金沢大学
KANAZAWA UNIVERSITY

ナノ構造の磁気異方性と電界効果
Magnetic anisotropy and its electric field effects in nano-structures

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PF研究会「磁性薄膜・多層膜を究める：
キャラクタリゼーションから新奇材料の創製へ」
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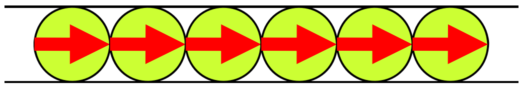
KEK研究本館小林ホール
KEK Tsukuba
October 15th 2011 (11:40-12:00)

Contents of the talk

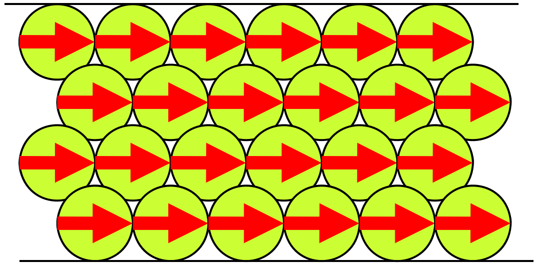
1. **Introduction**
2. **Magnetic anisotropy and Electric-field effect**
    - **2-1. Linear chains：Rashba effect**
    - **2-2. Films : dielectric/metal**
3. **Summary**

Microscopic origin of magnetic anisotropy



Magnetostatic contribution

$$E_{\text{d-d}} = \frac{1}{c^2} \sum_{\vec{R}_i, \vec{R}_j}^{i \neq j} \left\{ \frac{\vec{m}(\vec{R}_i) \cdot \vec{m}(\vec{R}_j)}{R_{ij}^3} - 3 \frac{\left[\vec{m}(\vec{R}_i) \cdot (\vec{R}_i - \vec{R}_j)\right]\left[\vec{m}(\vec{R}_j) \cdot (\vec{R}_i - \vec{R}_j)\right]}{R_{ij}^5} \right\}$$

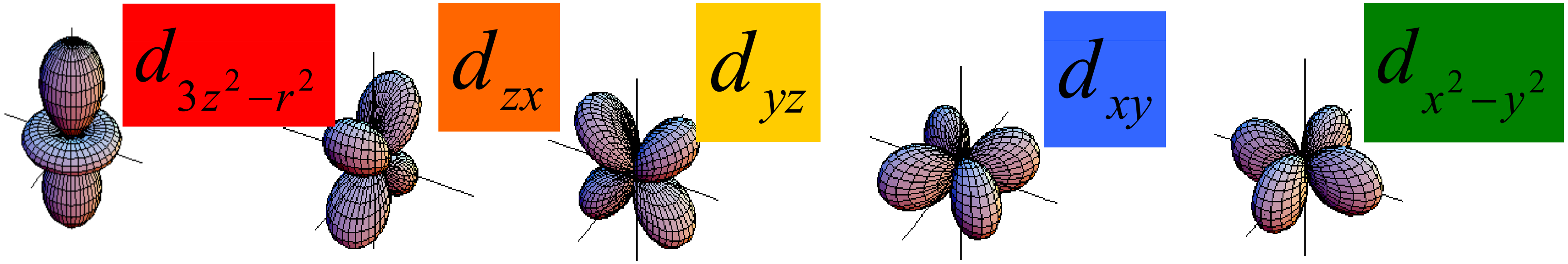


This depends on the arrangement of magnetic atoms, not so depend on electric field.

Electronic structure contribution

perturbation of spin-orbit interaction,
MA appears from an anisotropy of orbitals

$$H_{\text{SOI}} = \xi \, \vec{\ell} \cdot \vec{\sigma}$$



It is important to see the behavior of each angular orbitals.
Anisotropic occupation of electrons leads to MA.

Spin-orbit interaction

$$H_{SOI} = \frac{\hbar}{4m^2c^2}\vec{\sigma}\cdot\left(\underline{\mathrm{grad}}\; V(\vec{r})\times\vec{p}\right)$$

$\vec{\sigma}$ **Pauli's matrix**

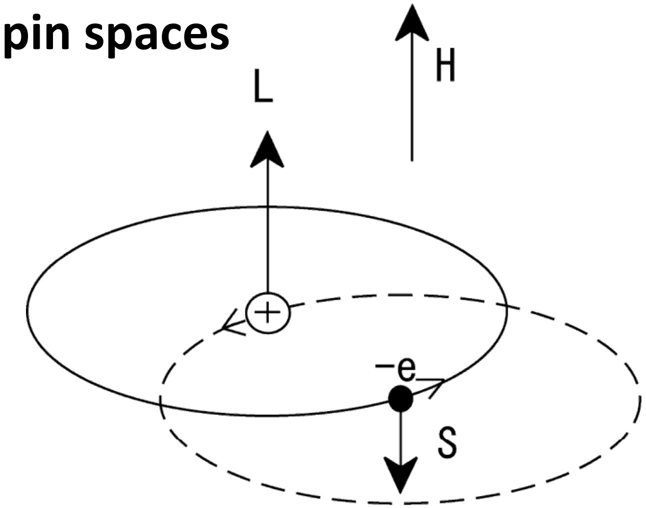
$$V(\mathbf{r}) \approx -\frac{Ze^2}{r} \qquad \mathrm{grad}\, V(r) \approx \frac{dV}{dr}\frac{\mathbf{r}}{r}$$

$$H_{SOI} = \underline{\xi\,\vec{\ell}\cdot\vec{\sigma} = \xi\left(\ell_x\sigma_x + \ell_y\sigma_y + \ell_z\sigma_z\right)}$$

connects orbital and spin spaces

$$\xi(r) = \frac{\hbar^2}{4m^2c^2r}\frac{dV}{dr}$$

2 **Biot-Savart law in the classical electromagnetics**



spin-orbit interaction

Origin of MAE in electronic structure

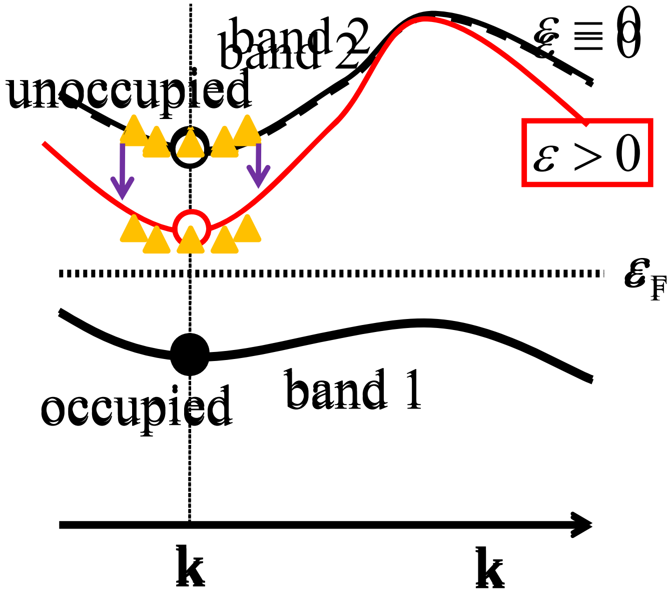
- **spin-orbit coupling contribution from band electrons**

