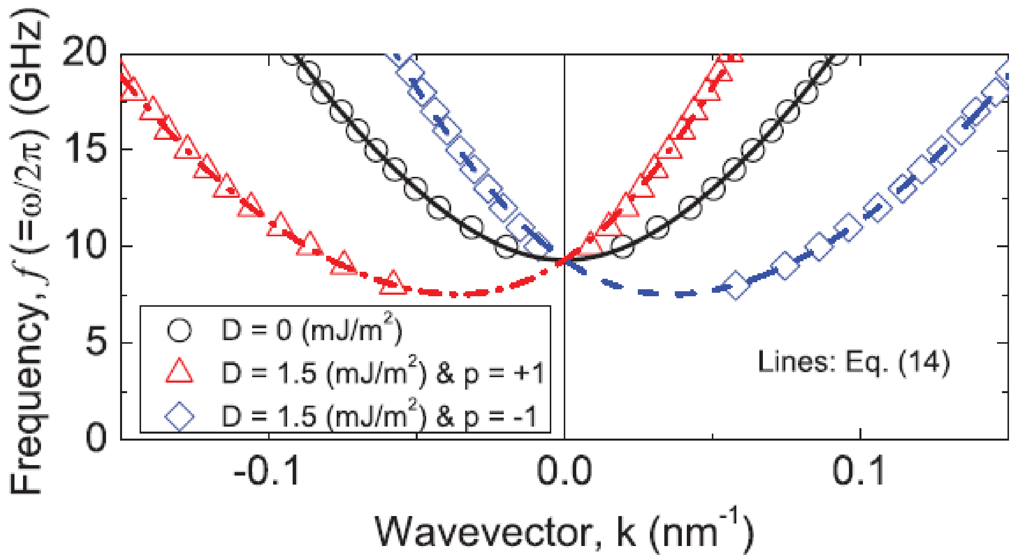
- By measuring spin-wave dispersion, one can determine the DMI strength "D"

Spin-wave propagation in the presence of DMI

- Moon, KJL, et al., PRB **88**, 184404 (2013)

$$\frac{\omega}{\gamma\mu_0} = \sqrt{(H + M_s/4 + Jk^2)(H + 3M_s/4 + Jk^2) - \frac{e^{-4|k|d} M_s^2}{16}(1 + 2e^{2|k|d})} + \boxed{pD^*k}$$

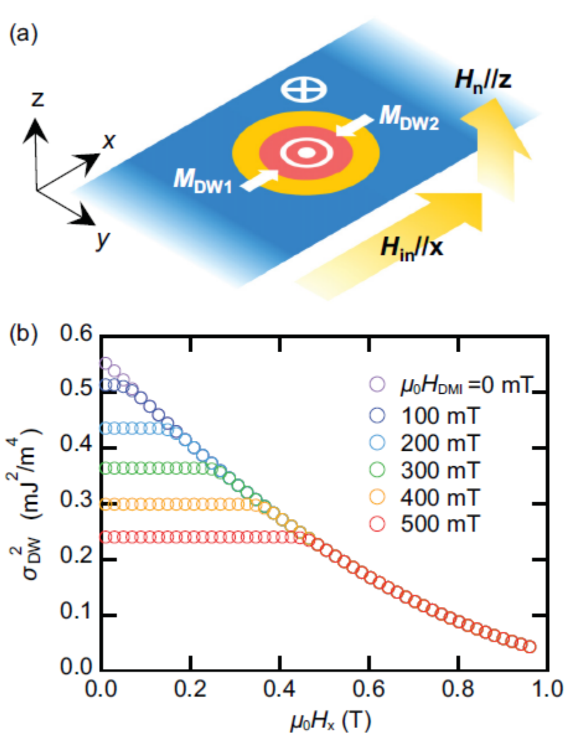
DMI contribution

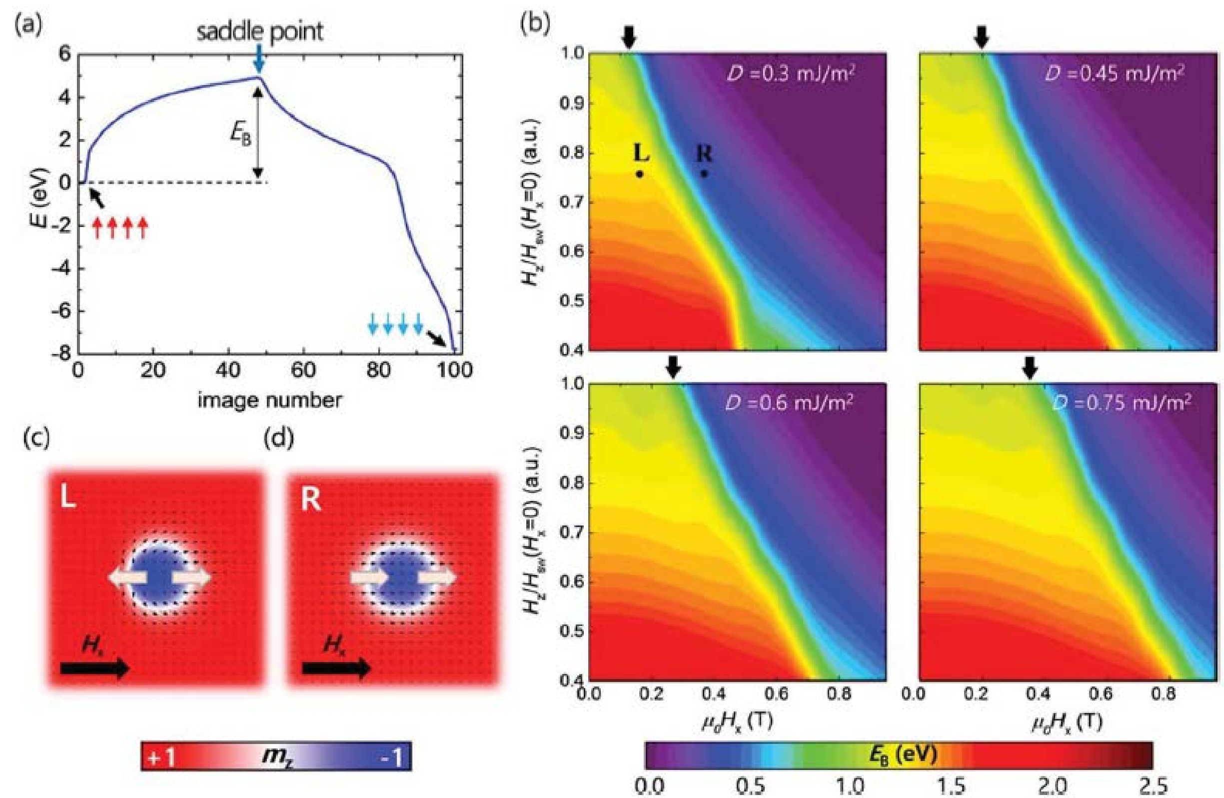


- Micromagnetic simulation confirms the validity of spin-wave dispersion
- Widely used to measure DMI [Nembach et al. Nat. Phys. **11**, 825 (2015); Cho et al, Nat. Commun. **6**, 7635 (2015); Lee, KJL, et al., Nano Lett. **16**, 62 (2016)]

Magnetic droplet nucleation in presence of DMI

- Kim, KJL, et al., PRB **95**, 220402 (R) (2017)
- Another way to determine the DMI ➔ Droplet nucleation field depends on the DMI





Atomistic LLG

- An example: Antiferromagnetic domain wall motion driven by spin-orbit torque [Shiino, KJL, et al., **PRL** 117, 087203 (2016)]

- Atomistic model

The Hamiltonian of the antiferromagnets is

$$\mathcal{H} = A_{\text{sim}} \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - K_{\text{sim}} \sum_i (\mathbf{S}_i \cdot \mathbf{e}_z)^2 - D_{\text{sim}} \sum_i \mathbf{e}_y \cdot (\mathbf{S}_i \times \mathbf{S}_{i+1}) + \frac{\mu_0}{8\pi} m_s \mu \sum_{i,j} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{3(\mathbf{S}_i \cdot \mathbf{r}_{ij})(\mathbf{S}_j \cdot \mathbf{r}_{ij})}{r^2} \right), \quad (1)$$

where $\mathbf{S}_i$ represents the normalized magnetic moment (i.e., $|\mathbf{S}_i| = 1$) at lattice site i, μ is the magnetic moment per lattice site, and $A_{\text{sim}}, K_{\text{sim}}, D_{\text{sim}}$ denote the exchange, anisotropy, and DMI energies, respectively. The last term represents the dipole-dipole interaction where $\mathbf{r}_{ij}$ is a distance vector between lattice sites i and j (i.e., $|\mathbf{r}_{ij}| = r$). The atomistic Landau-Lifshitz-Gilbert equation including spin-orbit torques is as follows:

