CMD Workshop 37 : Spintronics course
in Center for Spintronics Research Network (CSRN),
Graduate School of Engineering Science, Osaka University.

September 1, 2020

Spintronic Interface design
(スピントロニクス・インターフェース・デザイン)

Yoshio Miura

National Institute for Materials Science (NIMS)

Research Center for Magnetic and Spintronic Materials (CMSM)

Spin Theory Group

Topics

0. Introduction on spintronics

1. Spin-dependent transport in magnetic tunnel junctions with half-metallic Heusler alloys

Y. Miura, *et al*., PRB **83,** 214411 (2011).

2. Magneto-crystalline anisotropy at interfaces of Fe(001) with MgO and $MgAl_2O_4$

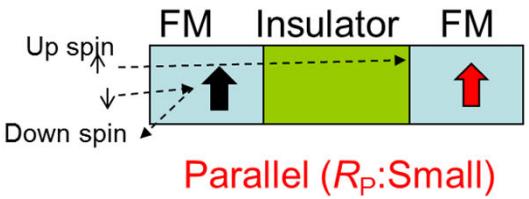
K. Masuda and Y. Miura, PRB **98**, 224421 (2018).

3. First-Principles Study on magnetic damping of Fe/MgO(001)

Y. Miura, in preparation

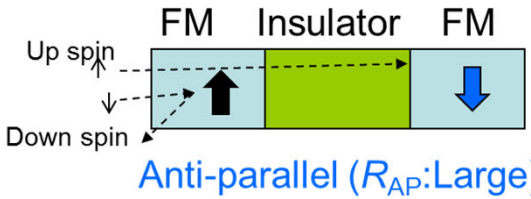
Instroduction

Magnetic tunnel junction (MTJs)



Parallel (R_P:Small)

(FM: Ferromagnetic metal)



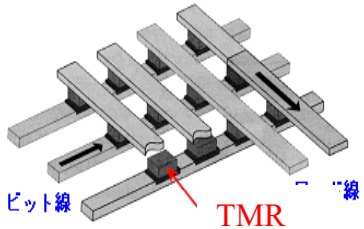
Anti-parallel (R_{AP}:Large)

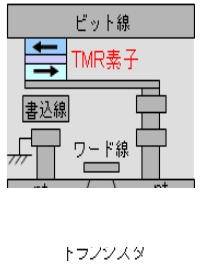
Tunneling magnetoresistance (TMR)

$$\text{TMR ratio} = \frac{R_{AP} - R_P}{R_{AP}}$$

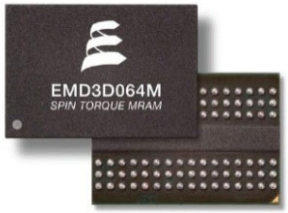
Magnetoresistive Random Access Memory (MRAM)

- Non volatile memory
- Fast writing speed (10～50ns)
- Low electricity consumption (～30μW)
- Long endurance (10 years)

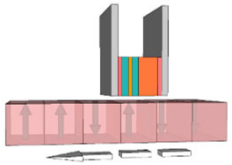




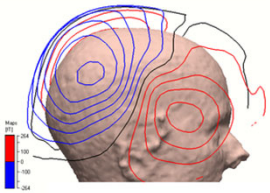
Everspin
64Mbit MRAM



Magnetic sensor



HDD read-out-head



Earth's magnetic field sensor・current sensor for car・biomagnetic sensor

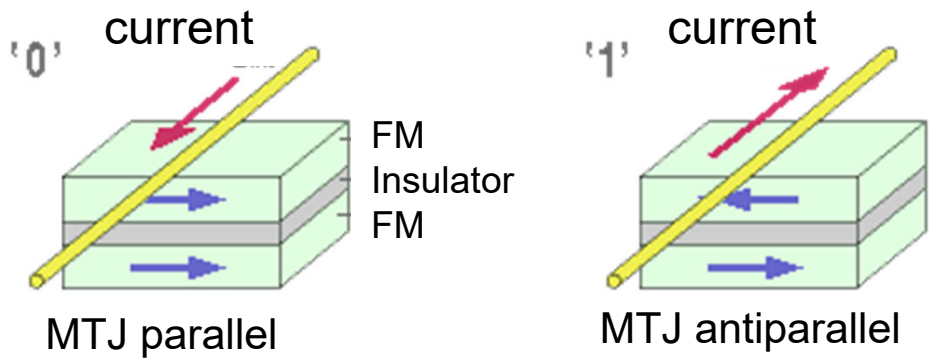
Corresponding to SQUID

Magnetization reversal in MTJs

1. Magnetic field by current

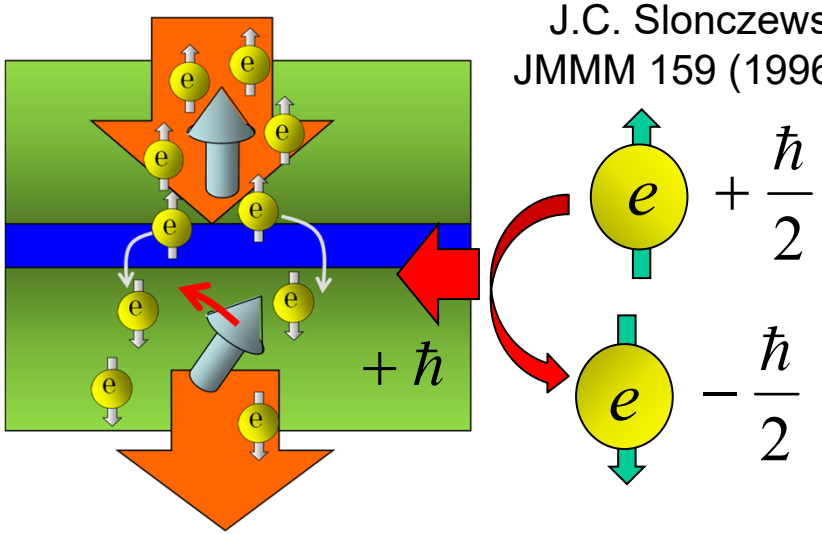
problem : ・complicate circuit.
・current∝1/device-size

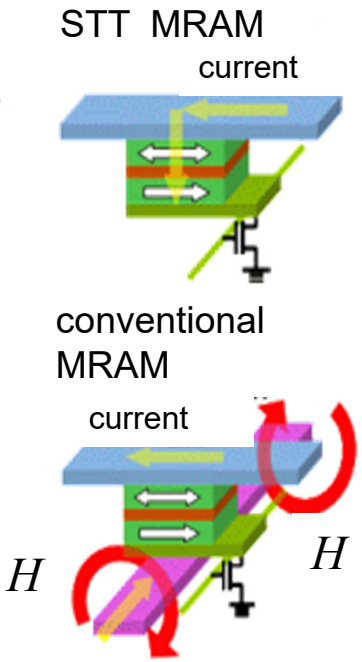
Effects of demagnetizing field increase the critical current for writing with decreasing size of device



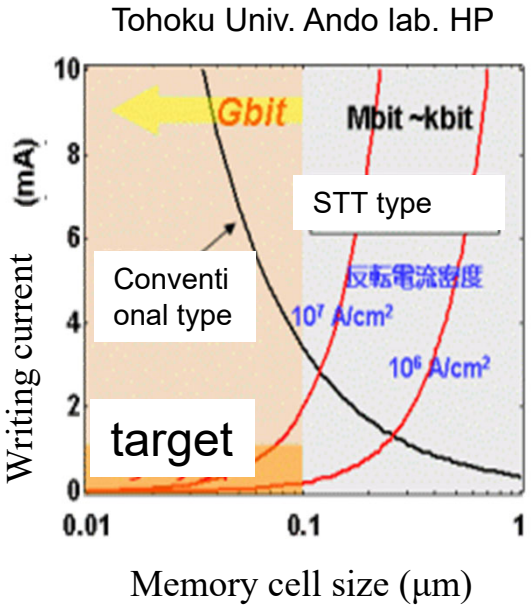
2. Spin transfer torque（STT）

The spin flip of conductive electron give the torque to the local spin moment due to the angular momentum conservation

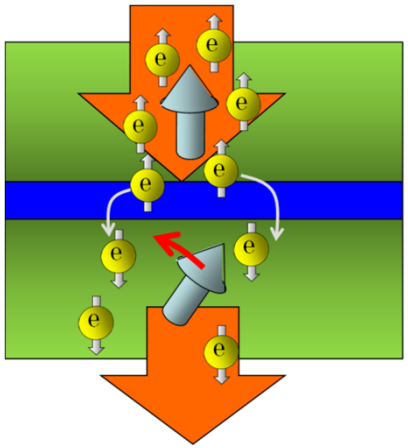


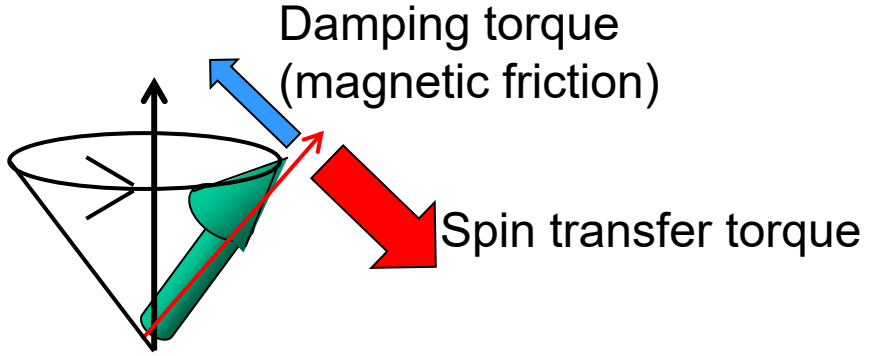


・simple circuit
・current∝device-size



Magnetization reversal by spin transfer torque (STT)





Reduction of critical current density (J_{c0})

$(10^7 \mathrm{A/cm^2} \Rightarrow 10^5 \mathrm{A/cm^2})$

$$J_{c0} \propto \alpha M_S [H_{\mathrm{anti}} \pm 4\pi M_S]\ t/P$$

J.C. Slonczewski, JMMM 159 (1996) L1.

α: Magnetic damping constant
M_S: Saturation Magnetization
$H_{\mathrm{anti}} \pm 4\pi M_S$: Effective anisotropy field
P: Spin polarization
t: Thickness of FM layer

1. High spin polarization (P)

2. Perpendicular magnetic anisotropy(PMA) H_{anti}-$4\pi M_s$

3. Low damping constant(α)

Topics

0. Introduction on spintronics

1. Spin-dependent transport in magnetic tunnel junctions with half-metallic Heusler alloys

Y. Miura, *et al*., PRB **83,** 214411 (2011).

2. Magneto-crystalline anisotropy at interfaces of Fe(001) with MgO and $MgAl_2O_4$

K. Masuda and Y. Miura, PRB **98**, 224421 (2018).

3. First-Principles Study on magnetic damping of Fe/MgO(001)

Y. Miura, in preparation

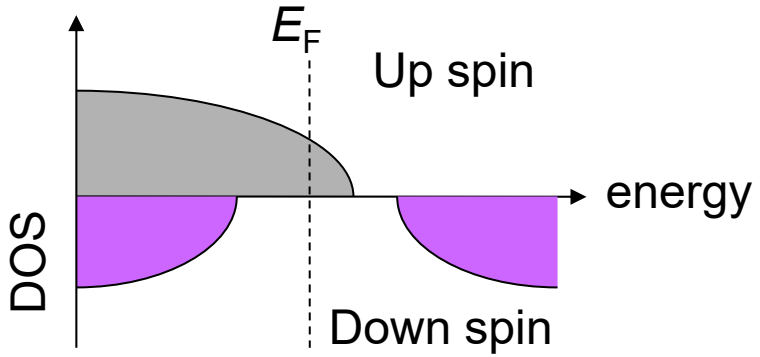
Introduction: Half-metallic ferromagnetic

Julliere model

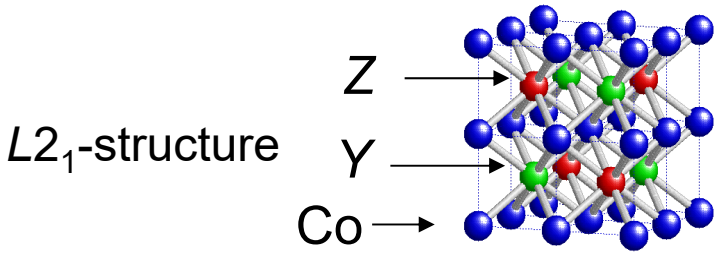
$$\mathrm{TMR} = \frac{G_\mathrm{P} - G_\mathrm{AP}}{G_\mathrm{P}} = \frac{2P_\mathrm{L} \cdot P_\mathrm{R}}{1 - P_\mathrm{L} \cdot P_\mathrm{R}}$$

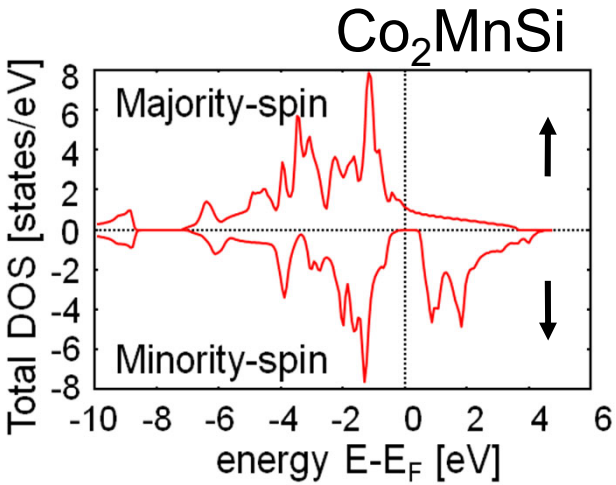
Spin-polarization at E_F $\quad P_{\mathrm{L(R)}} = \dfrac{D^{\uparrow}_{\mathrm{L(R)}} - D^{\downarrow}_{\mathrm{L(R)}}}{D^{\uparrow}_{\mathrm{L(R)}} + D^{\downarrow}_{\mathrm{L(R)}}}$

The Half-metallic ferromagnets

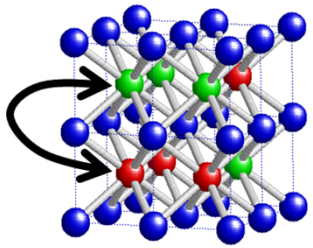


Co-based full Heusler alloys Co_2YZ (Y=Fe,Mn,Cr : Z=Si,Ge,Al,Ga)



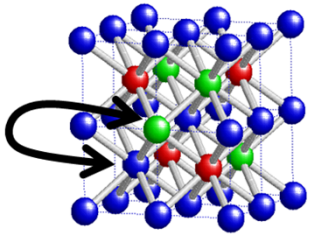


(1) B2-type disorder



$Co_2(Mn_{1-y}Si_y)(Si_{1-y}Mn_y)$

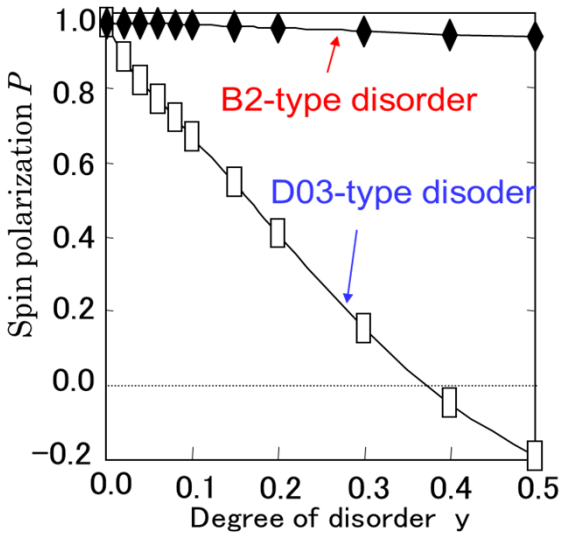
(2) D03-type disorder



$(Co_{2-y}Mn_y)(Mn_{1-y}Co_y)Si$

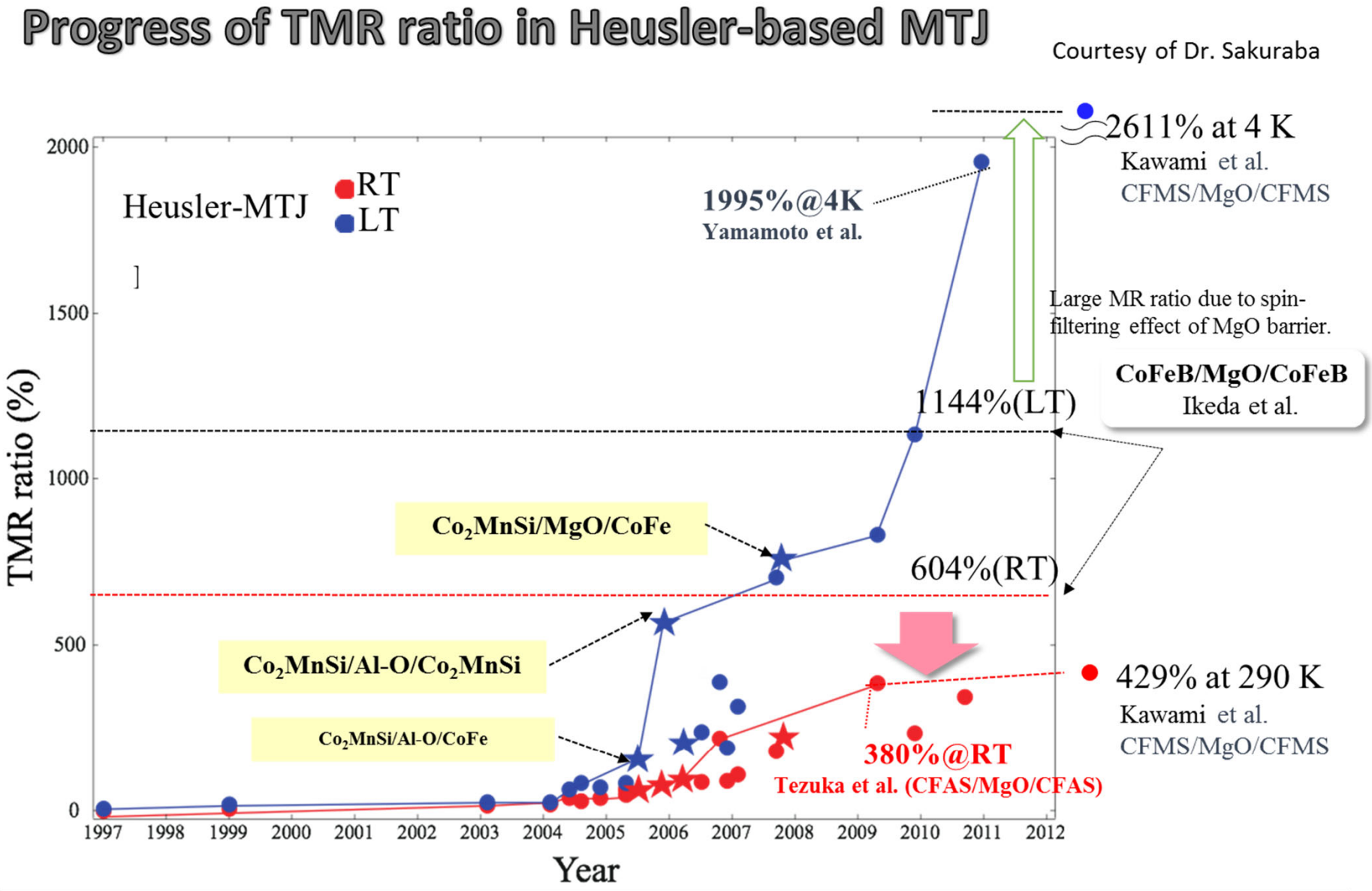
High Curie temperature (900K)

Simple fabrication process



Y. Miura, *et al.*, PRB, 69 (2004) 144413.

Problem in MTJs with half-metallic Heusler alloys

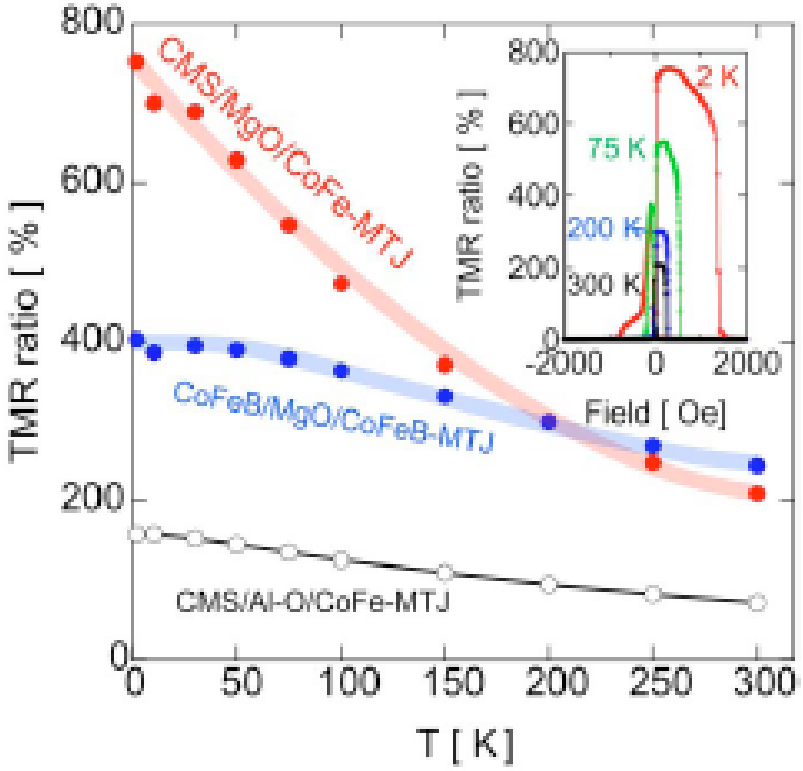


Heusler-based MTJ : Large temperature dependence of MR ratio is still a serious problem especially in CMS.

