Introduction to Numerical Micromagnetism.

Application to Mesoscopic Magnetic Systems

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Outline

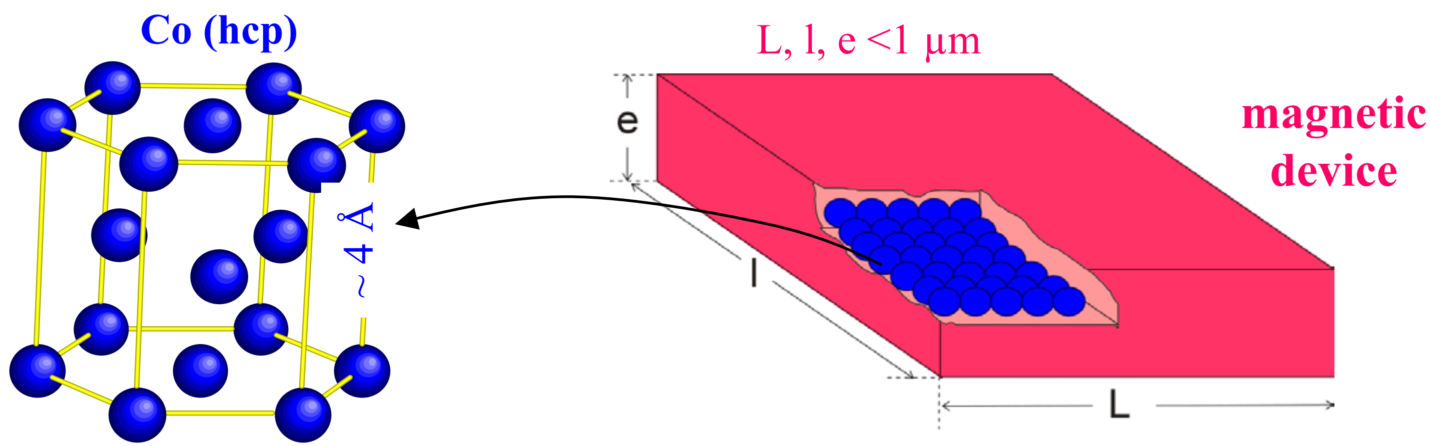
Micromagnetics – theoretical background
- hypothesis & limits
- total free energy minimization (variational principle)
- static and dynamic equations

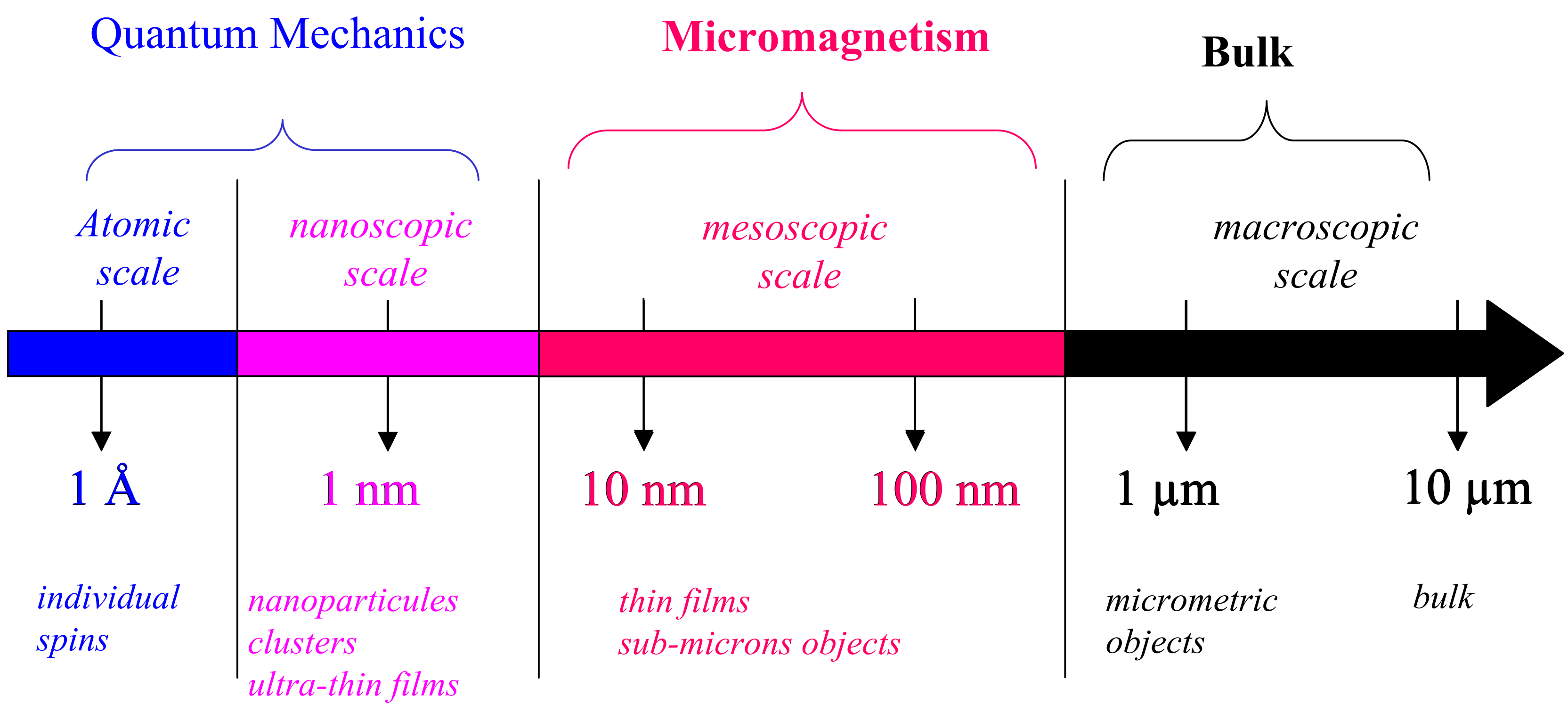
Micromagnetics – overview of the numerical implementation
- current state of the art
- finite difference approximation (fields & energies)
- errors & accuracy & validation

Application for mesoscopic ferromagnetic elements
- circular Co dots
- self-assembled epitaxial submicron Fe dots

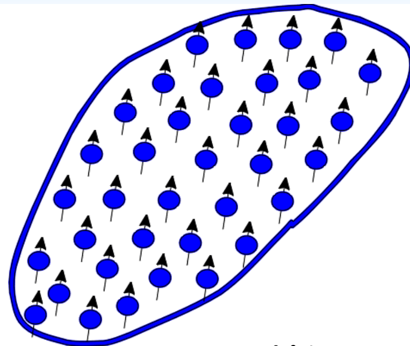
References

Length Scale

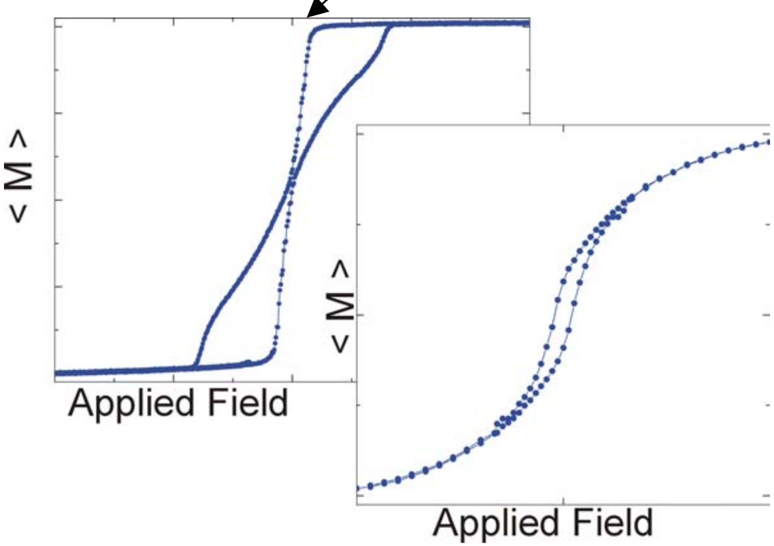




Experimental Scale

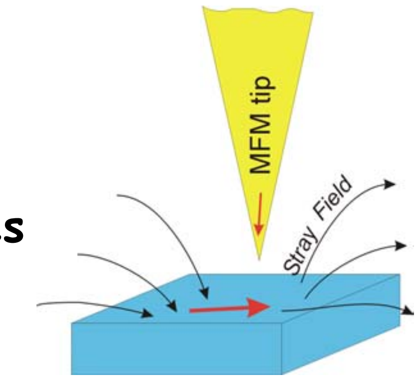


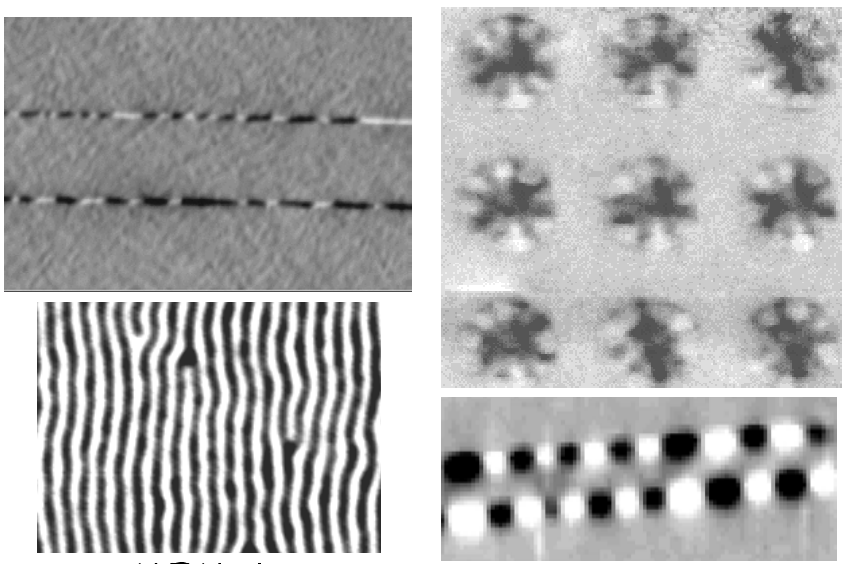
Macroscopic studies
Hysteresis curves



$\langle \vec{M} \rangle$ *Mean values of the magnetization*
MOKE, SQUID,...

Microscopic studies
Local imaging





MFM, Lorentz microscopy,...
- spatial resolution limited (>20 nm)
- several possible configurations

Vellekoop et al., JMMM. 190, 148 (1998).

Hypothesis

***1963 - W. F. Brown** Jr.*
- *1907 P. Weiss / magnetic domains*
- *1935 Landau-Lifshiz / domain walls*

- <u>Classical theory of continuous ferromagnetic material</u>

  - smooth spatial variation of the magnetization vector

- <u>Continuous functions (space & time)</u>

  - magnetization $\vec{M}(\vec{r},t)$
  - fields $\vec{H}(\vec{r},t)$
  - energies $E\left[\vec{m}\left(\vec{r},t\right)\right]$

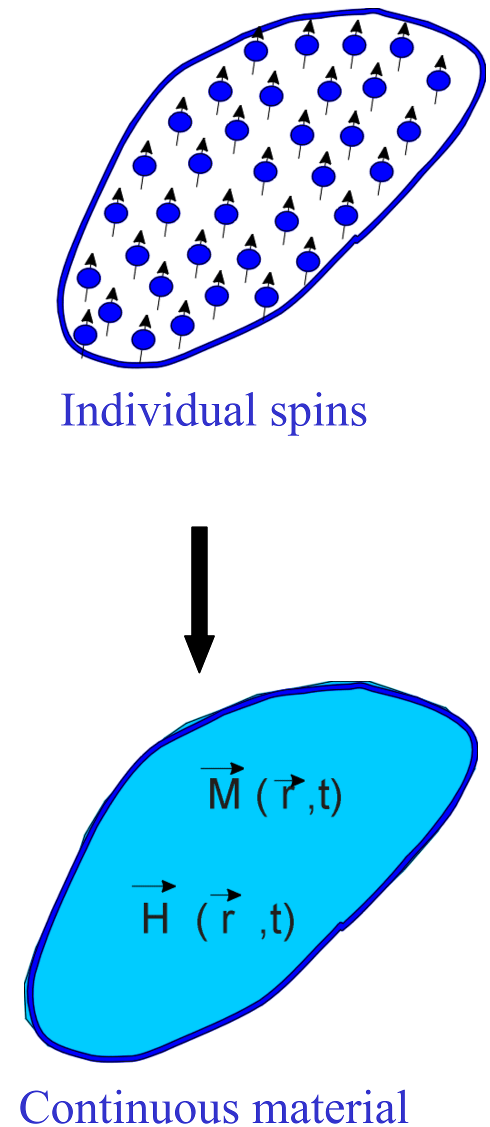
- <u>Magnetization</u> $\equiv$ <u>constant amplitude vector</u>

$$\vec{M}(\vec{r},t) = M_s \; \vec{m}(\vec{r},t)$$

$$\left|\vec{m}(\vec{r},t)\right| = 1$$

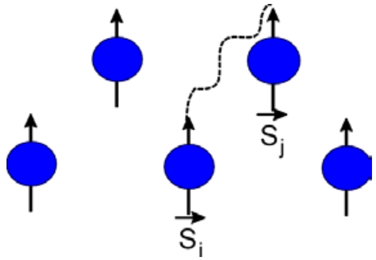
- <u>Thermal fluctuations neglected</u>

$$A_{ex}(T),\; M_s(T), K_u(T)$$



i **J. F. Brown**, Jr. : *Micromagnetics,* J. Wiley and Sons, New York (1963)

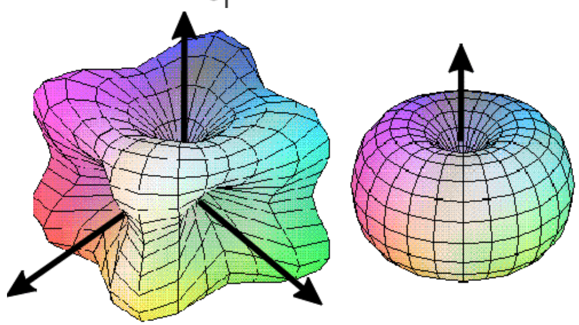
Total Free Energy (Gibb's free energy)