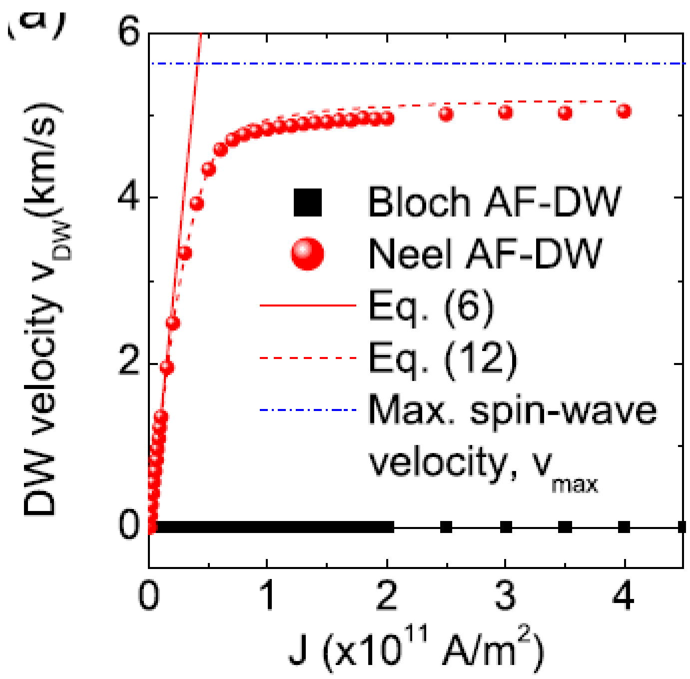
$$\frac{\partial \mathbf{S}_i}{\partial t} = -\gamma \mathbf{S}_i \times \mathbf{B}_{\text{eff}} + \alpha \mathbf{S}_i \times \frac{\partial \mathbf{S}_i}{\partial t} + \gamma B_{\text{D}} \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{e}_y) + \gamma B_{\text{F}} (\mathbf{S}_i \times \mathbf{e}_y), \quad (2)$$

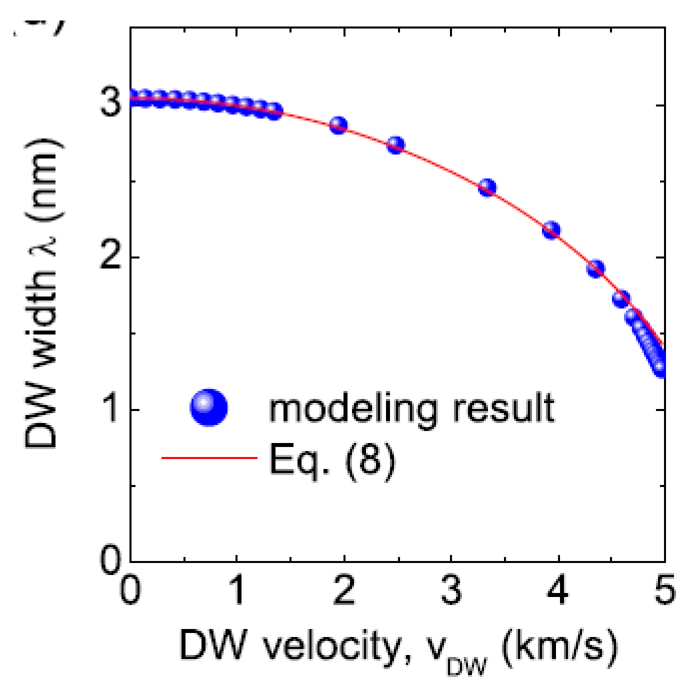
where $\mathbf{B}_{\text{eff}} = -\frac{1}{\mu} \frac{\delta \mathcal{H}}{\delta \mathbf{S}_i}$ is the effective field.

- All quantities are defined at discrete atomic lattices (no continuum approximation)

Antiferromagnetic domain wall motion

- Eq. (6): Non-relativistic $v_{\mathrm{DW}} = v_{\mathrm{AF}} = -\pi\gamma\lambda B_D/2\alpha$,
- Eq. (12): Relativistic $v_{\mathrm{DW}} = \dfrac{\gamma ald}{2}\sqrt{1-(\lambda/\lambda_{\mathrm{eq}})^2}$
- Eq. (8): Lorentz contraction of DW width $\lambda = \lambda_{\mathrm{eq}}\sqrt{1-(v_{\mathrm{DW}}/v_{\max})^2}$,





Rare-earth (RE)–transition metal (TM) Ferrimagnet

S = Angular momentum

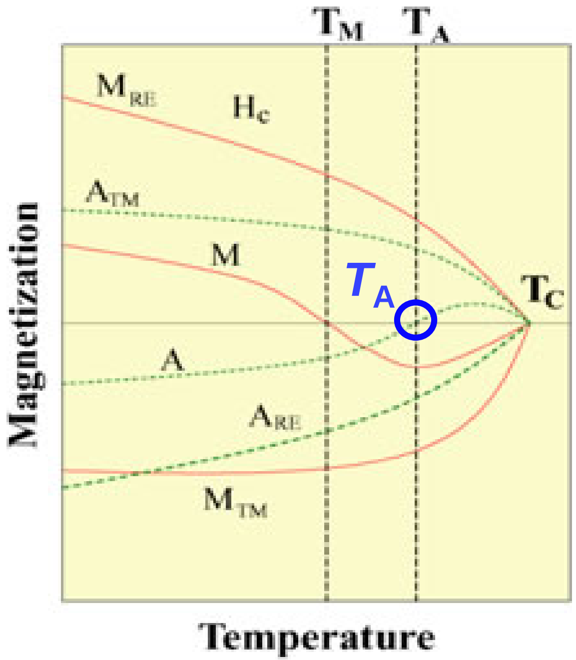
M = Magnetic moment

γ= Gyromagnetic ratio

$$\boldsymbol{S} = -\frac{\boldsymbol{M}}{\gamma} = -\frac{\hbar}{g_L \mu_B}\boldsymbol{M}$$

- Lande-g factor (g_L)

  ➔ 2.2 for Co, 2.0 for Gd



For RE-TM ferrimagnets, T_M ($\mathbf{M}_{tot}$ = 0 but $\mathbf{S}_{tot} \neq 0$) is different from $\mathbf{T_A}$ ($\mathbf{S}_{tot}$ = 0 but $\mathbf{M}_{tot} \neq 0$)

T_M: Magnetic moment compensation point

T_A: Angular moment compensation point ➔ Magnetization dynamics is antiferromagnetic at $\mathbf{T_A}$ + finite Zeeman coupling

Field-driven ferrimagnetic DW motion: Theory

Equations of Motion with two collective coordinates:

DW position X and DW angle ϕ

$$M\ddot{X} + G\dot{\phi} + \frac{M}{\tau}\dot{X} = F$$

$$I\ddot{\phi} - G\dot{X} + \frac{I}{\tau}\dot{\phi} = -\kappa \sin\phi \cos\phi$$

M : Mass

I : the moment of inertia

G : Gyrotropic coeff

τ : relaxation time

F : Force (external field)

κ : DW hard-axis anisotropy

- G = 2(S_1-S_2) x Area
- At T = T_A ➔ S_1-S_2 = δ_s = 0 ➔ G = 0

➔ X and ϕ are decoupled

Field-driven ferrimagnetic DW motion: Theory (2)

In the precessional regime

DW speed $$v_{DW} = \frac{\alpha s}{(\alpha s)^2 + {\delta_s}^2}(M_1 - M_2)\lambda H$$

Walker breakdown field $$H_{WB} = \frac{K_d \alpha s}{2\delta_s (M_1 - M_2)\lambda}$$