CMS: Co_2MnSi CFAS: $Co_2Fe(AlSi)$ CFMS: $Co_2(FeMn)Si$

Problem in MTJs with half-metallic Heusler alloys

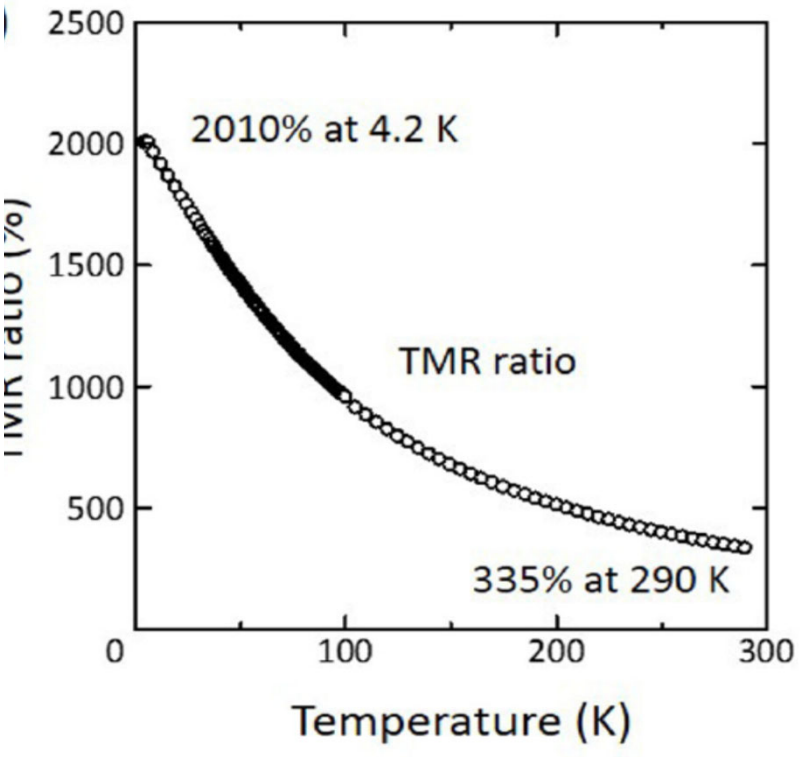
TMR ratio of MTJs with Co_2MnSi(CMS)



S. Tsunegi, *et al*., APL 93 (2008) 112506.

CMS/MgO/CMS(001)

B. Hu, et al., PRB **94** (2016) 094428.



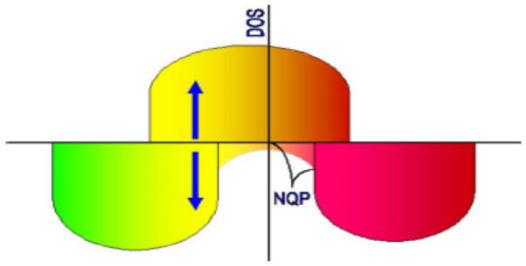
Present top data

Problem: Reduction of the TMR ratio at room temperature

in spite of high curie temperature of Co2MnSi: 985K

Introduction (theory)

1. Temperature dependence of bulk density of states owing to non-quasiparticle

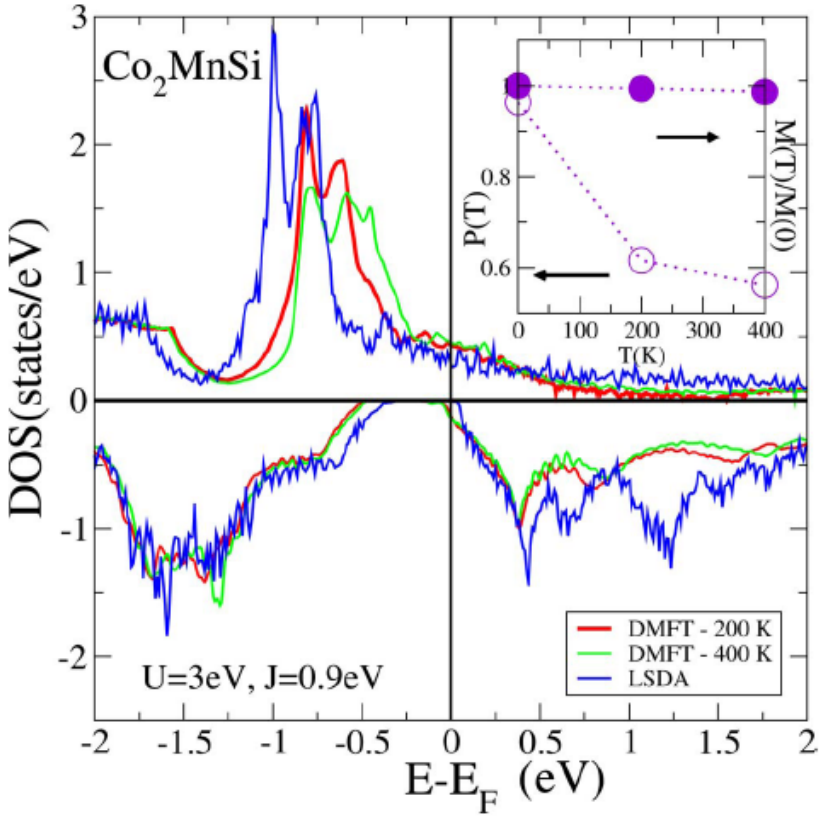


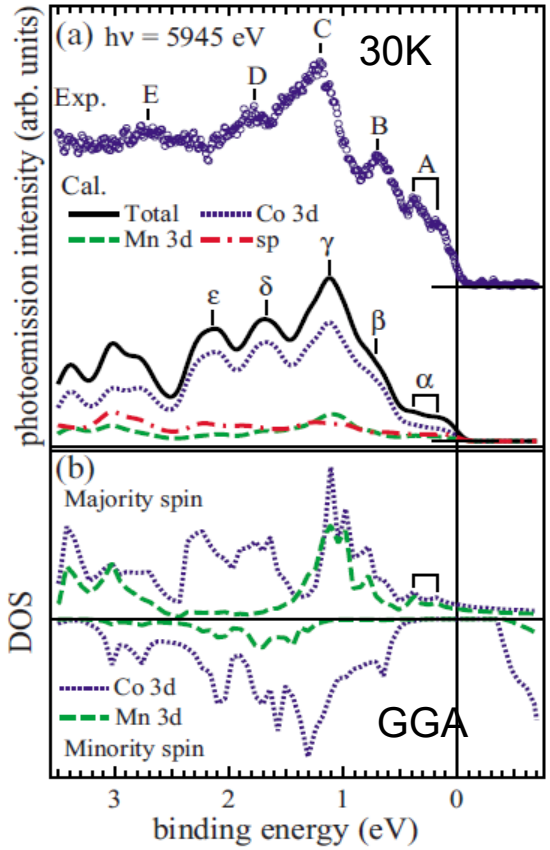
M. I. Katsnelson, *et al*., Rev. Mod. Phys. **80**, 315 (2008).

X-ray photoelectron spectroscopy of bulk CMS

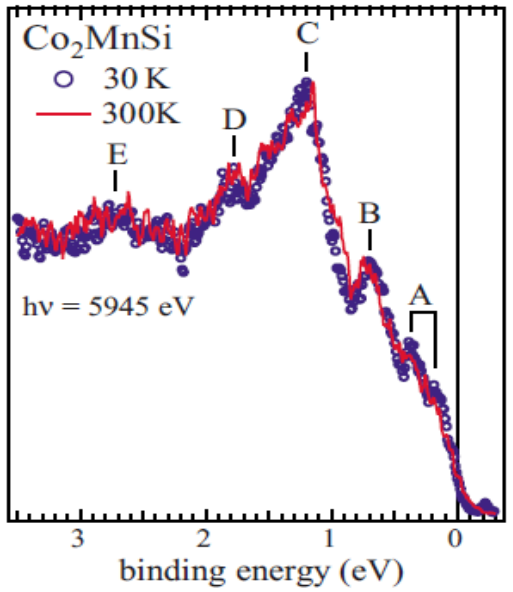
K. Miyamoto, *et al*., PRB. **79**, 100405(R) (2009).

Temperature dependence of total DOS of bulk CMS calculated from DMFT





Valence band electronic structures of bulk CMS

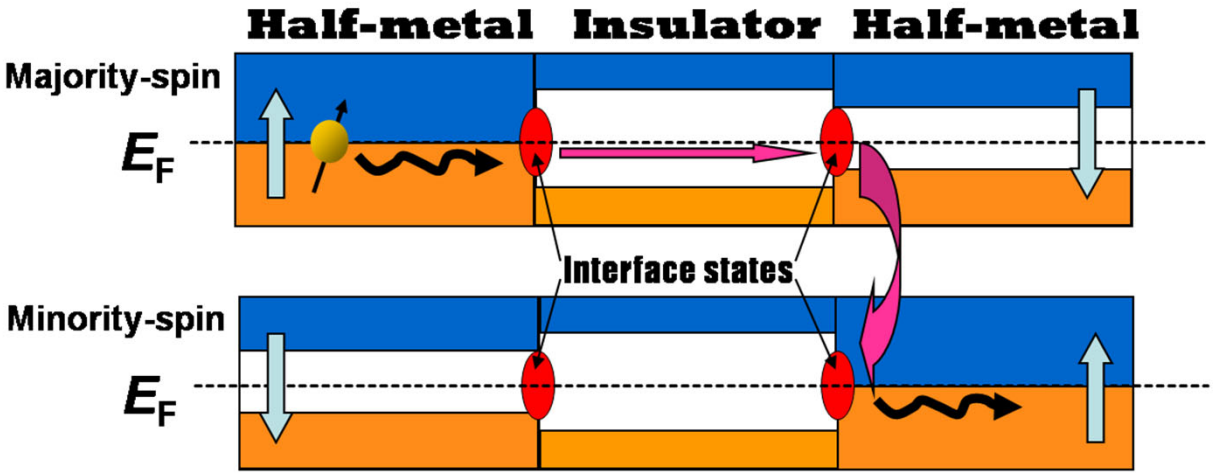


Introduction (theory)

2. Effects of the spin-flip scattering through the interface states promoted by magnetic excitation.

P. Mavropoulos, *et al*., PRB, 72 (2005) 174428.

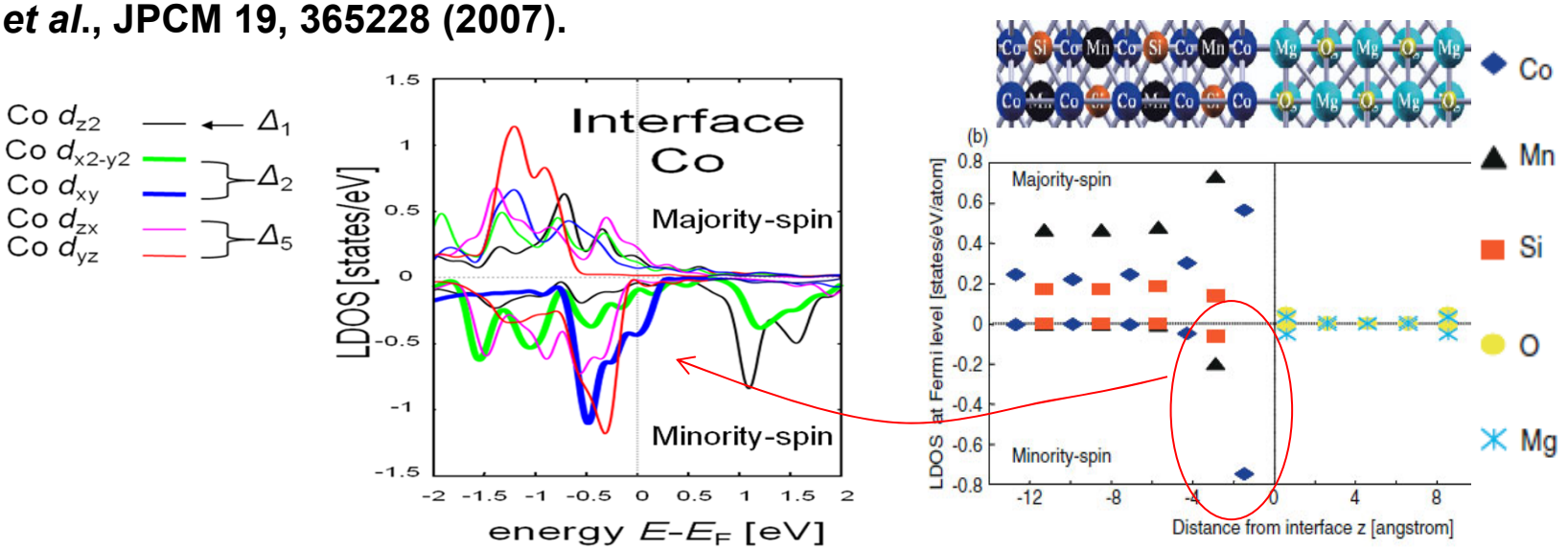
Anti-parallel magnetization



$Co_2MnSi/MgO(001)$

Y. Miura, *et al*., PRB 78, 064416 (2008).

Y. Miura, *et al*., JPCM 19, 365228 (2007).

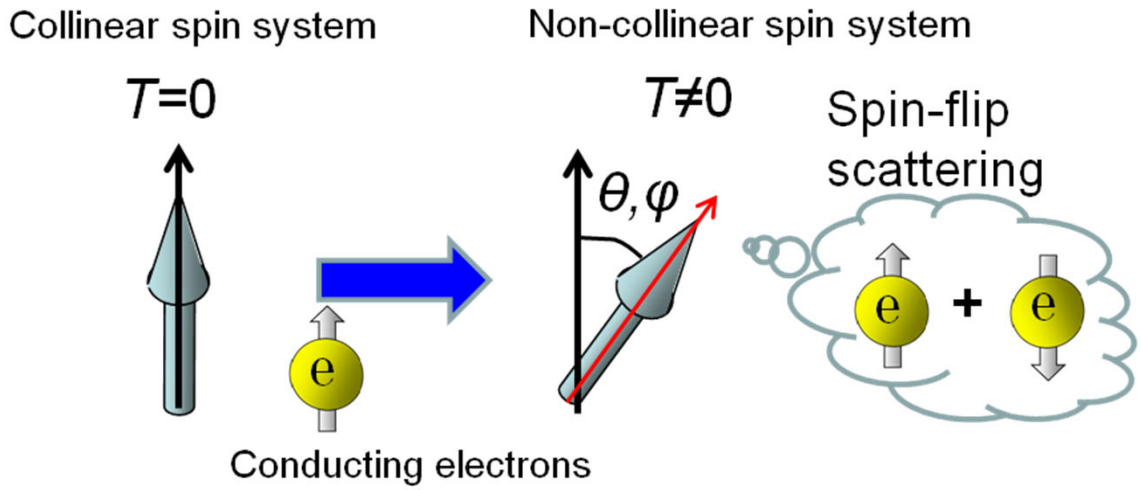


Purpose of this work

・To clarify a possible origin of reduction of TMR ratio at RT in MTJ with half-metallic Heusler alloys,

・We investigate effects of spin-flip scattering through the interface states at CMS/MgO junctions originating from non-collinear magnetic structures.

Thermal fluctuation of local spin-moments ⇒ Non-collinear magnetic structures



Calculation Method

Electronic structures

PWSCF http://www.pwscf.org/

- Plane-wave basis set
- Ultra-soft pseudopotential method
- GGA for Exchange-Correlation term

Transport calculations

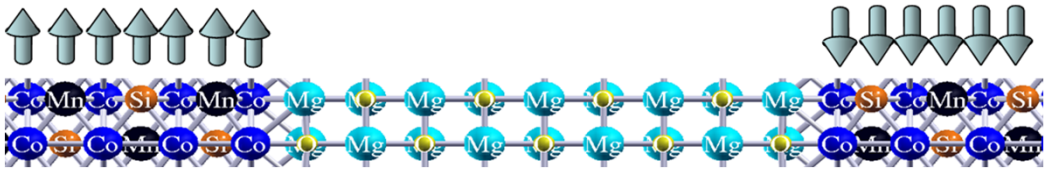
$$G = \frac{e^2}{h} \sum_{i}^{N} T_i$$

- Landauer formula
- Zero bias limet Ballistic Conductance

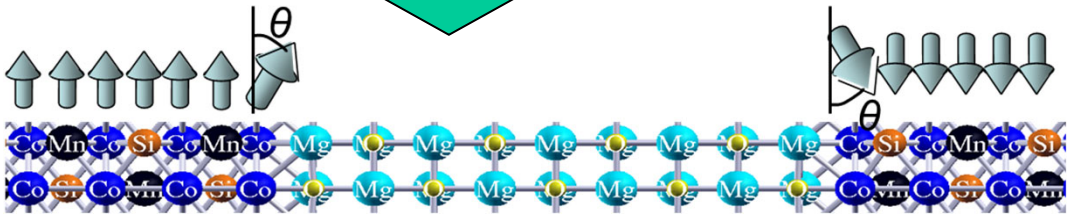
H. J. Choi and J. Ihm, PRB 59 (1999) 2267.
A. Smogunov, A. Dal Corso and E. Tosatti, PRB 70 (2004) 045417.

Conductance calculation in Non-collinear spin system

First, we perform electronic structure calculations in collinear spin system



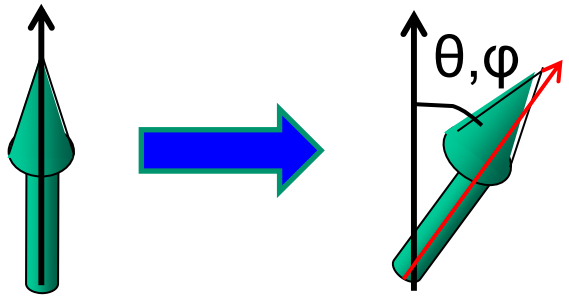
Then, we artificially rotate spin-quantum axis of local spin-moments to obtain density-matrix in non-collinear spin system.



The rotation of spin-quantum axis in NC spin system

The density matrix in non-collinear spin system is obtained from the inverse unitary transformation of spin-density in collinear spin system.

Collinear spin system($\mathbf{n}_i$) Non-collinear spin system($\mathbf{n}_{\alpha\beta}$)



$$n_{\alpha\beta}(\mathrm{r}) = \sum_{i=(\uparrow,\downarrow)} U^{+}_{\alpha i}\, n_i(\mathrm{r})\, U_{i\beta}$$

$$U = \begin{pmatrix} \exp\left(\frac{1}{2}i\varphi\right)\cos\left(\frac{1}{2}\theta\right) & \exp\left(-\frac{1}{2}i\varphi\right)\sin\left(\frac{1}{2}\theta\right) \\ -\exp\left(\frac{1}{2}i\varphi\right)\sin\left(\frac{1}{2}\theta\right) & \exp\left(-\frac{1}{2}i\varphi\right)\cos\left(\frac{1}{2}\theta\right) \end{pmatrix}$$

J. Kubler et al., J. Phys. F: Met. Phys. **18**, 469 (1988).

Local potential in Collinear spin system

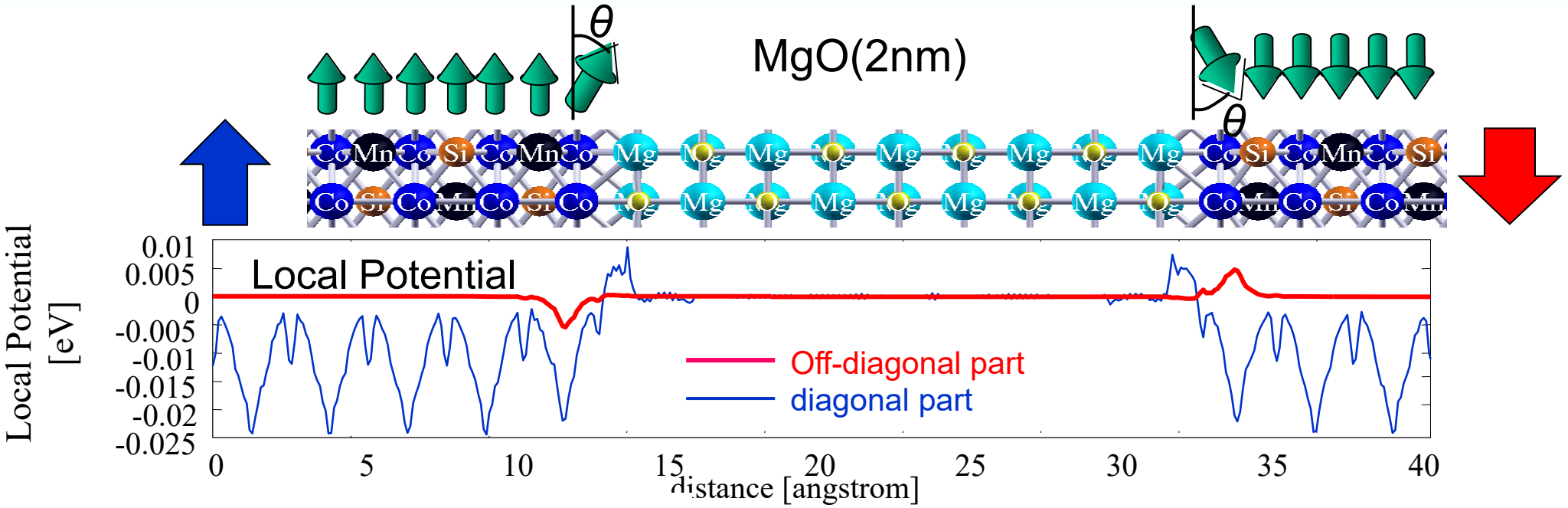
$$\begin{pmatrix} V_L(r)+V_H(r)+\frac{1}{2}\sum_{\alpha=(\uparrow,\downarrow)}\frac{\delta E_{XC}}{\delta n_\alpha}+\frac{1}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right) & 0 \\ 0 & V_L(r)+V_H(r)+\frac{1}{2}\sum_{\alpha=(\uparrow,\downarrow)}\frac{\delta E_{XC}}{\delta n_\alpha}-\frac{1}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right) \end{pmatrix}$$

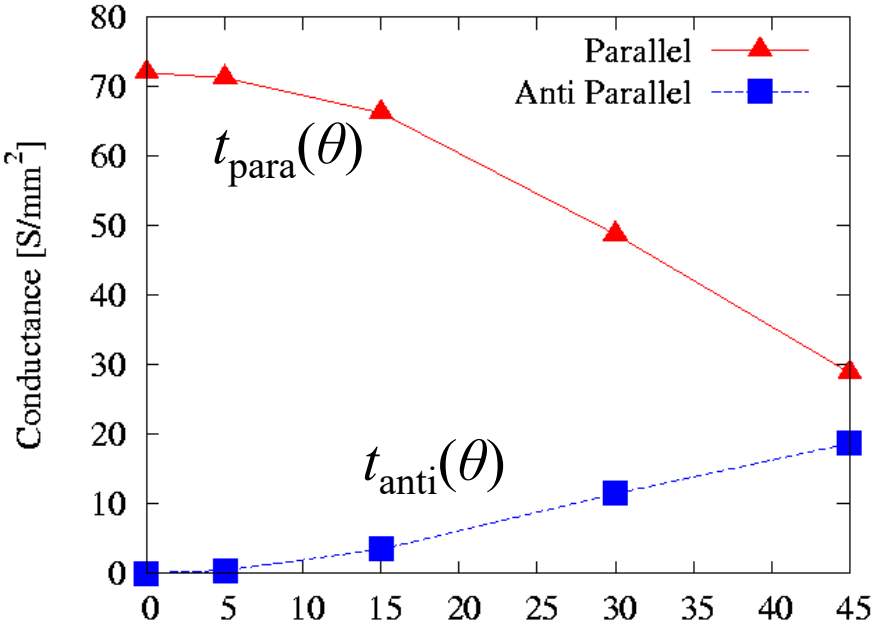
Local potential in Non-Collinear spin system