Exchange interaction
- *magnetic order* $(T<T_c)$ *(QM)*
- *parallels spins*

$$\int_V A_{ex}\left(\vec{\nabla}\vec{m}\right)^2 dV$$

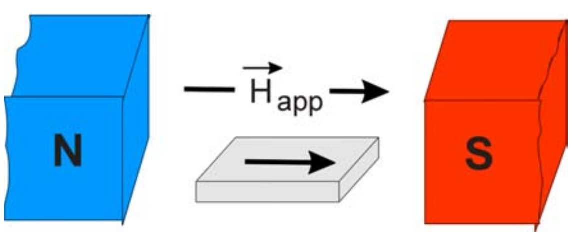
next neighbors



Magneto-crystalline anisotropy
- *the crystal symmetry axis*
- *easy direction*

$$\int_V K_1\left[1-(\vec{u}_K\cdot\vec{m})^2\right]dV$$

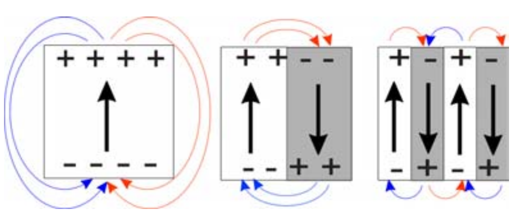
local interaction



Zeeman coupling
- *external applied field*
- *magnetization rotation*

$$-\mu_0 M_s\int_V\left[\vec{m}\cdot\vec{H}_{app}\right]dV$$

local interaction



Magnetostatic interaction
- *Maxwell's equations*
- *magnetic charges distribution*
- *magnetic domains formation*

$$-\frac{1}{2}\mu_0 M_s\int_V\left[\vec{m}\cdot\vec{H}_{dem}(\vec{m})\right]dV$$

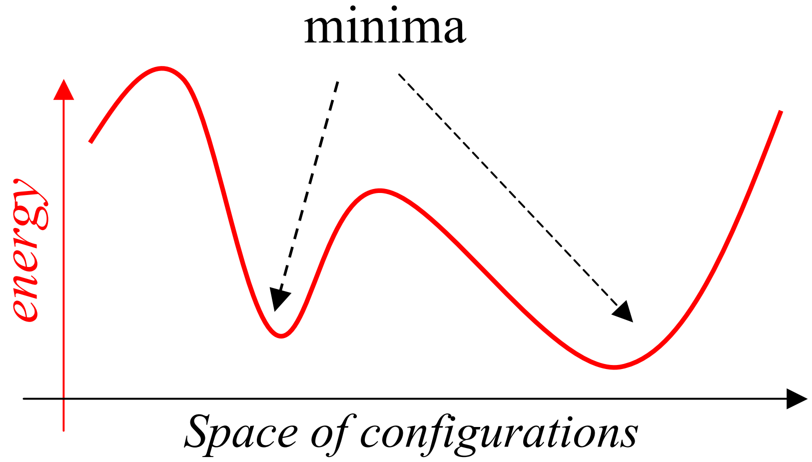
long range interaction

Others contributions : surface coupling, ….

Micromagnetic equations $\vec{m}(\vec{r})$

- **magnetization distribution**

$$\vec{m} = \left\{ \vec{m}(\vec{r}) \mid \vec{r} \in V, |\vec{m}| = 1 \right\}$$



- **total free energy functional**

$$E[\vec{m}] = \int_V \varepsilon(\vec{m}) dV$$

- **magnetic stable state** = minimum of the total free energy functional

$$\vec{m} \to \vec{m} + \delta\vec{m}$$

$$\vec{m}^2 = 1$$

$$\vec{m} \cdot \delta\vec{m} = 0$$

$$\delta E[\vec{m}] = 0$$

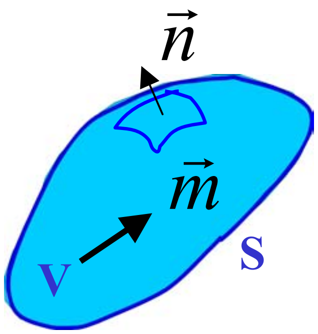
$$\delta^2 E[\vec{m}] > 0$$

$\Leftarrow$ **variational principle**

Micromagnetic equations – static equilibrium equations

$$\delta E = -\mu_0 M_s \int_V \boxed{\left(\vec{m}\times\vec{H}_{eff}\right)}\cdot\delta\vec{\theta}\; dV + 2A_{ex}\oint_S \boxed{\left(\vec{m}\times\frac{\partial\vec{m}}{\partial n}\right)}\cdot\delta\vec{\theta}\, dS$$

$$\delta\vec{m} = \delta\vec{\theta}\times\vec{m}$$



- **effective field**

$$\delta E = -\mu_0 M_s \int_V \delta\vec{m}\cdot\vec{H}_{eff}\, dV$$

$$\vec{H}_{eff} = \frac{2A_{ex}}{\mu_0 M_s}\Delta\vec{m} + \frac{2K_1}{\mu_0 M_s}\left(\vec{u}_K\cdot\vec{m}\right)\vec{u}_K + \vec{H}_{app} + \vec{H}_D + C\vec{m}$$

- **Brown’s equations**

$$\left[\vec{m}\times\vec{H}_{eff}\right]\left(\vec{r}\right) = \vec{0}\quad \forall\vec{r}\in V$$

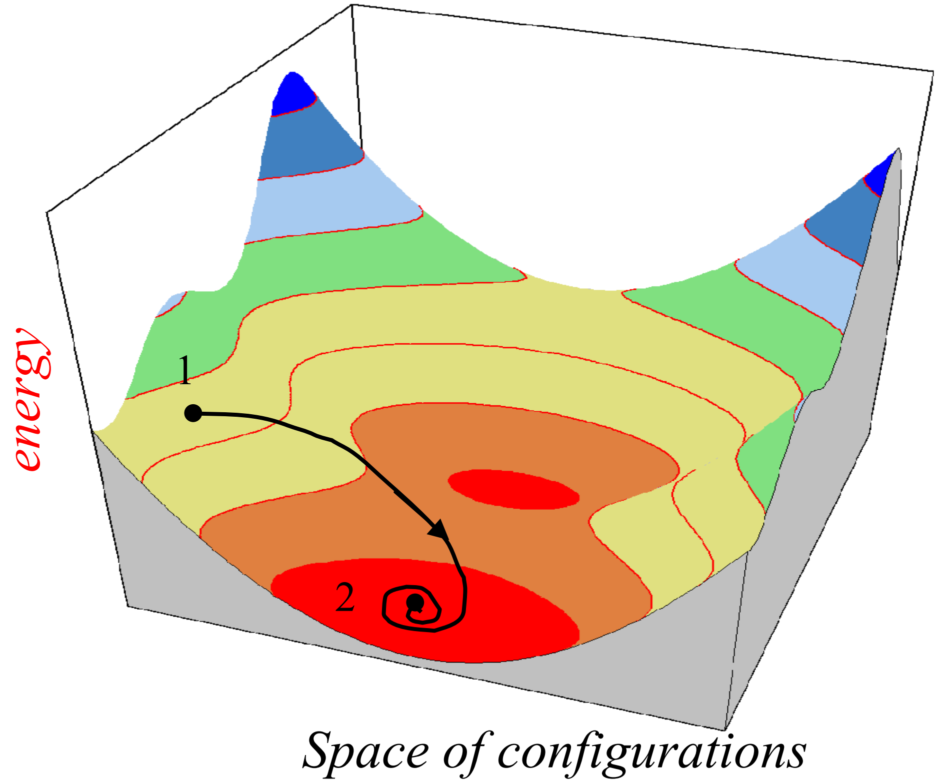
$$\frac{\partial\vec{m}}{\partial n} = 0,\ \vec{r}\in S$$

$$A_{ex,1}\frac{\partial\vec{m}_1}{\partial n} = A_{ex,2}\frac{\partial\vec{m}_2}{\partial n},\ \vec{r}\in S$$

i A. Hubert, R. Schäfer : *Magnetic Domains* (p. 149)
J. Miltat in *Applied Magnetism* (p. 221)

Micromagnetic equations $\vec{m}(\vec{r}, t)$

- **space & time dependence** $\rightarrow$ $\vec{m} = \left\{ \vec{m}(\vec{r},t) \mid \vec{r} \in V, t \geq 0, |\vec{m}| = 1 \right\}$

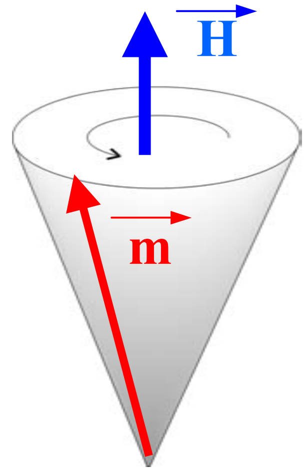


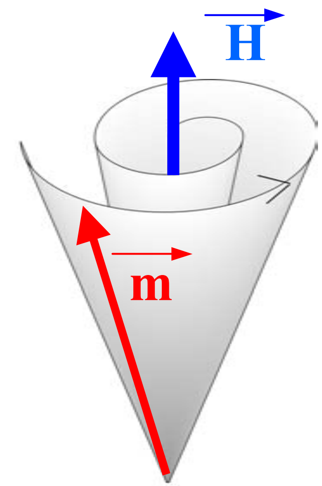
- **magnetization trajectory between two magnetic states**

Micromagnetic equations - dynamics

Landau-Lifshitz-Gilbert Equation (LLG)

$$(1+\alpha^2)\frac{\partial \vec{m}}{\partial t} = \overbrace{-\gamma\left(\vec{m}\times\mu_0\vec{H}_{eff}\right)}^{\text{precession}} \overbrace{-\ \alpha\gamma\left[\vec{m}\times\left(\vec{m}\times\mu_0\vec{H}_{eff}\right)\right]}^{\text{relaxation}}$$



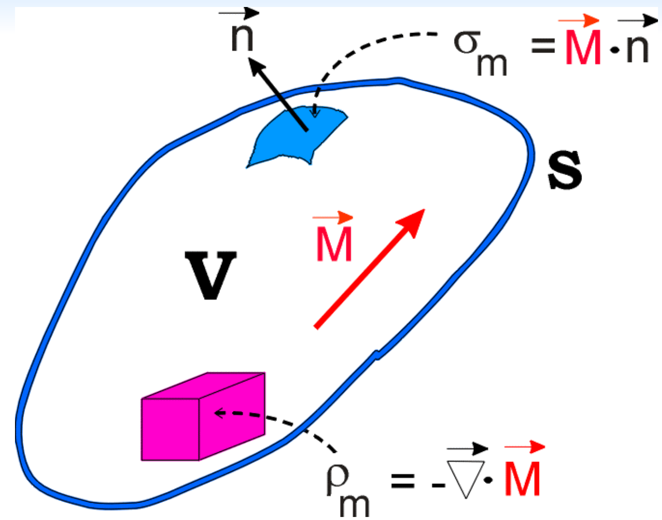


γ = gyromagnetic ratio $\qquad \gamma = \dfrac{g|e|}{2m_e} > 0 \qquad \gamma_0 = \mu_0\gamma = g\times 1.105\times 10^5\ m/(As)$

g = Landé factor $\qquad g \cong 2$

α = damping parameter $\qquad \alpha \cong 0.001 \div 1.0$

Magnetostatic Equations



- **Scalar potential formalism:** $\vec{H}_D = -\vec{\nabla}\phi$

3D $$\begin{cases} \Delta\phi(\vec{r}) = -\rho_m(\vec{r}) & \\ \phi_{\text{int}}(\vec{r}) = \phi_{ext}(\vec{r}) & \vec{r} \in S \\ \vec{n}\cdot\vec{\nabla}\left[\phi_{\text{int}} - \phi_{ext}\right](\vec{r}) = \sigma_m(\vec{r}) & \vec{r} \in S \\ \phi(\vec{r}) \to 0,\ |\vec{r}| \to \infty & \end{cases}$$

- **Green's function formalism :** $G(\vec{r}) = \dfrac{1}{4\pi|\vec{r}|}$ **&** $\vec{\nabla}G(\vec{r}) = -\dfrac{\vec{r}}{4\pi|\vec{r}|^3}$

$$\phi(\vec{r}) = \int_V \rho_m(\vec{r}\,')G(\vec{r}-\vec{r}\,')dV' + \oiint_S \sigma_m(\vec{r}\,')G(\vec{r}-\vec{r}\,')dS' \quad \vec{r} \in \Re^3$$

$$\vec{H}_D(\vec{r}) = \boxed{-\int_V \vec{\nabla}G(\vec{r}-\vec{r}\,')\rho_m(\vec{r}\,')dV'} \boxed{-\oiint_S \vec{\nabla}G(\vec{r}-\vec{r}\,')\sigma_m(\vec{r}\,')dS'}$$

i J. D. Jackson : *Classical electrodynamics*, New York (1962)

General Algorithm

$$\{\vec{m}(\vec{r},t_0)\}, K, A_{ex}, M_s, \vec{H}_{appl}$$

- Defining the problem
  - -geometry description
  - -material parameters
  - -initial conditions (time & space)

$$\rho = -\vec{\nabla}\cdot\vec{M}\,,\ \sigma = \vec{n}\cdot\vec{M}\,,\ \partial\vec{m}/\partial n = 0$$

$$\vec{H}_{eff} = \vec{H}_{app} + \vec{H}_D + \vec{H}_{ex} + \vec{H}_k$$

$$\varepsilon = \varepsilon_H + \varepsilon_D + \varepsilon_{ex} + \varepsilon_k$$

- State characterization
  - -magnetic charges
  - -magnetostatic field
  - -fields & energy terms

$$(1+\alpha^2)\frac{\partial\vec{m}}{\partial t} = -\gamma\left(\vec{m}\times\mu_0\vec{H}_{eff}\right) - \alpha\gamma\left[\vec{m}\times\left(\vec{m}\times\mu_0\vec{H}_{eff}\right)\right]$$

- LLG time integration
  - - amplitude conservation

$$\left|\vec{m}\times\vec{H}_{eff}\right| / M_s^{\max} \le \varepsilon rr$$

- Check equilibrium criteria

false: t→t+δt

true:

$$\{\vec{m}\}_{eq},\ E_{eq}$$

- Stable state- numerical solution

Solution

static & dynamic equations

✓non-linear $\leftarrow$ $|\vec{m}| = 1$

✓non-local $\leftarrow$ $\vec{H}_D$

✓coupled partial differential $\leftarrow$ ∂, ∂^2

Second order integro-differential equations

analytical treatment

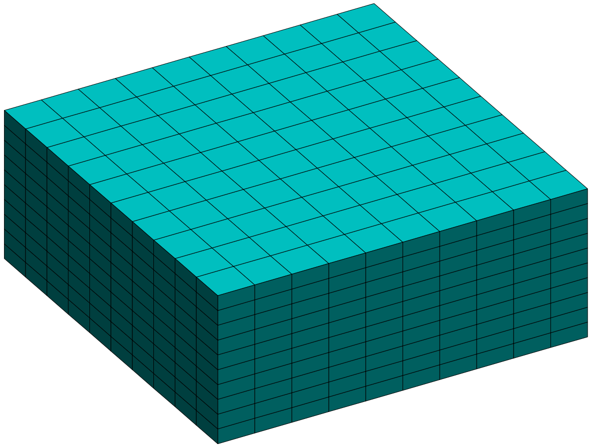
- macrospin approximation
- Bloch domain wall in bulk
- by linearisation
  - near the saturation limit
  - nucleation and switching of domains
  - ferromagnetic resonance

numerical treatment

- powerful and efficient tools (if some rules are respected!)