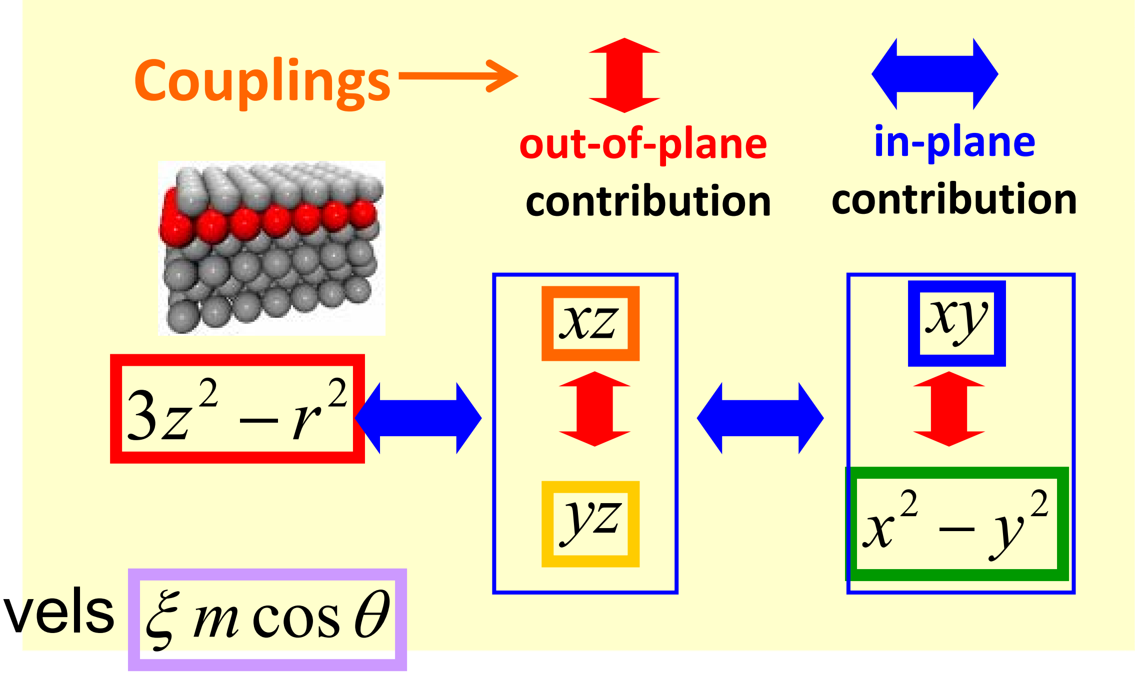
(A) 2nd perturbative contributions

$$\underline{\mathrm{MAE}=E_x-E_z}\approx(\xi)^2\sum_{o,u}\frac{\left|\langle o_\downarrow|\ell_z|u_\downarrow\rangle\right|^2-\left|\langle o_\downarrow|\ell_x|u_\downarrow\rangle\right|^2}{\varepsilon_u^\downarrow-\varepsilon_o^\downarrow}$$

matrix element

z	$\langle xz\|\ell_z\|yz\rangle=1$ $\langle x^2-y^2\|\ell_z\|xy\rangle=2$
x	$\langle 3z^2-r^2\|\ell_x\|yz\rangle=\sqrt{3}$ $\langle xy\|\ell_x\|xz\rangle=1$ $\langle x^2-y^2\|\ell_x\|yz\rangle=1$
y	$\langle 3z^2-r^2\|\ell_y\|xz\rangle=\sqrt{3}$ $\langle xy\|\ell_y\|yz\rangle=1$ $\langle x^2-y^2\|\ell_y\|xz\rangle=1$





Couplings →

out-of-plane contribution

in-plane contribution

$3z^2-r^2$

xz

yz

xy

x^2-y^2

(B) Existence of partly-occupied degenerate levels $\boxed{\xi\, m\cos\theta}$

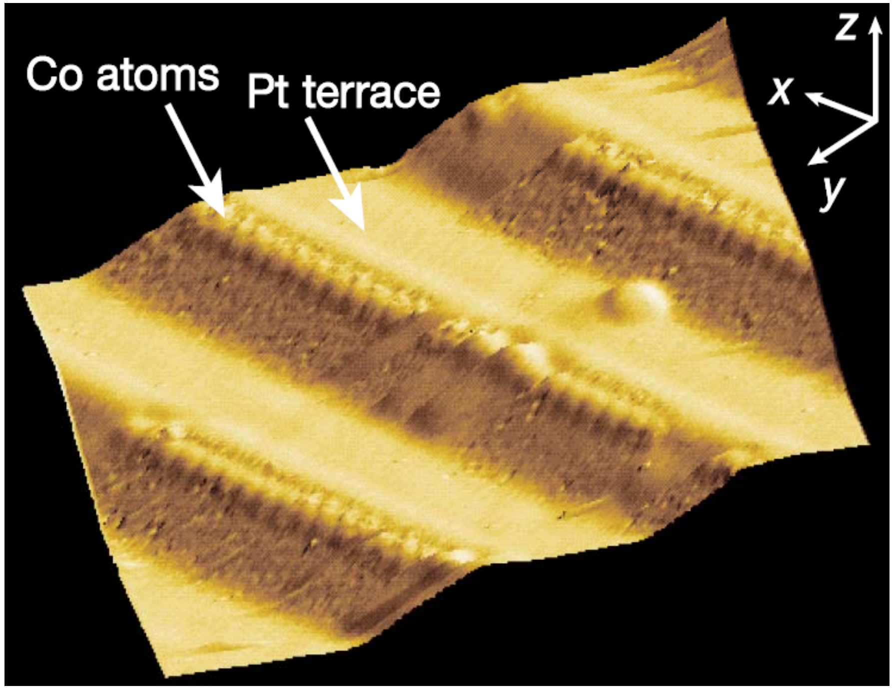
Low dimentional system **D. S. Wang, R. Wu, and A. J. Freeman, Phys. Rev. B 47,14932 (1993).**

Nano magnetic structures on surface

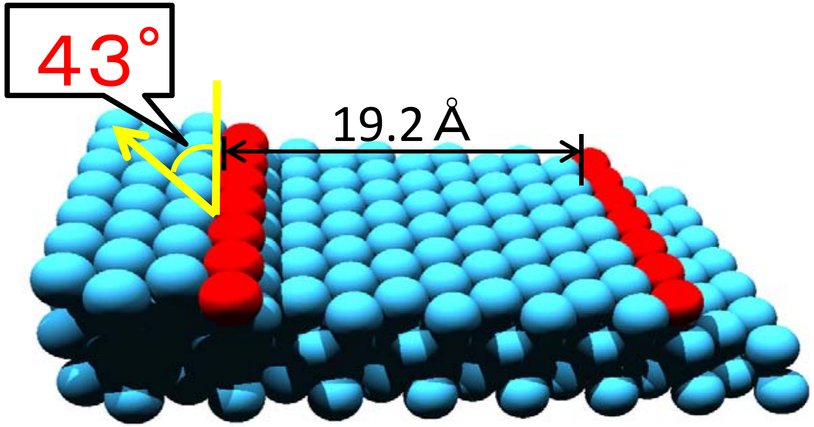
The magnetism of the low-dimensional system with a supported material (magnetism in nano-scaled systems) has been studied extensively.