- At T = T_M ➔ M_1-M_2 = 0

  ➔ v_{DW1} = v_{DW2} = 0

& DW motion changes its direction at T_M

- **At T = T_A ➔ δ_s = 0 & M_1-M_2 ≠ 0**

  ➔ v_{DW} = maximum & $H_{WB} \rightarrow \infty$

$$\alpha S = \alpha_1 S_1 + \alpha_2 S_2$$

α : damping constant

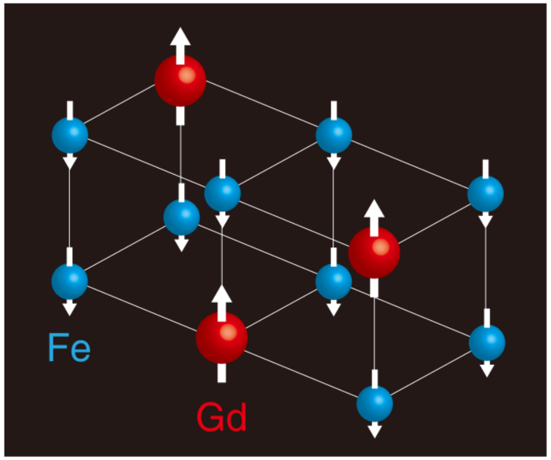
λ : DW width

H : external field

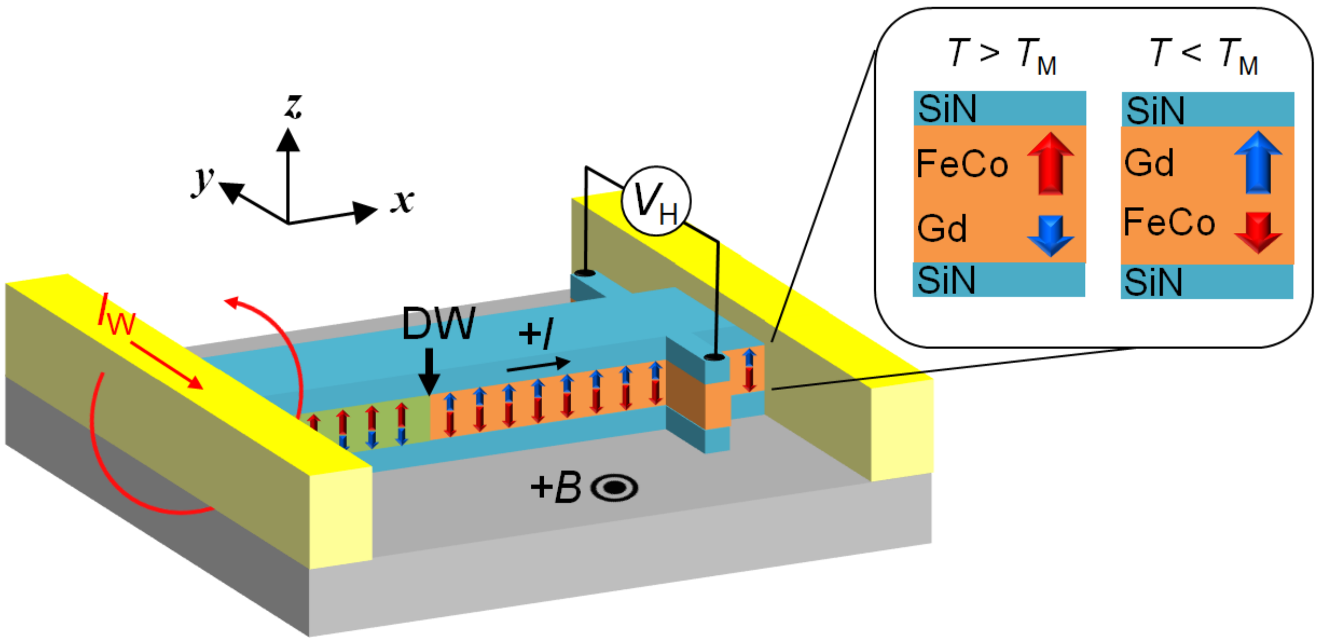
K_d : DW hard-axis anisotropy

Field-driven DW Experiment: FeCoGd

Kim et al., Nat. Mater. 16, 1187 (2017)

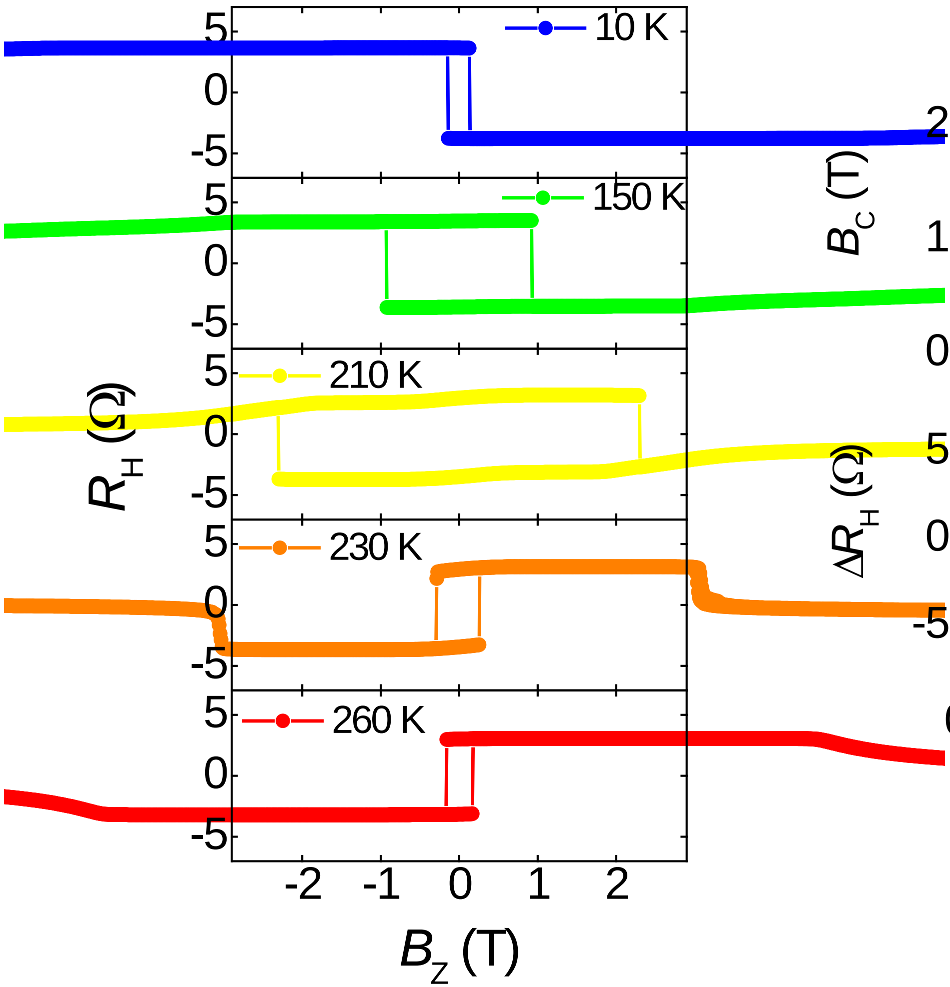


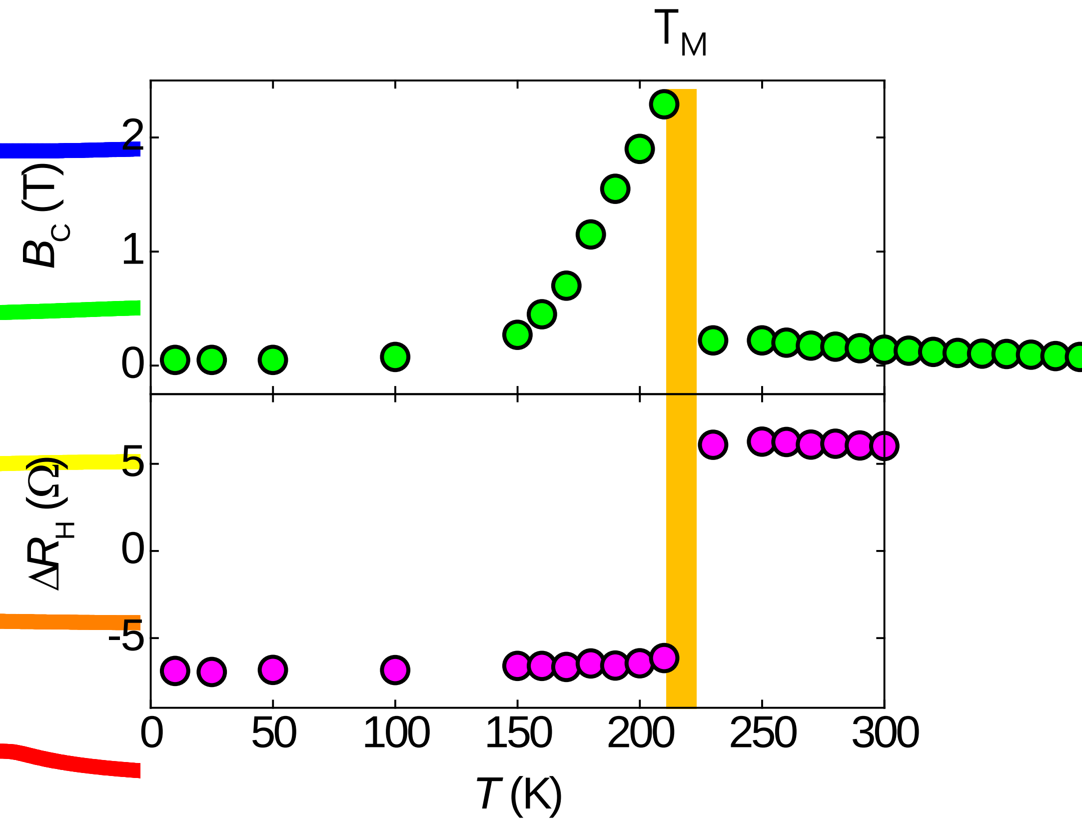
Done by T. Ono's group



Determination of T_M

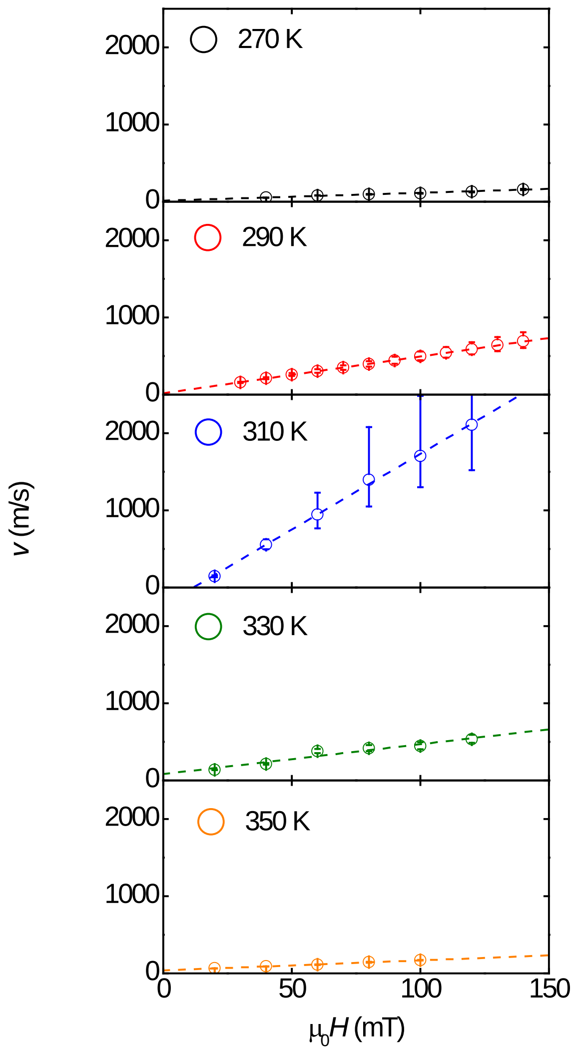
T_M : Magnetization compensation temperature