Current State of the Art

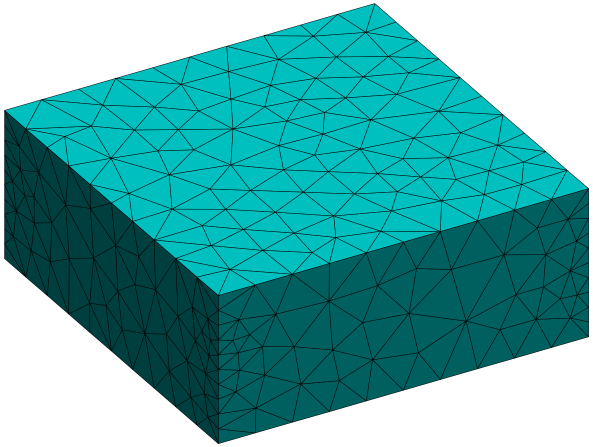
- Finite difference approximation (FDA)



-regular mesh
-restrictive geometry

W.F. Brown Jr (1965)
Schabes et al., (1988)
Berkov et al.
Bertram et al.
Donahue et al.
Miltat et al.
Nakatani et al.
Toussaint et al.
Scheinfein et al.
J. -G. Zhu et al.…………

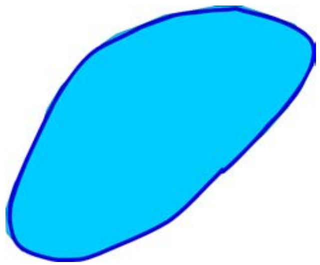
- Finite element method (FEM / BEM)



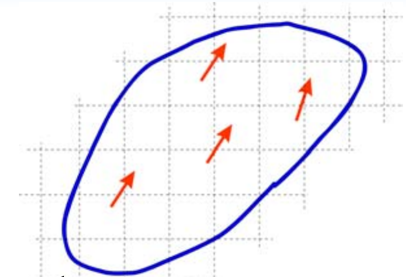
-irregular meshes
-adaptive mesh refinement

Fredkin & Koehler
Fidler & Schrefl
Hertel & Kronmuller
Ramstöck et al.
…….

Finite Difference Approximation (FDA)



Numerical discretisation



$$\vec{m} = \{ \vec{m}(\vec{r}) \mid \vec{r} \in V, |\vec{m}| = 1 \}$$

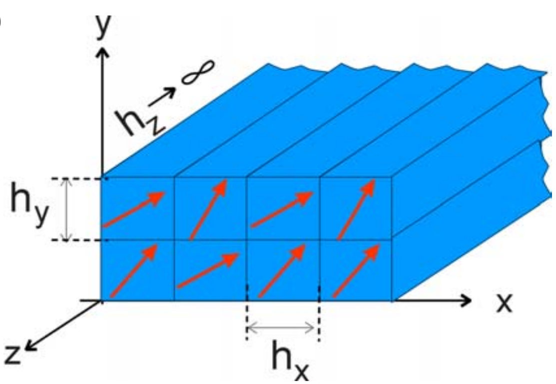
$$\vec{H}_{eff} = \{ \vec{H}_{eff}(\vec{r}) \mid \vec{r} \in V \}$$

$$\vec{m} = \{ \vec{m}_i \mid i = 1..N, |\vec{m}_i| = 1 \}$$

$$\vec{H}_{eff} = \{ \vec{H}_{eff,i} \mid i = 1..N \}$$

N – total number of mesh nodes

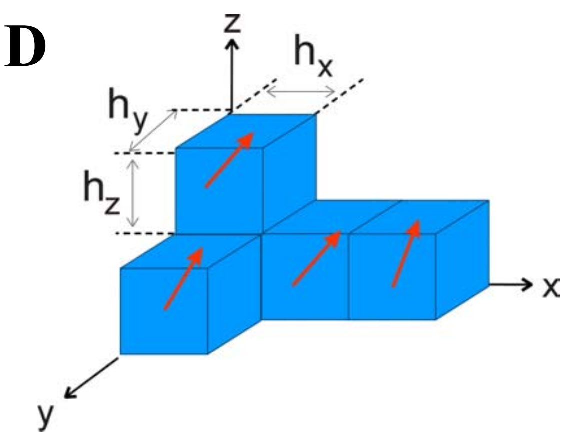
2D



-infinite prisms

: e.g. thin films

3D



-orthorhombic cells

: dots, wires, platelets, …

Finite Difference Aproximation (FDA)

$$E[\vec{m}]=\int_V \left\{ \begin{array}{l} A_{ex}\left[\vec{\nabla}\vec{m}(\vec{r})\right]^2+K_1\left[1-\left(\vec{u}_K\cdot\vec{m}(\vec{r})\right)^2\right]- \\ -\mu_0 M_s\left[\vec{m}(\vec{r})\cdot\vec{H}_{app}(\vec{r})\right]-\frac{1}{2}\mu_0 M_s\left[\vec{m}(\vec{r})\cdot\vec{H}_{dem}(\vec{m}(\vec{r}))\right] \end{array} \right\} dV$$

$$\vec{H}_{eff}=\frac{2A_{ex}}{\mu_0 M_s}\Delta\vec{m}+\frac{2K_1}{\mu_0 M_s}\left(\vec{u}_K\cdot\vec{m}\right)\vec{u}_K+\vec{H}_H+\vec{H}_D$$

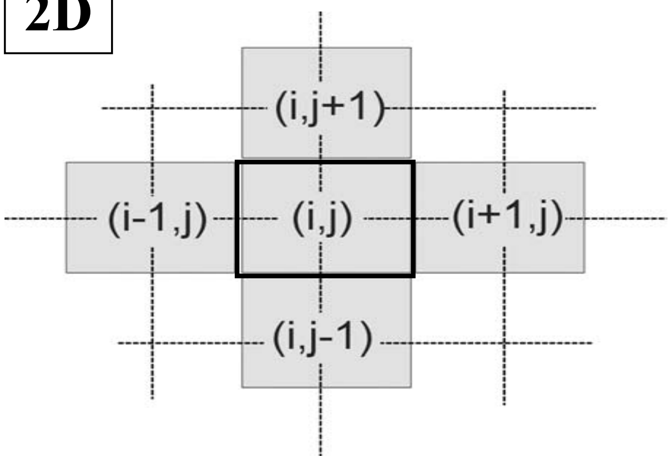
magnetic charges

$$\rho_m=-M_s\left(\vec{\nabla}\cdot\vec{m}\right)$$

$$\sigma_m=M_s\left(\vec{m}\cdot\vec{n}\right)$$

Taylor expansion

2D



$$m(i+1,j)=m(i,j)+\frac{\partial m}{\partial x}(i,j)h_x+\frac{1}{2}\frac{\partial^2 m}{\partial x^2}(i,j)h_x^2+O(h_x^3)$$

$$m(i-1,j)=m(i,j)-\frac{\partial m}{\partial x}(i,j)h_x+\frac{1}{2}\frac{\partial^2 m}{\partial x^2}(i,j)h_x^2+O(h_x^3)$$

$$\frac{\partial m}{\partial x}(i,j)\cong\frac{m(i+1,j)-m(i-1,j)}{2h_x}$$

$$\frac{\partial^2 m}{\partial x^2}(i,j)\cong\frac{m(i+1,j)-2m(i,j)+m(i-1,j)}{h_x^2}$$

The accuracy is dependent on the Taylor expansion order !

i M. Labrune, J. Miltat, JMMM **151**, 231 (1995).

General Algorithm

$$\{\vec{m}(\vec{r},t_0)\}, K, A_{ex}, M_s, \vec{H}_{appl}$$

$$\downarrow$$

$$\rho = -\vec{\nabla}\cdot\vec{M},\ \ \sigma = \vec{n}\cdot\vec{M},\ \ \partial\vec{m}/\partial n = 0$$

$$\vec{H}_{eff} = \vec{H}_{app} + \vec{H}_D + \vec{H}_{ex} + \vec{H}_k$$

$$\varepsilon = \varepsilon_H + \varepsilon_D + \varepsilon_{ex} + \varepsilon_k$$

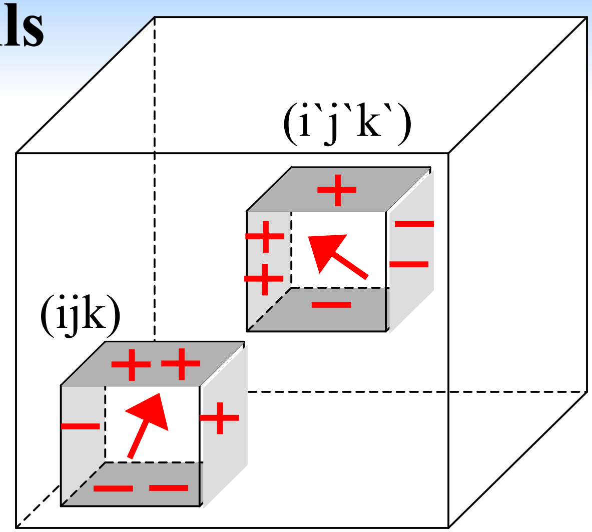
- Defining the problem
  -geometry description
  -material parameters
  -initial conditions
  (time & space)
- State characterization
  -magnetic charges
  -magnetostatic field
  -fields & energy terms

Exchange	$E_{ex}[\vec{m}],\ \vec{H}_{ex}[\vec{m}]$	*local terms direct evaluation*
Magnetocrystalline anisotropy	$E_K[\vec{m}],\ \vec{H}_K[\vec{m}]$	
Zeeman	$E_H[\vec{m}],\ \vec{H}_{app}[\vec{m}]$	
Magnetostatic	$E_D[\vec{m}],\ \vec{H}_D[\vec{m}]$	*long range interaction*

-the stray field energy calculation involves amounts up to
a six-fold integration (90% of the computation time)

Stray field (H_D) → constant magnetization cells

i W.F. Brown Jr., A.E. LaBonte: JAP 36, 1380 (1965)
A.E. LaBonte: J. Appl. Phys. 38, 3196 (1967)
Schabes et al., JAP **64**, 1347 (1988).



$$\vec{m}_{ijk} = cst$$

Volume charges $\cancel{\rho_m = -M_s\left(\vec{\nabla}\cdot\vec{m}\right)}$

Surface charges $\sigma_m = M_s\left(\vec{m}\cdot\vec{n}\right)$

$$E_D = \frac{\mu_0}{8\pi}\oiint_S\oiint_S \frac{\sigma_m(\vec{r})\sigma_m(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}dSdS' = \frac{1}{2}\mu_0 M_s^2 \sum_{I=1}^{Ncells} \vec{m}_I \cdot \left\langle \vec{H}_D \right\rangle_I V_{cell}$$

-mean stray field upon the cell I

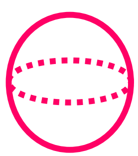
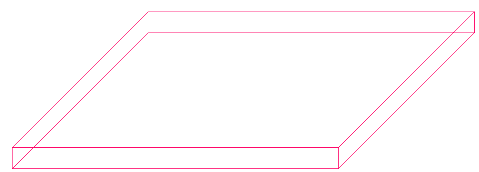
$$\left\langle \vec{H}_D(\vec{r}_I)\right\rangle = -M_s \sum_{J=1}^{N} \begin{pmatrix} N_{xx} & N_{xy} & N_{xz} \\ N_{yx} & N_{yy} & N_{yz} \\ N_{zx} & N_{zy} & N_{zz} \end{pmatrix}_{(\vec{r}_I-\vec{r}_J)} \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix}_{\vec{r}_J}$$

[N] = demagnetizing factor

Demagnetizing Factor (N)

$$\vec{H}_D = -\left[\overleftrightarrow{N}\right]\vec{M} = -\begin{pmatrix} N_{xx} & N_{xy} & N_{xz} \\ N_{yx} & N_{yy} & N_{yz} \\ N_{zx} & N_{zy} & N_{zz} \end{pmatrix}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix}$$

N is a tensor with the trace : $\mathrm{N}_{xx} + \mathrm{N}_{yy} + \mathrm{N}_{zz} = 1$

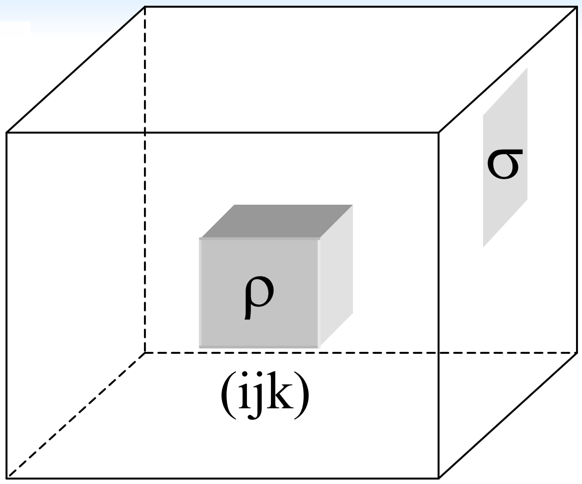
Sphere	**Thin film ∞**	**Cylinder ∞**
		
$\mathrm{N} = 1/3$	$\mathrm{N}_{\parallel} = 0$ $\mathrm{N}_{\perp} = 1$	$\mathrm{N}_{\parallel} = 0$ $\mathrm{N}_{\perp} = 1/2$

! General: a uniformly magnetized ferromagnetic body gives rise to a non-uniform stray field.

! Exception : the ellipsoid

Stray field (H_D) → volume + surface charges

K. Ramstöck et al., JMMM **135** , 97 (1994)



Volume charges $\rho_m = -M_s\left(\vec{\nabla}\cdot\vec{m}\right)$

Surface charges $\sigma_m = M_s\left(\vec{m}\cdot\vec{n}\right)$

Stray field evaluated in the center of each cell.

$$\vec{H}_D(\vec{r}_I) = -\sum_{J=1}^{Nvol}\int_{V_J}\vec{\nabla}G(\vec{r}_I-\vec{r}\,')\rho_m\left(\vec{r}\,'\right)dV' - \sum_{J}^{Nsurf}\oiint_{S_J}\vec{\nabla}G(\vec{r}_I-\vec{r}\,')\sigma_m\left(\vec{r}\,'\right)dS'$$

- Constant and/or linear volume and/or surface charges

- Evaluation of a sum with a huge number of terms : N X N terms !
  Computation time?