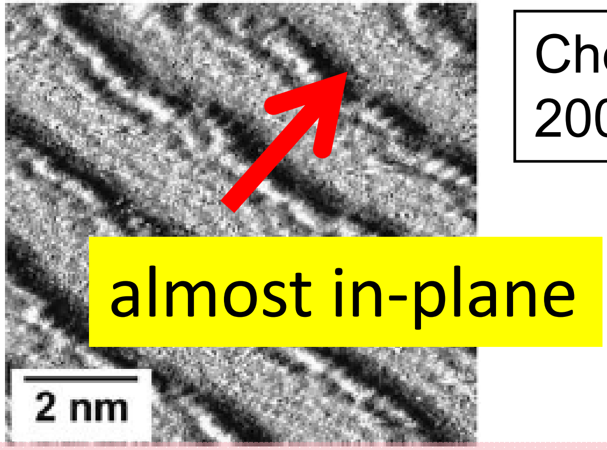
FePt alloys are a promising magnetic material for ultra high density recording media due to their large perpendicular magnetic anisotropy energy (MAE).

nano-scale structure v.s. magnetic anisotropy



Co nano-wire on Pt(997) surface.
P. Gambardella *et.al*, Nature 416 (2002) 301.

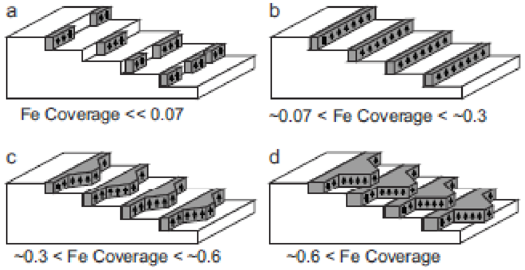




Cheng *et al*., 2005

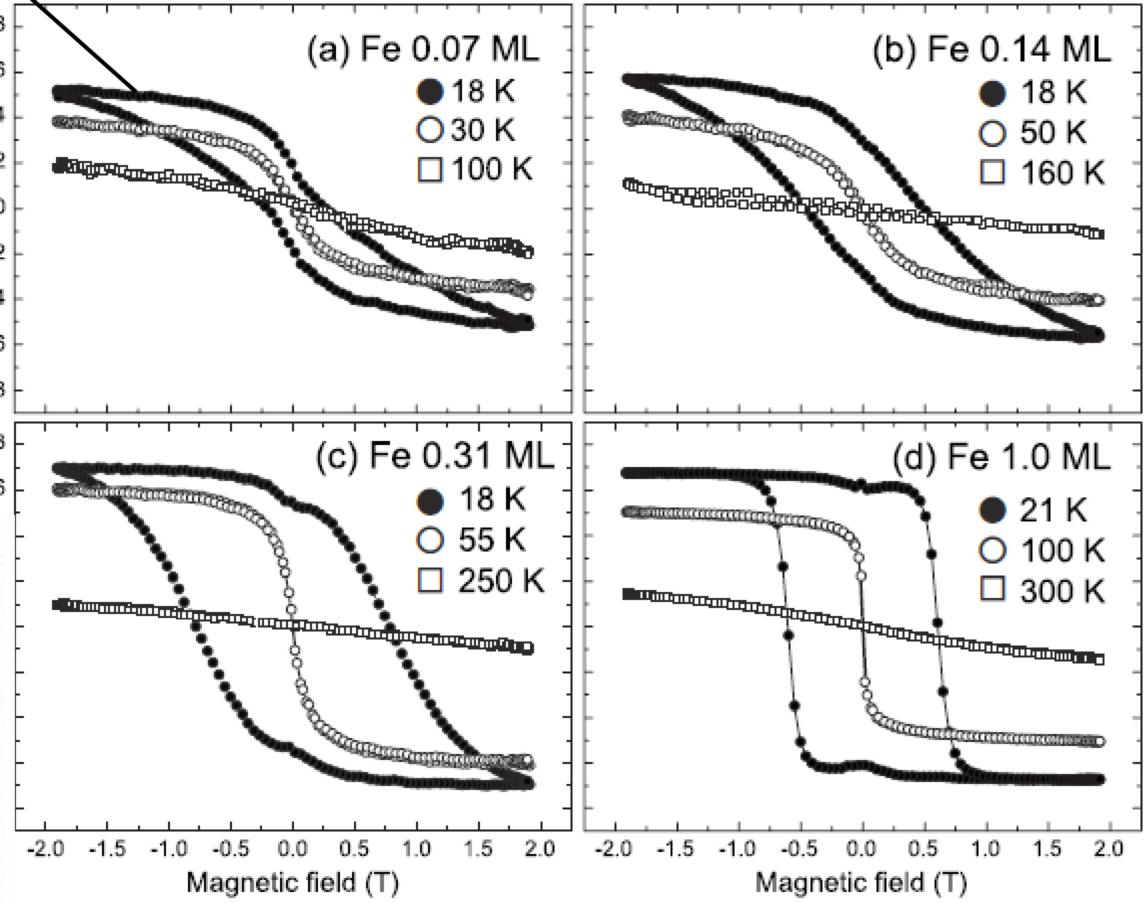
STM Fe 0.15ML on Pt(997)

Fe atomic layer on Au(788) surface

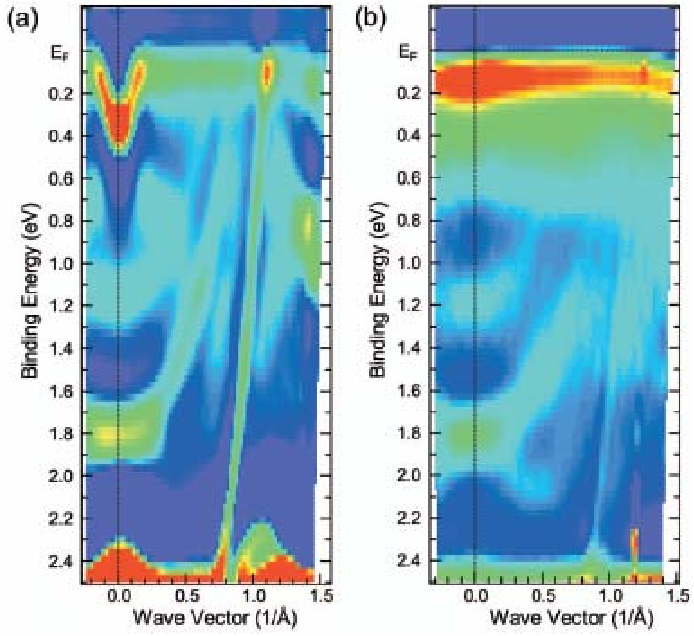


single Fe-chain

Shiraki *et al*., PRB **78**, 11548 (2008)



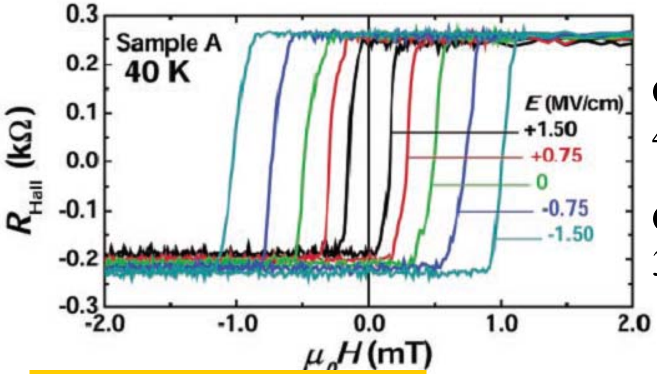
Fe(0.08ML)/Au(788)



The magnetic easy axis has
a perpendicular component.