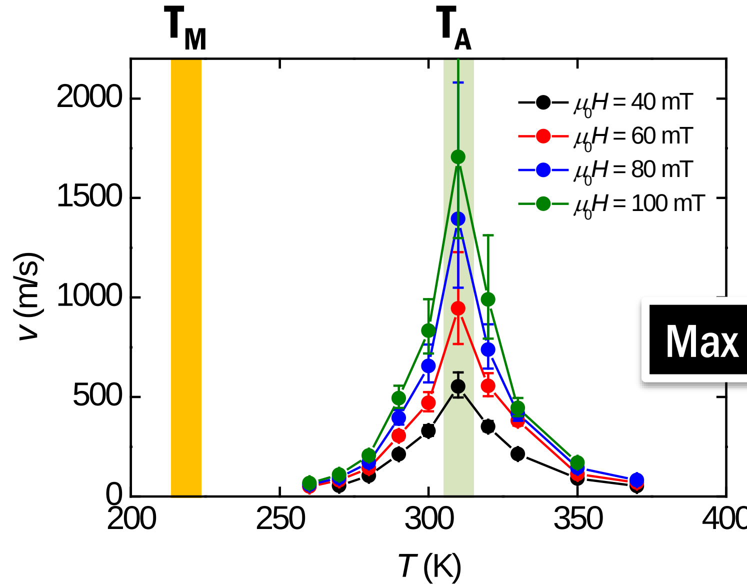




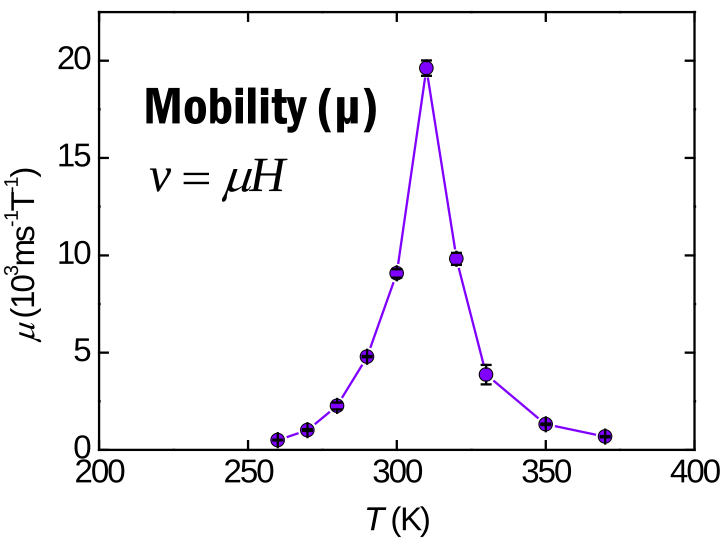
T_M is found to be 220 K

DW velocity: Experiment

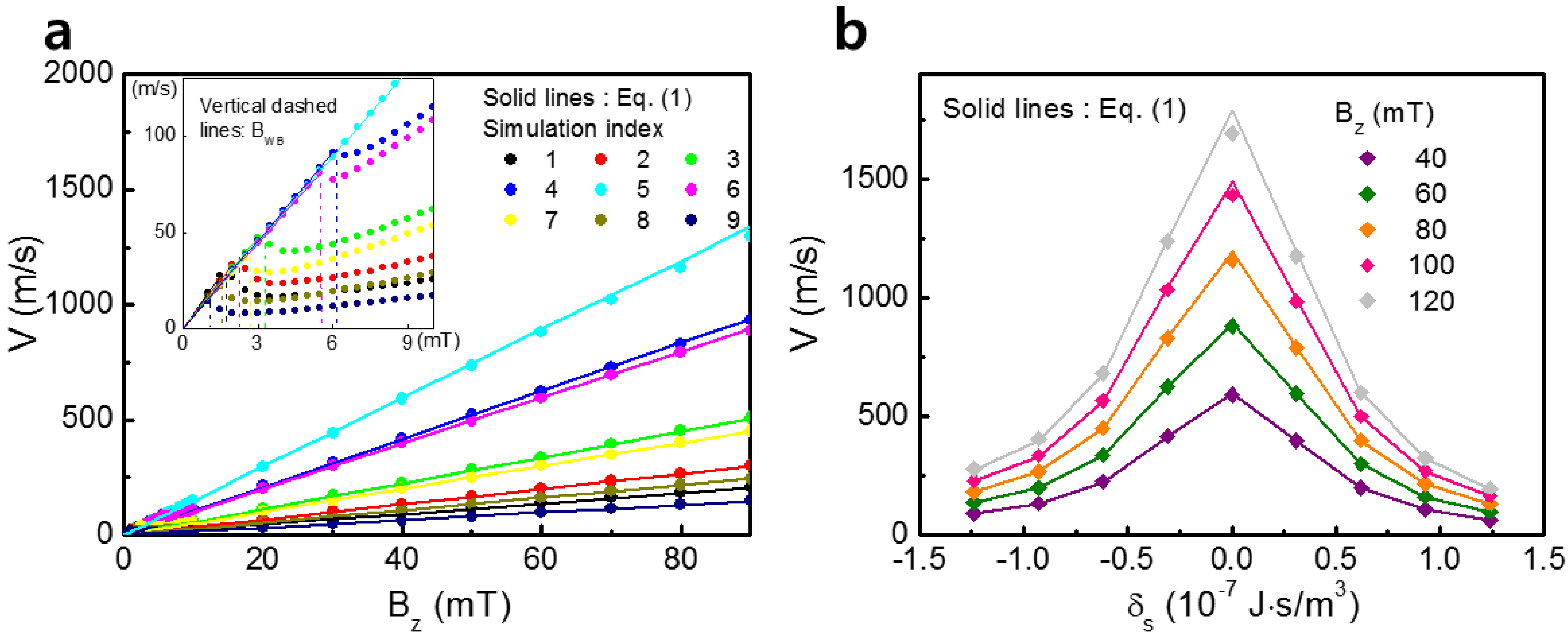




Max speed: 1.7 km/s



DW velocity: Modeling

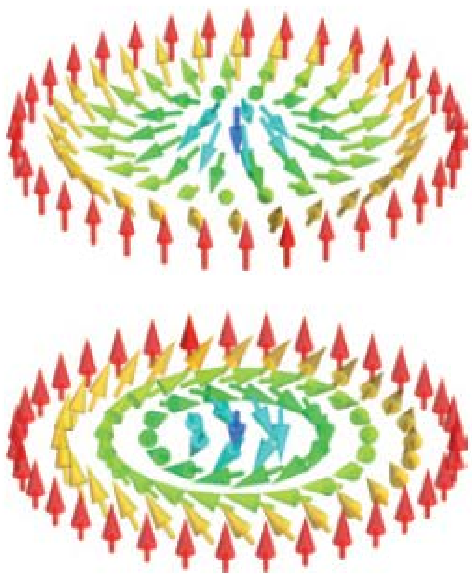


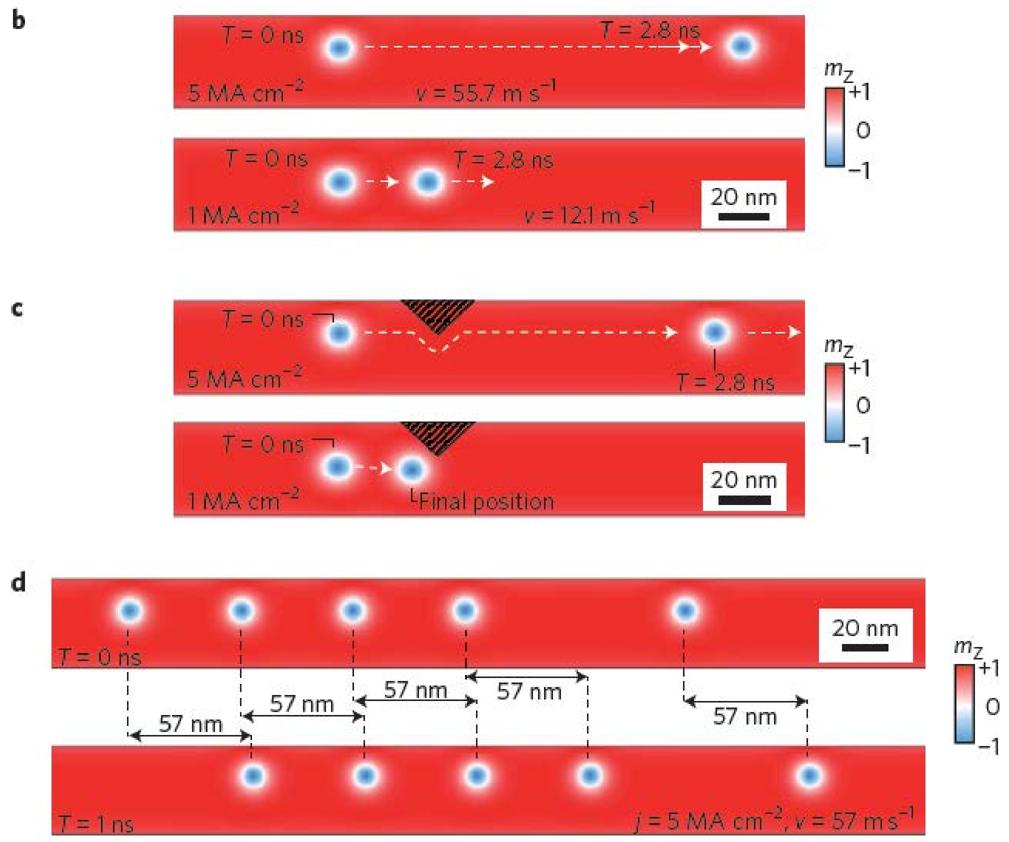
- Solid lines : $v_{DW} = \dfrac{\alpha s}{(\alpha s)^2 + {\delta_s}^2}(M_1 - M_2)\lambda H$

- Simulation index 5 = T_A (δ_s = 0)

Magnetic Skyrmions

A. Fert et al., "Skyrmions on the track", **Nat. Nano.** (2013)

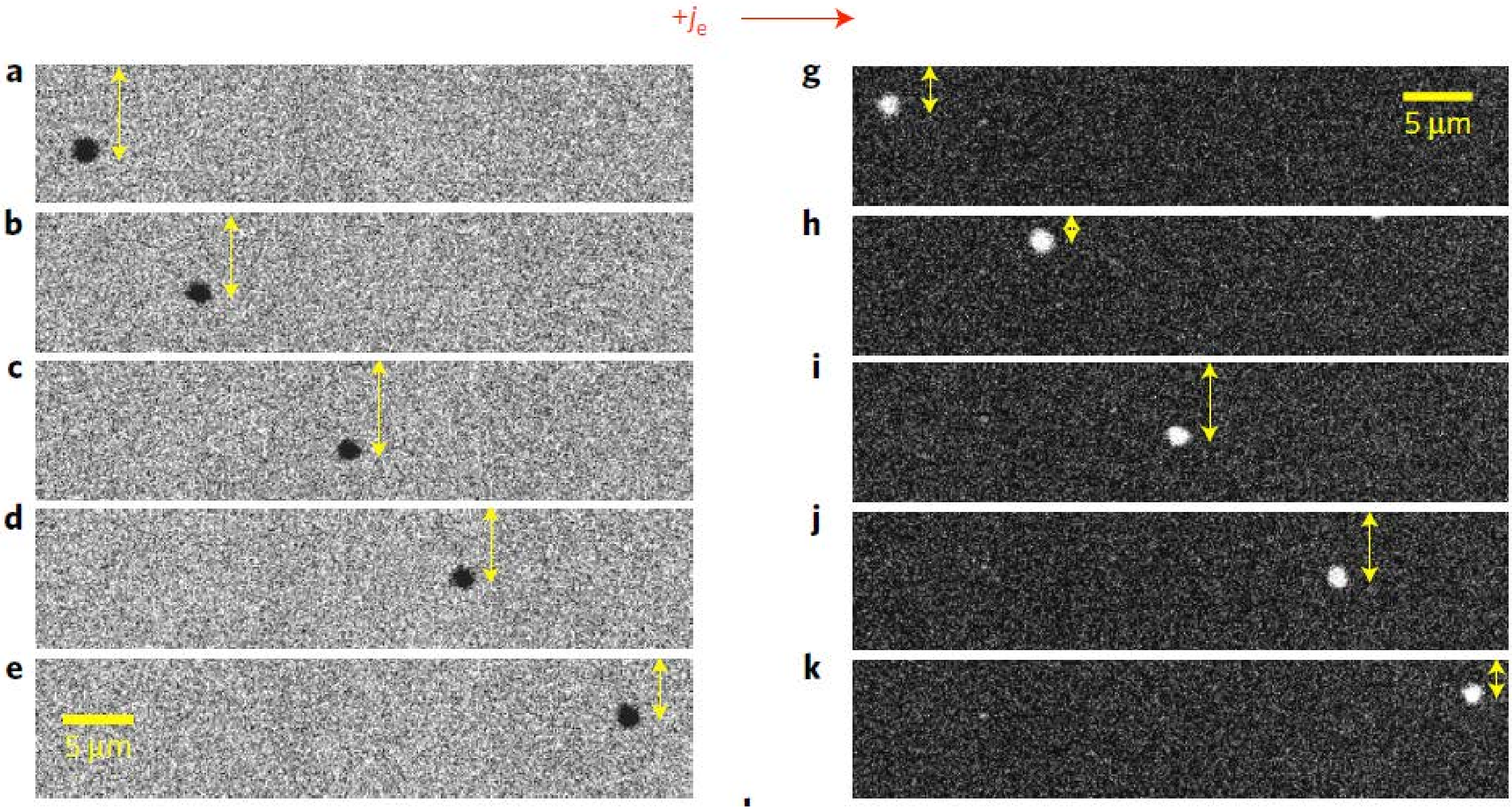




- **Skyrmions: small (~ 10 nm), fast, move at low current, defect-insensitive**

Skyrmion Hall effect

W. Jiang et al., Nat. Phys. (2017); K. Litzius et al., Nat. Phys. (2017)



- **Transverse deflection of skyrmion ~ the Hall effect**

Charge Hall effect vs Skyrmion Hall effect