Fourier Transform implementation (TF)

$$\vec{H}_D(\vec{r}) = -\int_V \vec{\nabla} G(\vec{r}-\vec{r}\,')\rho_m(\vec{r}\,')dV' - \oint_S \vec{\nabla} G(\vec{r}-\vec{r}\,')\sigma_m(\vec{r}\,')dS'$$

$$\vec{H}_D(\vec{r}) = -\left[\vec{\nabla} G \otimes \rho_m\right](\vec{r}) - \left[\vec{\nabla} G \otimes \sigma_m\right](\vec{r})$$

Theorem of the Convolution Product

$f, g : \left[-\infty, +\infty\right] \rightarrow \Re$

$$(f \otimes g)(x) = \int_{-\infty}^{+\infty} g(x-x')f(x')dx'$$

$$\Rightarrow \quad \mathrm{TF}\left[f \otimes g\right] = \mathrm{TF}\left[f\right] \cdot \mathrm{TF}\left[g\right]$$

1 $\mathrm{TF}\left[\vec{\nabla} G\right]$

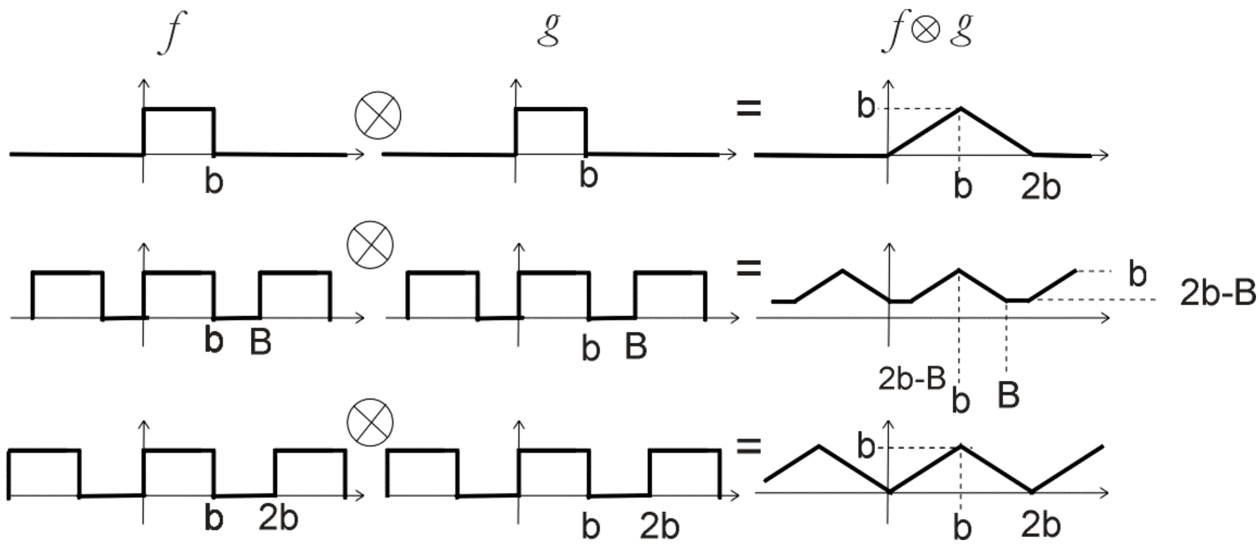
2 $\rho_m(\vec{r})$, $\sigma_m(\vec{r})$

3 $\mathrm{TF}[\rho_m]$, $\mathrm{TF}[\sigma_m]$

4 $\vec{H}_D = \mathrm{TF}^{-1}\left[TF\left[\vec{\nabla} G\right] \cdot TF\left[\rho_m\right] + TF\left[\vec{\nabla} G\right] \cdot TF\left[\sigma_m\right]\right]$

Discrete Fourier Transform & FFT

-Discrete functions (charges, interaction function,..)
-Discrete Fourier Transform → periodicity
-Zero padding technique allows to deal with non-periodic systems



- no. operations / iteration ↘ $N^2 \rightarrow N \log_2 N$

  N*=*8* X *8* X *8 ***262144 → 4607***

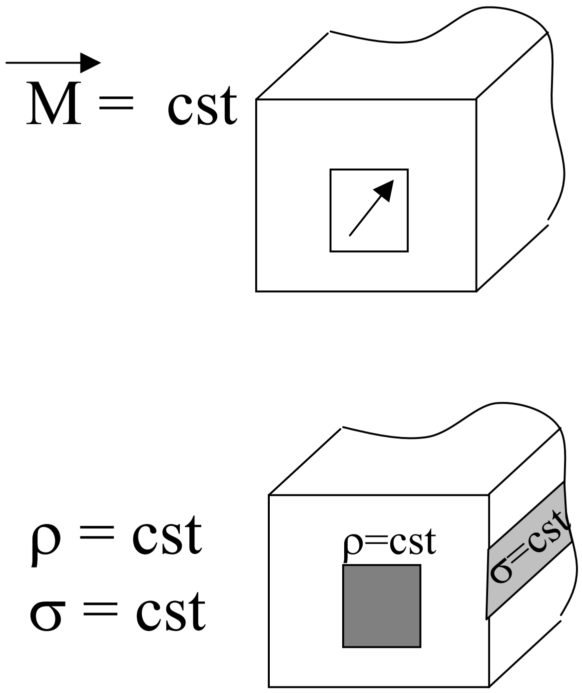
- $\mathrm{TF}\left[\vec{\nabla} G\right]$ is evaluated once at the beginning of the simulation

- regular mesh & double the size of the real system

i **FFT** - T.W.Cooley et al, (1965); **FFTW** - M. Frigo et al, MIT, (1997)

Stray field (H_D) – comparison

D. Berkov et al., IEEE Trans. Mag. **29**(6) 2548 (1993)



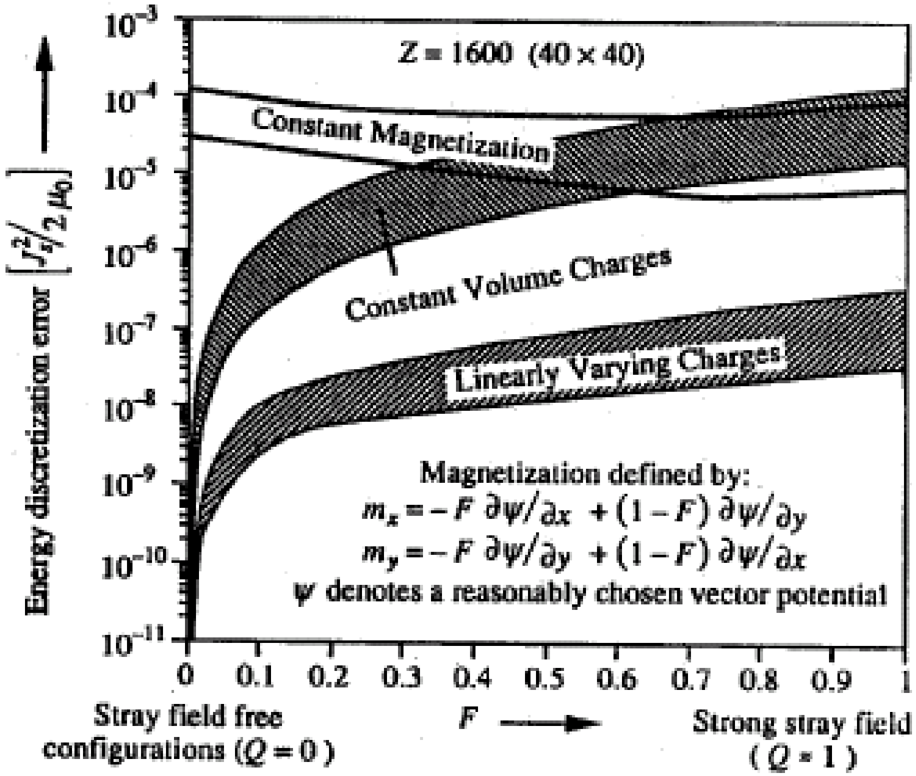


Fig. 1. Energy discretization error for configurations as defined in the inset where the parameter F generates a completely stray-field-free configuration for $F = 0$ and configurations of strong field for $F = 1$. The bands indicate the range of results obtained for many computer experiments.

Soft magnetic material : constant volume charges is the appropriated approximation!

- package **GL_FFT®** by JC Toussaint (LLN)

General Algorithm

$$\{\vec{m}(\vec{r}, t_0)\}, K, A_{ex}, M_s, \vec{H}_{appl}$$

$$\rho = -\vec{\nabla} \cdot \vec{M}, \ \sigma = \vec{n} \cdot \vec{M}, \ \partial\vec{m}/\partial n = 0$$

$$\vec{H}_{eff} = \vec{H}_{app} + \vec{H}_D + \vec{H}_{ex} + \vec{H}_k$$

$$\varepsilon = \varepsilon_H + \varepsilon_D + \varepsilon_{ex} + \varepsilon_k$$

$$(1+\alpha^2)\frac{\partial\vec{m}}{\partial t} = -\gamma\left(\vec{m} \times \mu_0 \vec{H}_{eff}\right) - \alpha\gamma\left[\vec{m} \times \left(\vec{m} \times \mu_0 \vec{H}_{eff}\right)\right]$$

- Defining the problem
  -geometry description
  -material parameters
  -initial conditions
  (time & space)
- State characterization
  -magnetic charges
  -magnetostatic field
  -fields & energy terms
- LLG time integration
  - amplitude conservation

LLG integration scheme & numerical stability

Explicit scheme

$$\frac{\partial \vec{m}}{\partial \tau} = -\vec{m}(\tau)\times\vec{H}(\tau)$$

$$\tau = \frac{\mu_0 \gamma t}{1+\alpha^2}$$ ← normalized time

$$\vec{H}(\tau) = \vec{H}_{eff}(\tau) + \alpha\ \vec{m}(\tau)\times\vec{H}_{eff}(\tau)$$

$$\boxed{\vec{m}(\tau+\delta\tau) = \vec{m}(\tau)\cos(H\delta\tau) + \frac{\sin(H\delta\tau)}{H}\left[\vec{H}\times\vec{m}(\tau)\right] + (1-\cos(H\delta\tau))\frac{\vec{H}\cdot\vec{m}(\tau)}{H^2}\vec{H}}$$

- Amplitude of the magnetization is implicitly conserved. $|\vec{m}| = 1$
- The field $\vec{H}(t)$ varies slowly in time.
- Fast integration method
- von Neumann analysis → critical time step for stability $\delta t < \frac{1}{2}\frac{\alpha}{\gamma\mu_0 M_s}\left(\frac{h}{l_{ex}}\right)^2$

$$\alpha = 0.1,\ M_s = 8\times10^5\ A/m\ ,\ \ h/l_{ex} = 1/2 \Longrightarrow \delta t_{\lim} \cong 70\ fs$$

Toussaint et al., *Proceedings of the 9th International Symposium Magnetic Anisotropy and Coercivity in Rare-Earth Transition Metal Alloys 2, 59 (1996)*

General Algorithm

$$\{\vec{m}(\vec{r},t_0)\}, K, A_{ex}, M_s, \vec{H}_{appl}$$

$$\rho = -\vec{\nabla}\cdot\vec{M},\ \ \sigma = \vec{n}\cdot\vec{M},\ \ \partial\vec{m}/\partial n = 0$$

$$\vec{H}_{eff} = \vec{H}_{app} + \vec{H}_D + \vec{H}_{ex} + \vec{H}_k$$

$$\varepsilon = \varepsilon_H + \varepsilon_D + \varepsilon_{ex} + \varepsilon_k$$

$$(1+\alpha^2)\frac{\partial\vec{m}}{\partial t} = -\gamma\left(\vec{m}\times\mu_0\vec{H}_{eff}\right) - \alpha\gamma\left[\vec{m}\times\left(\vec{m}\times\mu_0\vec{H}_{eff}\right)\right]$$

$$\left|\vec{m}\times\vec{H}_{eff}\right| / M_s^{\max} \le \varepsilon rr$$

false: $t \rightarrow t+\delta t$

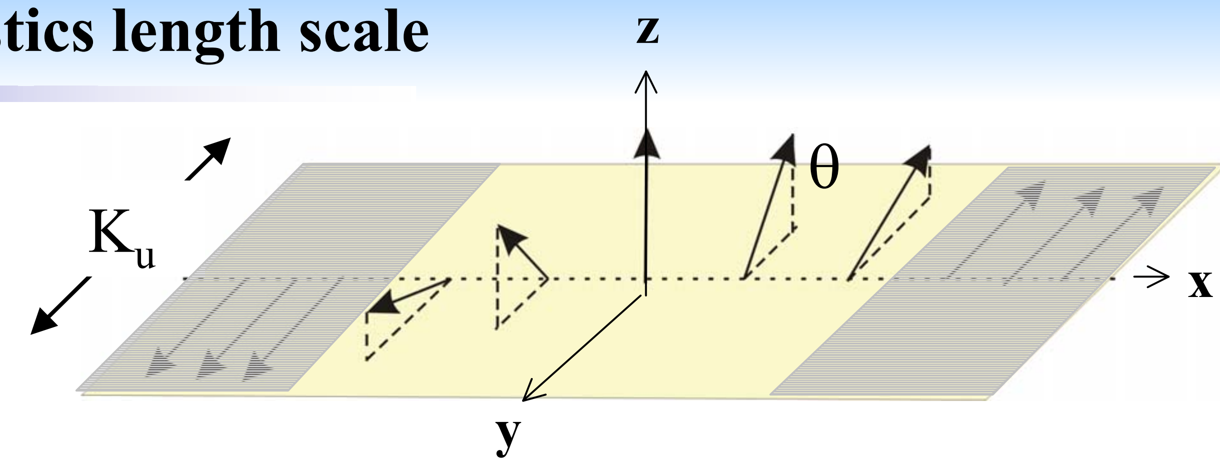
true:

$$\{\vec{m}\}_{eq},\ E_{eq}$$

- Defining the problem
  -geometry description
  -material parameters
  -initial conditions
  (time & space)
- State characterization
  -magnetic charges
  -magnetostatic field
  -fields & energy terms
- LLG time integration
  - amplitude conservation
- Check equilibrium criteria
- Stable state- numerical solution

Mesh size & characteristics length scale

Bloch wall parameter



$$\Delta_0 = \sqrt{\frac{A_{ex}}{K_u}}$$

Infinite Bloch wall

$$\varepsilon(\theta) = K_u (\sin\theta)^2 + A_{ex}\left(\frac{\partial\theta}{\partial x}\right)^2 \Rightarrow \theta(x) = \pm 2 \arctan\left[\exp\left(\frac{x}{\Delta_0}\right)\right]$$

Exchange length

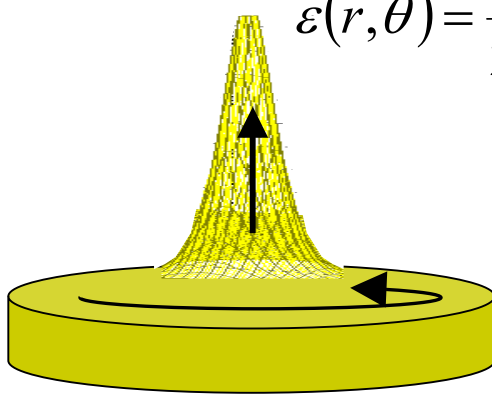
$$l_{ex} = \sqrt{\frac{2A_{ex}}{\mu_0 M_s^2}}$$

$$\varepsilon(r,\theta) = \frac{1}{2}\mu_0 M_s^2 (\cos\theta)^2 + A_{ex}\left(\frac{\partial\theta}{\partial x}\right)^2 + \frac{1}{r^2} A_{ex} (\sin\theta)^2$$

$$\Downarrow$$

$$\theta(r) \cong \arccos\left[\exp\left(-\frac{r}{l_{ex}}\right)\right]$$

‘vortex’ in a full disk



! Mesh size < Δ_0 , l_{ex}

	M_s(A/m)	A_{ex}(J/m)	K_u(J/m^3)	Δ_0 (nm)	l_{ex}(nm)
Co	1400 X 10^3	(1.5÷3) X 10^{-11}	500 X 10^3	5.5 ÷ 7.7	3.4 ÷ 4.8
NiFe	800 X 10^3	1. X 10^{-11}	1 X 10^3	100.	4.9