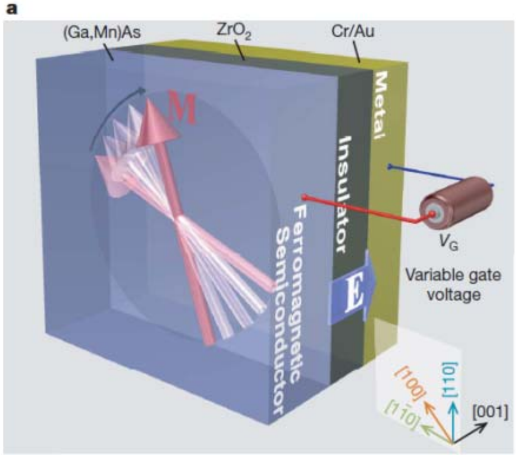
Fujisawa *et al*., PRB **75**, 245423 (2007)

Toward electric field assisted magnetization reversal, there are some pioneering works on magnetic state control by electric field



Ohno et. al., Nature 408, 948 (2000).

Chiba et. al., Science 301, 943 (2003).



Chiba et. al., Nature. 455, 515 (2008).

(In, Mn)As

magnetic semico.

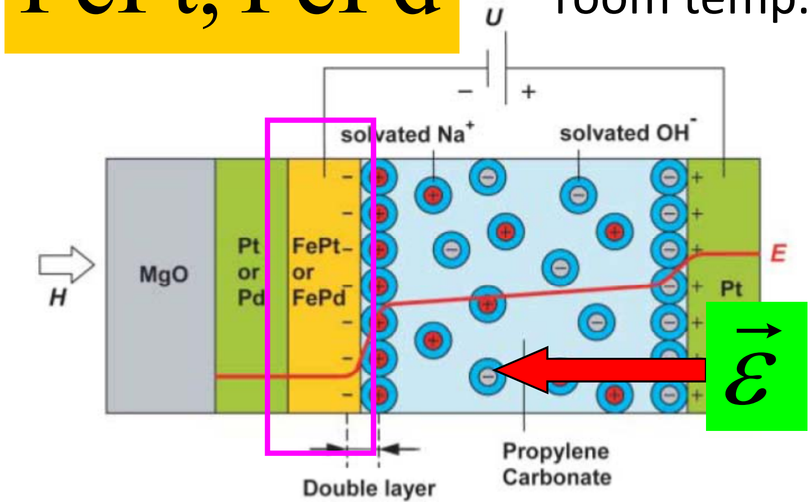
(Ga, Mn)As

metallic layer
with dielectric mat.

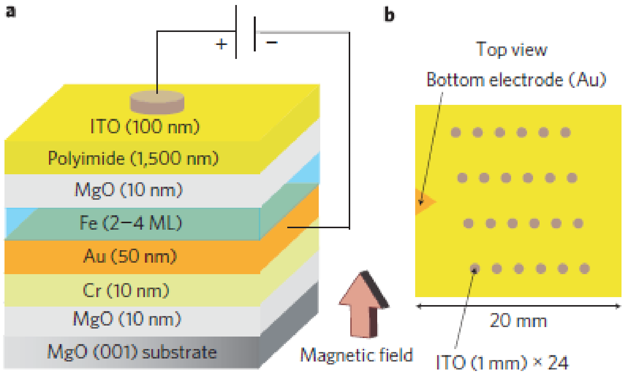
FePt, FePd

room temp.

MgO/Fe/Au(001)

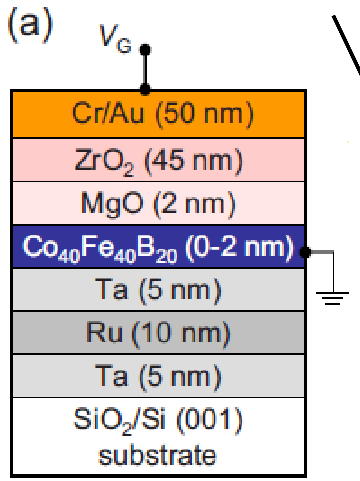


Weisheit et al., Science 315, 349 (2007)



Maruyama et. al., Nature Nanotech. 4, 158 (2009)

Recent works on the electric field effect of magnetic anisotropy energy



$\varepsilon_{\mathrm{ZrO_2}} = 23 \longrightarrow$

$\varepsilon_{\mathrm{MgO}} = 10 \longrightarrow$

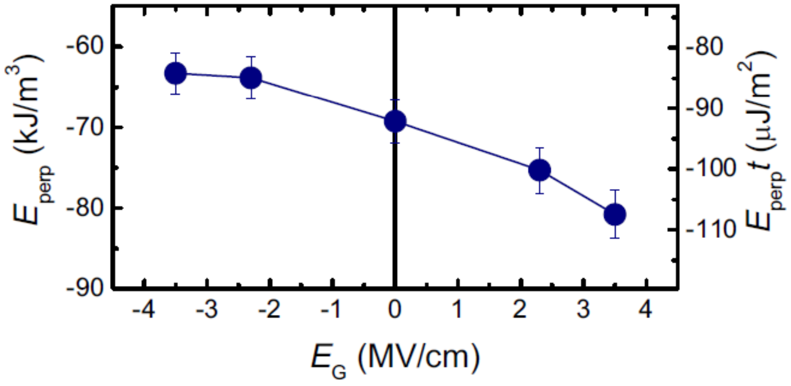
Electic Field (in MgO)

$$\longrightarrow E_G = \varepsilon_{\mathrm{ZrO_2}} \mathrm{V}_G \big/ \left(\varepsilon_{\mathrm{MgO}} d_{\mathrm{ZrO_2}} + \varepsilon_{\mathrm{ZrO_2}} d_{\mathrm{MgO}} \right)$$

$$E_{perp} = -\frac{M_{\mathrm{S}}}{R^{\mathrm{AHE}}_{\mathrm{Hall,max}}} \int H \, dR^{\mathrm{AHE}}_{\mathrm{Hall}}$$