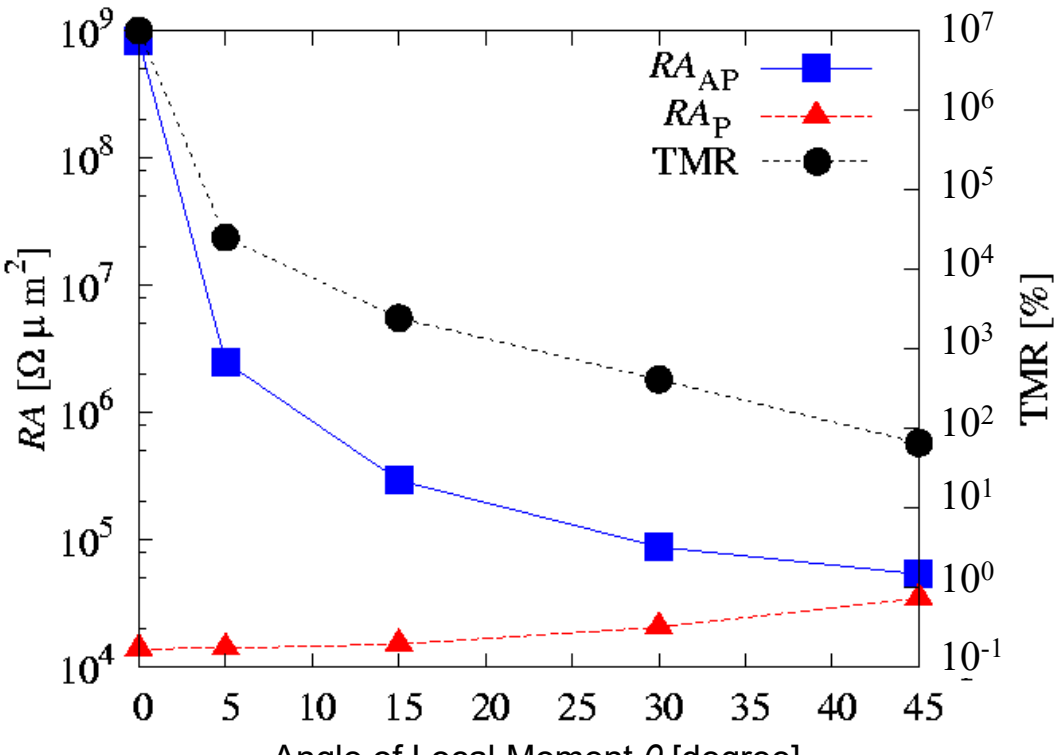
$$\begin{pmatrix} V_L(r)+V_H(r)+\frac{1}{2}\sum_{\alpha=(\uparrow,\downarrow)}\frac{\delta E_{XC}}{\delta n_\alpha}+\frac{1}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right)\cos\theta & \frac{1}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right)\sin\theta\cos\phi+\frac{i}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right)\sin\theta\sin\phi \\ \frac{1}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right)\sin\theta\cos\phi-\frac{i}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right)\sin\theta\sin\phi & V_L(r)+V_H(r)+\frac{1}{2}\sum_{\alpha=(\uparrow,\downarrow)}\frac{\delta E_{XC}}{\delta n_\alpha}-\frac{1}{2}\left(\frac{\delta E_{XC}}{\delta n_\uparrow}-\frac{\delta E_{XC}}{\delta n_\downarrow}\right)\cos\theta \end{pmatrix}$$

Y. Miura, et al., Phys. Rev. B **83,** 214411 (2011).

Transport in non-collinear spin MTJs





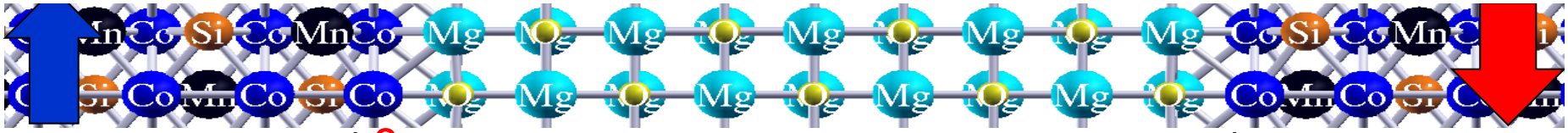


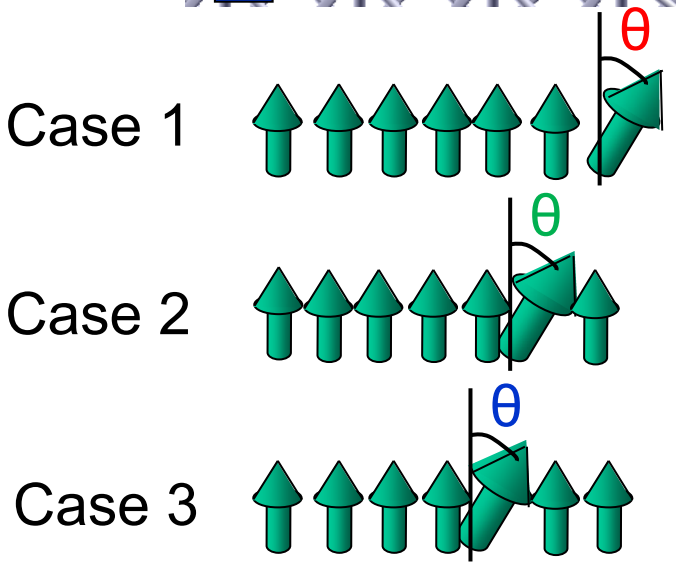
Angle of Local Moment θ [degree]

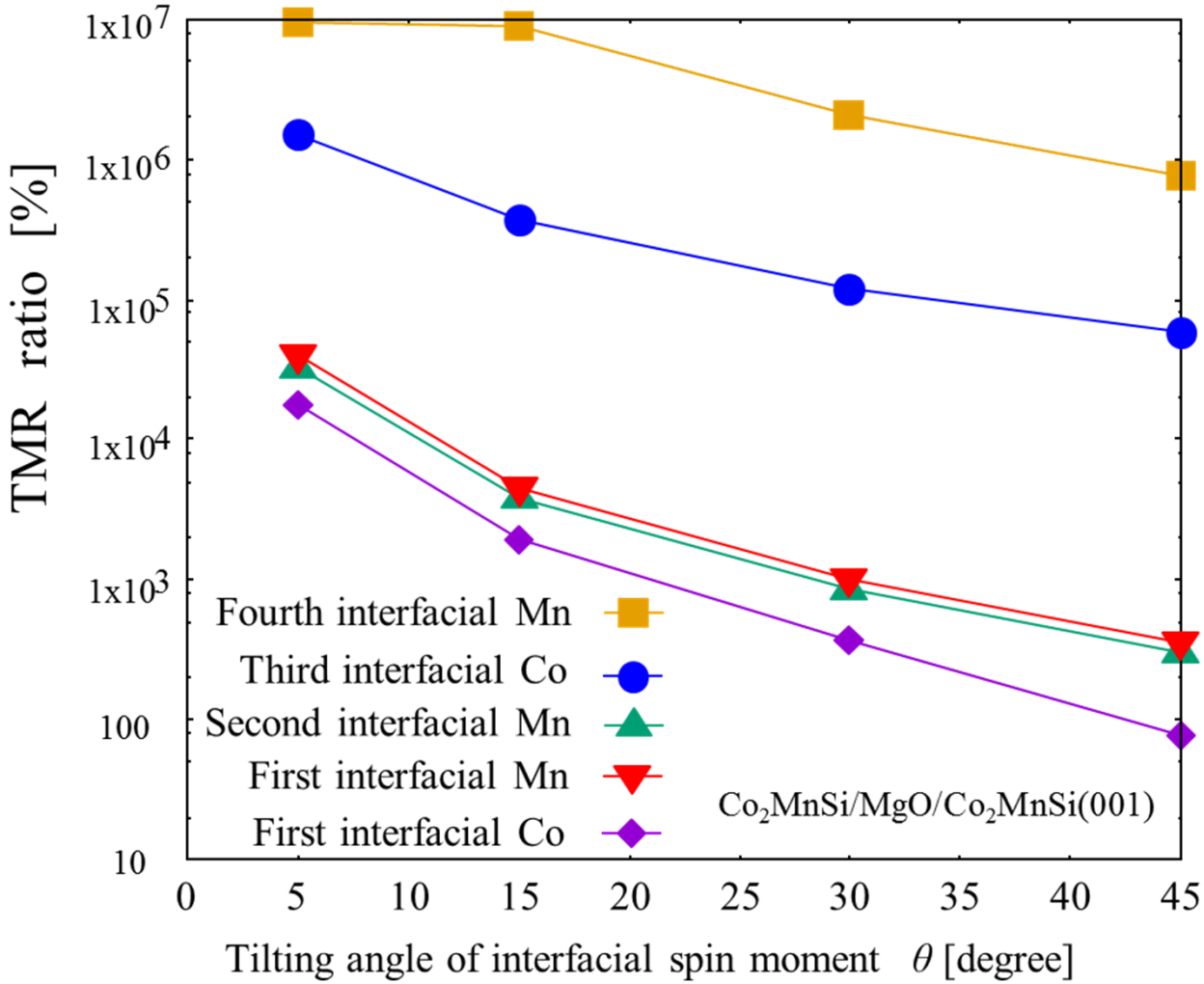
Angle of Local Moment θ [degree]

Y. Miura, et al., Phys. Rev. B **83,** 214411 (2011).

Effects of sub-interfacial non-collinear spin to TMR







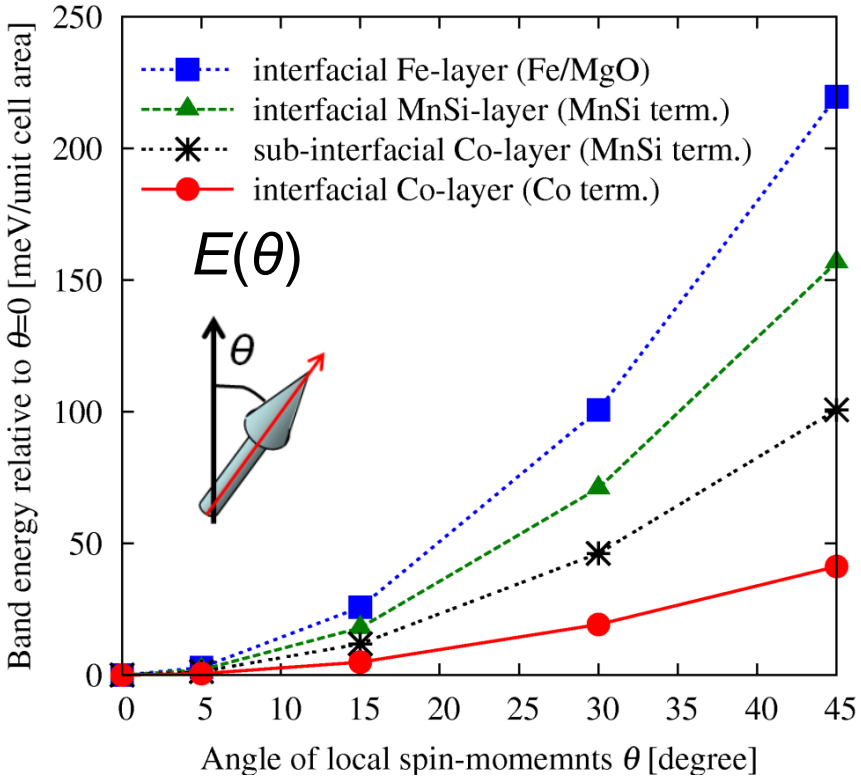
Noncollinear magnetic structures of the first and the second interfacial layer strongly reduce TMR.

Noncollinear magnetic structure of the third and forth interfacial layer show relatively small reduction of TMR.

Exchange stiffness constant at CMS/MgO(001)

Increase of band energy of Non-collinear Spin ⇒ Strength of exchange coupling

$E(\theta)=A(1-\cos\theta)$ $A \propto JM^2$



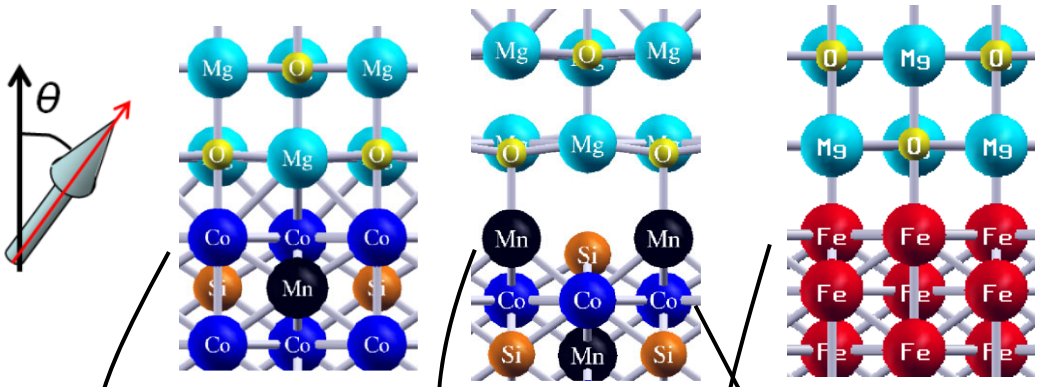
A. Sakuma, *et al.*, JAP **105**, 07C910 (2009).

Off-diagonal part of local potential

$$V_{\alpha\beta(\alpha\neq\beta)}(\mathrm{r})=\left(\frac{\delta E_{XC}}{\delta n_{\uparrow}}-\frac{\delta E_{XC}}{\delta n_{\downarrow}}\right)\sin\theta$$

CMS/MgO(001) **Fe/MgO(001)**

Co-term. **MnSi-term.**



Exchange stiffness of interfacial atoms

A [meV/u.c.a.]	Co^1	Mn^1	Fe^1	Co^2
Bulk (CMS or Fe)	414	529	600	414
MgO interface	145	565	753	347
ΔA [meV/u.c.a.]	−269	+34	+153	−67

Interfacial local spin-moment

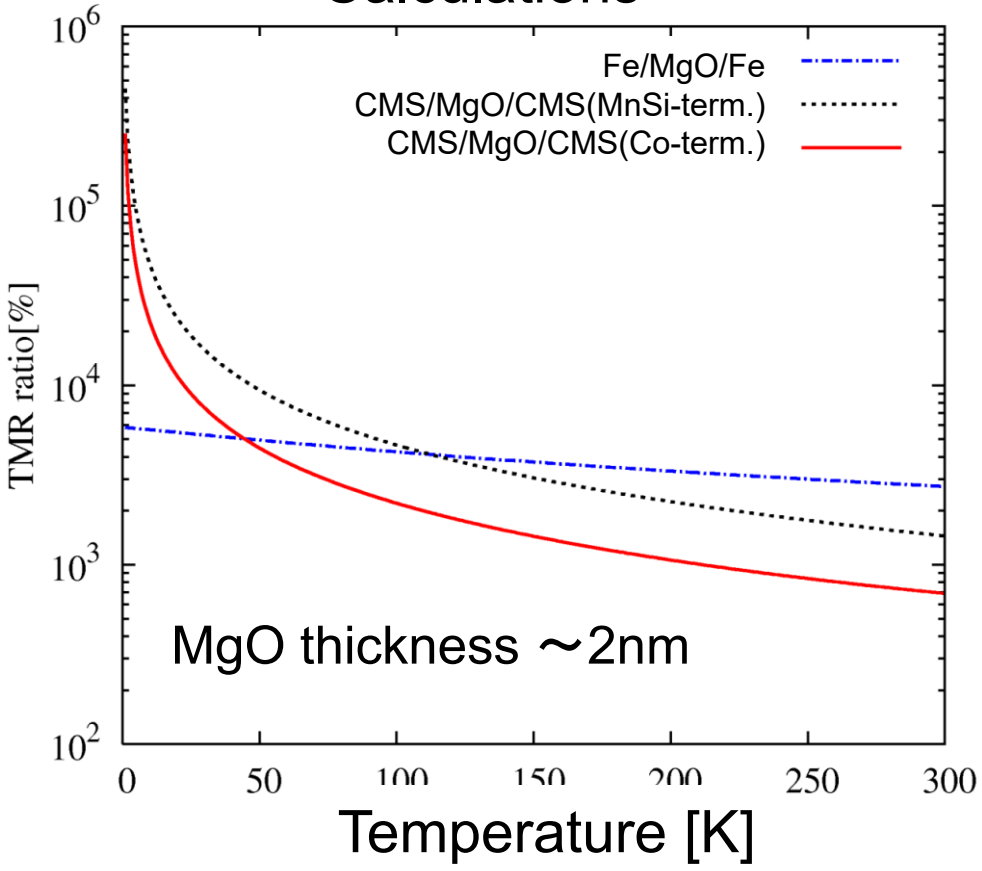
$M[\mu_B]$	Co^1	Mn^1	Fe^1
Bulk (CMS or Fe)	0.93	3.31	2.35
MgO interface	0.54	4.06	2.98
$\Delta M[\mu_B]$	−0.39	+0.75	+0.63

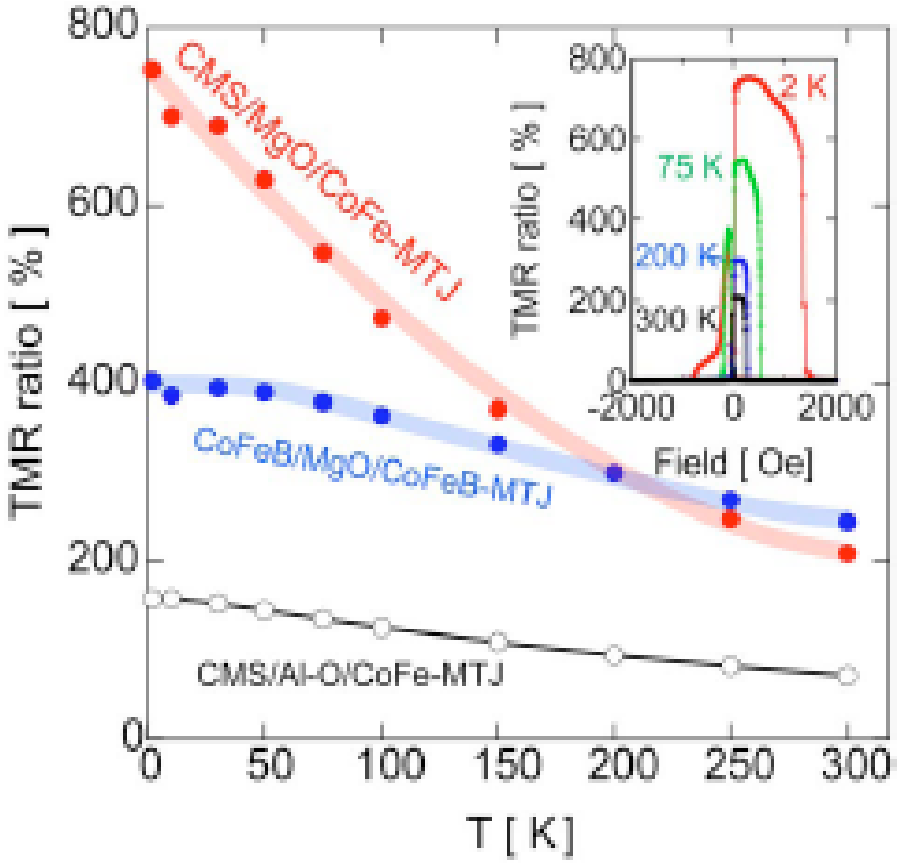
TMR ratio at finite temperature

Boltzmann average of tunneling conductance

$$t^{(\mathrm{para,anti})}(T) = \frac{\int t_{(\mathrm{para,anti})}(\theta)\exp[-2E(\theta)/k_BT]\sin\theta d\theta}{\int \exp[-2E(\theta)/k_BT]\sin\theta d\theta}$$

Calculations

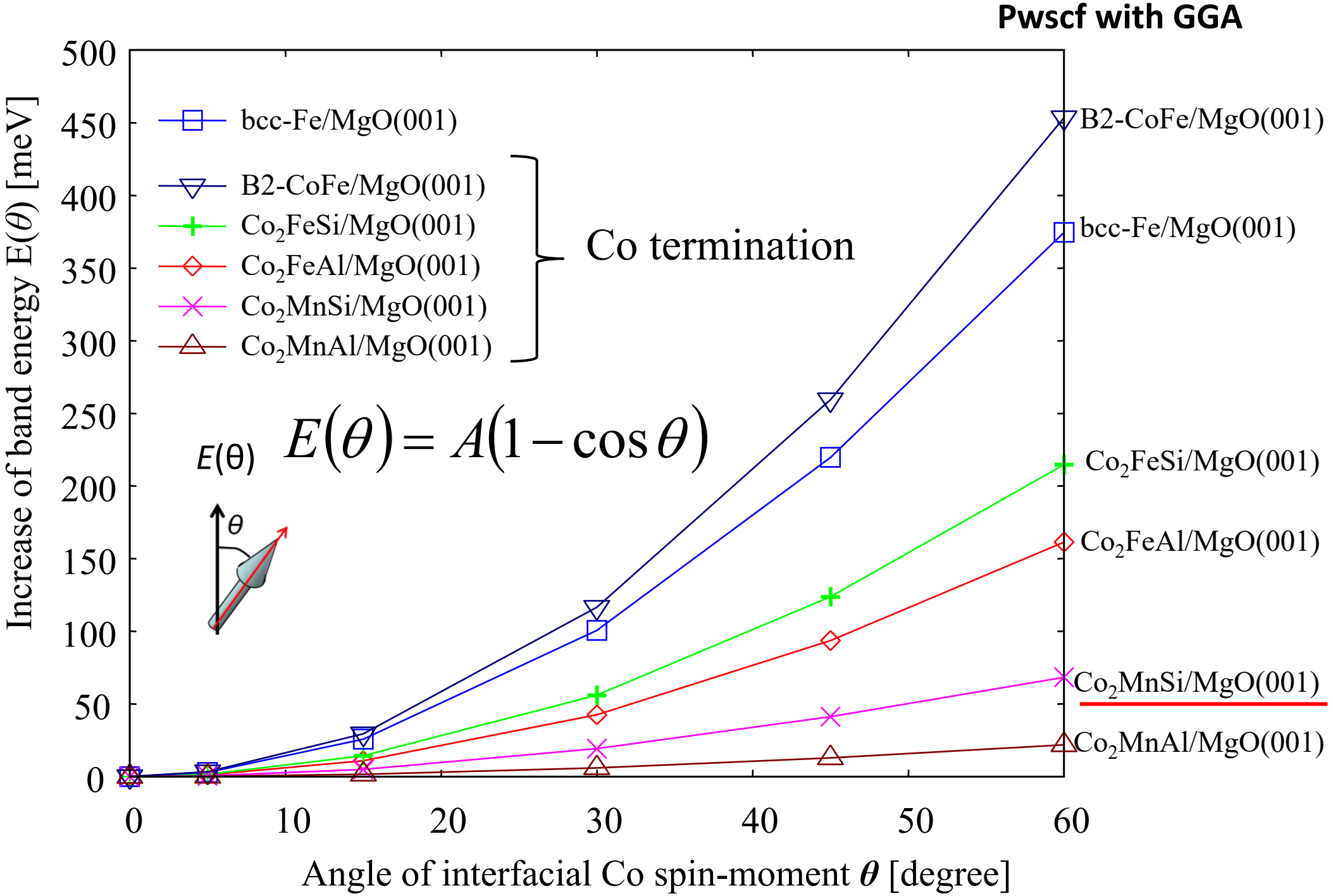




S. Tsunegi, *et al.*, APL 93 (2008) 112506.

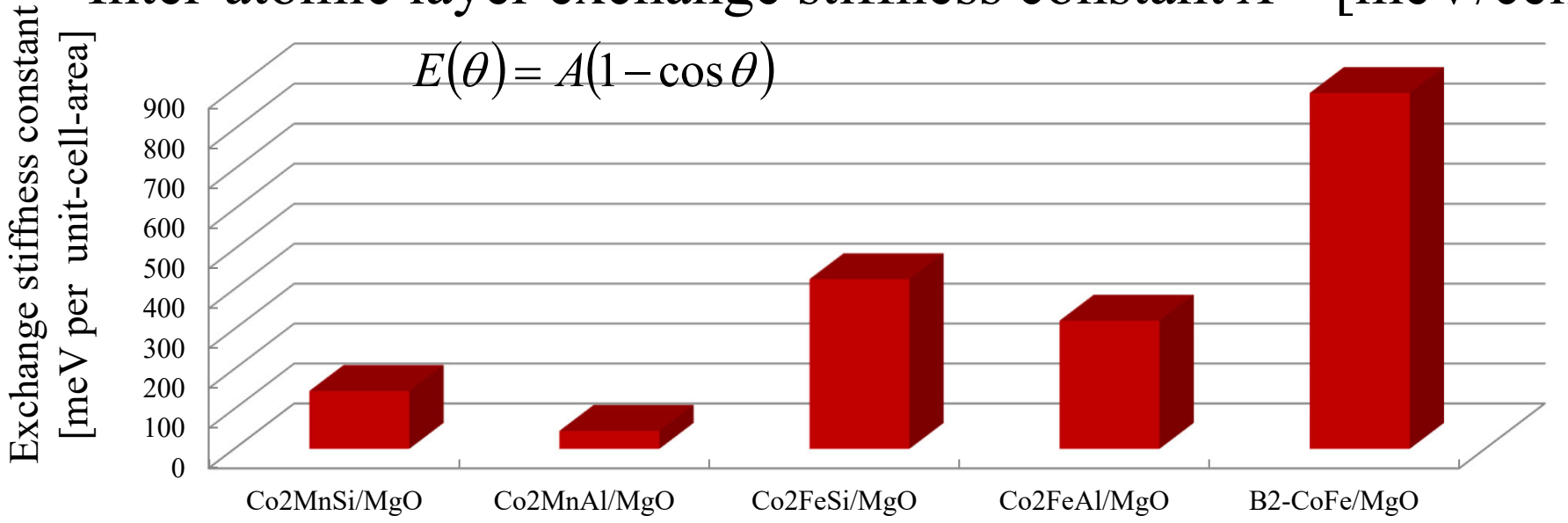
Reduction TMR ratio at RT in CMS/MgO/CMS MTJ can be attributed to a spin-flip scattering at interfacial region caused by thermal fluctuation.