Charge Hall effect

Elementary charge

External magnetic field

Lorentz force: $Q\dot{\boldsymbol{R}} \times \boldsymbol{B}$

Topological charge

Fictitious magnetic field

$$Q \equiv \int dxdy\boldsymbol{n} \cdot (\partial_x \boldsymbol{n} \times \partial_y \boldsymbol{n})/4\pi$$

$$\boldsymbol{B} = -4\pi s_{\mathrm{net}} \hat{\boldsymbol{z}}$$

Net spin density

Skyrmion Hall effect

Vanishing skyrmion Hall effect for antiferromagnet ($s_{net} = \delta_s = 0$)

Barker & Tretiakov, PRL **116**, 147203; Zhang, Zhou, & Ezawa, NCOMM **7**, 10293 (16)

Current-driven bubble elongation in GdFeCo/Pt

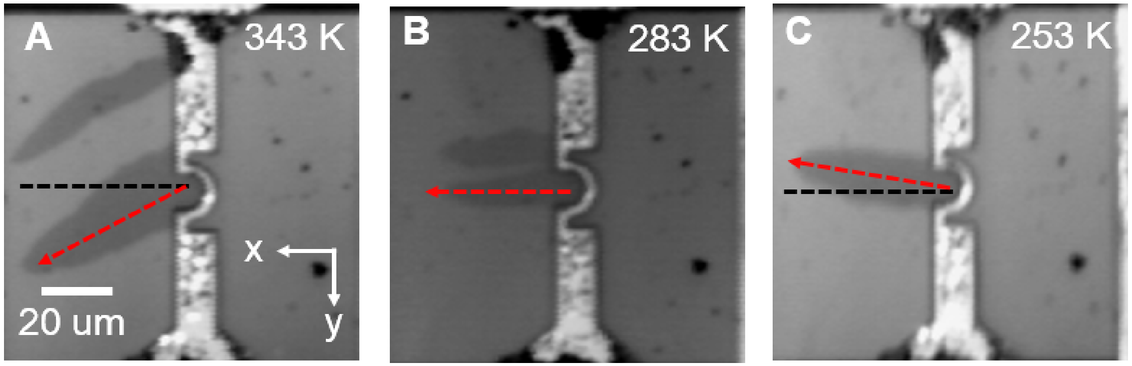
Hirata et al., Nat. Nanotechnol. 14, 232 (2019)

DMI field = 63 mT >> DW hard-axis anisotropy field = 0.9 mT

➔ Well-defined topological charge Q

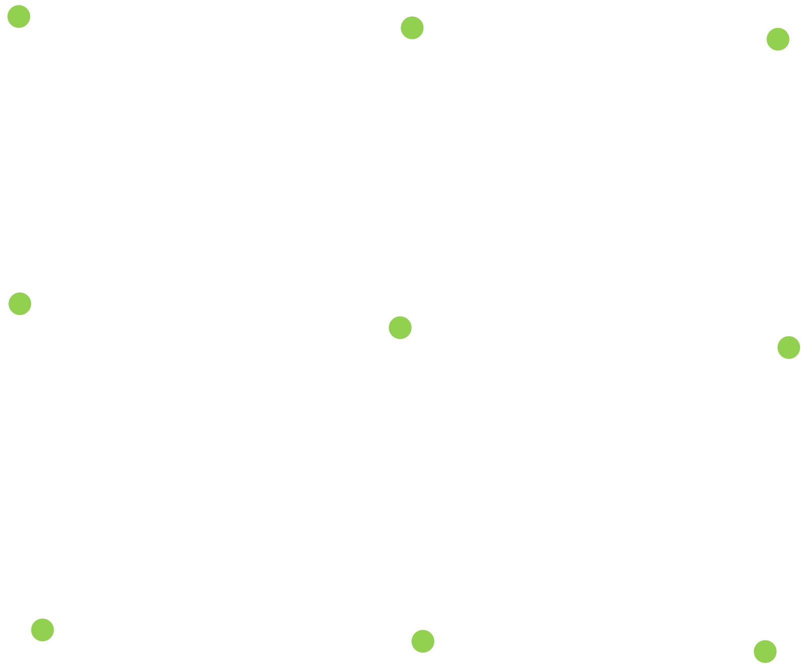
Bubble elongation ~ half skyrmion motion