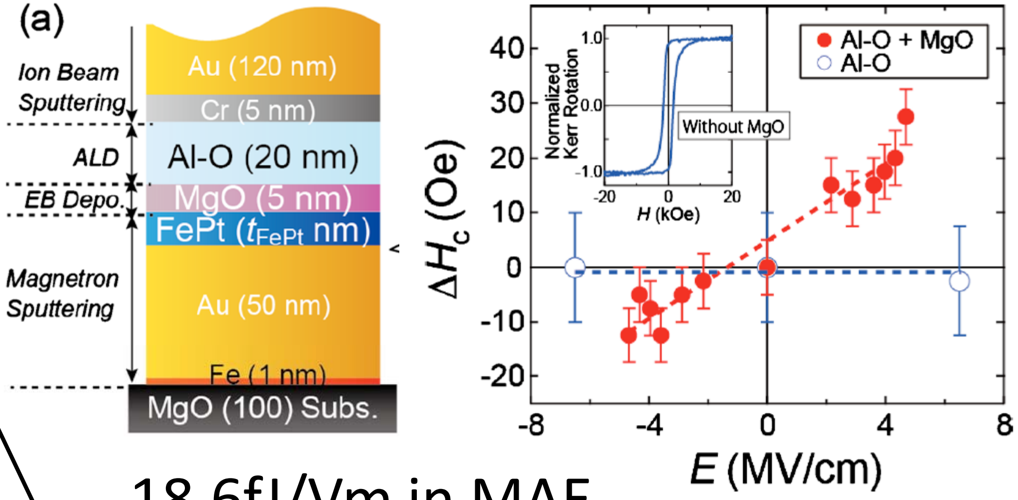
$33\mu\mathrm{J/m^2}$ in $1\mathrm{V/nm}$

$\uparrow$ **Anomalous Hall Resistance**



M. Endo et. al., APL **96**, 212503 (2010)

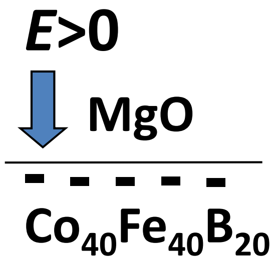
Seki et al., APL **98**, 212505 (2011)

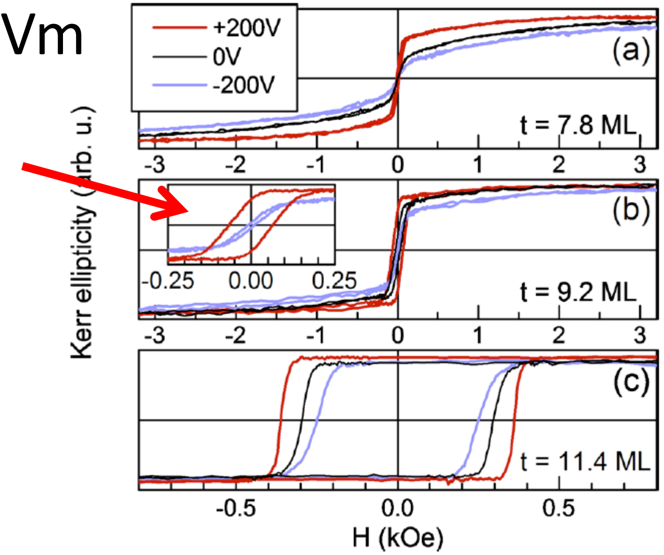


18.6fJ/Vm in MAE

MgO/(Fe/Pd)$_n$(001) n=3-4

602fJ/Vm

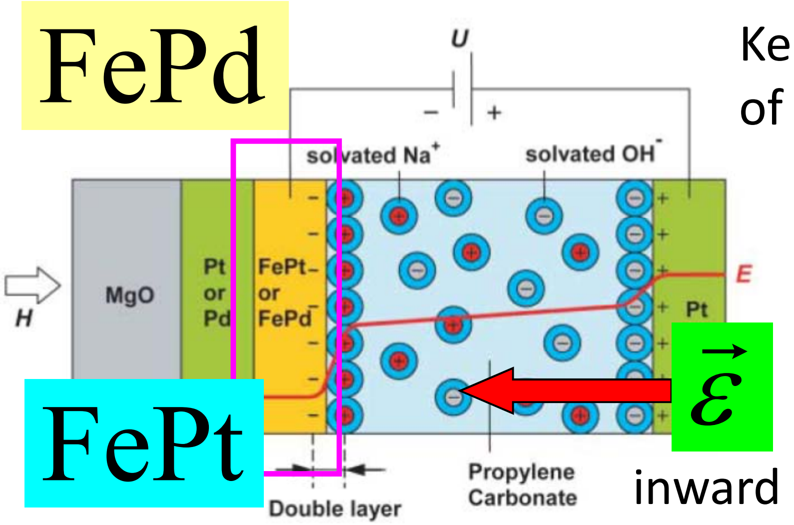




Bonell et al., APL **98**, 232510 (2011)

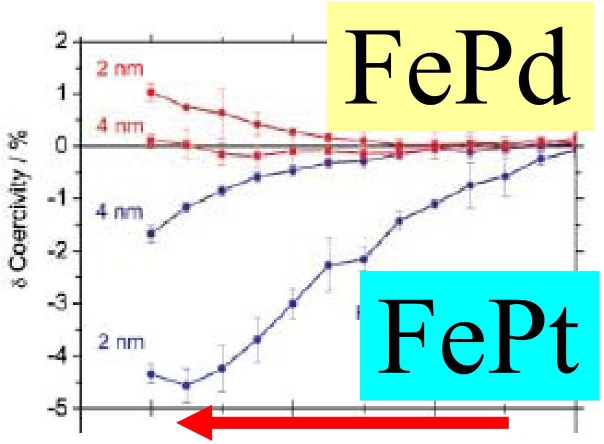
Electric field effect of magnetic anisotropy energy

M. Weisheit, S. Fähler, A. Marty, Y. Souche, C. Poinsignon, and D. Givord, Science 315, 349 (2007)



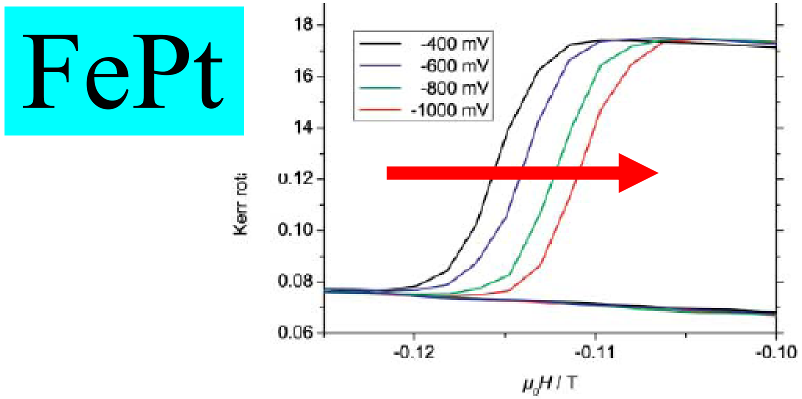
Kerr rotation
of surface magnetism

inward electric field



For 2nm-thick system of
FePt, 4.5% change of
coercivity
in the difference of 600mV.