Exchange coupling for other Heusler alloys

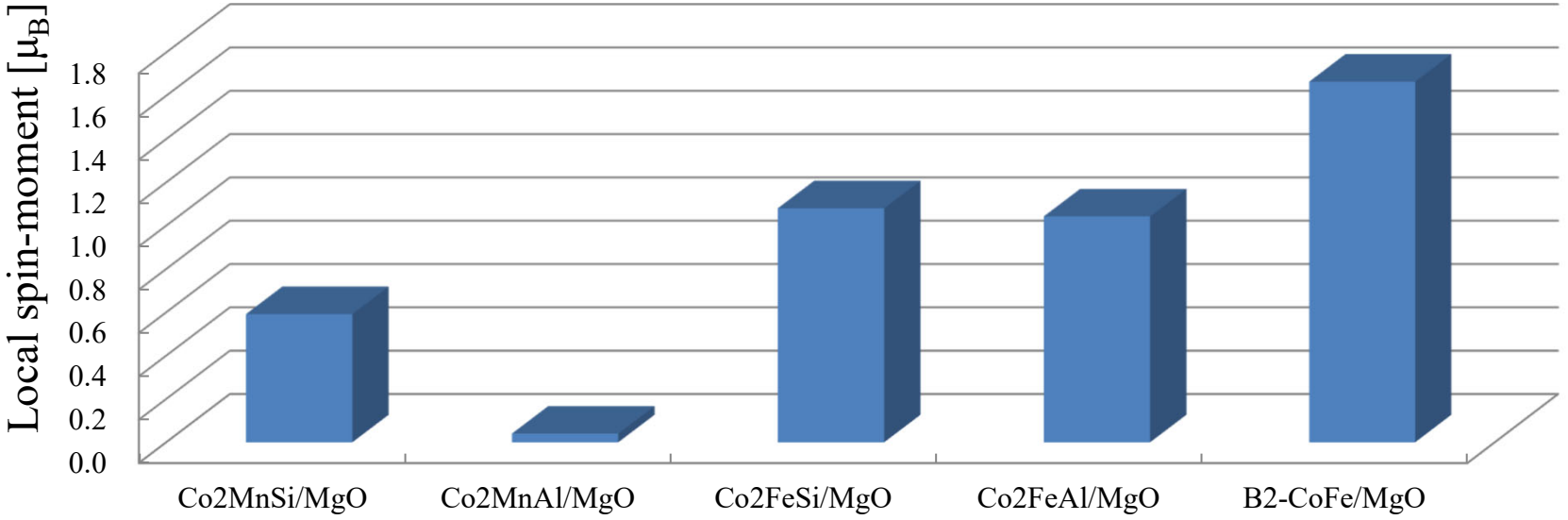


Exchange stiffness constant at Co termination

Inter-atomic layer exchange stiffness constant A [meV/cell area]



Interfacial Co spin-moment at Co termination [μ_B] $A \propto JM^2$



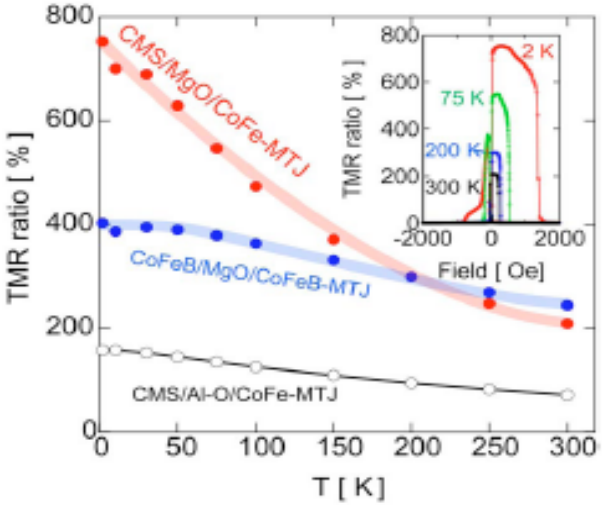
Enhancement of interfacial Co spin-moment is effective to obtain large exchange coupling.

Comparison with Experimental results on TMR at LT and RT

$Co_2MnSi/MgO(001)$

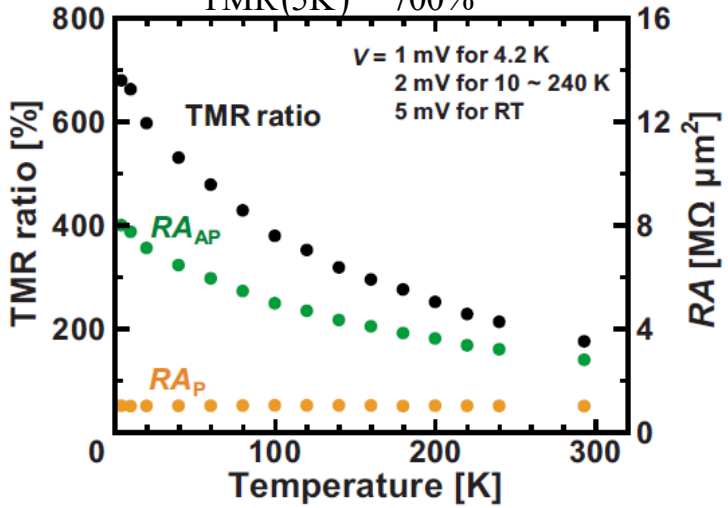
S. Tsunegi, *et al*., APL 93 (2008) 112506.

$$\frac{\mathrm{TMR(RT)}}{\mathrm{TMR(2K)}} = \frac{217\%}{753\%} = 0.29$$



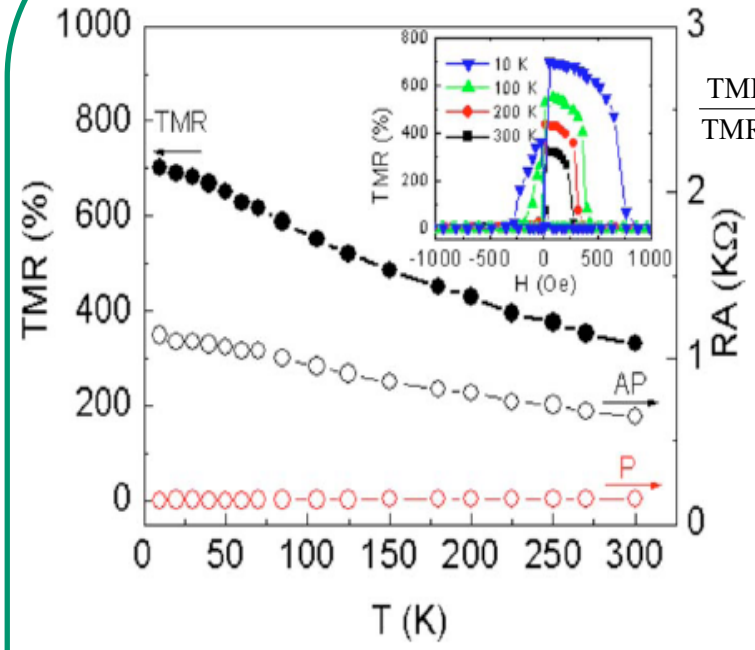
T. Ishikawa, *et al*., APL 94 (2009) 092503.

$$\frac{\mathrm{TMR(RT)}}{\mathrm{TMR(5K)}} = \frac{180\%}{700\%} = 0.26$$



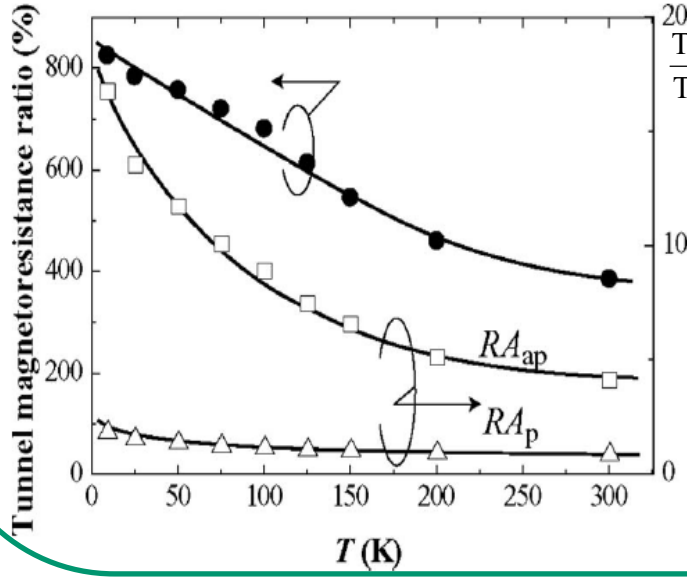
$Co_2Fe(Al,Si)/MgO(001)$

W. Wang, *et al*., APL 95 (2009) 182502.



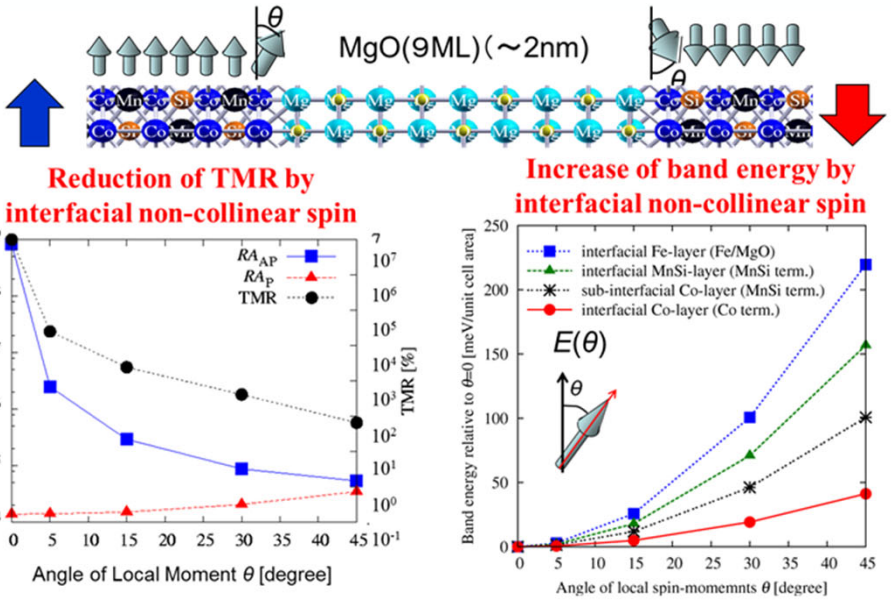
$$\frac{\mathrm{TMR\,(RT\,)}}{\mathrm{TMR\,(10K\,)}} = \frac{330\%}{700\%} = 0.47$$

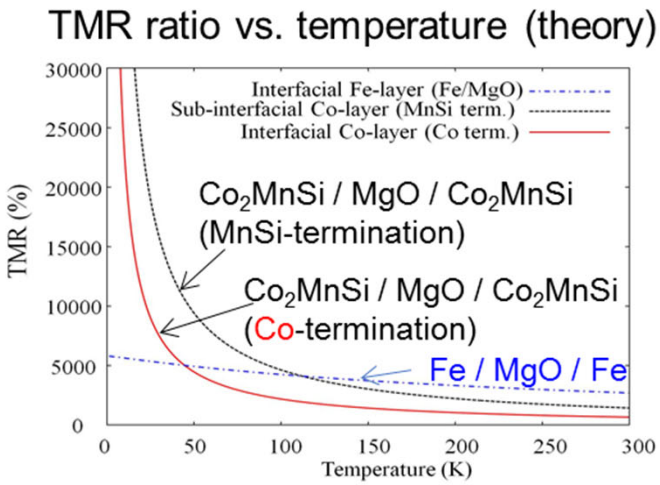
N. Tezuka, *et al*., APL 94 (2009) 162504.



$$\frac{\mathrm{TMR(RT)}}{\mathrm{TMR(9K)}} = \frac{386\%}{832\%} = 0.46$$

Summary of the first topic





◇ Spin-flip scattering at 1ML of interfacial non-collinear magnetic structures strongly affect the spin-dependent conductance and TMR ratio.

◇ Interfacial Co-layer is easy to fluctuate at RT due to the small exchange stiffness at CMS/MgO(001) junctions.

◇ The reduction of the TMR ratio at RT can be attributed to spin-flip scattering at interfacial region caused by thermal fluctuation of interfacial Co-layers.

To raise the TMR ratio at RT, we have to insert CoFe-layer to enhance the interfacial exchange stiffness of CMS/MgO junction.

Topics

0. Introduction on spintronics

1. Spin-dependent transport in magnetic tunnel junctions with half-metallic Heusler alloys

Y. Miura, *et al*., PRB **83**, 214411 (2011).

2. Magneto-crystalline anisotropy at interfaces of Fe(001) with MgO and $MgAl_2O_4$

K. Masuda and Y. Miura, PRB **98**, 224421 (2018).

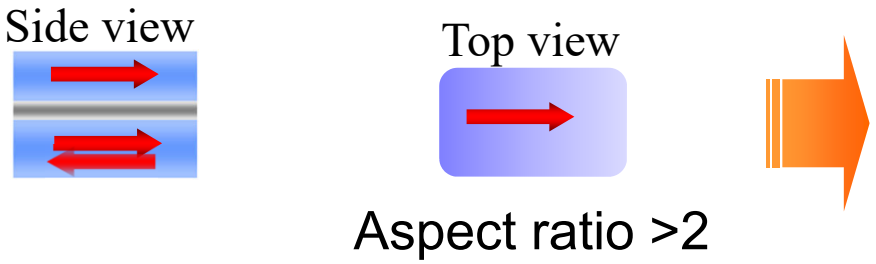
3. First-Principles Study on magnetic damping of Fe/MgO(001)

Y. Miura, in preparation

Thermal stability of magnetization in MTJs

To achieve ultra high density MRAM

In-plane MTJ



Perpendicular MTJ

For 10 year's write endurance

Thermal stability factor $\frac{K_u V}{k_B T} \geq 60$

K_u : uniaxial magnetic anisotropy

Large K_u is required with decreasing volume towards scaling down of device dimensions

Examples of Perpendicular MTJ

Using $L1_0$-type FePt, CoPt, CoFePd alloys and its multilayered structures

[1] M. Yoshikawa, *et al.*, IEEE Trans. Magn. vol.**44** 2573 (2008). (Toshiba)

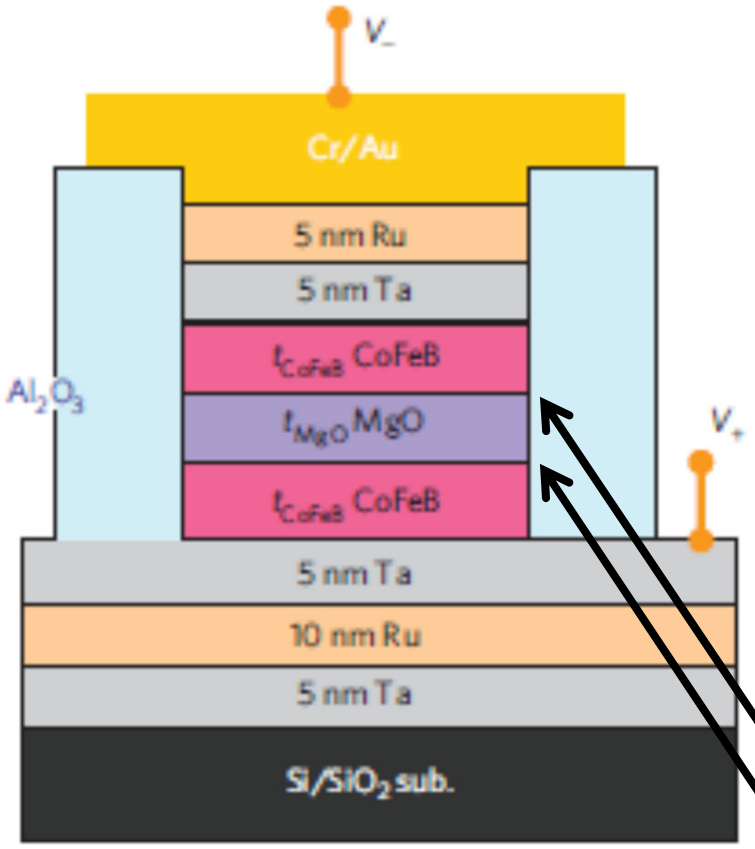
[2] K. Yakushiji, *et al.*, APEX vol. **3** 053003 (2010). (AIST)

[3] K. Mizunuma *et al.*, APEX vol. **4** 023002 (2011). (Tohoku)

Interfacial Perpendicular Magnetic Anisotropy (PMA) for MgO

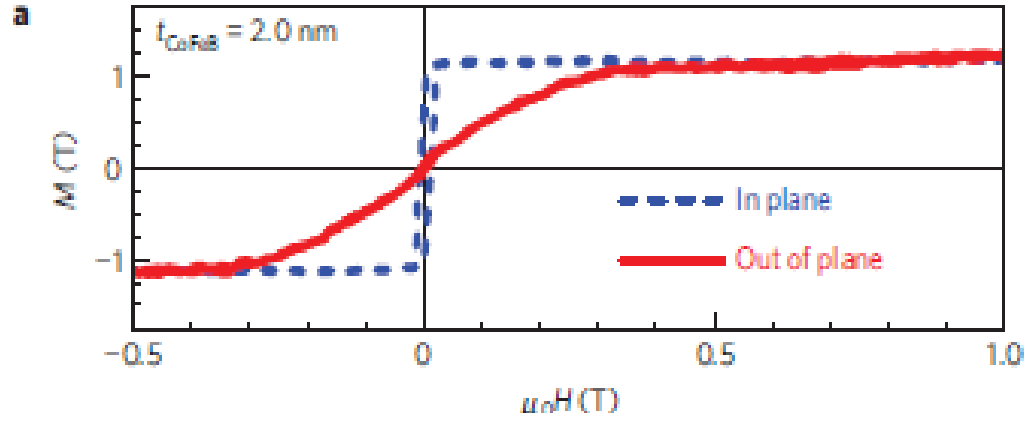
S. Ikeda, *et al*., Nature Materials **9**, 721 (2010).