Validation Tests

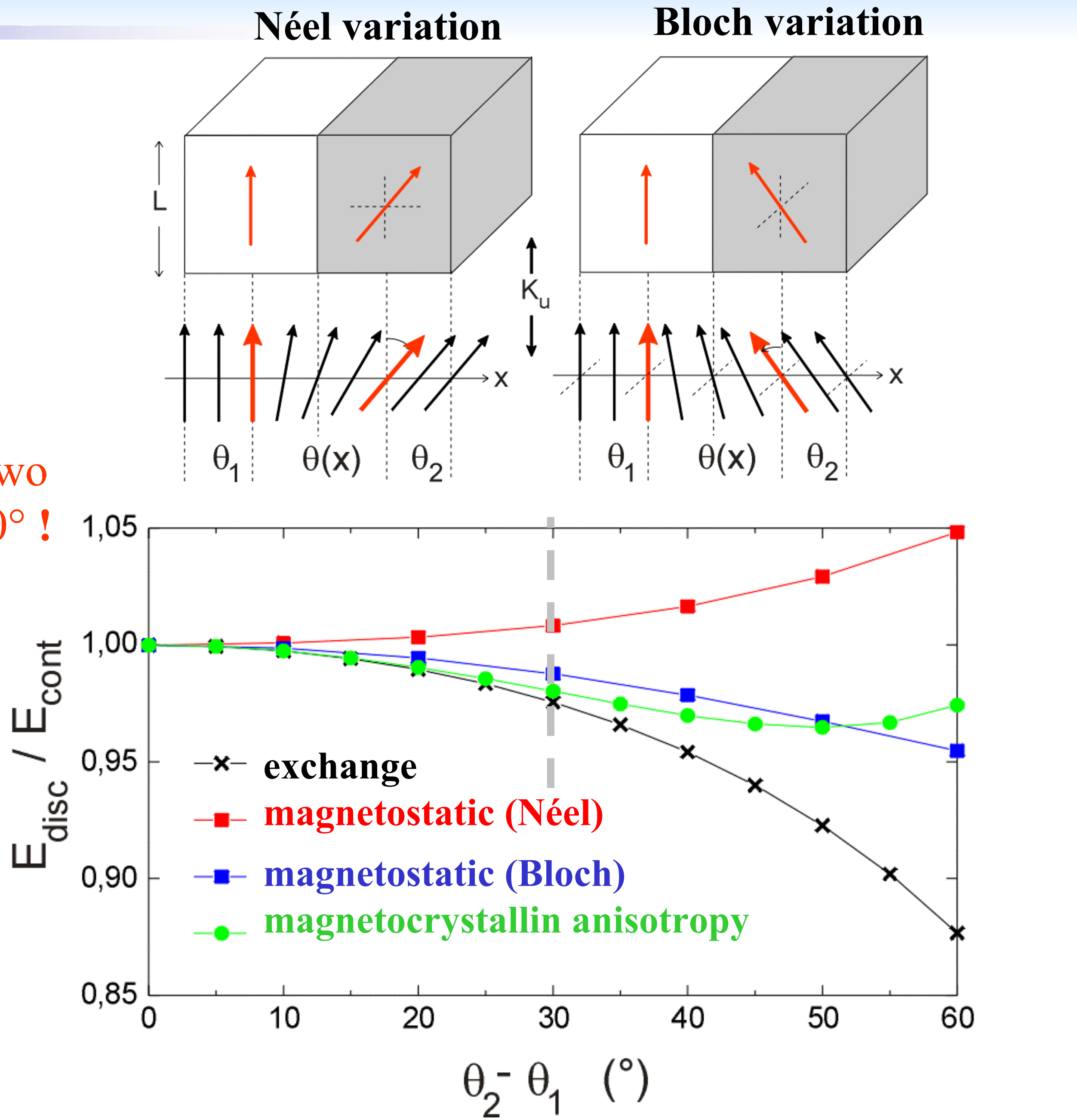
Numerical results
&
Analytical results

↓

Angular deviation between two adjacent cells smaller than 30° !

$$|\theta_2 - \theta_1| < 30°$$

$$err < 5\%°$$



Mesh effects

Vortex state in a circular dot

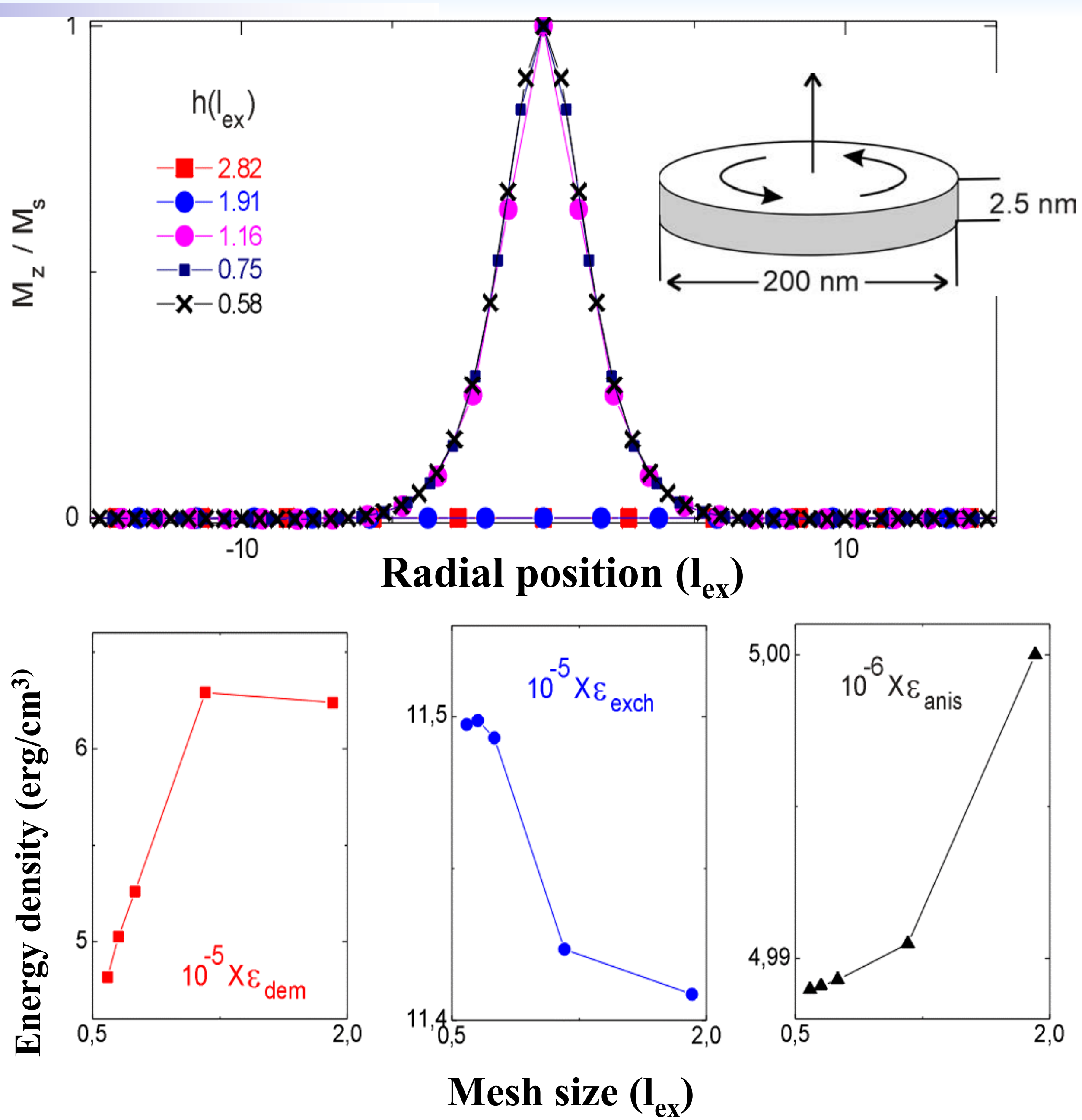
$$M_s = 1400\times10^3\, A/m$$

$$K_u = 500\times10^3\, J/m^3$$

$$A_{ex} = 1.4\times10^{-11}\, J/m$$

$$\Delta_0 = 5.29\, nm$$

$$l_{ex} = 3.37\, nm$$



Validation tests

Standard problems (NIST)

Standard problem 1,2,3: static calculus

Standard problem 4 : dynamic calculus

http://www.ctcms.nist.gov/~rdm/mumag.org.html

Simulation & experience

MFM, Lorentz microscopy,....

Magnetization curves…

Check points

Check different equilibrium criteria…

Check different discretisations (doest it converge smoothly to limit value…

Check different field steps…

Break the symmetry…

Free Open Source & Commercial software

- **OOMMF** (Object Oriented MicroMagnetic Framework), **M.Donahue** & **D. Porter**
  http://math.nist.gov/oommf/

  SimulMag (PC Micromagnetic Simulator), developed by **J. Oti**
  http://math.nist.gov/oommf/contrib/simulmag/

  GDM2 (General Dynamic Micromagnetics), developed by **B. Yang**
  http://physics.ucsd.edu/~drf/pub/

- **LLG** Micromagnetics **Simulator**, developed by **M. R. Scheinfein**
  http://llgmicro.home.mindspring.com/

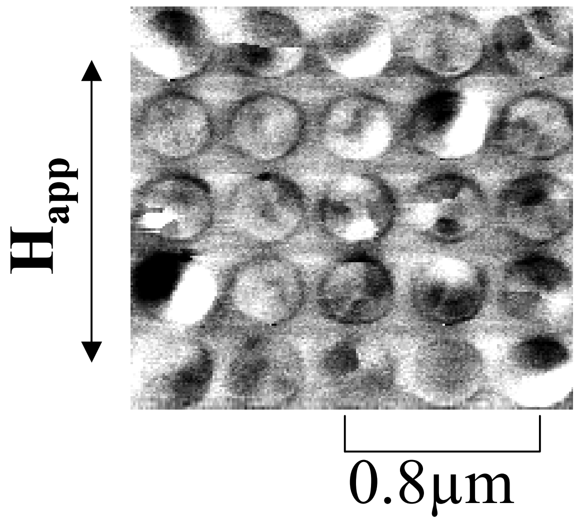
  MagFEM3D, developed by **K. Ramstöck**
  http://www.ramstock.de/

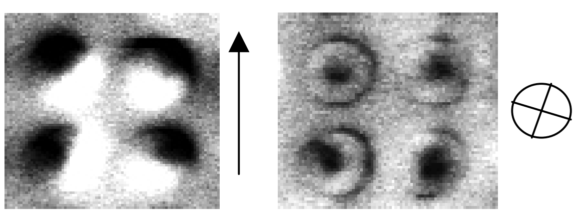
  MicroMagus, developed by **D. V. Berkov, N. L. Gorn**
  http://www.micromagus.de/

  Magsimus, Euxine Technologies
  http://www.euxine.com/

Circular Co Disks

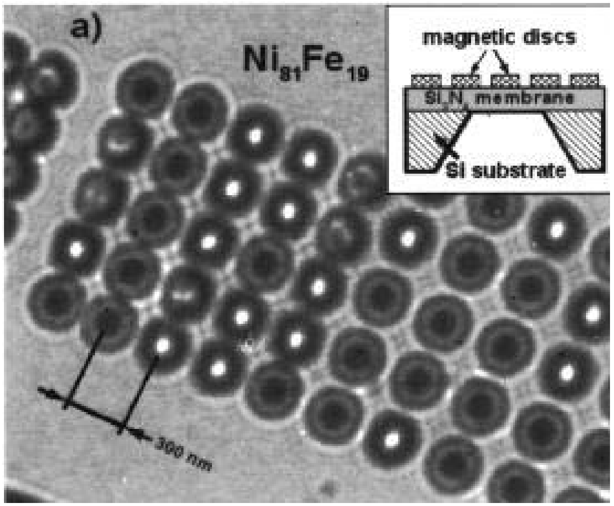
Co(0001)



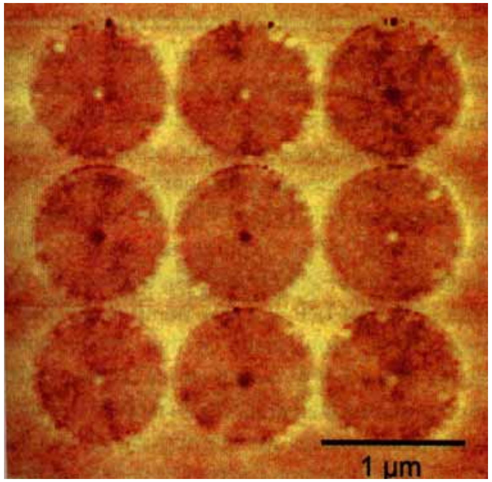


M. Demand et al. JAP. **87**, 5111 (2000)

NiFe

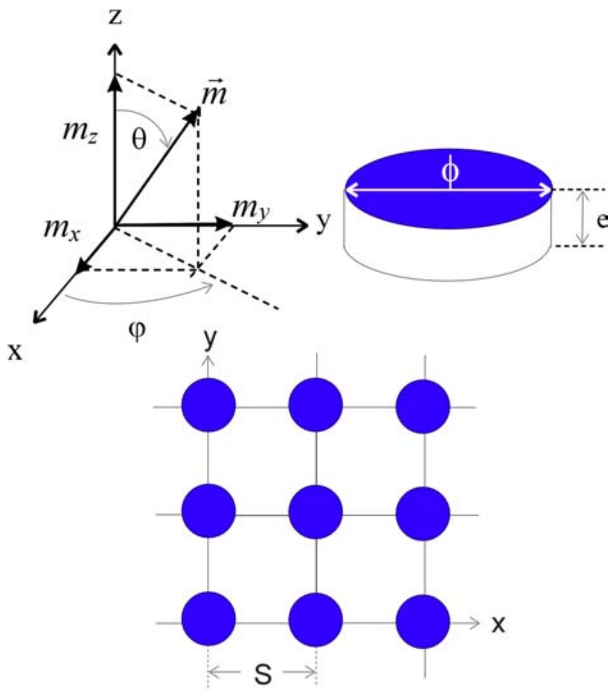


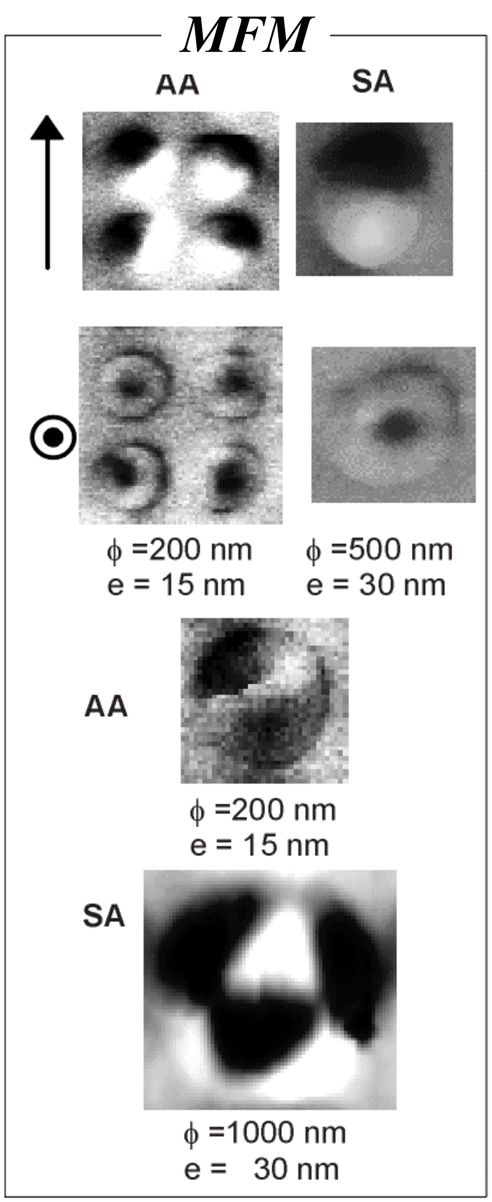
J. Raabe et al. JAP **88**, 4437 (2000)