Coercivity decreases by the inward electric field

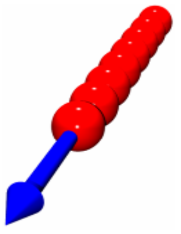


chains   Fe-chain/Pt(111) and Fe-chain/Pt(664)

Rashba effect

MAE of Fe-chain/Pt(664) surface

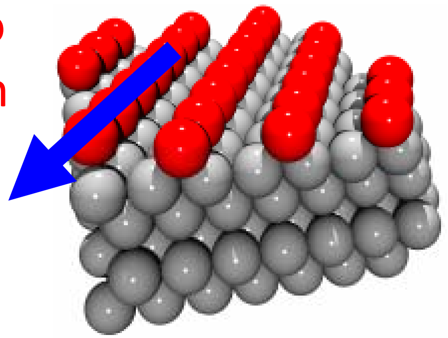
-3.23 meV/Fe



bare
Fe-chain

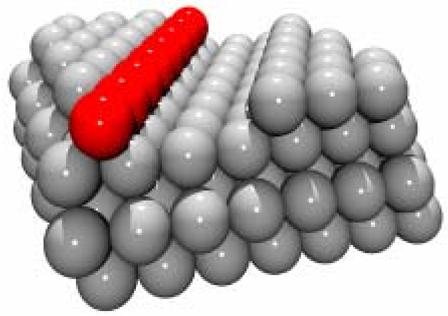
parallel to
the chain

-2.25 meV/Fe



Fe-chain/Pt(111)

1.19 meV/Fe

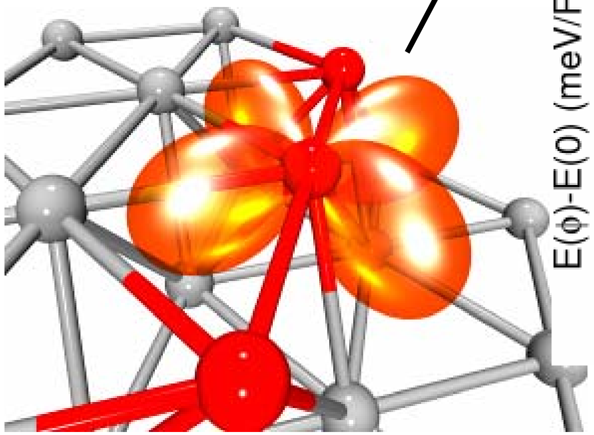


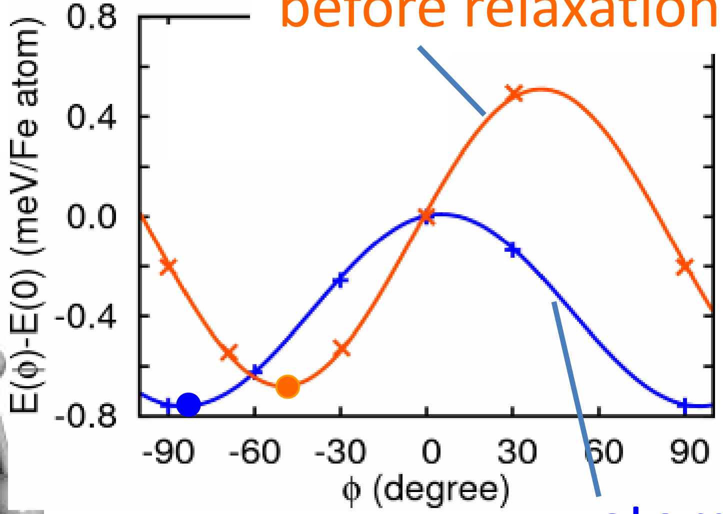
Fe-chain/Pt(664)