- CoFeB/MgO/CoFeB(001)

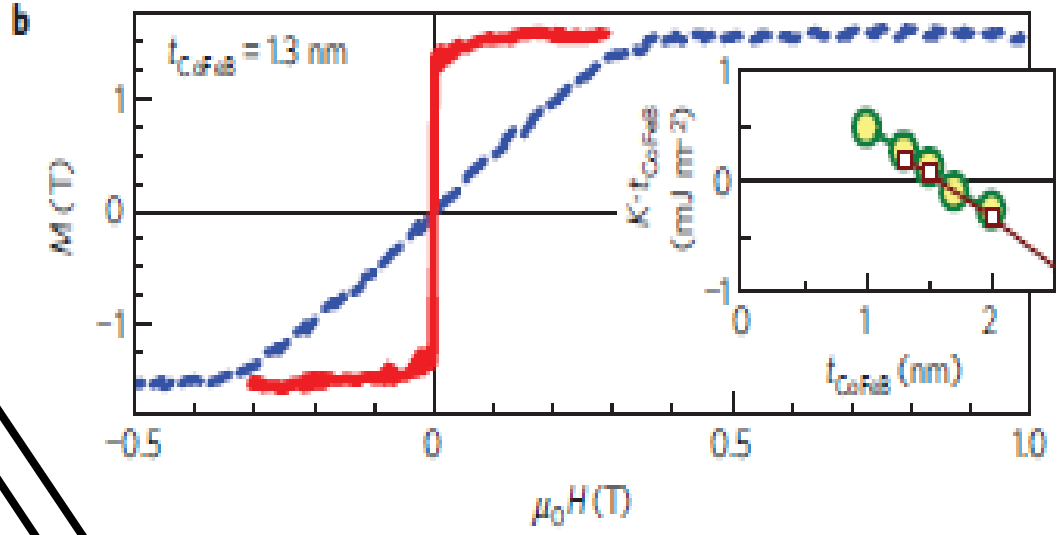


TMR ratio of 120% at 300K

In-plane magnetization (t_{CoFeB}=2.0nm)



Perpendicular magnetization (t_{CoFeB}<1.3nm)

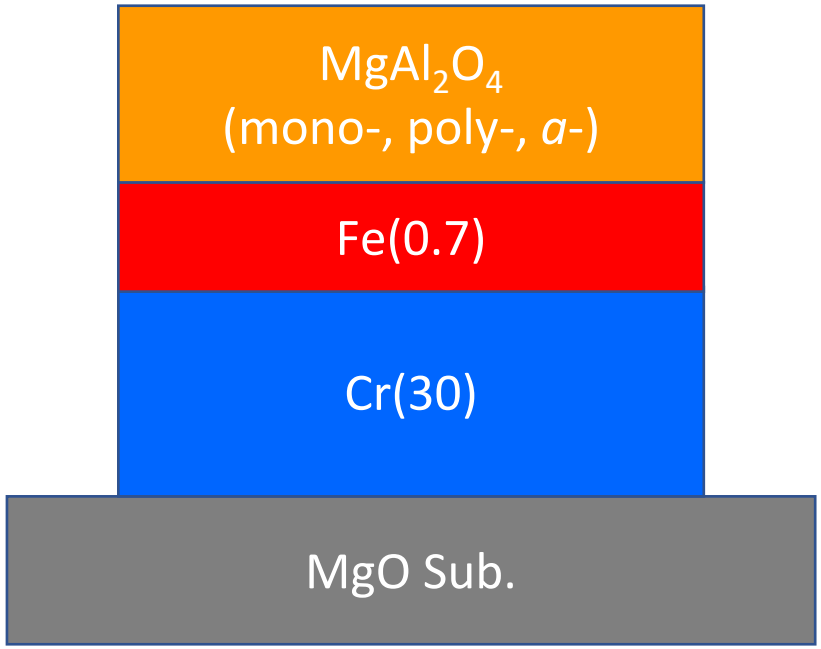


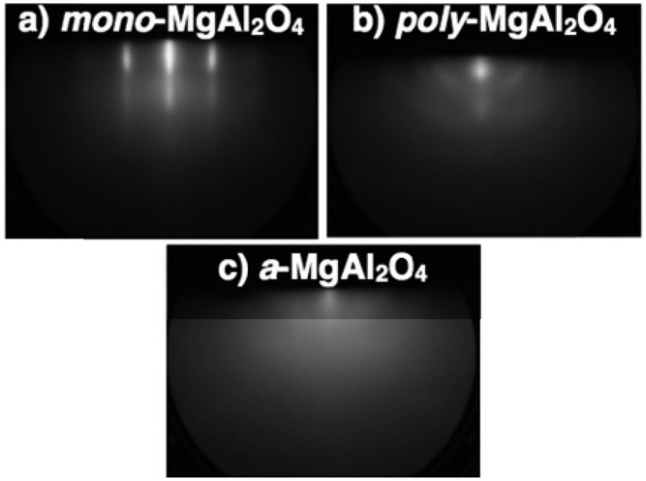
Interfacial perpendicular MCA of Fe/MgO(001), which is K_i=1.30 mJ/m^2

Interfacial Perpendicular Magnetic Anisotropy(PMA) for $MgAl_2O_4$(MAO)

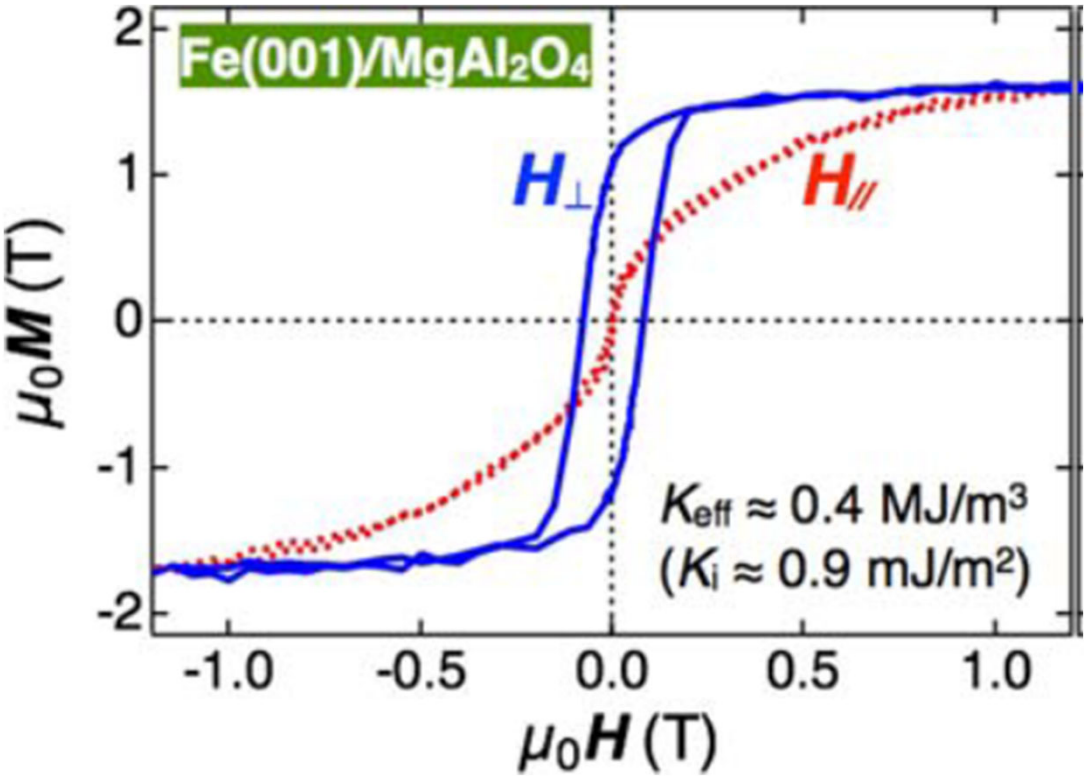
Multilayer structure

Annealed @350-450℃





Lattice mismatch between
bcc-Fe and $MgAl_2O_4$ is 0.2%.



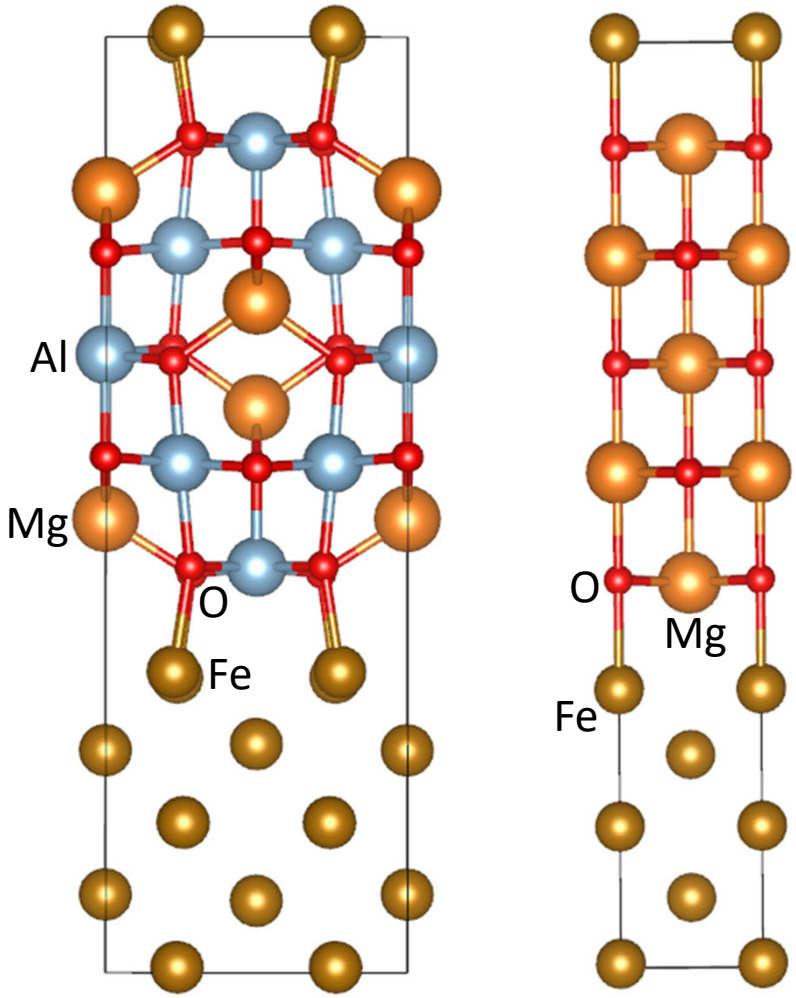
J. Koo, *et.al.*, Phys. status solidi RRL **8**, 841 (2014).

Ki of Fe/MgO(001) is 1.4mJ/m2,
J. W. Koo, *et al.*, Appl. Phys. Lett. 103, 192401 (2013).

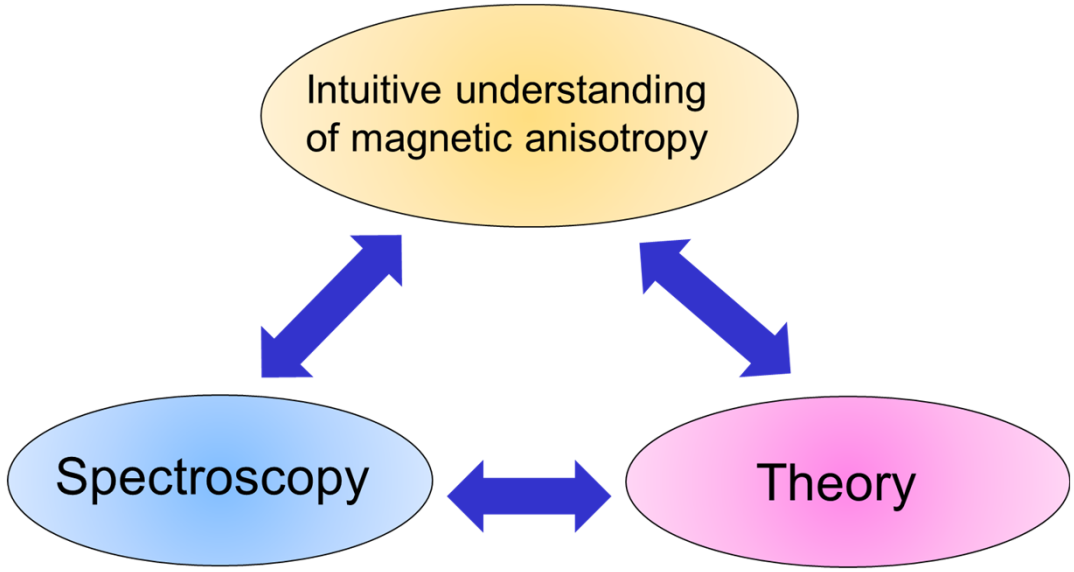
Purpose of this work

We study interfacial magnetocrystalline anisotropy (MAE) in Fe/MgAl2O4 and Fe/MgO by means of first-principles calculations based on density functional theory.

$Fe/MgAl_2O_4(2a_{Fe})$ $Fe/MgO\ (a_{Fe},a_{MgO})$



・origin of interfacial perpendicular magnetocrystalline anisotropy (PMA)



・XMCD Measurement (orbital and spin moment , quadrupole moment)

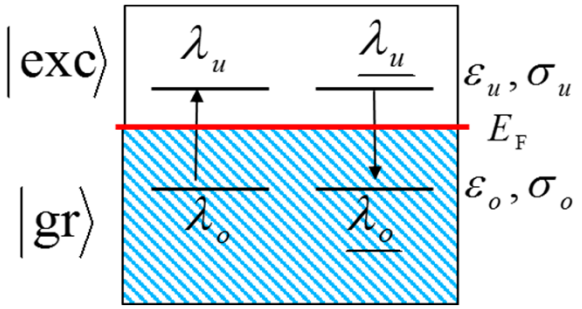
・First-principles calculations
・2nd order perturbation of SOI

Second order perturbation of spin-orbit interaction (SOI)

Bruno, PRB **39**, 865 (1989).
Wang, Wu, Freeman, PRB **47**, 14932 (1993).
van der Laan, JPCM 10, 3239 (1998).

$$\delta E = -\sum_{\text{exc}} \frac{\left|\langle \text{exc}|H^{\text{SO}}|\text{gr}\rangle\right|^2}{\varepsilon_{\text{exc}} - \varepsilon_{\text{gr}}} \qquad H^{\text{SO}} = \xi \vec{L} \cdot \vec{S}$$

$$|\text{gr (exc)}\rangle = \sum_{\mu,\sigma} c_{i,\mu,\sigma}\, |i,\mu\rangle$$



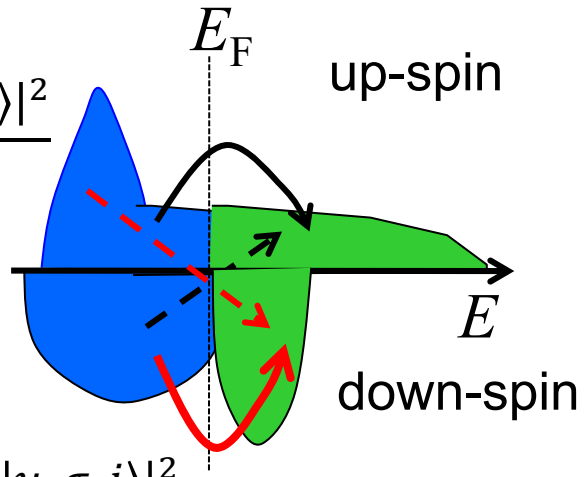
μ : local atomic orbital index
i,j : index of atomic position

Magneto-crystalline anisotropy (MCA) energy

$$\Delta E^{\text{MCA}} = \delta E[\text{in-plane}] - \delta E[\text{perpendicuar}]$$

$$\Delta E^{\text{MCA}}(i) = \sum_{\sigma,\sigma'} (-1)^{\delta_{\sigma'\sigma}} \xi_i^2 \sum_{o,\,u} \frac{|\langle o,\sigma'|L_z|u,\sigma,i\rangle|^2 - |\langle o,\sigma'|L_x|u,\sigma,i\rangle|^2}{\varepsilon_{u,\sigma'} - \varepsilon_{o,\sigma}}$$

$$= \Delta E^{\text{MCA}}_{\uparrow\Rightarrow\uparrow}(i) + \Delta E^{\text{MCA}}_{\downarrow\Rightarrow\downarrow}(i) + \Delta E^{\text{MCA}}_{\uparrow\Rightarrow\downarrow}(i) + \Delta E^{\text{MCA}}_{\downarrow\Rightarrow\uparrow}(i)$$

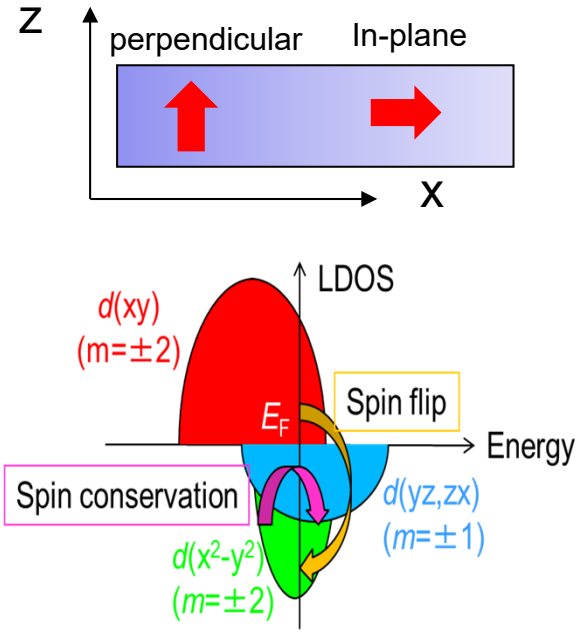


Orbital moment $\quad \langle L^z \rangle = 4\xi_i \sum_{o,\,u} \frac{|\langle o,\uparrow|L_z|u,\uparrow,i\rangle|^2 - |\langle o,\downarrow|L_z|u,\sigma,i\rangle|^2}{\varepsilon_{u,\sigma'} - \varepsilon_{o,\sigma}}$

Spin conserving term and spin flip term in magnetic anisotropy

Spin conserving term

$$\Delta E^{\mathrm{MCA}}_{\downarrow\Rightarrow\downarrow}(i) = +\xi_i^2 \sum_{o,\,u} \frac{|\langle u,\downarrow|L_z|o,\downarrow,i\rangle|^2}{\varepsilon_{u,\downarrow}-\varepsilon_{o,\downarrow}} - \xi_i^2 \sum_{o,\,u} \frac{|\langle u,\downarrow|L_x|o,\downarrow,i\rangle|^2}{\varepsilon_{u,\downarrow}-\varepsilon_{o,\downarrow}}$$



$L_z Y_l^m = m Y_l^m$

Contributed to PMA energy, if there are *d* orbitals with the same magnetic quantum number *m* exist around E_F.

$L_x Y_l^m \propto Y_l^{m\pm1}$

Contributed to PMA energy, if there are *d* orbitals with *m* and m±1 exist around E_F.

$\langle zx,\downarrow|L_z|yz,\downarrow\rangle = 1$

$\langle x^2-y^2,\downarrow|L_z|xy,\downarrow\rangle = 2$

$\langle xy,\downarrow|L_x|zx,\downarrow\rangle = 1$

$\langle x^2-y^2,\downarrow|L_x|zx,\downarrow\rangle = 1$

$\langle 3z^2-r^2,\downarrow|L_x|yz,\downarrow\rangle = \sqrt{3}$

Spin flip term

$$\Delta E^{\mathrm{MCA}}_{\downarrow\Rightarrow\uparrow}(i) = -\xi_i^2 \sum_{o,\,u} \frac{|\langle u,\uparrow|L_z|o,\downarrow,i\rangle|^2}{\varepsilon_{u,\uparrow}-\varepsilon_{o,\downarrow}} + \xi_i^2 \sum_{o,\,u} \frac{|\langle u,\uparrow|L_x|o,\downarrow,i\rangle|^2}{\varepsilon_{u,\uparrow}-\varepsilon_{o,\downarrow}}$$

2nd order perturbation energy

$$\Delta E^{\mathrm{MCA}} \approx \frac{\xi}{4\mu_{\mathrm{B}}}\left(\Delta m^{\mathrm{orb}}\right) + \frac{21}{2\mu_{\mathrm{B}}}\frac{\xi^2}{\Delta E_{\mathrm{ex}}}\left(m^T\right)$$

Orbital moment anisotropy term
⇒Spin-conserving term

Magnetic dipole (Quadupole moment) term
⇒Spin-flip term

Bruno, PRB **39**, 865 (1989).
Wang, Wu, Freeman, PRB **47**, 14932 (1993).
van der Laan, JPCM 10, 3239 (1998).

Intuitive understanding of magneto-crystalline anisotropy (MCA)

P. Bruno, PRB **39**, 865 (1989).
G. Laan, JPCM **10**, 3239 (1998).

$$\Delta E^{\mathrm{MCA}} \approx \frac{\xi}{4\mu_{\mathrm{B}}}\left(\Delta m^{\mathrm{orb}}\right) + \frac{21}{2\mu_{\mathrm{B}}}\frac{\xi^2}{\Delta E_{\mathrm{ex}}}\left(m^T\right)$$

Orbital moment term

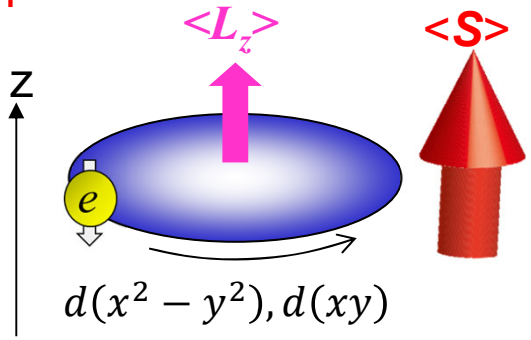
Magnetic dipole term

$$\Delta m^{\mathrm{orb}} = \langle L^z \rangle - \langle L^x \rangle$$

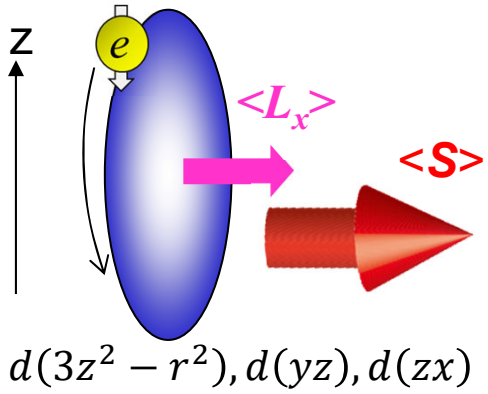
$$m^T = \langle T^z \rangle = -\langle \mathrm{Q}^z \mathrm{S} \rangle$$

Orbital moment term

$$H^{\mathrm{SO}} = -\xi \vec{L} \cdot \vec{S}$$



Perpendicular magnetic anisotropy



In-plane magnetic anisotropy

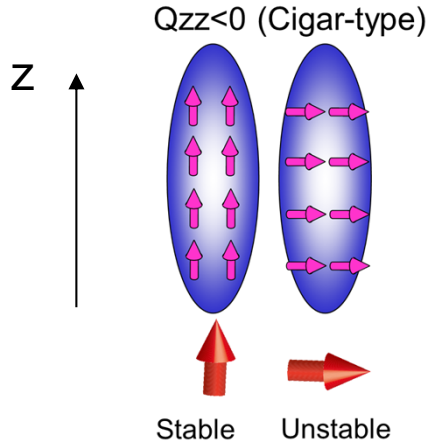
Magnetic dipole term *T* ⇒Quadrupole moment of spin density

$$\vec{T} \approx -\frac{2}{7}\boldsymbol{Q}\hat{S} \quad \Rightarrow \quad T^z \approx -\frac{2}{7}\sum_{i=1}^{5} Q_i^z S^i$$

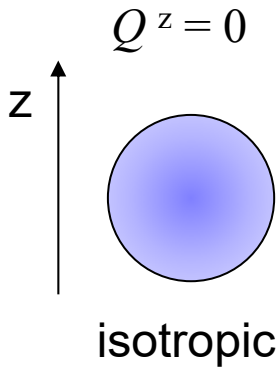
Q: Quadrupole moment of spin density

$Q^z < 0$ ($T^z > 0$)⇒ Prolate distribution

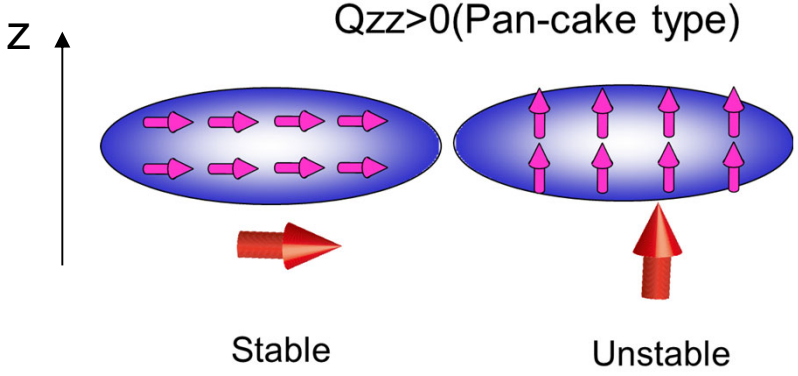
$Q^z > 0$ ($T^z < 0$) ⇒ Oblate distribution