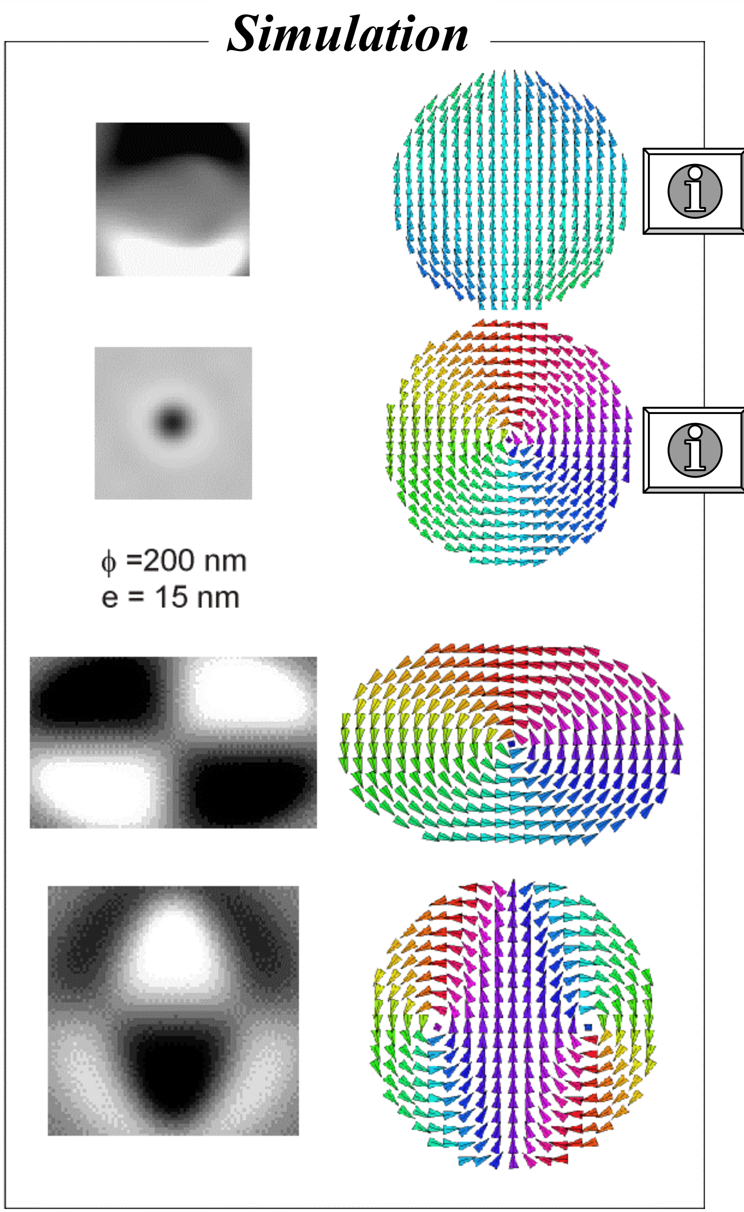


T. Shinjo et al. Science **289**, 930 (2000)

Magnetic Stable States







Material Parameters

$$M_s = 1400 \times 10^3 \, A/m$$

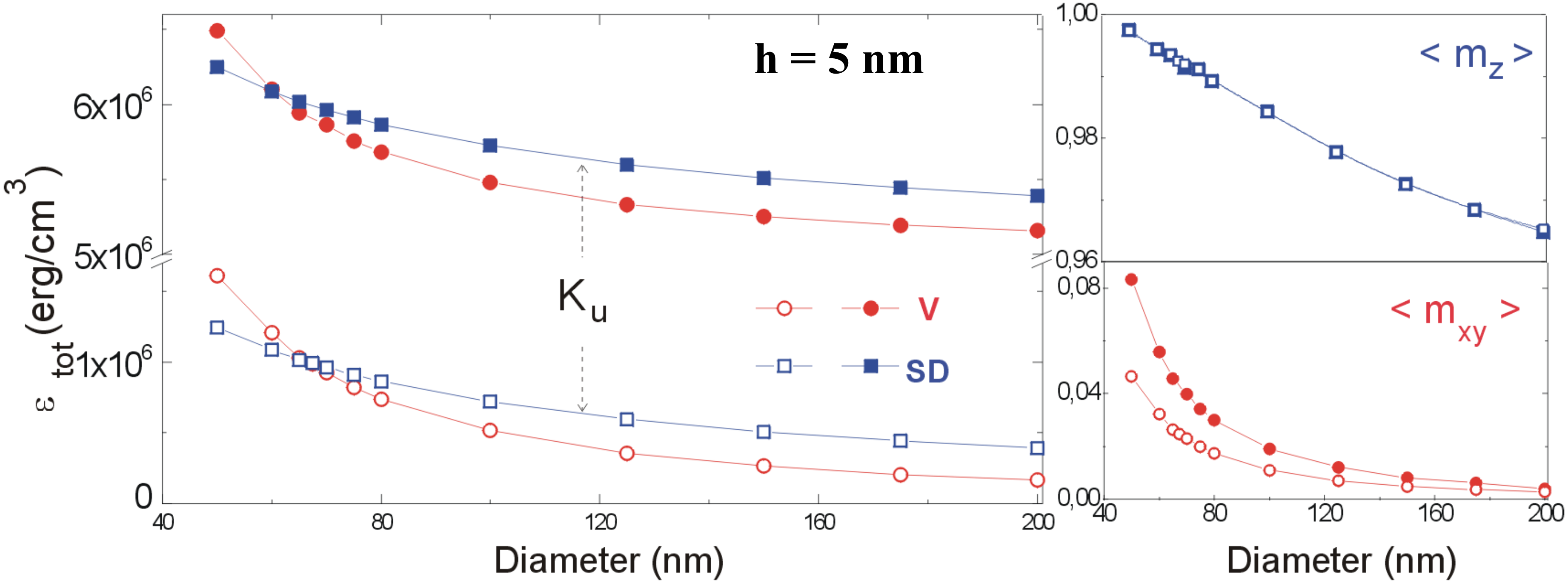
$$A_{ex} = 1.4 \times 10^{-11} \, J/m$$

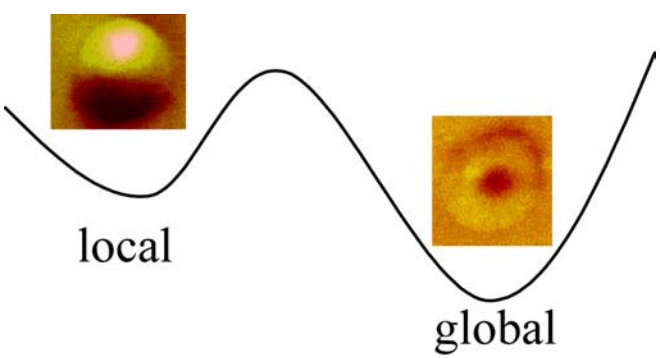
$$K_u = 500 \times 10^3 \, J/m^3$$

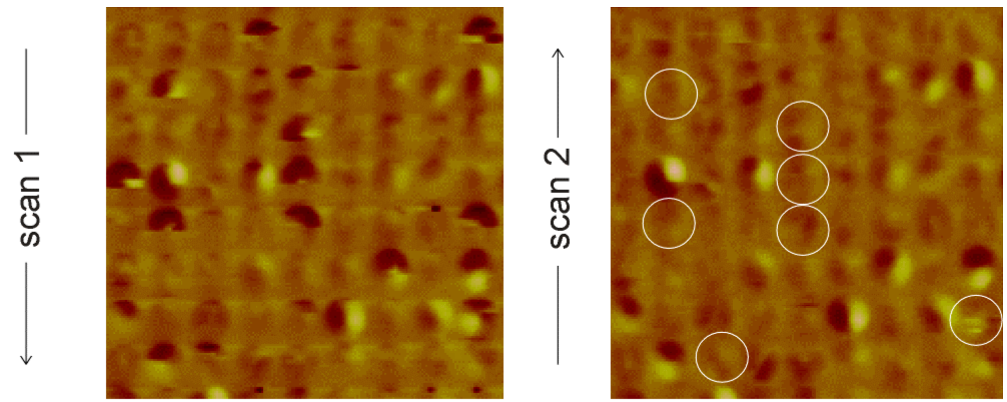
$$h_x = h_y = h_z = 2.5 \, nm$$

i Demand et al., JAP (2000), Prejbeanu Ph.D. thesis, Natali et al. PRL(2002)

Sizes & energies



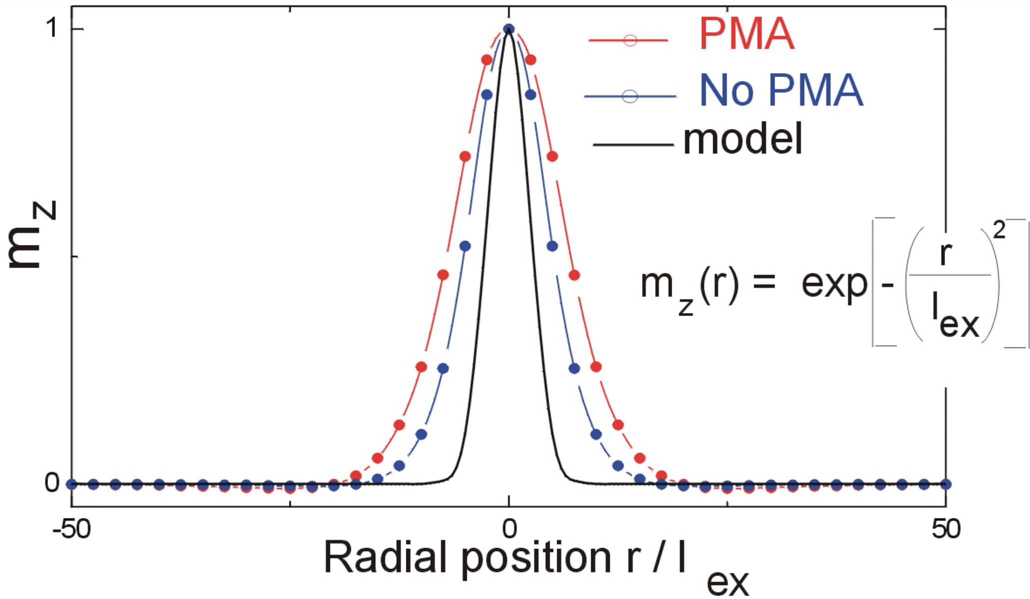




Lift scan height 50nm

ϕ= 200 nm
h = 15 nm

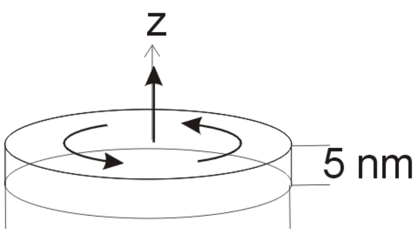
Internal vortex structure

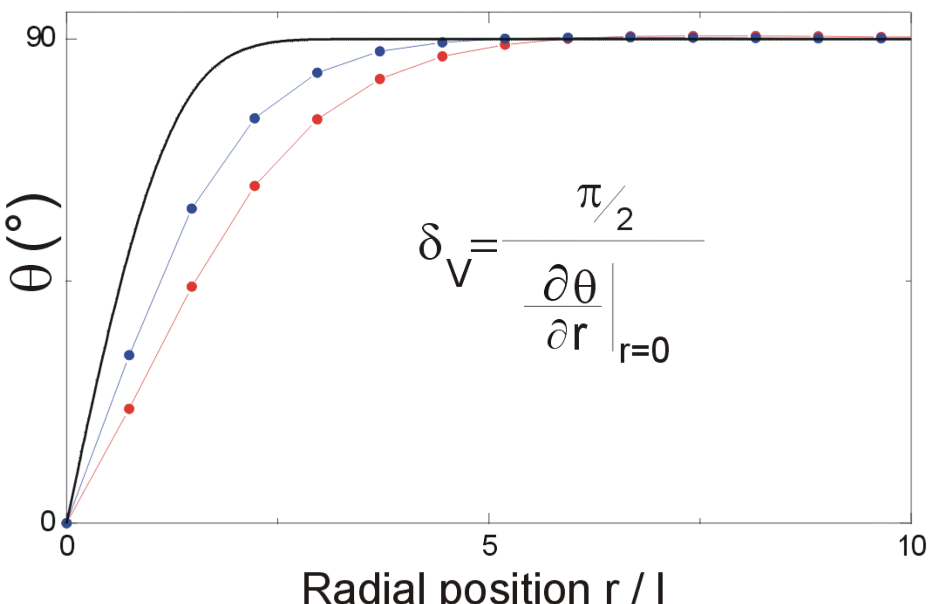


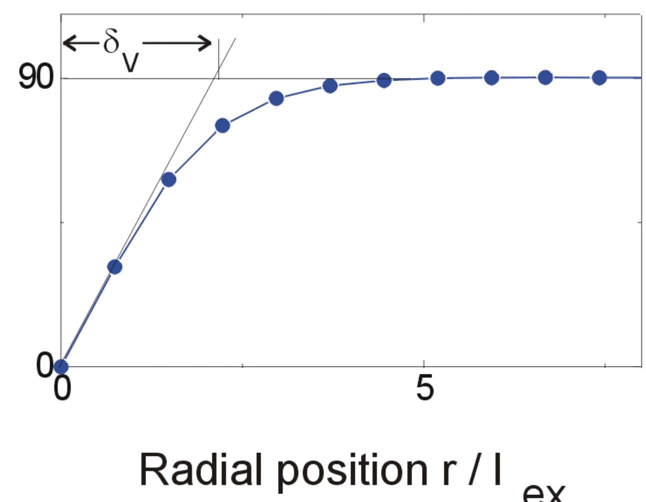
$$\left(K_u \neq 0 \;\;\&\;\; K_u \perp\right)$$