perpendicular to the chain

hybridization of 3*d* orbitals between Fe and Pt atoms

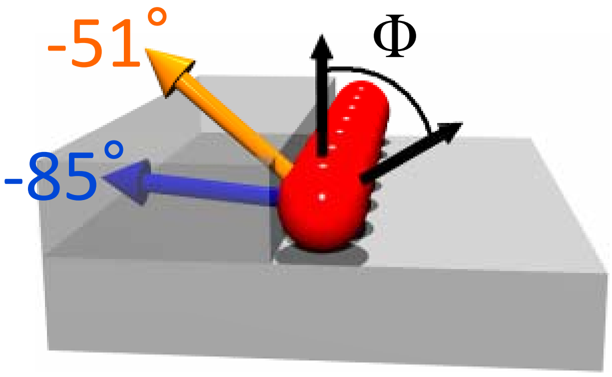
yz orbital





before relaxation

atomic relaxation

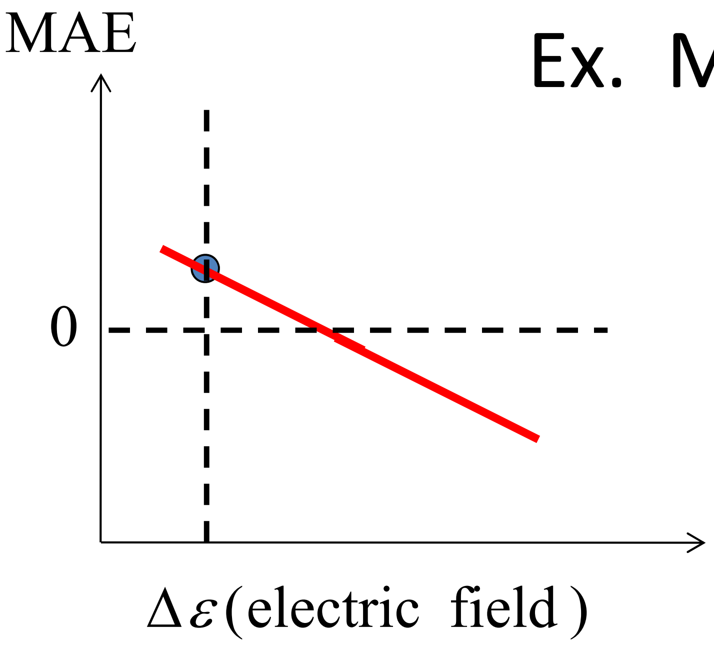


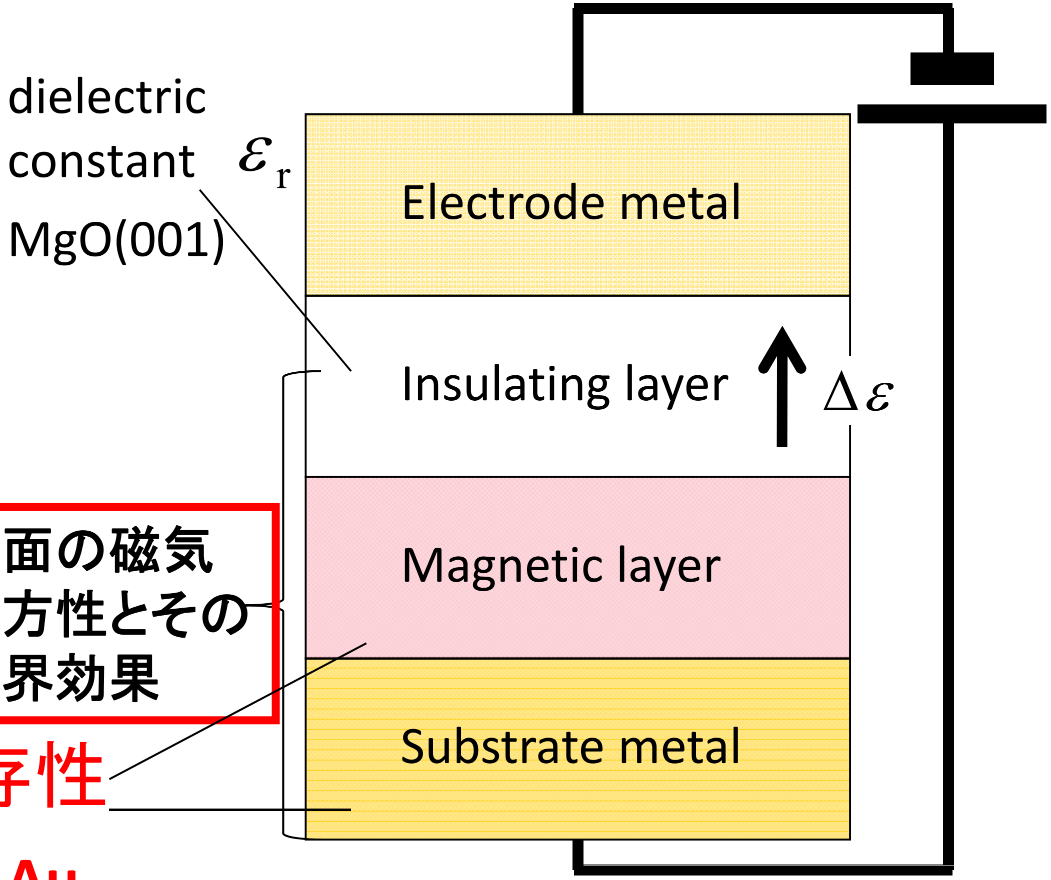
exp. -80°
(Repetto et al., 2006)

磁気異方性エネルギーの電界効果

Electric field effects on MAE

Ex. MgO/X/M(001)



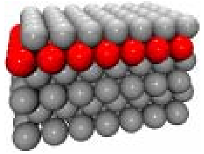


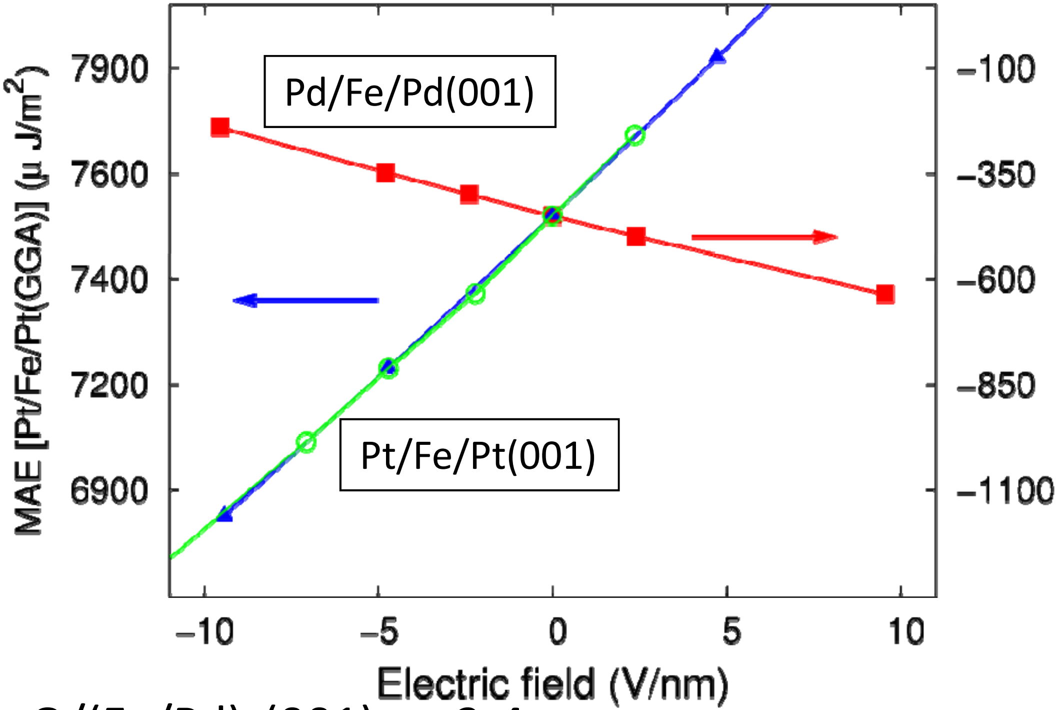
界面の磁気異方性とその電界効果

物質依存性、界面依存性

Fe, Co, Ni, FeCo, **Pt**, **Pd**, **Au**

Inverse of EF effects: Pd/Fe/Pd(001), comparison with Pt/Fe/Pt(001)





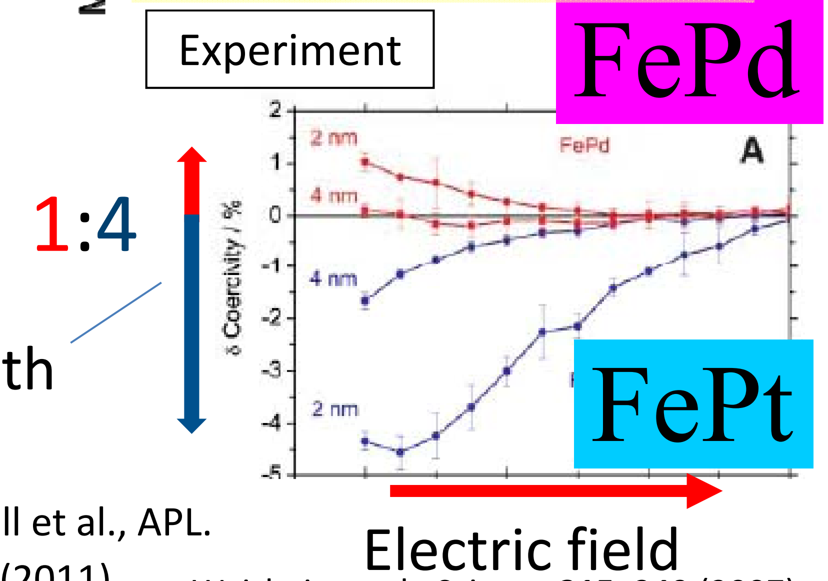
Pd/Fe/Pd(001) **Pd**

-21 fJ/Vm

Pt/Fe/Pt(001) **Pt**

+78 fJ/Vm (GGA)

$$\frac{\gamma_{\mathrm{Pd}}}{\gamma_{\mathrm{Pt}}} \approx \frac{-21}{78} = -0.27$$



MgO/(Fe/Pd)$_n$(001) n=3-4

$$\gamma_{\mathrm{Pd}}^{\mathrm{exp}} = -602\ \mathrm{fJ/Vm} \quad \approx -21\varepsilon_r^{\mathrm{MgO}}\ \mathrm{fJ/Vm}$$

Minus slope : qualitative agreement with the experiment of Weisheit et al.