Perpendicular magnetic anisotropy



isotropic

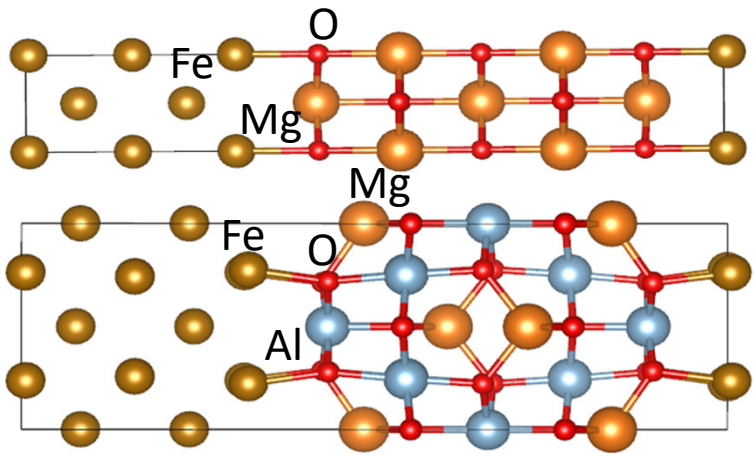


In-plane magnetic anisotropy

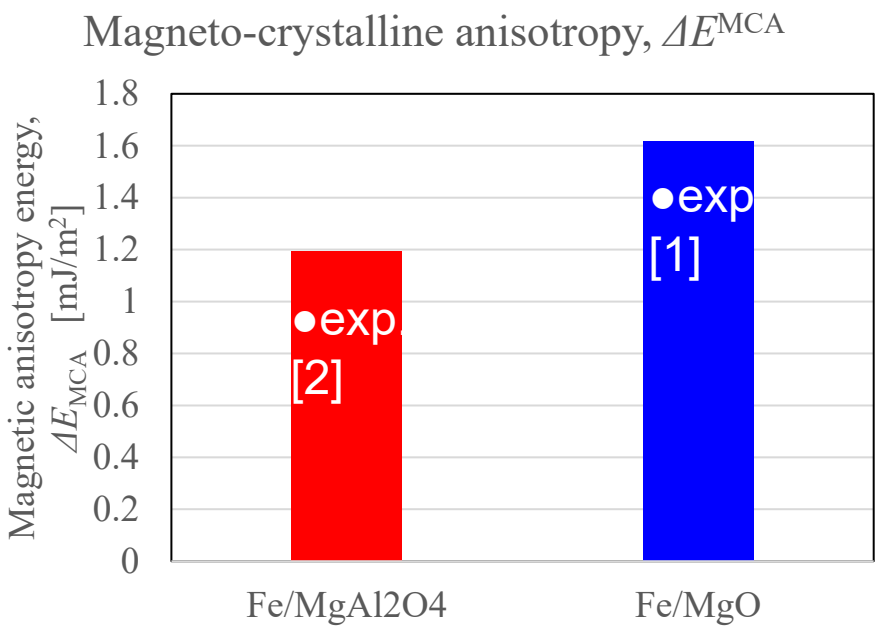
MCA energy for $Fe/MgAl_2O_4$(MAO) and Fe/MgO

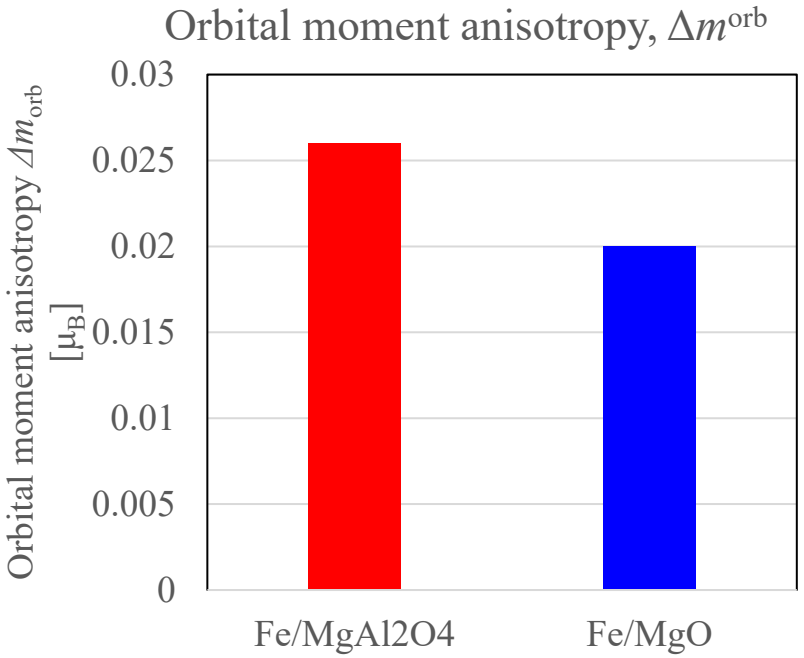
Fe/MgO(001)
($a_{||}=a_{Fe}$)

$Fe/MgAl_2O_4$(MAO)(001)
($a_{||}=2a_{Fe}$)



K. Masuda and Y. Miura, PRB **98**, 224421 (2018).





[1] J. W. Koo, *et al.*, Appl. Phys. Lett. 103, 192401 (2013).

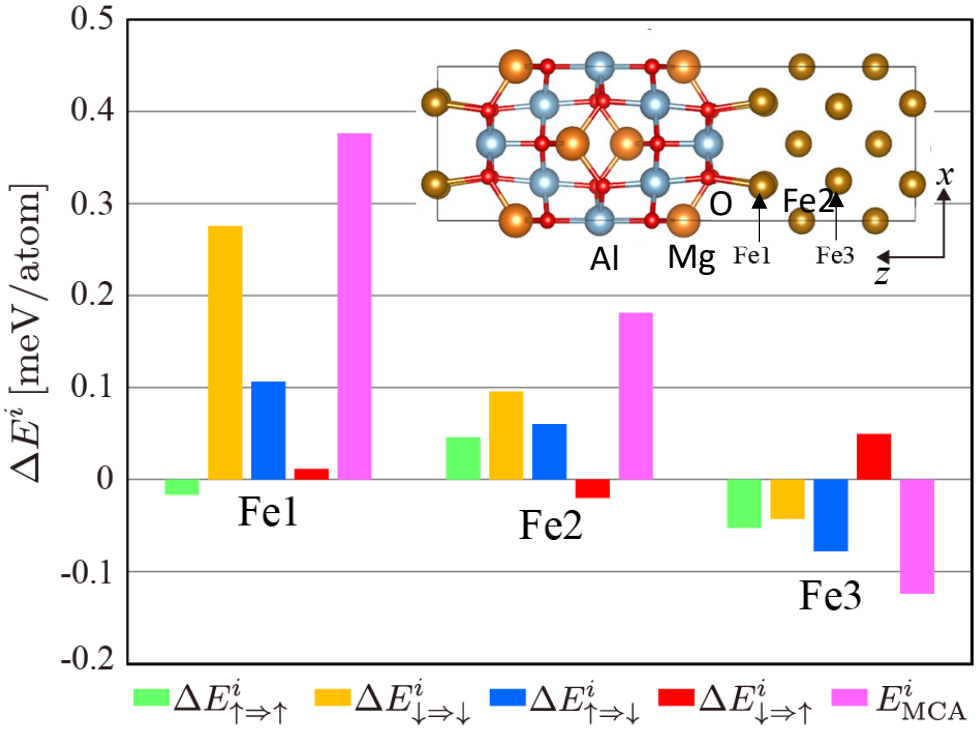
[2] J. W. Koo, *et.al.*, Phys. status solidi RRL **8**, 841 (2014).

$$\Delta E^{\mathrm{MCA}} \approx \frac{\xi}{4\mu_{\mathrm{B}}}\left(\Delta m^{\mathrm{orb}}\right) + \frac{21}{2\mu_{\mathrm{B}}}\frac{\xi^2}{\Delta E_{\mathrm{ex}}}\left(m^T\right)$$

Spin-decomposed PMA energy of Fe/$MgAl_2O_4$(MAO) and Fe/MgO

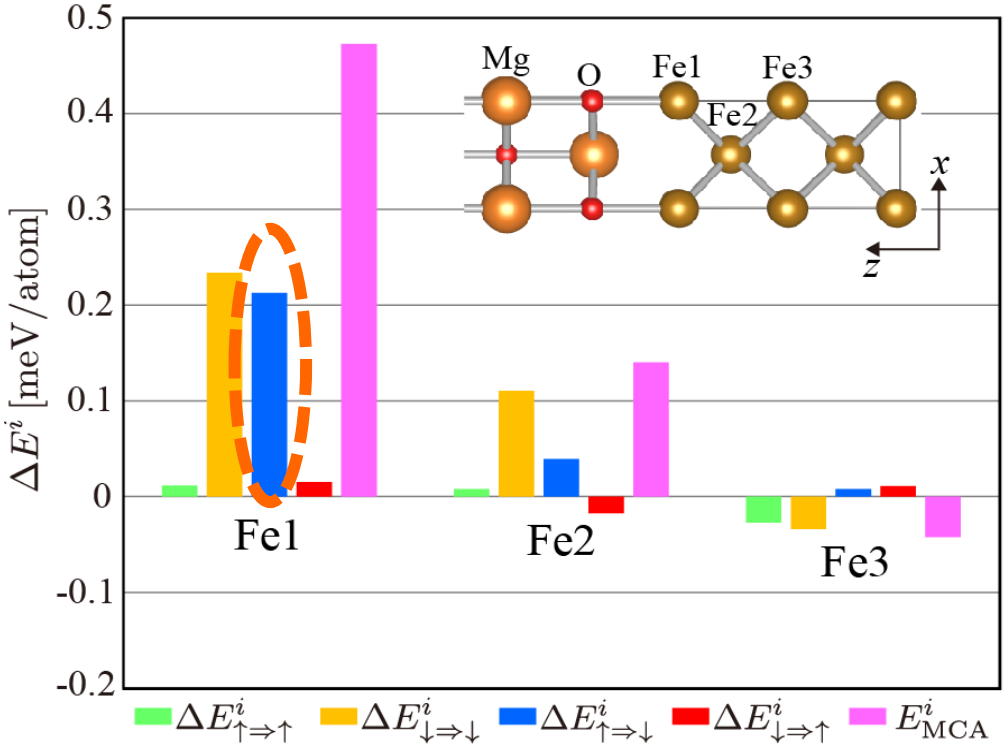
Fe/$MgAl_2O_4$(MAO) $a=a_{Fe}$

$\Delta E^{MCA}=1.2[mJ/m^2]$



Fe/MgO $a=a_{Fe}$

$\Delta E^{MCA}=1.6[mJ/m^2]$



- Interfacial Fe mainly contributes to Perpendicular (Positive) MCA
- Spin conservation term $\Delta E^{MCA}_{\downarrow\Rightarrow\downarrow}(i)$ mainly contributes to Perpendicular MCA.
- For Fe/MgO, the spin flip term $\Delta E^{McA}_{\uparrow\Rightarrow\downarrow}(i)$ also contributes to Perpendicular MCA.

Magnetic dipole term of $Fe/MgAl_2O_4$ and Fe/MgO

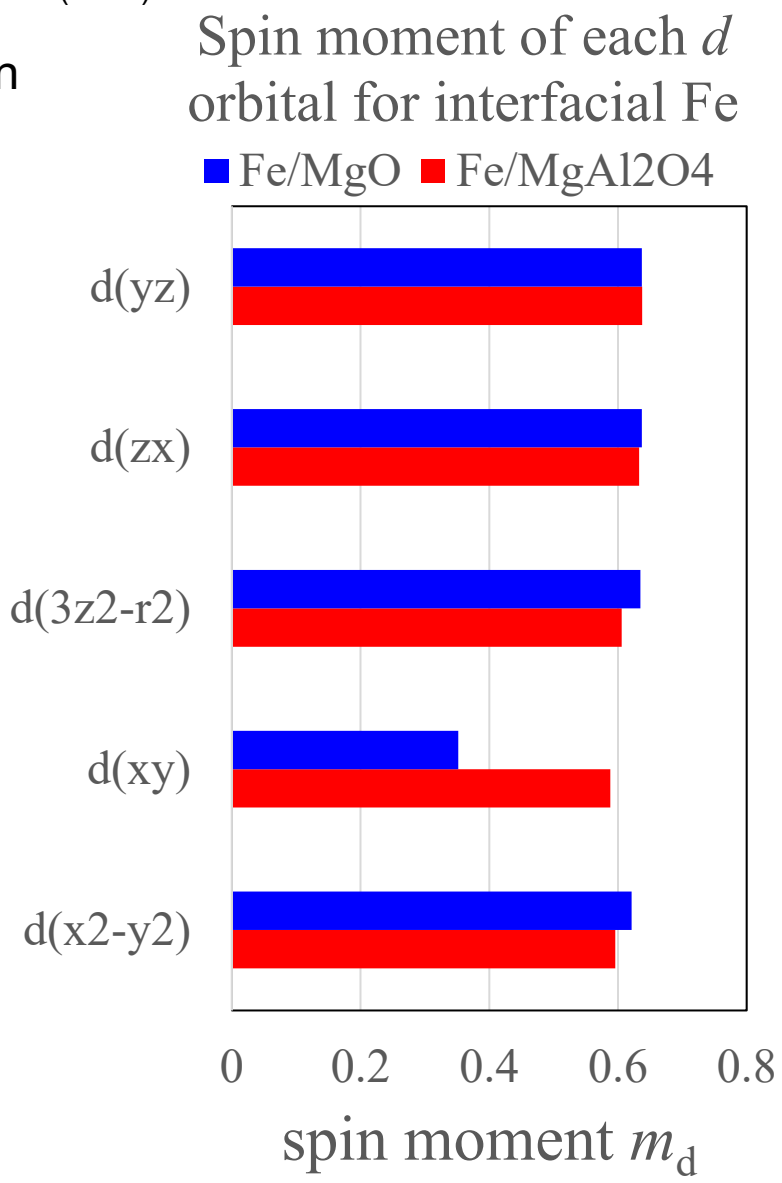
$$m^T = T^z \approx -\frac{2}{7}\left(-16m^{3z^2-r^2} - 8m^{zx} - 8m^{yz} + 16m^{xy} + 16m^{x^2-y^2}\right)$$

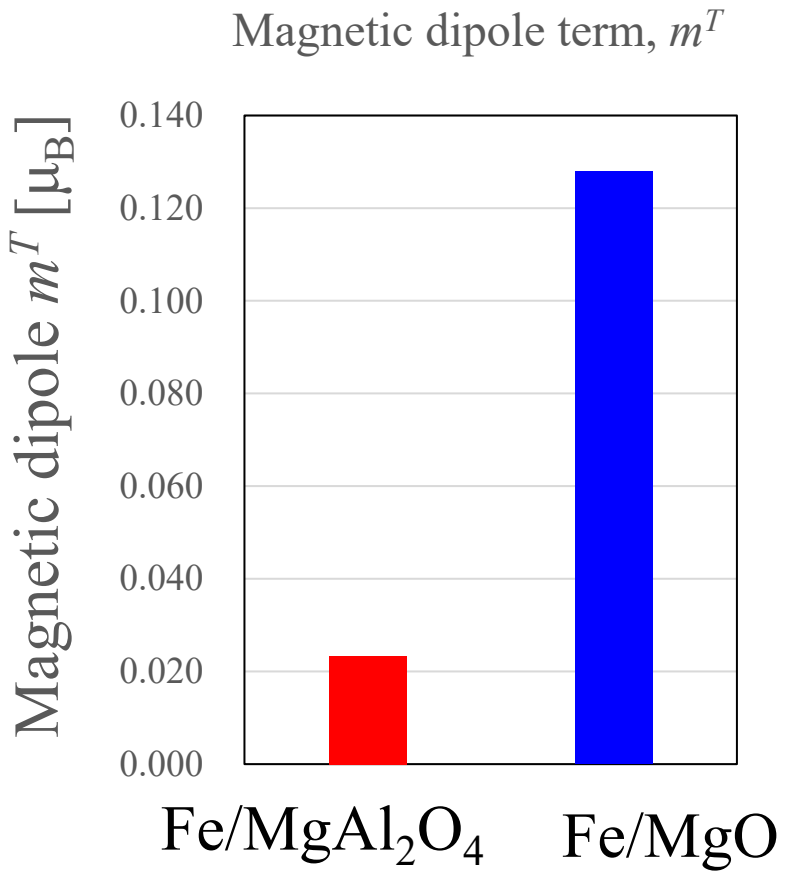
J. Stöhr and H. König, PRL **75**, 3748 (1995).

$$m^T = \langle T^z \rangle = -\langle Q^z S \rangle$$

Quadrupole distribution of *d* orbitals

Orbital i	$\alpha = x, y$ or z $4\left(7\,Q_\alpha^i\right)$
d_{yz}	−8, −8, 16
d_{xz}	−8, 16, −8
$d_{3z^2-r^2}$	−16, 8, 8
d_{xy}	16, −8, −8
$d_{x^2-y^2}$	16, −8, −8



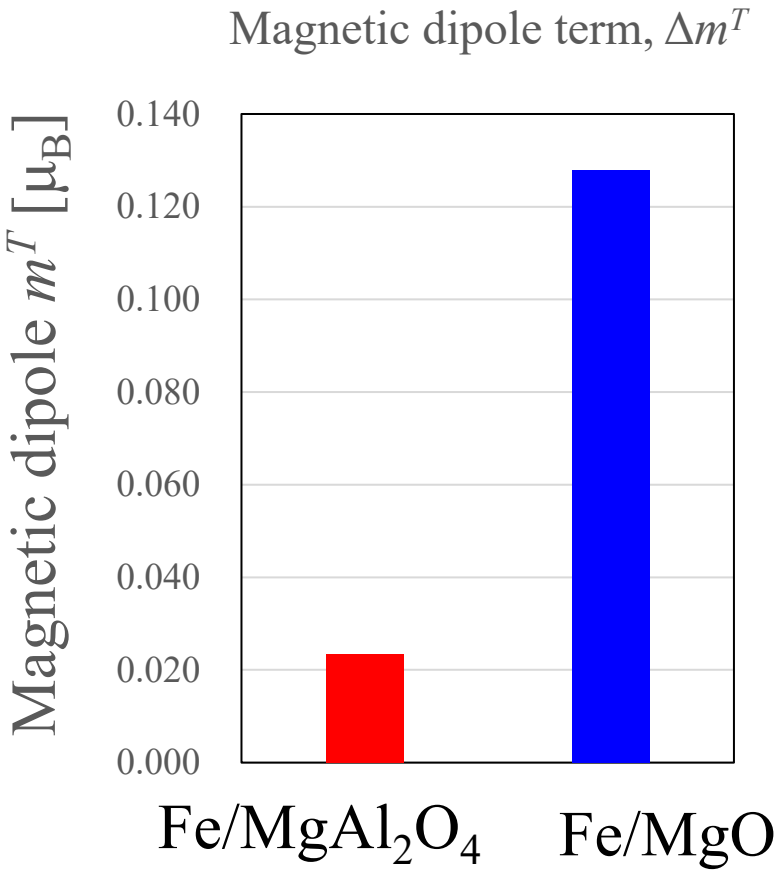


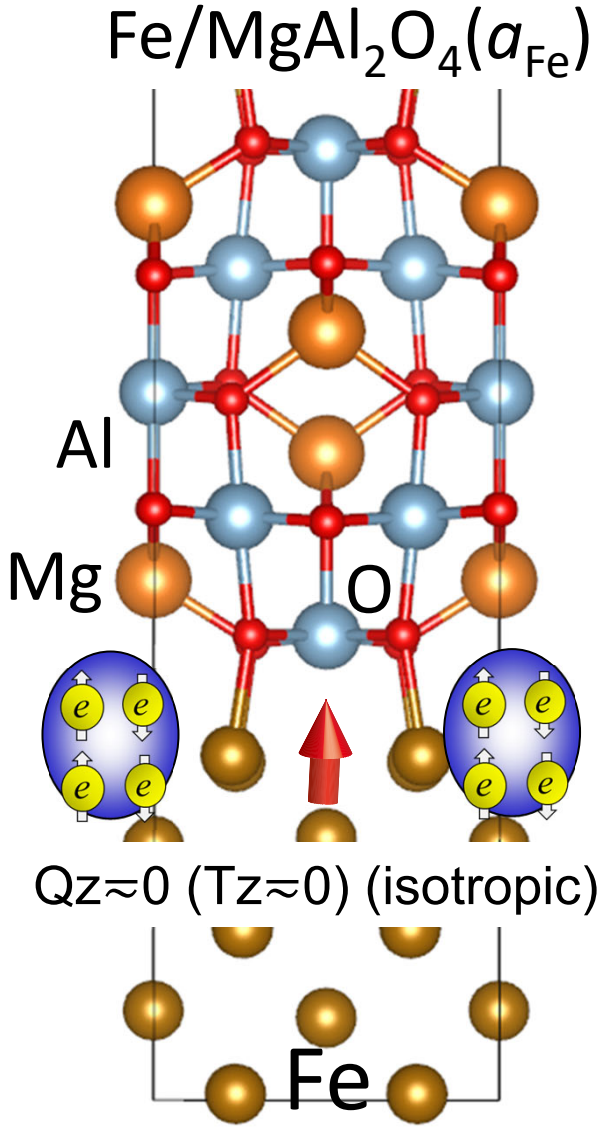
Magnetic dipole term of $Fe/MgAl_2O_4$ and Fe/MgO

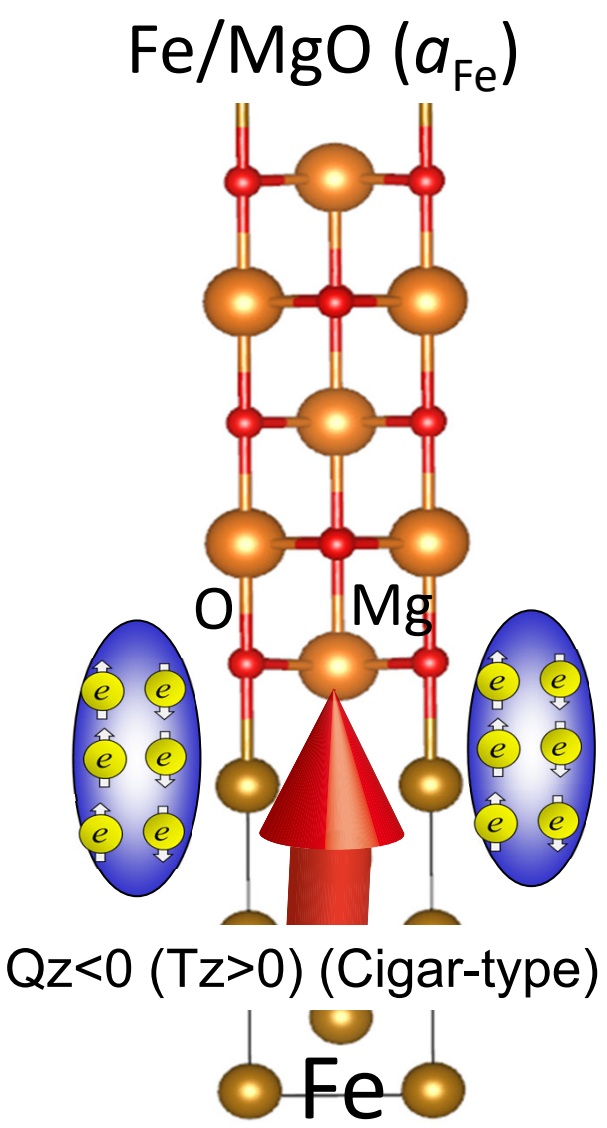
$$\langle T^z \rangle \approx -\frac{2}{7}\sum_{i=1}^{5} Q_i^z S^i = -\frac{2}{7}\left(-16m^{3z^2-r^2} - 8m^{zx} - 8m^{yz} + 16m^{xy} + 16m^{x^2-y^2}\right)/16$$

J. Stöhr and H. König, PRL **75**, 3748 (1995).

$$m^T = \langle T^z \rangle = -\langle Q^z S \rangle$$







Summary of the second topic

- $Fe/MgAl_2O_4(001)$ show Perpendicular MCA, which is slightly smaller than that of Fe/MgO(001).

- For Fe/MgO(001), not only spin conservation term $\Delta E_{\downarrow\Rightarrow\downarrow}$ but also spin-flip term $\Delta E_{\uparrow\Rightarrow\downarrow}$ contributes to Perpendicular MCA, resulting in larger MCA energy than that of $Fe/MgAl_2O_4$.

- Cigar type quadrupole moment additionally increases the Perpendicular MCA of Fe/MgO, but not for $Fe/MgAl_2O_4$(MAO).

The quadrupole moment of spin-density is essential to understand the magneto-crystalline anisotropy (MCA) especially for ferromagnetic interfaces.