Elongation angle vs temperature (Experiment)



Elongation angle ≈ 0 at T_A ➔ Vanishing skyrmion Hall effect for s_{net} = 0

Elongation angle vs temperature (Modeling)

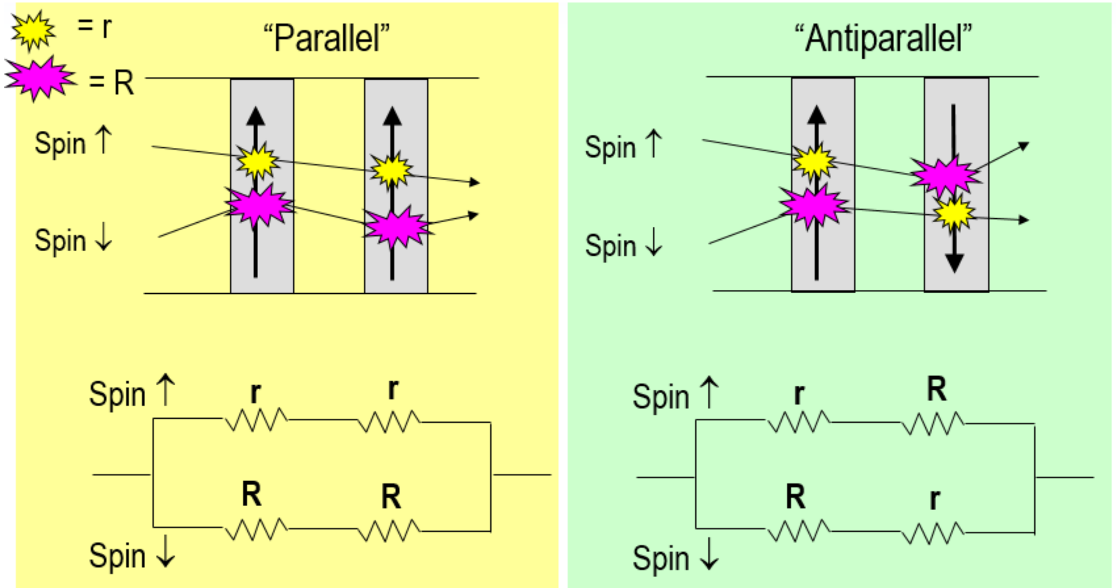


Elongation angle ≈ 0 at T_A ➔ Consistent with experiment & theory

Spin drift-diffusion model

- Spin transport is an important branch of spintronics
- Giant magnetoresistance (GMR: A. Fert and P. Grünberg, Nobel prize in physics, 2007)
- How to understand GMR?

- Two-current model
- Spin-flip scattering is ignored



$$R_P = \left(\frac{1}{2r} + \frac{1}{2R}\right)^{-1} = 2\left(\frac{Rr}{R+r}\right)$$

$$R_{AP} = \left(\frac{1}{r+R} + \frac{1}{R+r}\right)^{-1} = \left(\frac{R+r}{2}\right)$$

$$\mathbf{R_P < R_{AP}}$$

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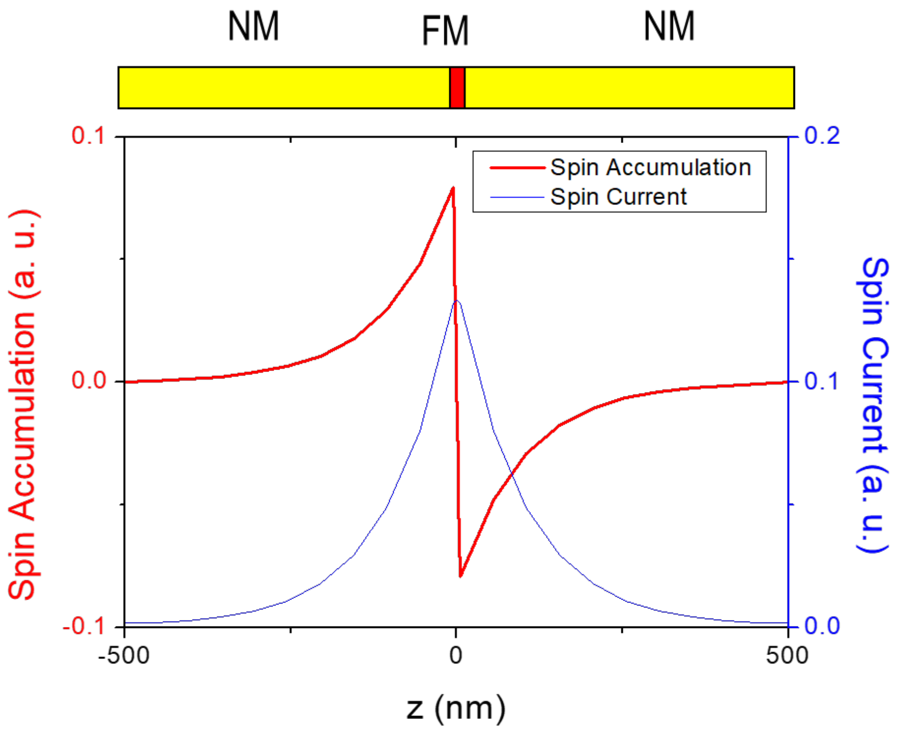
Valet-Fert theory [PRB 48, 7099 (1993)]

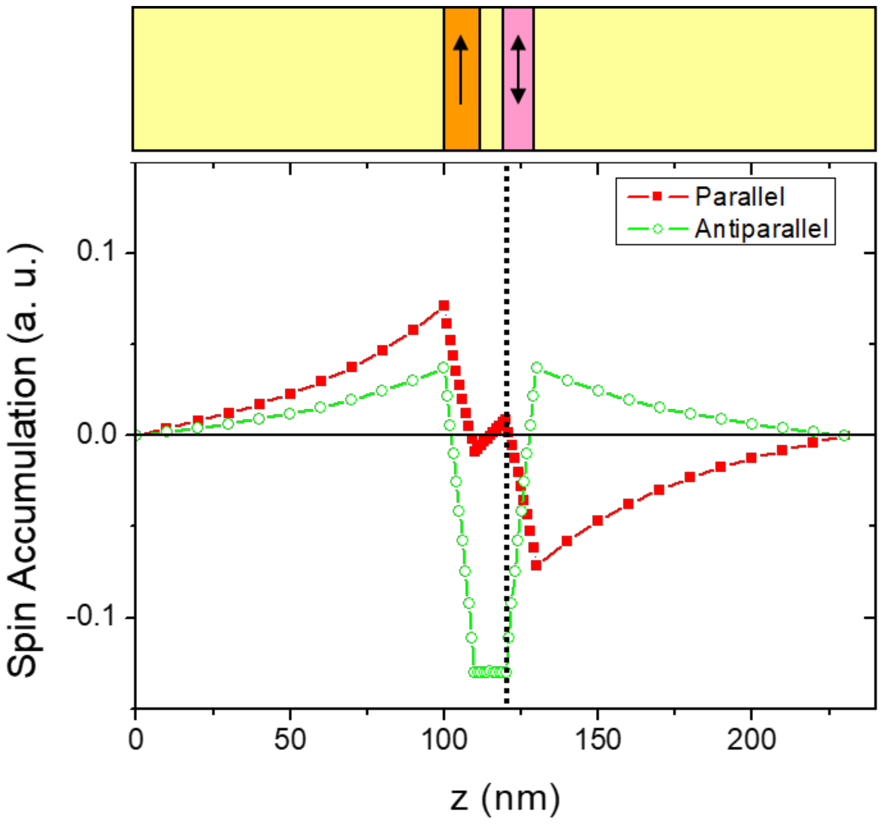
- Spin-flip scattering is included for longitudinal (**s** || **m**) spin current
- Spin drift: $$J_s = \frac{\sigma_s}{e} \frac{\partial \bar{\mu}_s}{\partial z}$$
- Spin diffusion $$\frac{e}{\sigma_s} \frac{\partial J_s}{\partial z} = \frac{\bar{\mu}_s - \bar{\mu}_{-s}}{l_s^2}$$
- s = ↑ or ↓
- J_s = spin current & μ_s = spin chemical potential ~ spin accumulation
- σ_s = spin-dependent conductivity
- l_s = spin-diffusion length