$$\downarrow$$

enhancement of the vortex

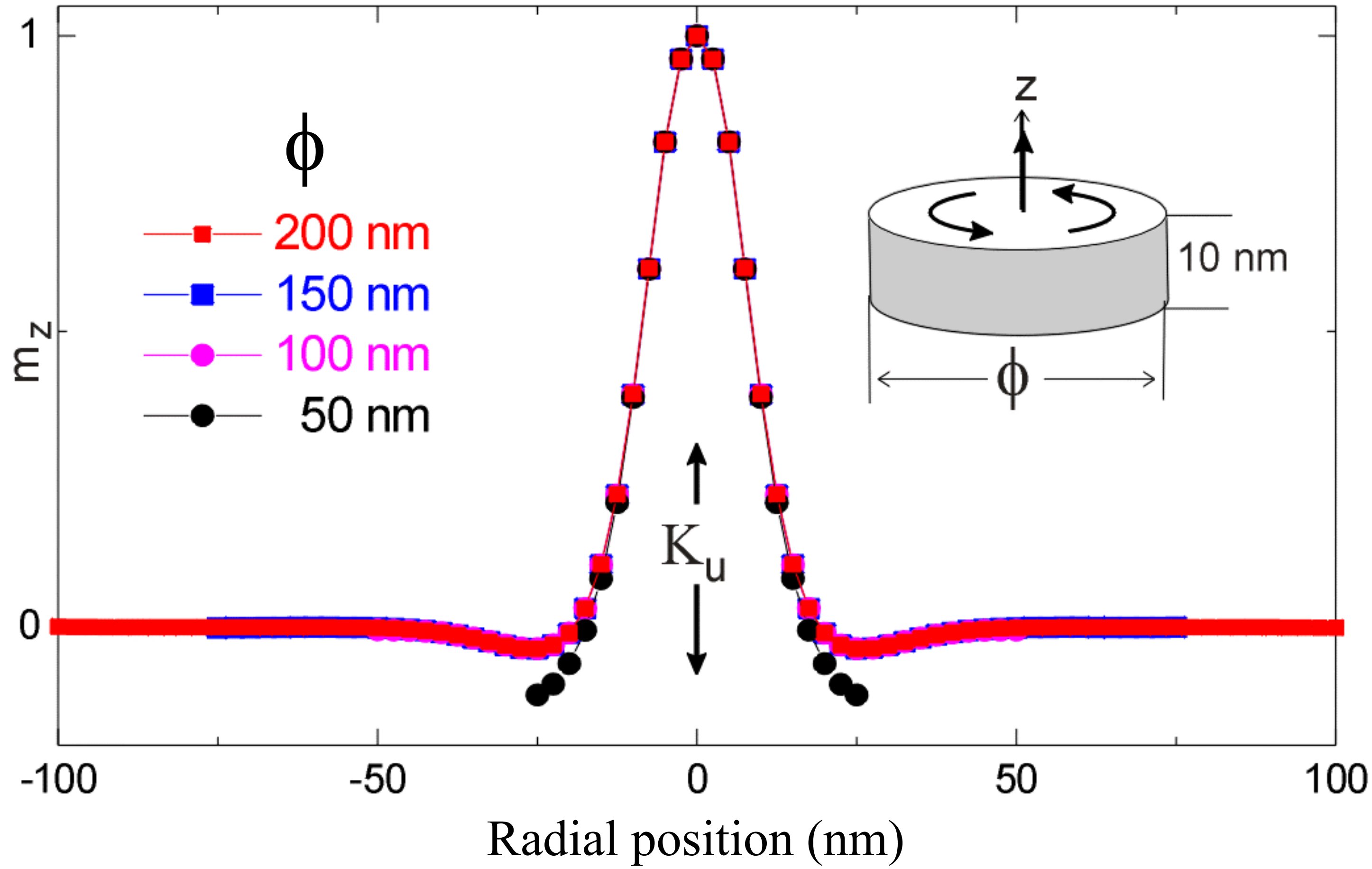




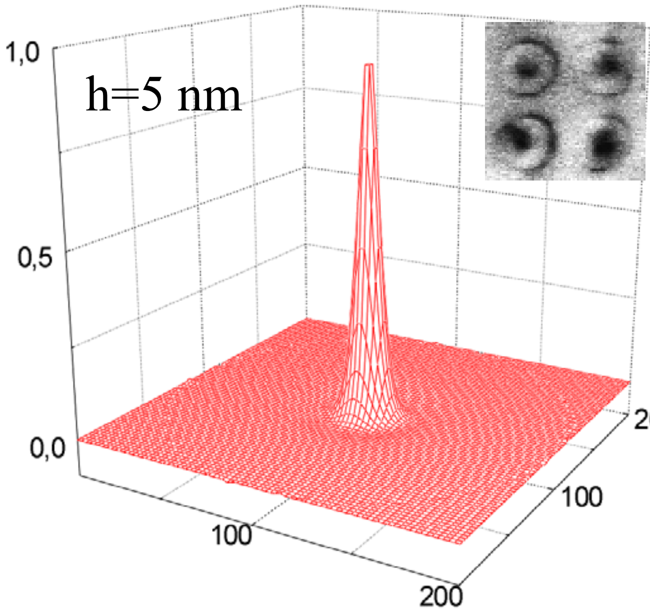


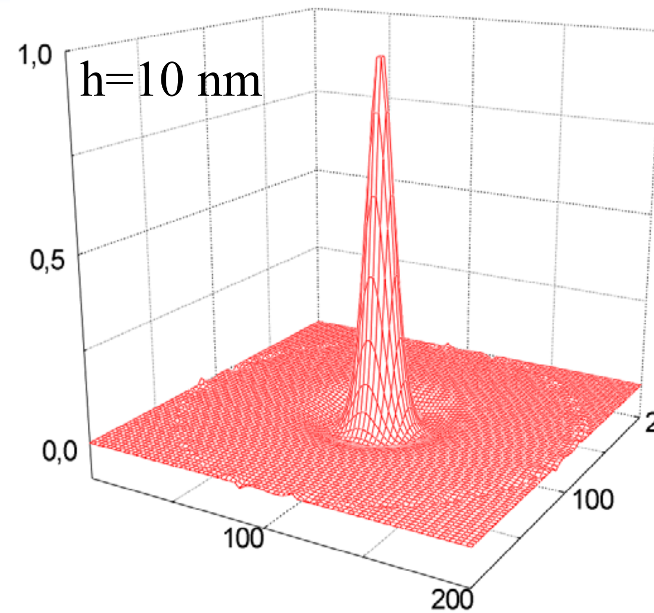
J. Miltat in Applied Magnetism, R. Gerber et al Eds. Kluwer (1994)

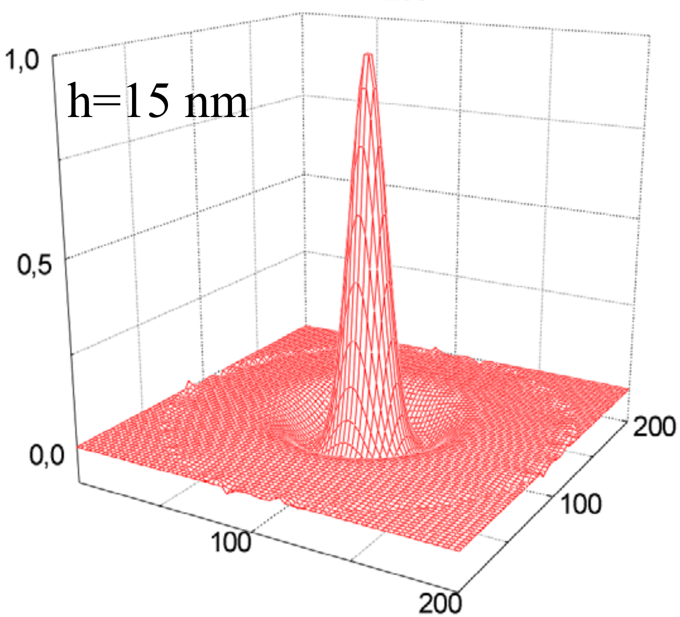
Diameter effects (ϕ)

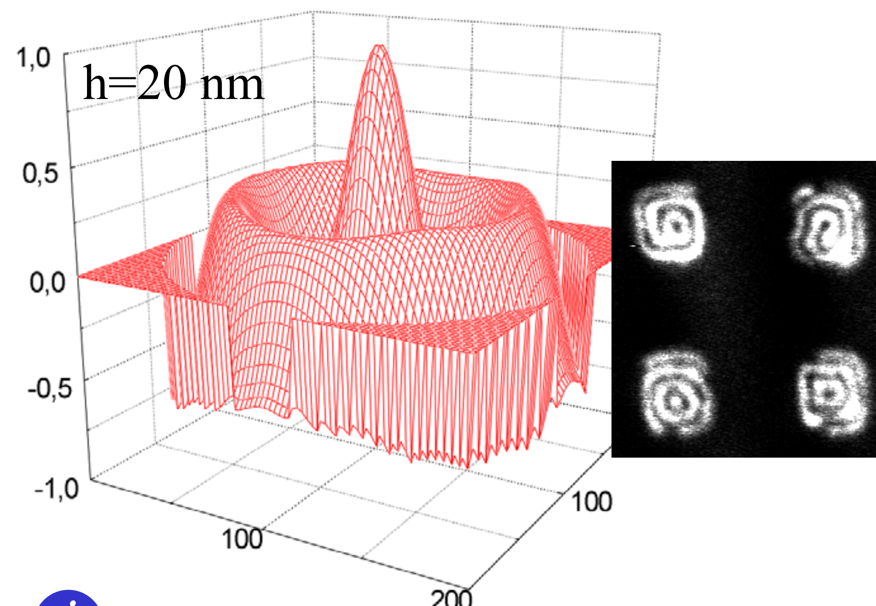


Thickness effects (h)





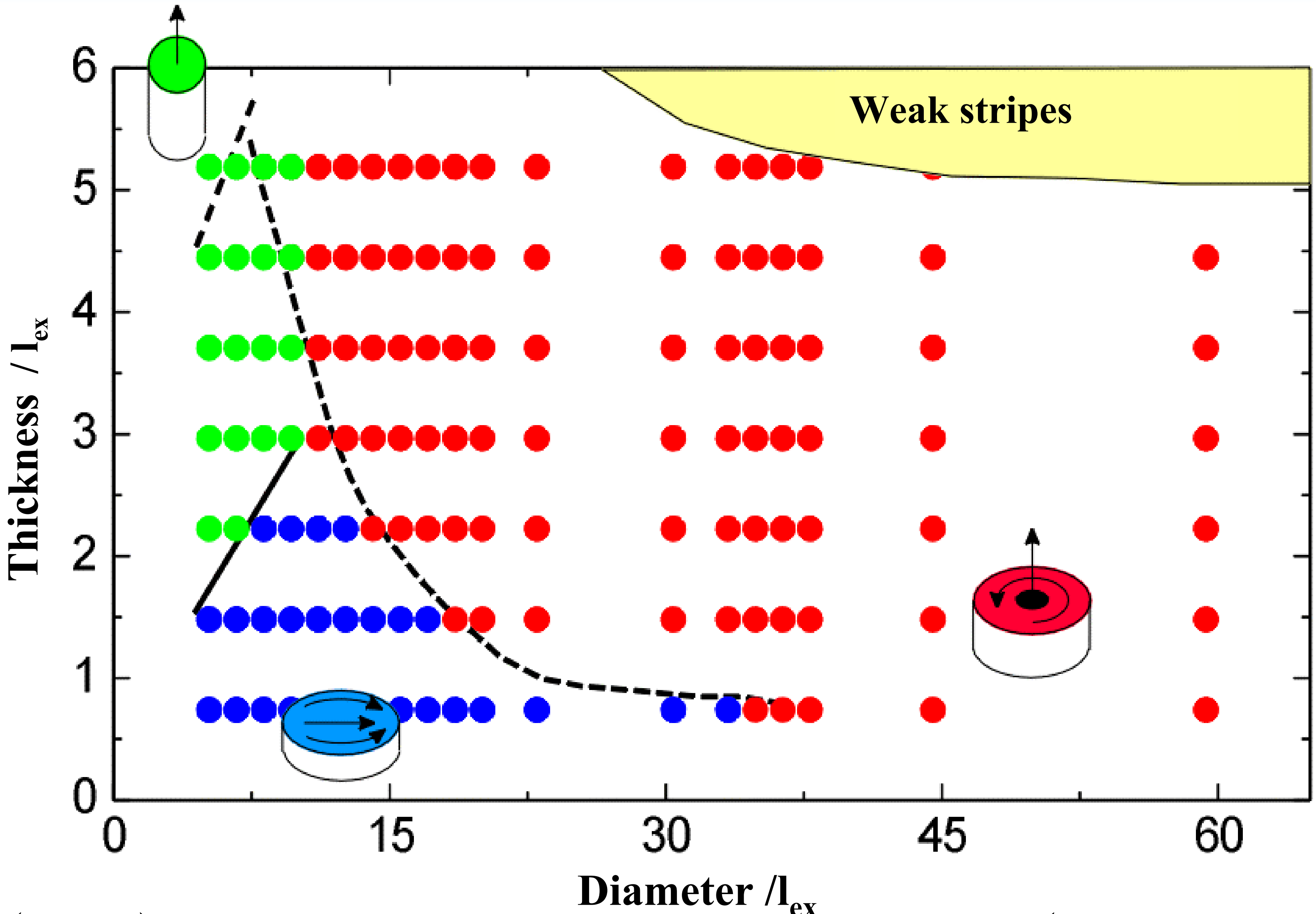




i Demand et al., JAP. 87, 5111 (2000).