Topics

0. Introduction on spintronics

1. Spin-dependent transport in magnetic tunnel junctions with half-metallic Heusler alloys

Y. Miura, *et al*., PRB **83,** 214411 (2011).

2. Magneto-crystalline anisotropy at interfaces of Fe(001) with MgO and $MgAl_2O_4$

K. Masuda and Y. Miura, PRB **98**, 224421 (2018).

3. First-Principles Study on magnetic damping of Fe/MgO(001)

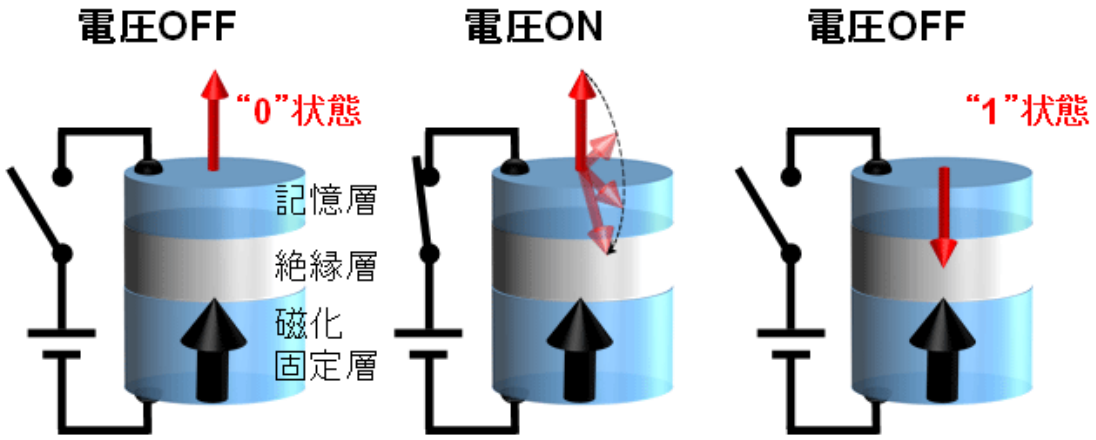
Y. Miura, in preparation

Voltage-driven dynamic switching in MTJ

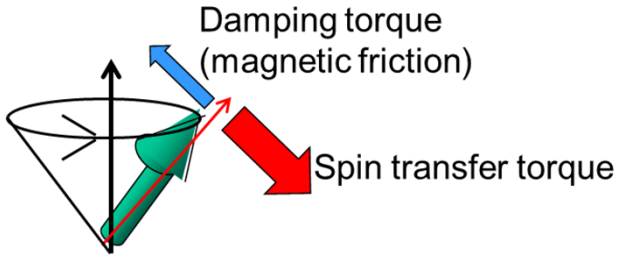
Applied Physics Express **9**, 013001 (2016)
http://doi.org/**10.7567/APEX.9.013001**

Evaluation of write error rate for voltage-driven dynamic magnetization switching in magnetic tunnel junctions with perpendicular magnetization

Yoichi Shiota*, Takayuki Nozaki, Shingo Tamaru, Kay Yakushiji, Hitoshi Kubota, Akio Fukushima, Shinji Yuasa, and Yoshishige Suzuki



From website of Sahashi's ImPACT project in JST



Write Error Rate (WER)

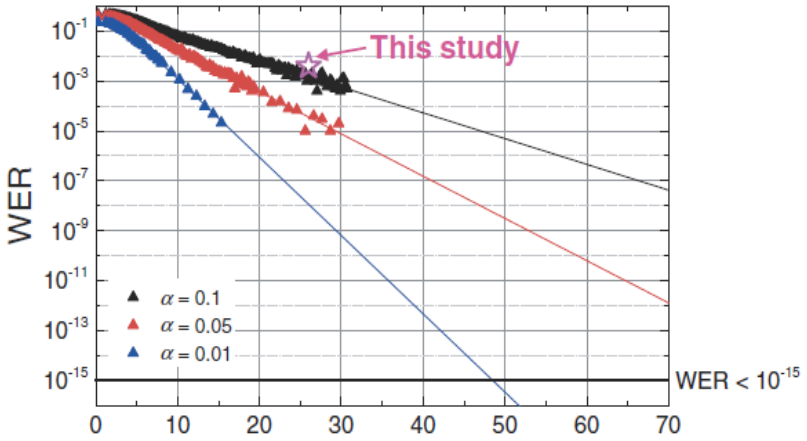


Fig. 4. Calculated WER as a function of Δ for fixed tilted magnetization angle and half precession period τ_{pulse} for various damping constants.

Pulsed bias voltage changes PMA of interface of FM layer and promote the precession motion of the magnetization.

➡ By removing the voltage with a proper pulse duration, such as a half precession period, magnetization switching can be achieved.

➡ Basically, no current flow

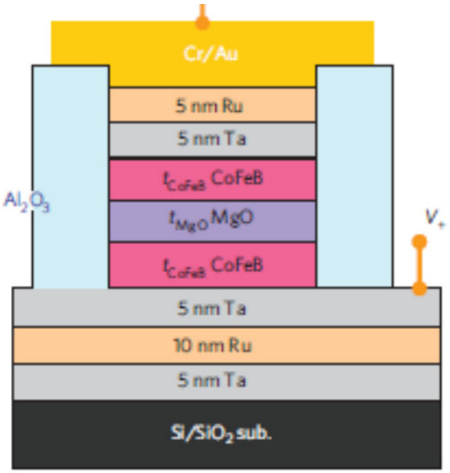
Large Ku and Small damping α can reduce the WER

Experiments electric field effects of PMA and magnetic damping

APPLIED PHYSICS LETTERS **105**, 052415 (2014)

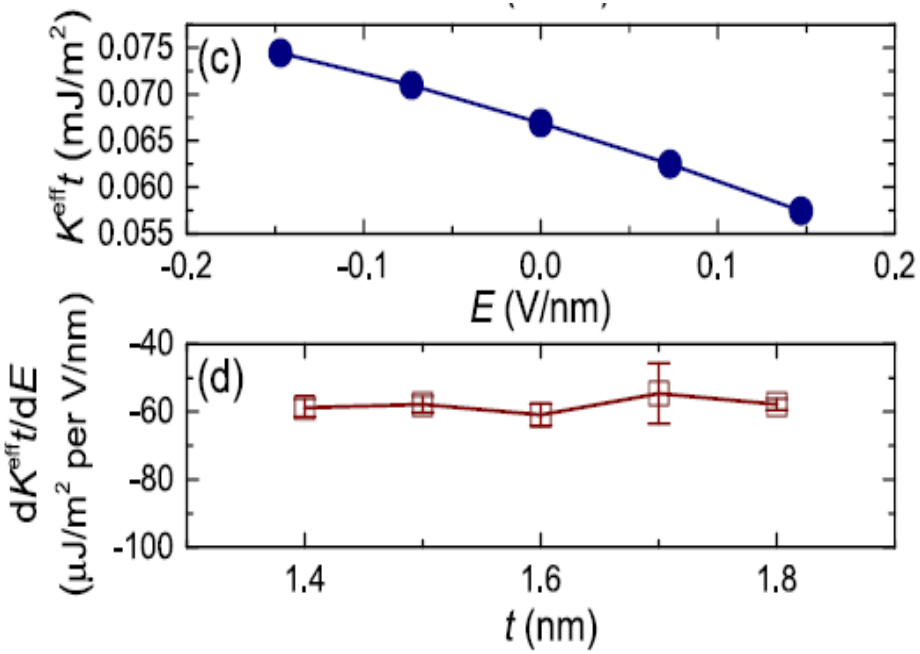
Electric-field effects on magnetic anisotropy and damping constant in Ta/CoFeB/MgO investigated by ferromagnetic resonance

A. Okada,[1] S. Kanai,[1] M. Yamanouchi,[1,2] S. Ikeda,[1,2] F. Matsukura,[3,2,a)] and H. Ohno[1,2,3]
[1]*Laboratory for Nanoelectronics and Spintronics, Research Institute of Electrical Communication, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan*
[2]*Center for Spintronics Integrated Systems, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan*
[3]*WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan*



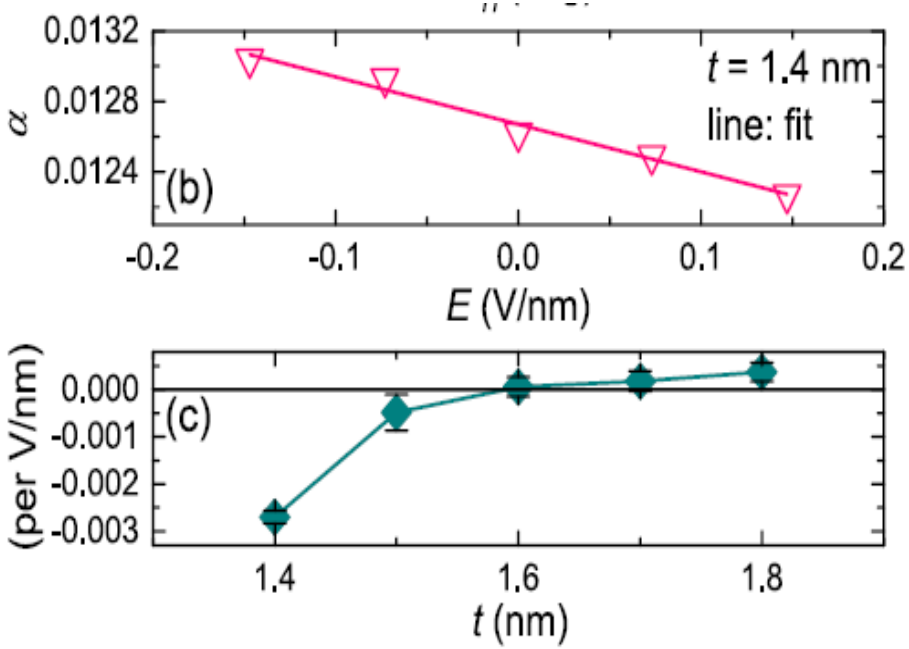
-21% of magnetic damping α is changed by 1V/nm EF for t=1.4nm

Magnetic anisotropy change by EF



EF dependence is insensitive to thickness of FM layer

Magnetic damping change by EF

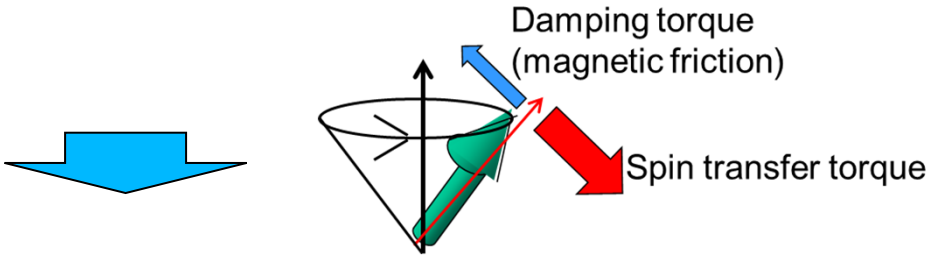


Large thickness dependence of FM layer

Purpose of this work

If PMA and magnetic damping can be simultaneously reduced by applied voltage, we can drastically reduce power consumption and write error rate in magnetization reversal of MRAM.

Voltage dependence of magnetic damping is hardly investigated.



This work investigates the voltage dependence of magnetic damping and magnetic anisotropy of Fe/MgO interface based on the first-principles calculation.

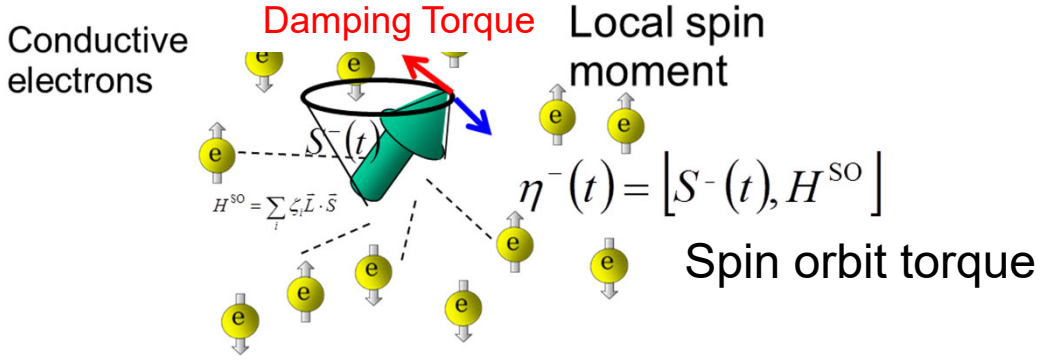
Origin of Magnetic Damping α

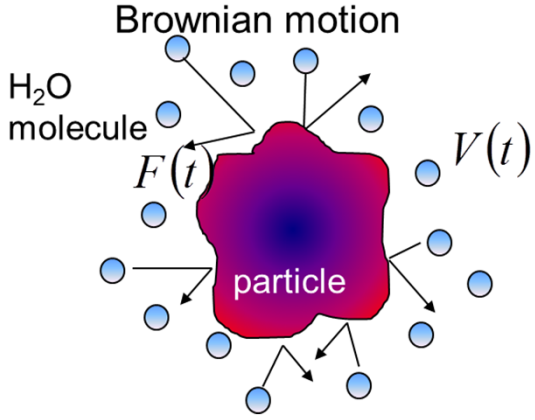
- Electronic system
- Phonon
- Atomic disorder
- Other extrinsic factors

Kambersky's torque correlation model

V. Kambersky, Czechoslovak Journal of Physics B **26**, 1366 (1976).

Precession motion of local spin moment





Generalized Langevin equation for magnetization dynamics

$$\frac{dS^-(t)}{dt}=-i\Omega S^-(t)-i\eta^-(t)-\int_0^t P^{-1}\left\langle\left[\eta^-(t'),\eta^+\right]\right\rangle_0 S^-(t)dt'$$

Precession-tem

Spin-torque term from SOI

Damping-term

Magnetic susceptibility $\chi^+(\omega)=-\frac{\mu_0(g\mu_B)^2}{\hbar V}\frac{P}{\omega+i0-(\Omega-\Delta)-P^{-1}F(\omega+i0)}$

Green function of Torque operator $F(\omega+i0)=-i\int_{-\infty}^{\infty}\left\langle\left[\eta^-(t),\eta^+\right]\right\rangle_0\theta(t)e^{i(\omega+i0)t}dt$

Magnetic susceptibility from LLG equation $\chi^+(\omega)=-\frac{\gamma M_s}{\omega-\gamma H_{eff}+i\alpha\omega}$

Magnetic damping constant (comparing macroscopic formula) $\alpha=-\lim_{\omega\to 0}\frac{\gamma}{\hbar\mu_0 V M_S}\mathrm{Im}\left[\frac{1}{\omega}F(\omega+i0)\right]$

First-principles calculation of damping constant

V. Kambersky, Czechoslovak Journal of Physics B **26**, 1366 (1976).

$$\alpha = \frac{g^2 \mu_0 \mu_B^2}{\pi \hbar V \gamma M_S} \sum_{\vec{k}} \sum_{nm} \left| \Gamma_{nm}^{-}(\vec{k}) \right|^2 \frac{\delta}{\left(E_F - E_{n\vec{k}}\right)^2 + \delta^2} \frac{\delta}{\left(E_F - E_{m\vec{k}}\right)^2 + \delta^2}$$

$$\gamma = \mu_0 g \mu_B / \hbar$$

Eigenstates at each k-point and band

Matrix elements of torque operator

$$\Gamma_{nm}^{-}(\vec{k}) = \left\langle n, \vec{k} \left| \zeta \left[S^{-}, H^{SO} \right] \right| m, \vec{k} \right\rangle$$

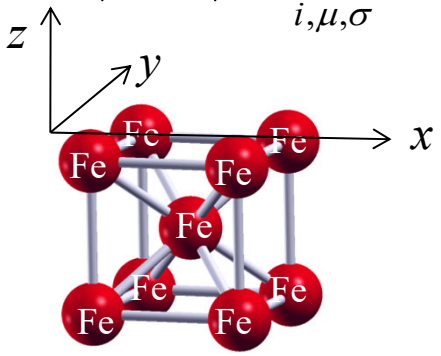
$$H_{SO} = \xi \vec{L} \cdot \vec{S}$$ Spin-orbit interaction

$$\left| m, \vec{k} \right\rangle = \sum_{i,\mu,\sigma} c_{i\mu}^{\vec{k}m\sigma} \left| i\mu \right\rangle$$

matrix elements of torque operator based on the local atomic orbital

VASP code

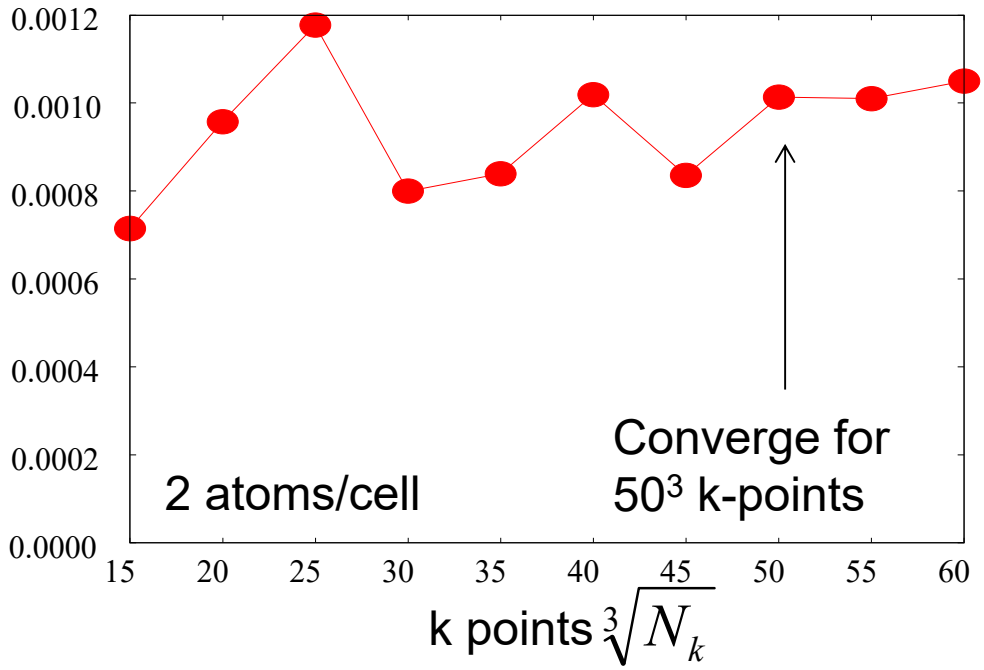
Bulk-Fe



α=0.0011 (this work)

α=0.0013 (by Gilmore)

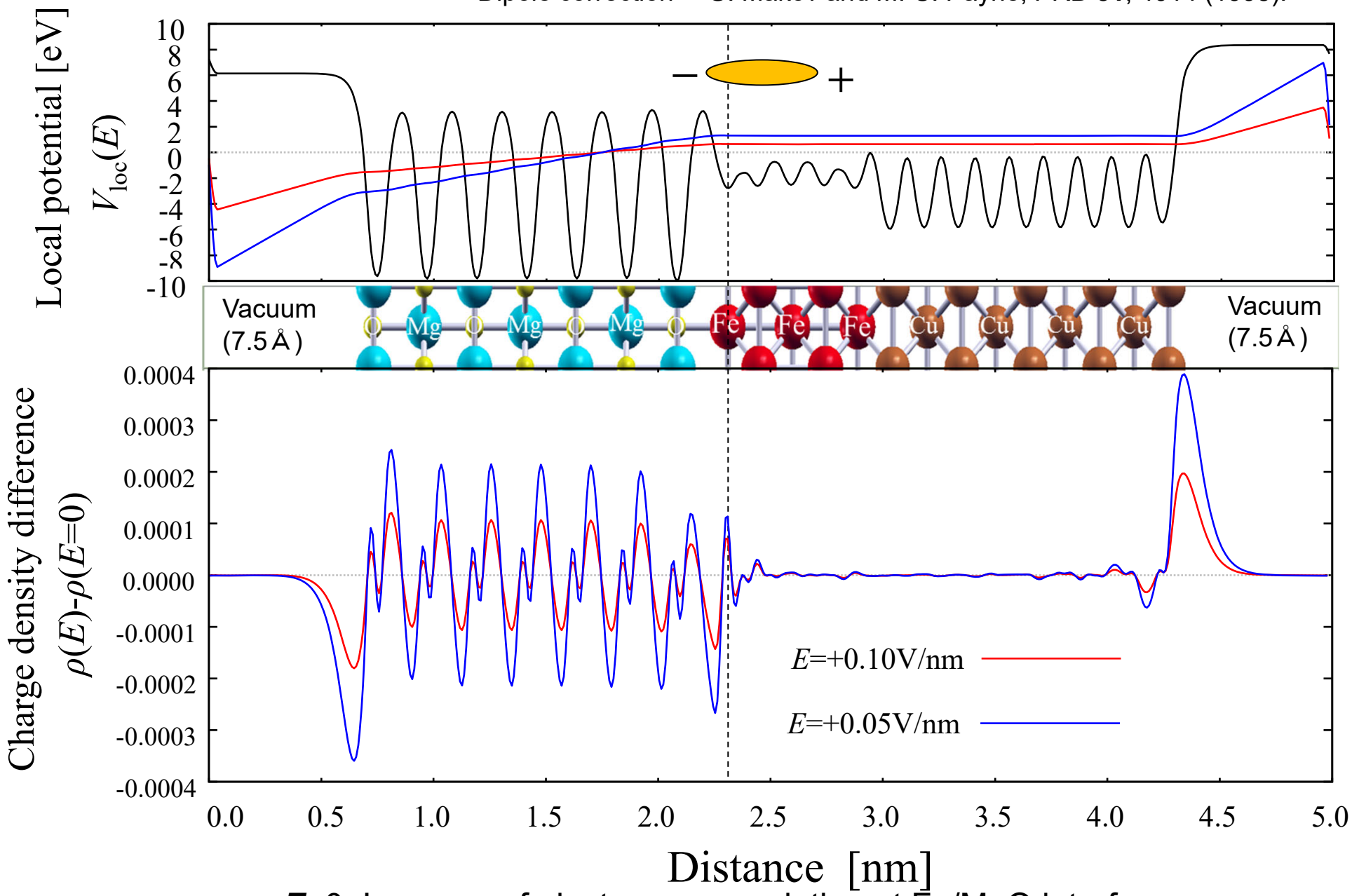
K. Gilmore, PRL **99,** 027204 (2007)



⇒For Fe/MgO(001) interface, I considered 50x50 k-points.

Potential and charge for model system

Dipole correction⇒ G. Makov and M. C. Payne, PRB **51**, 4014 (1995).