Spin drift-diffusion model

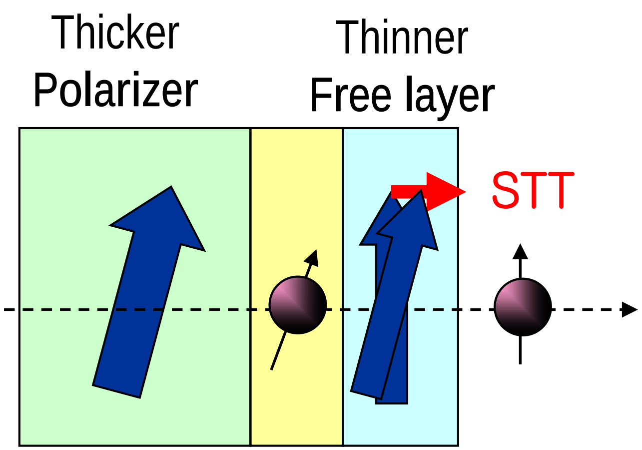
Single FM



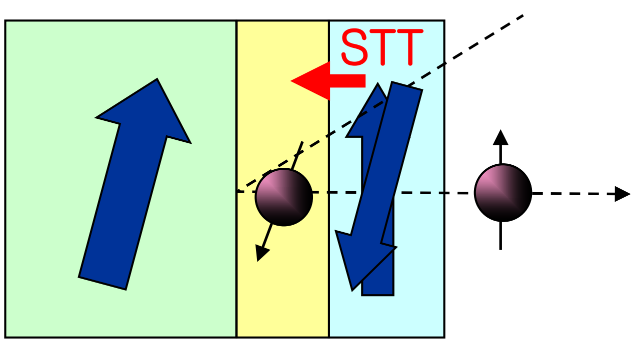
Spin valve



What about transverse spin current? STT



Free M aligns P to Polarizer M



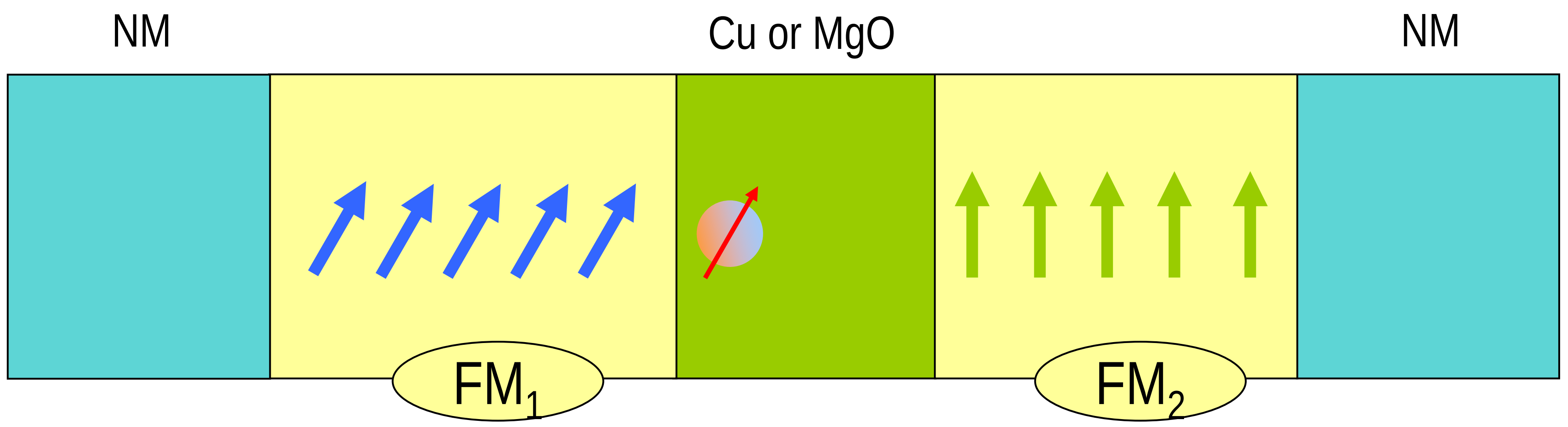
Free M aligns AP to Polarizer M

- Angular momentum conservation
  - Spin angular momentum (incoming s-el') + local magnetic momentum (localized d-el') = CONSTANT
- STT ∝ (Details of scattering matrix at interface) x (Transverse spin accumulation)
- Bi-stable switching (P or AP) depending on the current sign.

[1] J.C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996)

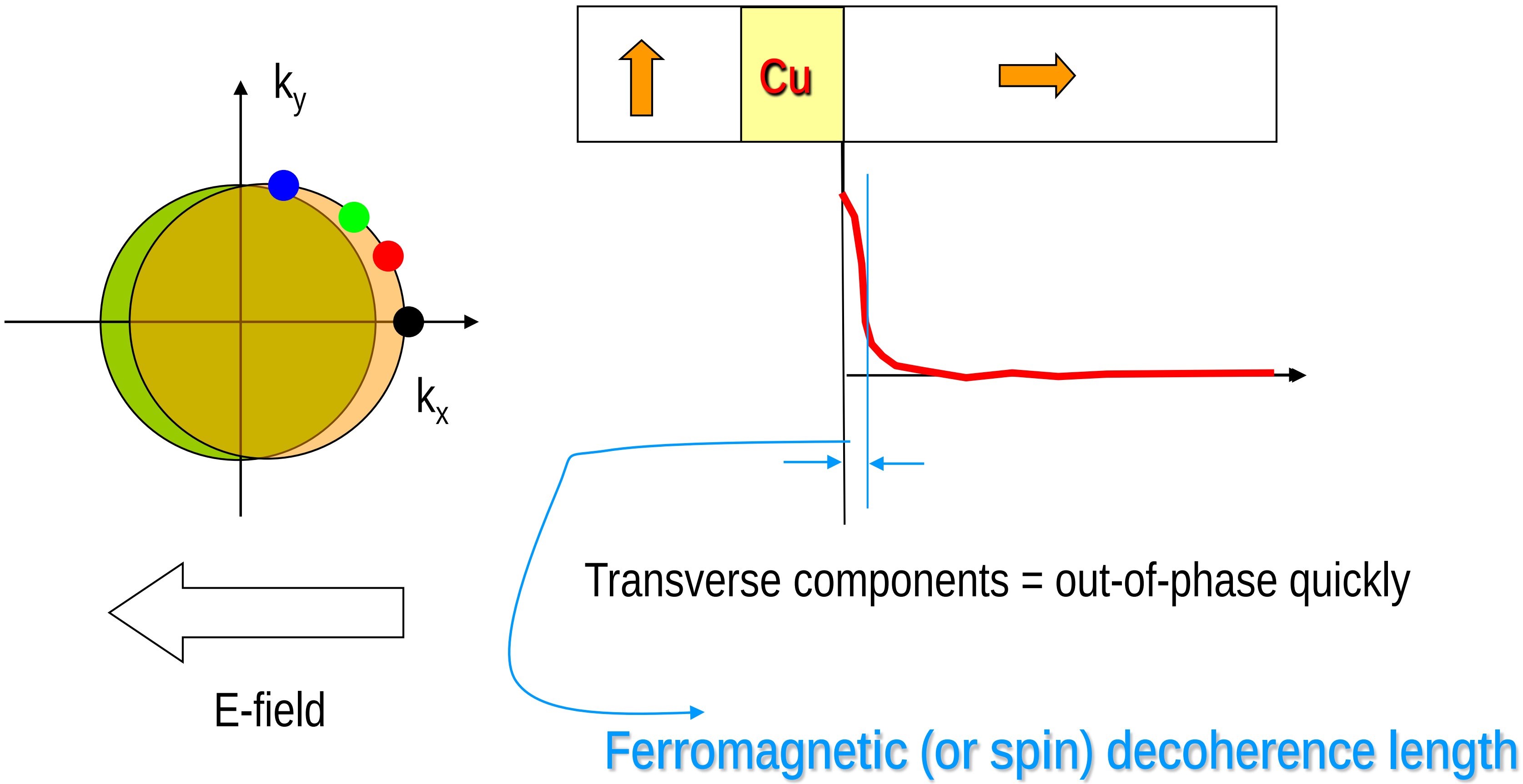
[2] L. Berger, Phys. Rev. B **54**, 9353 (1996)

Spin precession due to s-d exchange



• The s-electron spin precesses around the **M** (d-electron) of FM_2 when **M**'s of FM_1 and FM_2 are not collinear.