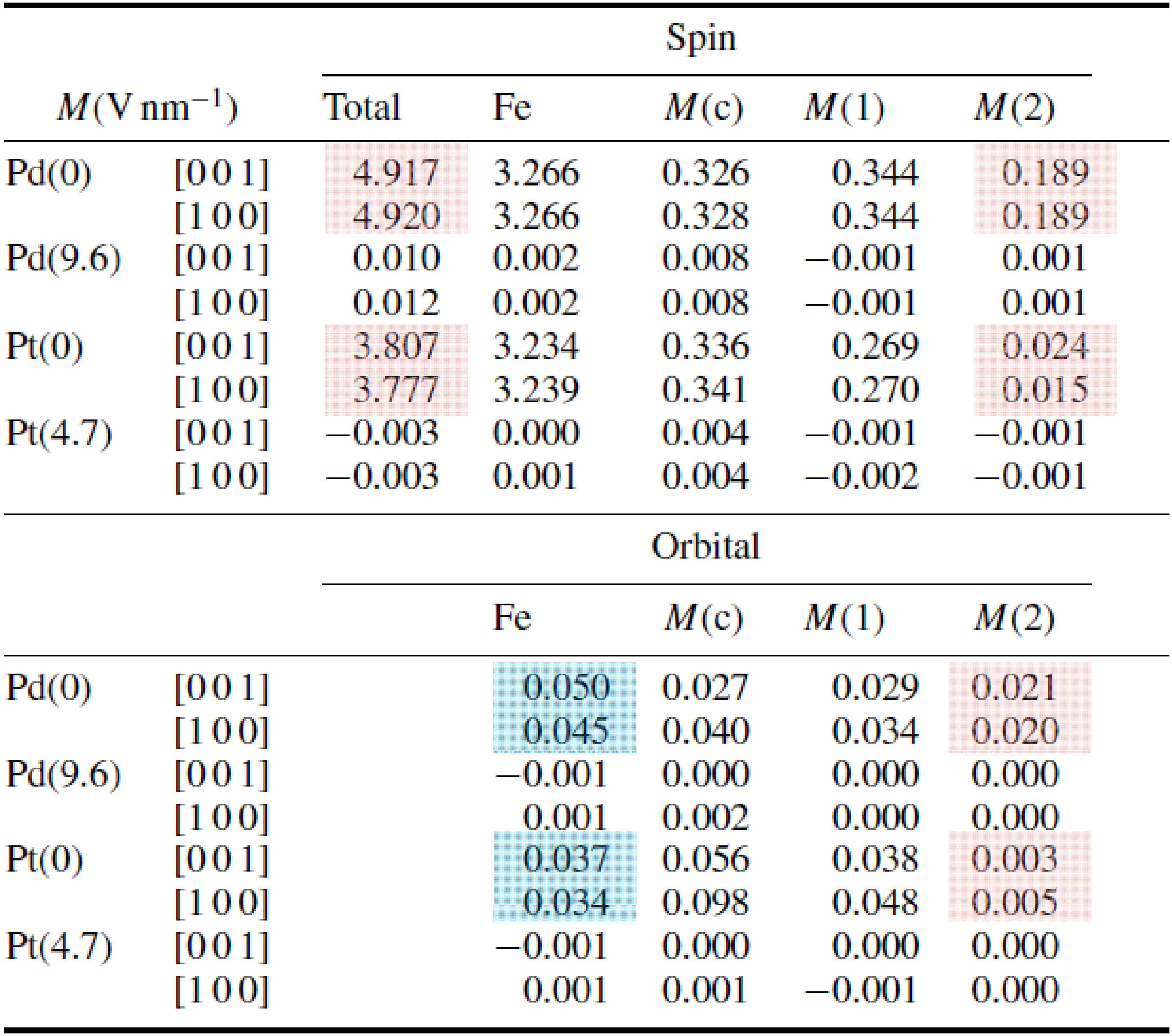
S. Haraguchi, M. Tsujikawa, J. Gotou, and TO,
J. Phys. D: Appl. Phys., **44** (2011) 064005.

exp.) Bonell et al., APL.
8, 232510 (2011)

Weisheit et. al., Science **315**, 349 (2007)

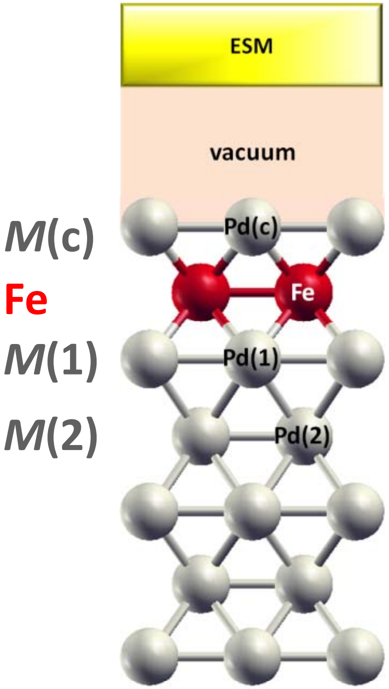
Magnetic moments (in μ_B)

Pd/Fe/Pd(001)
Pt/Fe/Pt(001)



M (V nm^{-1})		Spin Total	Spin Fe	Spin M(c)	Spin M(1)	Spin M(2)
Pd(0)	[0 0 1]	4.917	3.266	0.326	0.344	0.189
	[1 0 0]	4.920	3.266	0.328	0.344	0.189
Pd(9.6)	[0 0 1]	0.010	0.002	0.008	−0.001	0.001
	[1 0 0]	0.012	0.002	0.008	−0.001	0.001
Pt(0)	[0 0 1]	3.807	3.234	0.336	0.269	0.024
	[1 0 0]	3.777	3.239	0.341	0.270	0.015
Pt(4.7)	[0 0 1]	−0.003	0.000	0.004	−0.001	−0.001
	[1 0 0]	−0.003	0.001	0.004	−0.002	−0.001

		Orbital Fe	Orbital M(c)	Orbital M(1)	Orbital M(2)
Pd(0)	[0 0 1]	0.050	0.027	0.029	0.021
	[1 0 0]	0.045	0.040	0.034	0.020
Pd(9.6)	[0 0 1]	−0.001	0.000	0.000	0.000
	[1 0 0]	0.001	0.002	0.000	0.000
Pt(0)	[0 0 1]	0.037	0.056	0.038	0.003
	[1 0 0]	0.034	0.098	0.048	0.005
Pt(4.7)	[0 0 1]	−0.001	0.000	0.000	0.000
	[1 0 0]	0.001	0.001	−0.001	0.000



S. Haraguchi, et al.,
JPDAP, **44** (2011) 064005.

まとめ

密度汎関数法に基づいた第一原理計算による、磁性薄膜の電子状態と磁気異方性エネルギーの計算結果を紹介した。

〇SOIから寄与するMAEは、フェルミ準位付近の電子構造に敏感である。

〇面内磁化の場合、フェルミ準位付近には、磁性層のラシュバ効果による分散の非対称性が現れた。

〇MAE電界効果の大きい薄膜の探索：FePt

〇不純物元素や不規則構造（膜厚方向および膜内方向）の効果の解析も必要となる。