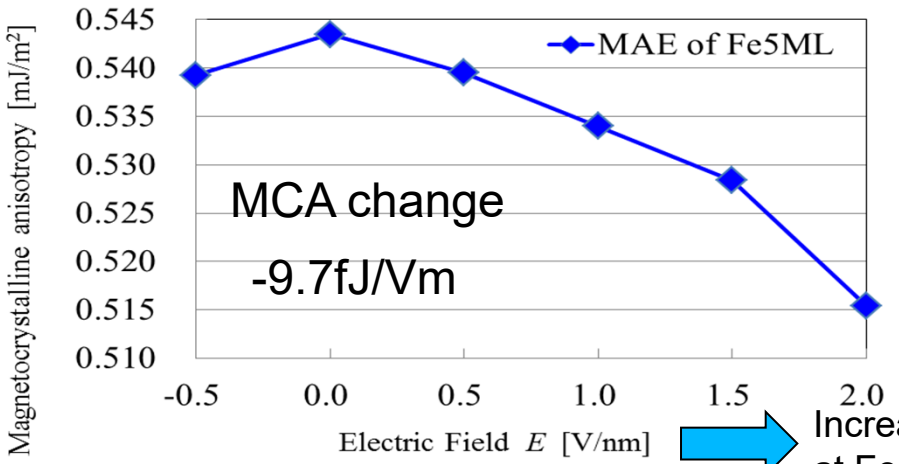


E>0 :Increase of electron accumulation at Fe/MgO interface

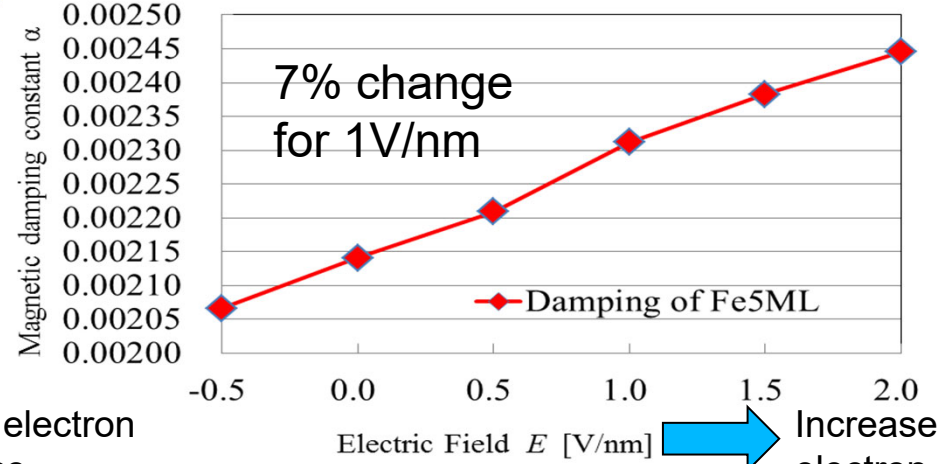
E<0 :Decrease of electron accumulation at Fe/MgO interface

Voltage dependence of MCA and damping α of Fe surface and Fe/MgO interface

Fe(001) surface



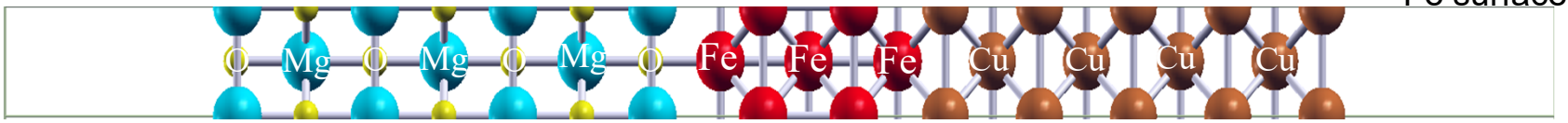
Increase of electron at Fe surface

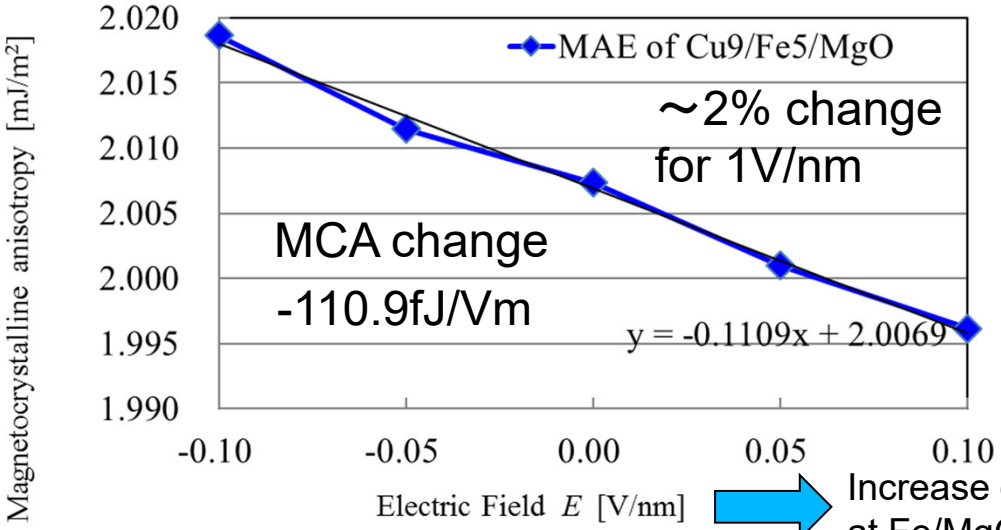


Increase of electron at Fe surface

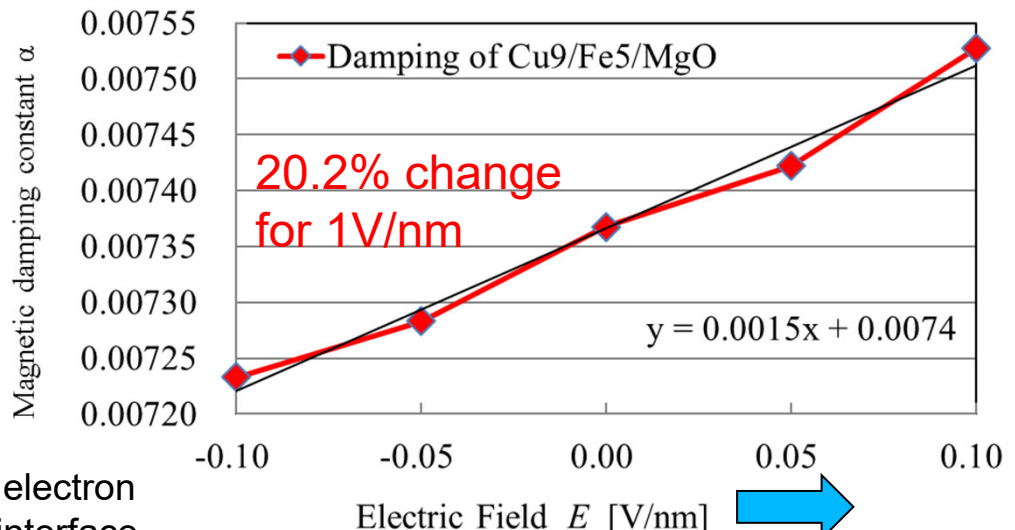
C. G. Duan, *et al.*, PRL **101**, 137201 (2008).

Fe/MgO(001) interface





Increase of electron at Fe/MgO interface



Increase of electron at Fe/MgO interface

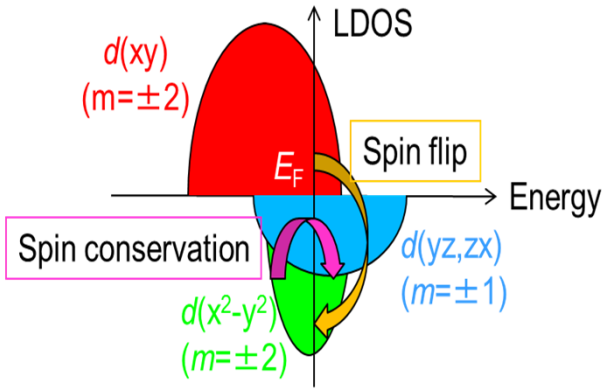
Decomposition of magnetic damping α

Torque operator $\Gamma^- = \left[S^-, H^{SO}\right] = \zeta\left(S^z L^- - S^- L^z\right)$

Spin conservation (Orbital deexcitation) term

$\left\langle u^\sigma \middle| L^- \middle| o^\sigma \right\rangle$

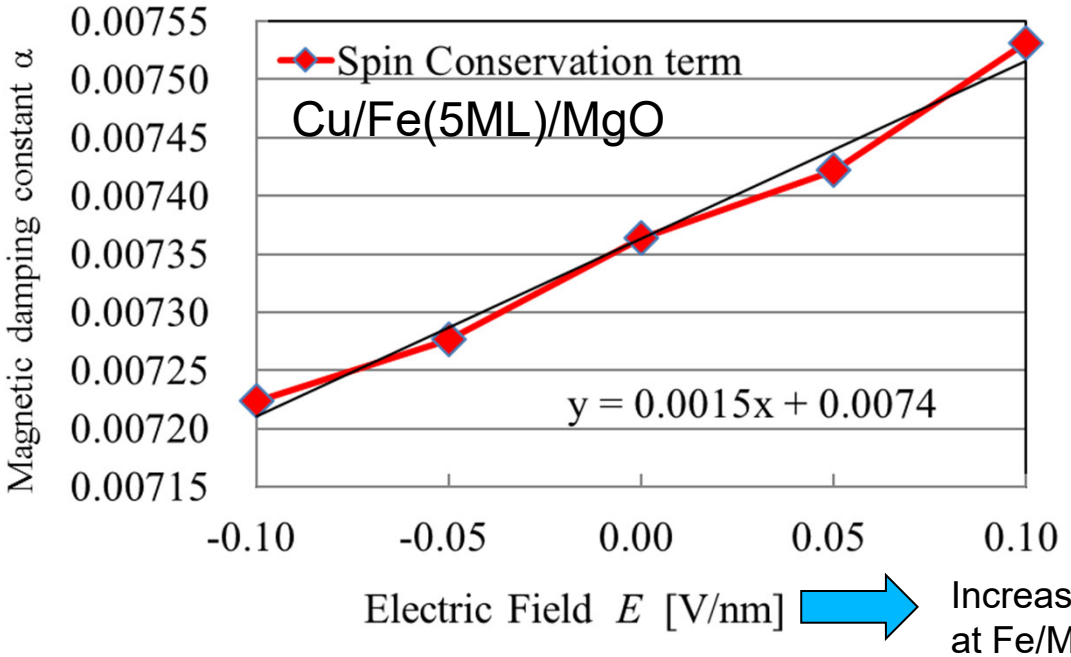
The matrix elements are non-zero for atomic orbitals between different magnetic quantum number, such as d(yz,zx)-d(z^2), d(yz,zx)-d(x^2-y^2), d(yz,zx)-d(xy)



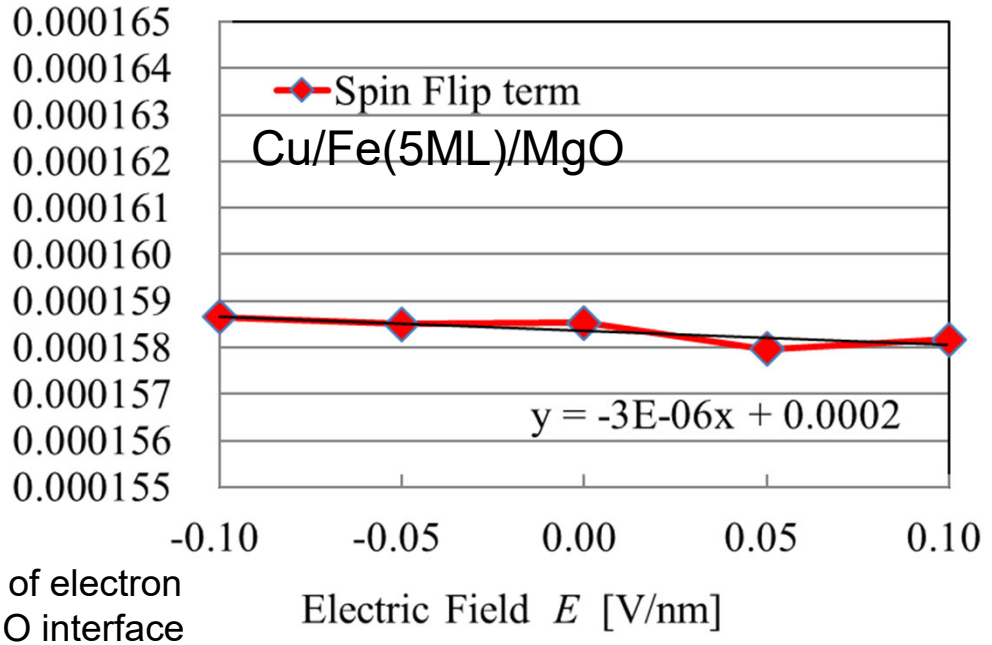
Spin flip (Orbital conservation) term

$\left\langle u^{-\sigma} \middle| L_Z \middle| o^\sigma \right\rangle$

The matrix elements are non-zero for atomic orbitals between same magnetic quantum number, such as d(yz)-d(zx),d(x^2-y^2)-d(xy)

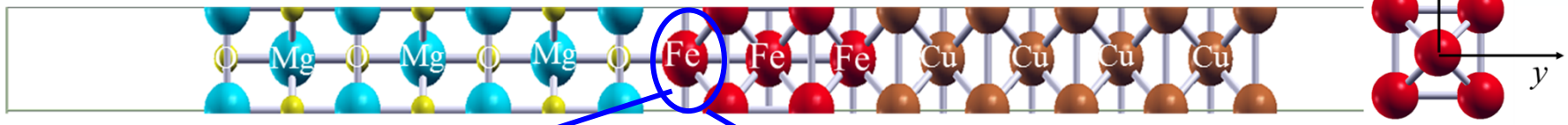


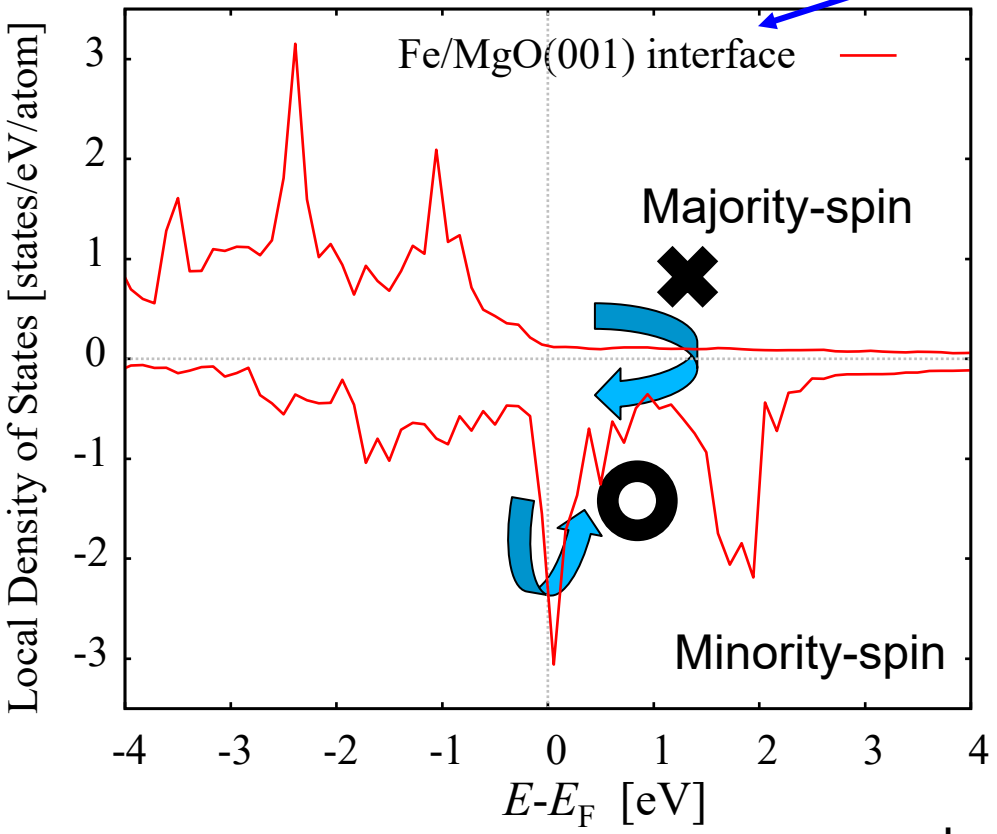
Increase of electron at Fe/MgO interface

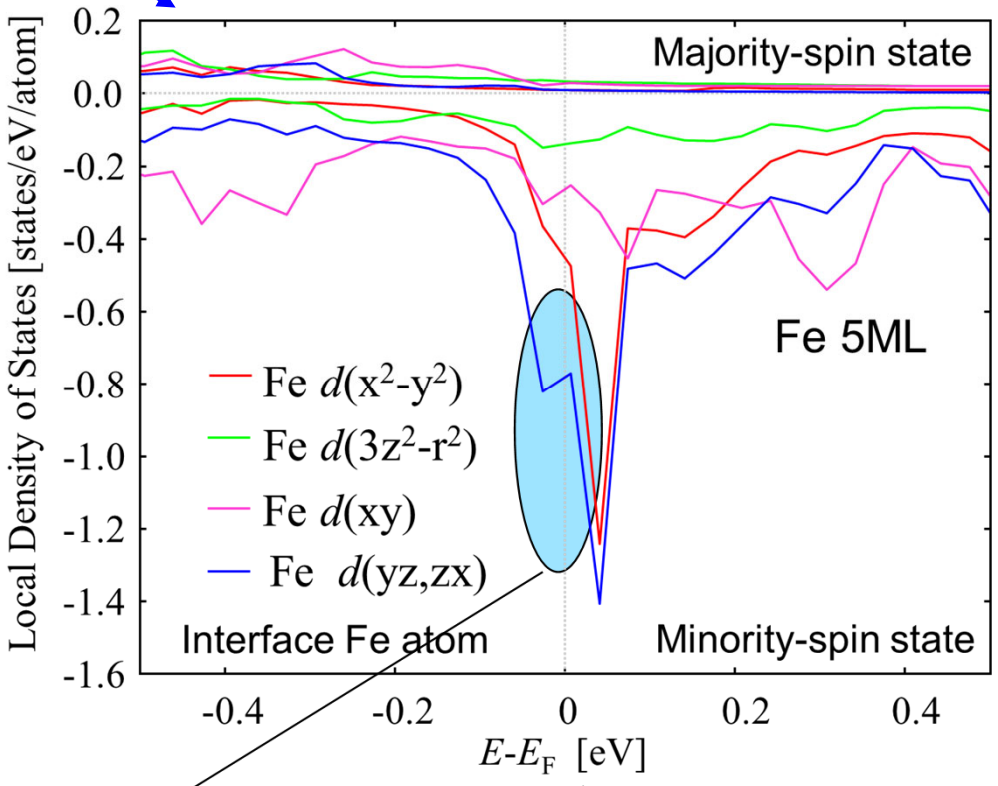


Origin of electric filed dependence

Fe/MgO(001) interface







Large matrix element of $\langle d(x^2-y^2)|L^-|d(yz,zx)\rangle$

Increase damping with increasing EF

Second order perturbation of SOI

D. Wang, et al., PRB **47**, 14932 (1993).

$$E_{\mathrm{PMA}} \propto (\xi)^2 \sum_{o,u,k} \frac{\left|\langle o,k,\downarrow|L_z|u,k,\downarrow\rangle\right|^2 - \left|\langle o,k,\downarrow|L_x|u,k,\downarrow\rangle\right|^2}{\varepsilon^{\downarrow}_{u,k} - \varepsilon^{\downarrow}_{o,k}}$$

$$L_x = \tfrac{1}{2}\left(L^- + L^+\right)$$

The $\langle d(x^2\text{-}y^2)|L^-|d(yz)\rangle$ increase the damping, but decrease the PMA.⇒opposite EF dependence

Summary of the third topic

First principles study on voltage control of magnetic anisotropy (VCMA) and magnetic damping in Fe/MgO interface

・For Fe/MgO(001) surface, the magnetic damping increases with increasing the electron accumulation at interface (positive EF).

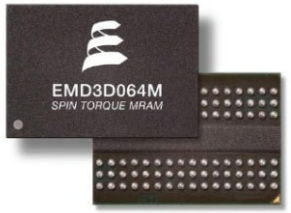
(20% of damping constant α can be changed by EF=1[V/nm] for Fe/MgO(001))

・It is opposite to that of Perpendicular MCA.

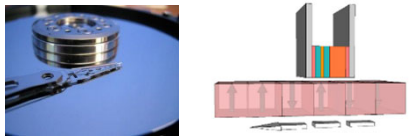
・The voltage dependence of magnetic damping of Fe/MgO(001) can be attributed to the spin conservation term.

Summary of this talk

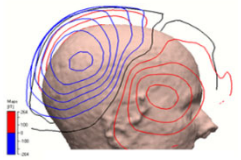
MRAM



Magnetic censer



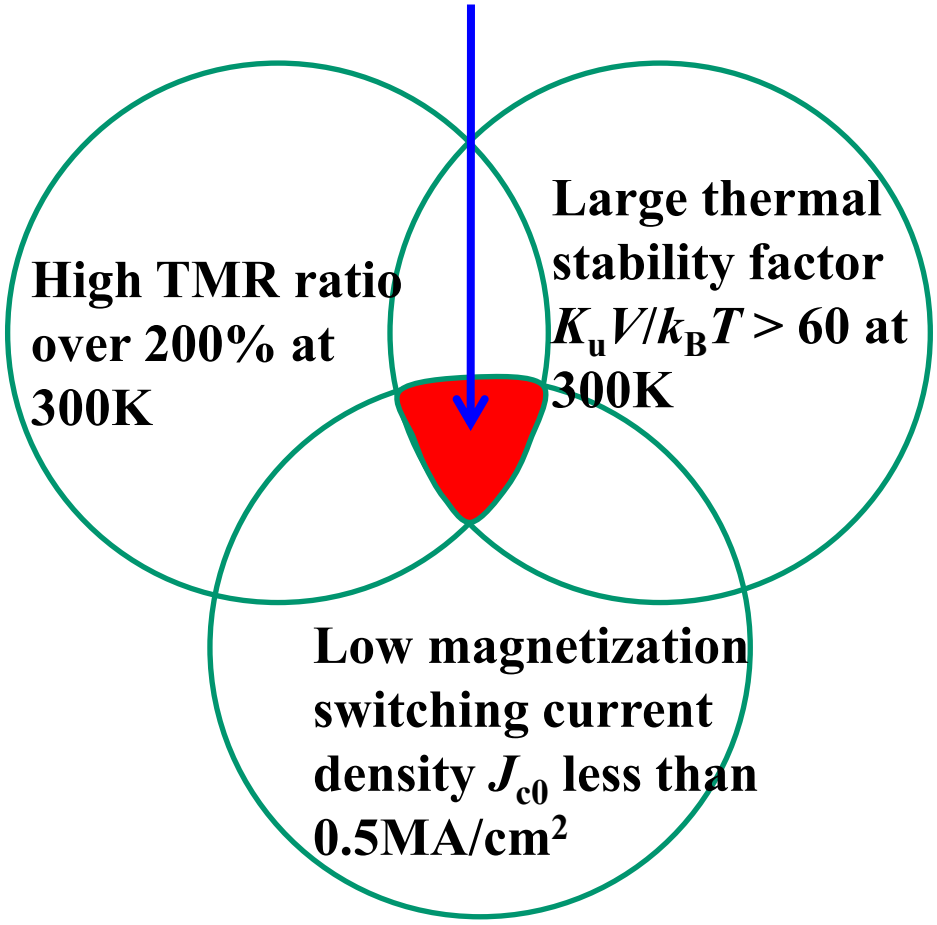
HDD read-out-head



Earth's magnetic field censer・current censer for car・biomagnetic censer

Corresponding to SQUID

Required performance for pMTJs



Required properties for spintronic materials