For all current-carrying electrons



- Spin-transfer torque = Surface torque in fully metallic SV

Boundary condition for transverse spin current

- Neglecting spin-orbit coupling effect, the spin coherence length of transverse spin current in FM is extremely short ➔ Quantum BC at NM/FM interface assuming no transverse spin current in FM [Brataas et al., Eur. Phys. J. B **22**, 99 (2001)]
- Charge current J_e:

$$J_e(\pm t_F/2) = (G_\uparrow + G_\downarrow)\Delta\mu_e/e + (G_\uparrow - G_\downarrow)\mathbf{m}\cdot(\boldsymbol{\Delta\mu}_S/e)$$

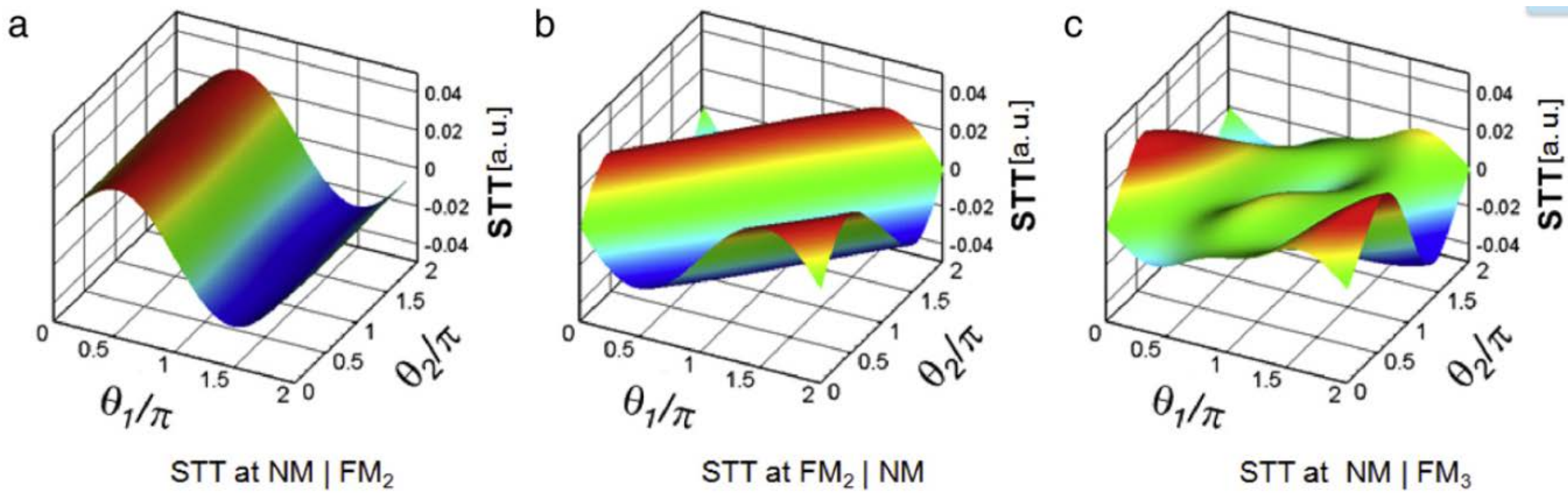
- Spin current J_s (1st line: longitudinal, 2nd line: transverse):

$$\mathbf{J}_S(\pm t_F/2) = -(\hbar/2e^2)\left[(G_\uparrow + G_\downarrow)\mathbf{m}\cdot\boldsymbol{\Delta\mu}_S + (G_\uparrow - G_\downarrow)\Delta\mu_e\right]\mathbf{m}$$
$$+ \mathrm{Re}(G_{\uparrow\downarrow})(\hbar/2e^2)(2\boldsymbol{\Delta\mu}_S \times \mathbf{m} \pm \hbar\partial\mathbf{m}/\partial t) \times \mathbf{m}$$

- G_s = spin-dependent interface conductance
- $\Delta\mu$ = pontential drop over the interface
- $G_{\uparrow\downarrow}$ = spin-mixing conductance [Im($G_{\uparrow\downarrow}$) is ignored]

Angular dependence of STT

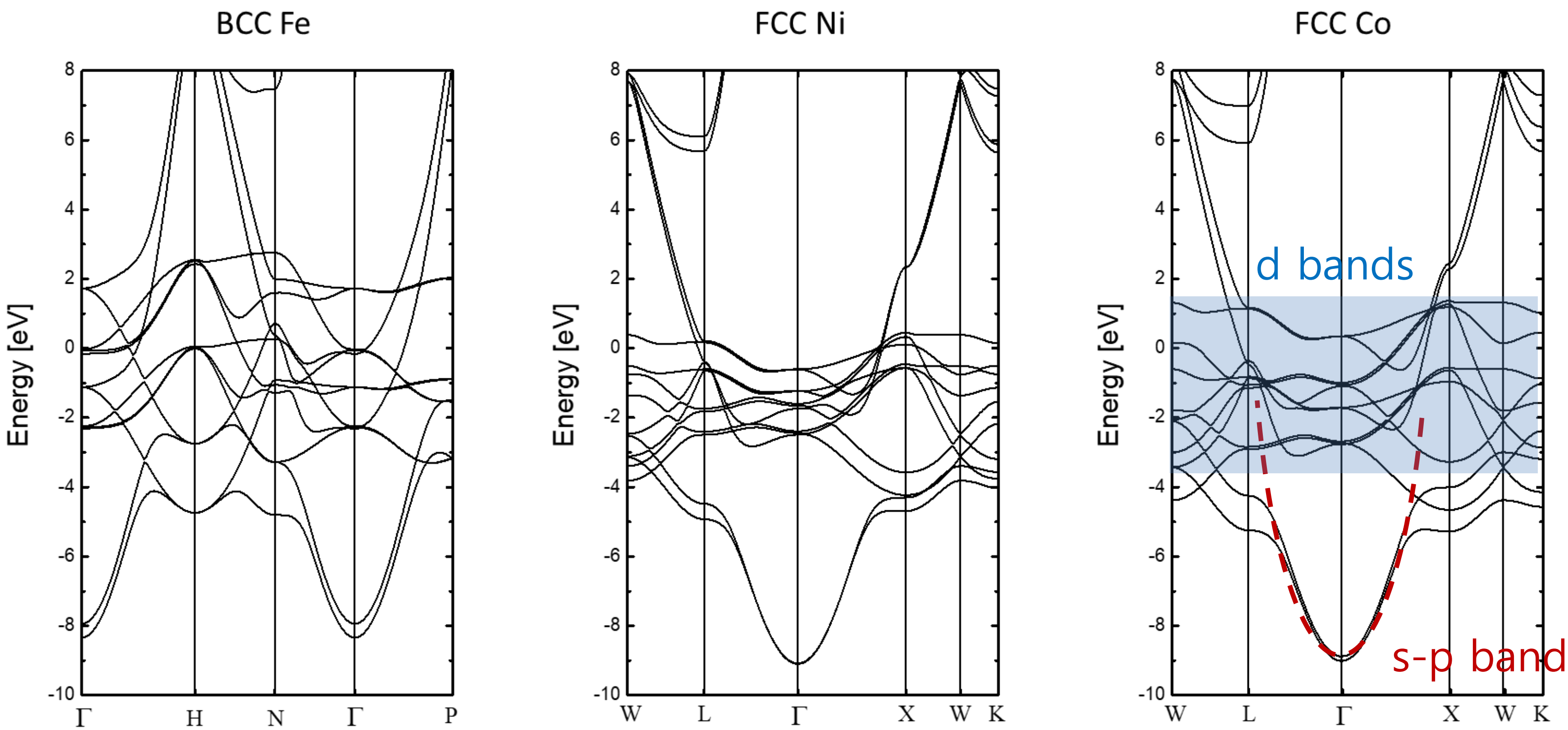
- KJL et al., Phys. Rep. **531**, 89 (2013)
- STT in NM | FM1 | NM | FM2 | NM | FM3 multilayer
- θ_1 and θ_2 are the magnetization angles of FM2 and FM3 with respect to the magnetization angle of FM1, respectively.



Band structure calculation

- First-principles: electronic structure at equilibrium based on the Density Functional Theory (DFT)
- In magnetism: Spin moment, Orbital moment, Magnetic Anisotropy, Exchange, DMI, …
- Various codes depending on the type of basis function, the way to describe the exchange-correlation, etc
- An example: OpenMX http://www.openmx-square.org/
- DFT + norm-conserving pseudopotentials + pseudo-atomic localized basis functions

Band structures of 3d FMs



Transport calculation

- Calculate non-equilibrium quantities such as spin current and spin density based on a model Hamiltonian or ab initio band
- An example: Kubo formula: spin Hall conductivity

$$\sigma_{SH} = \frac{e}{\hbar}\sum_n \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, f_{n\mathbf{k}}\Omega_n^s(\mathbf{k})$$

$$\Omega_n^s(\mathbf{k}) = 2\hbar^2 \sum_{m\neq n} \mathrm{Im}\left[\frac{\langle u_{n\mathbf{k}}|j_y^s|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|v_x|u_{n\mathbf{k}}\rangle}{(E_{n\mathbf{k}} - E_{m\mathbf{k}} + i\eta)^2}\right]$$

- $f_{n\mathbf{k}}$ = Fermi-Dirac distribution function
- $|u_{n\mathbf{k}}\rangle$ = a periodic part of the Bloch state (eigenvalue = $E_{n\mathbf{k}}$)
- v_x = x component of the velocity operator
- j_y^s = y component of the spin current operator

Anomalous & Planar Hall currents in FMs

- Calculate spin current with spin polarization along **m** of FMs
- Two effects can be identified (we consider spin flow in z-direction & **E** in x-direction)
- Anomalous Hall effect: $\propto \mathbf{m}\times\mathbf{E}\big|_z = \mathbf{m}\times\mathbf{x}\big|_z = -m_y$
- Planar Hall effect: $\propto (\mathbf{m}\cdot\mathbf{E})\mathbf{m}\big|_z = (\mathbf{m}\cdot\mathbf{x})\mathbf{m}\big|_z = m_x m_z$