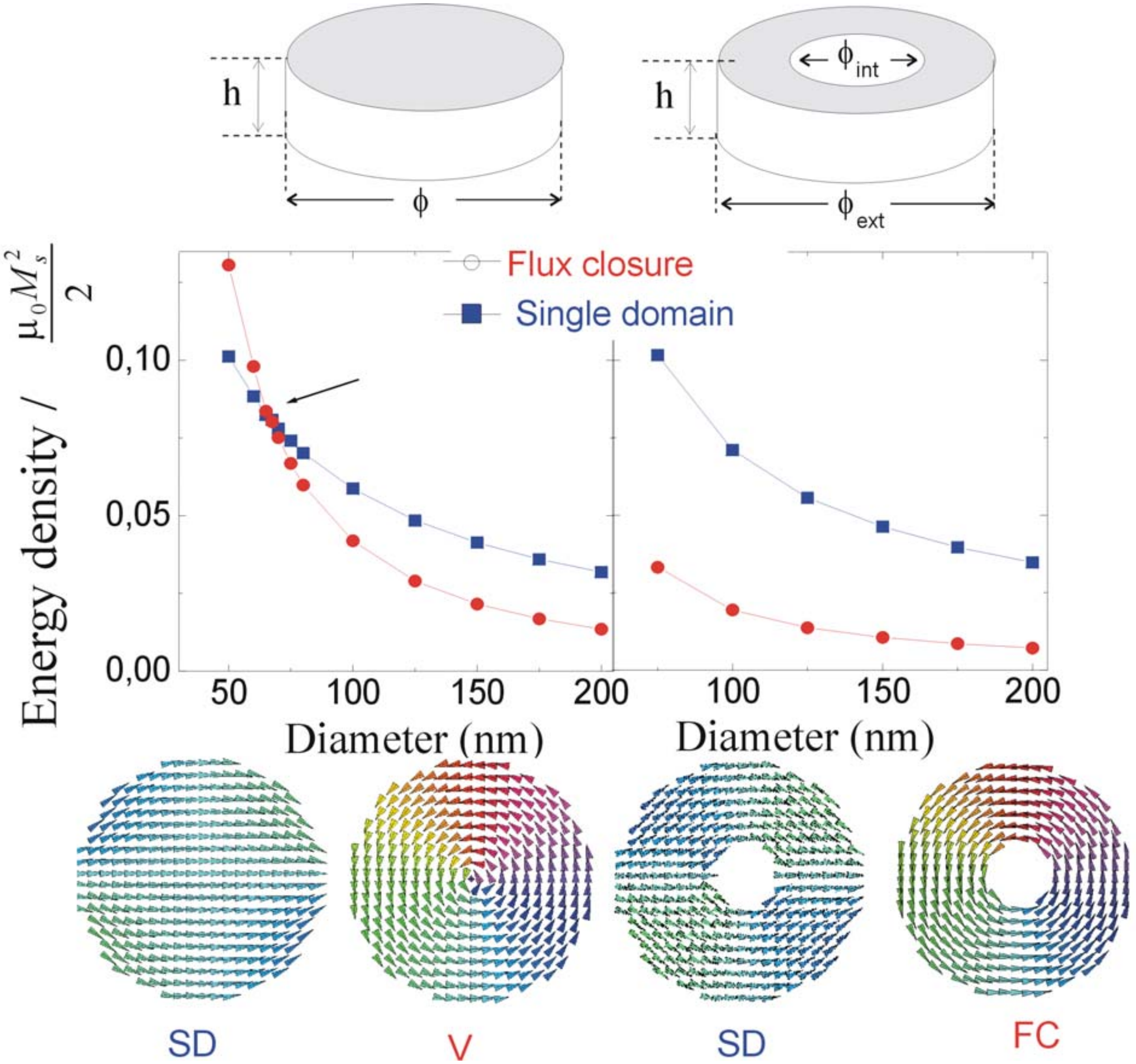
i Hehn et al., Science 272, 1782 (1996).

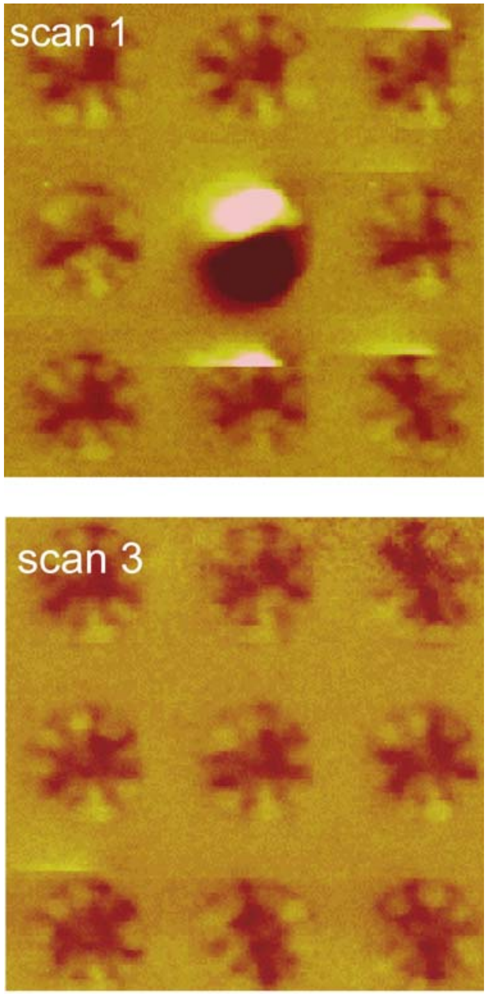
Ground state phase diagram



○ $(K_u = 0)$ ● $(K_u \neq 0 \quad \& \quad K_u \perp)$

Comparison disks & rings





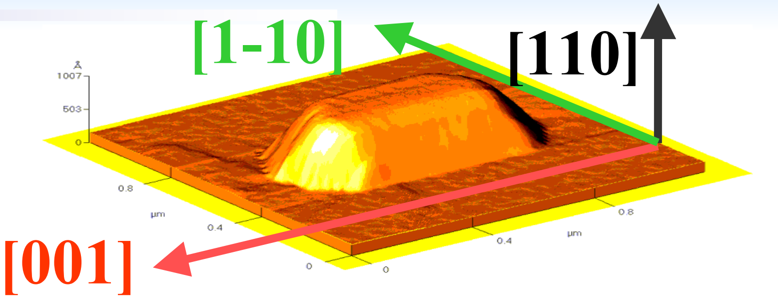
ϕ_e = 600 nm
ϕ_i = 200 nm
e = 20 nm
h_{tip} = 40 nm

i S. Li et al. PRL (2001)

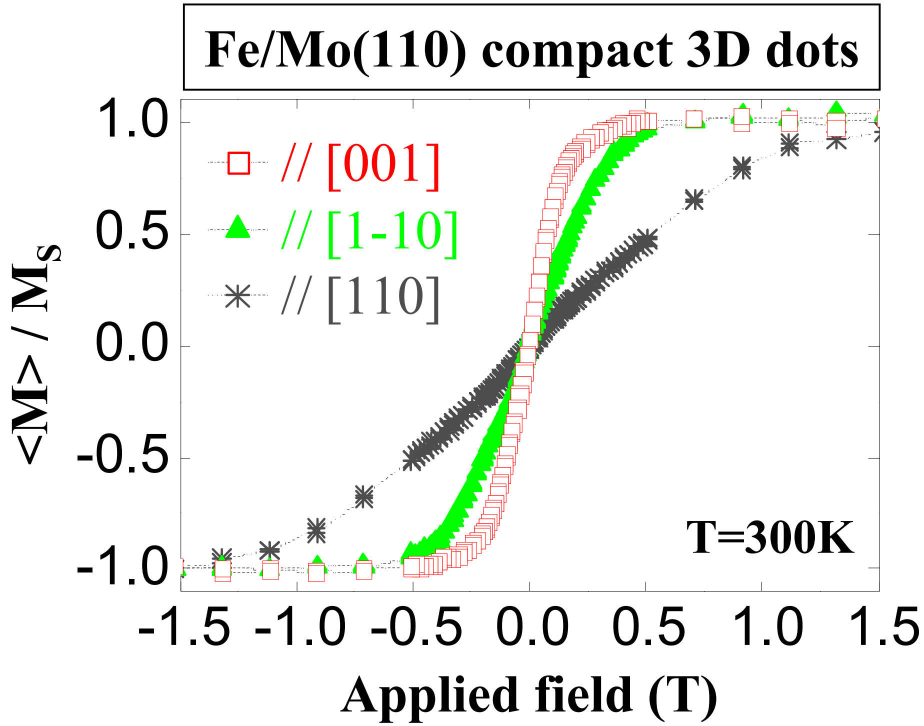
Self-assembled Epitaxial Submicron Fe Dots

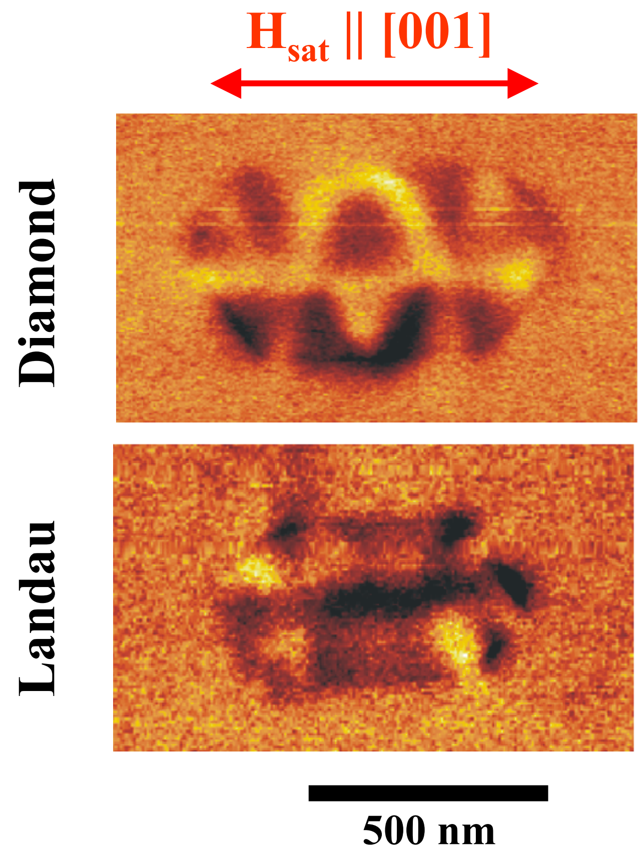
P. O. Jubert, J.C. Toussaint
O. Fruchart, C. Meyer
Laboratoire Louis Néel, Grenoble

Y Samson
CEA / DRFMC / SP2M / NM, Grenoble



L~550nm, w~350nm, h~65nm

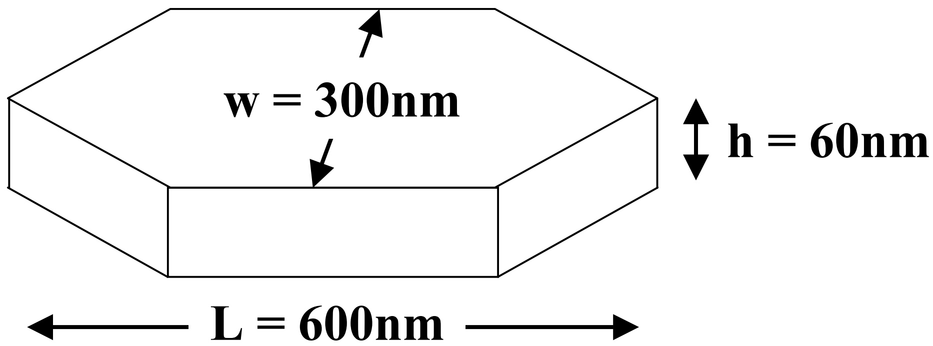




P.O. Jubert et al. PRB **64**, 115419 (2001)

Remanent Configurations ($H_{app}=0$)

Ideal shape : **hexaplot**



Fe bulk parameters

$$M_s = 1750\times10^3\,A/m$$

$$A_{ex} = 2.\times10^{-11}\,J/m$$

$$K_1 = 4.81\times10^4\,J/m^3$$

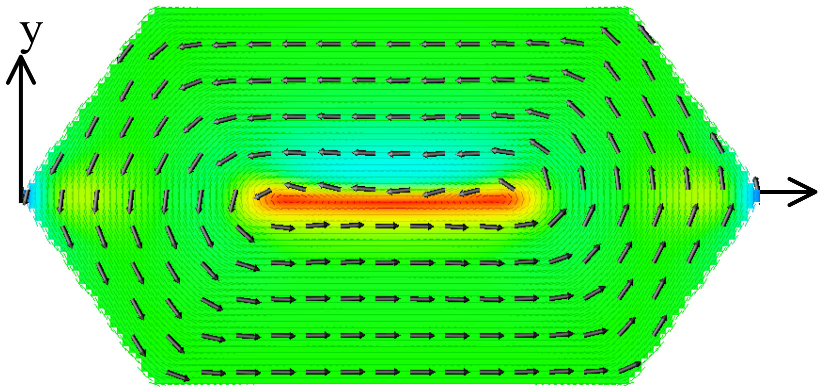
$$\pi\Delta_0 \cong 7nm$$

$$\pi l_{ex} \cong 10nm$$

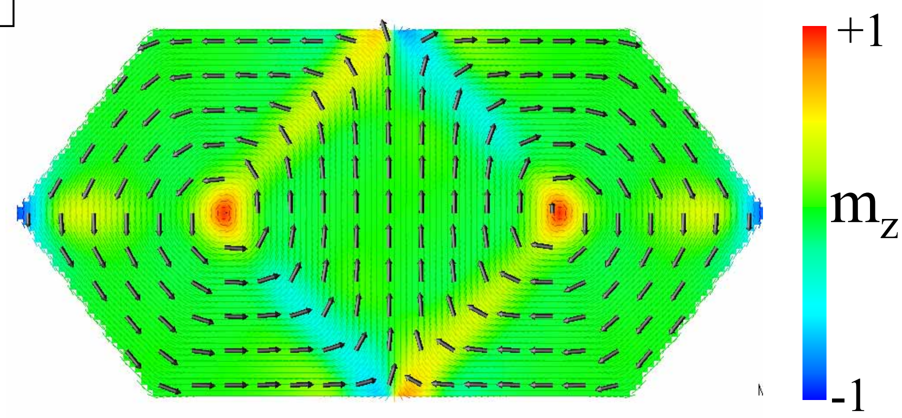
Mesh : $4.68\times4.68\times3.75\,nm^3$

z = h/2

Landau state

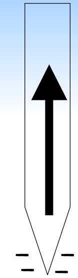


Diamond State

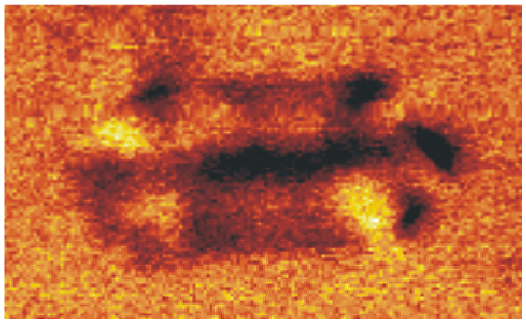
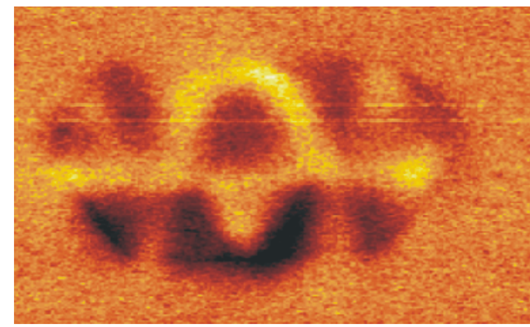
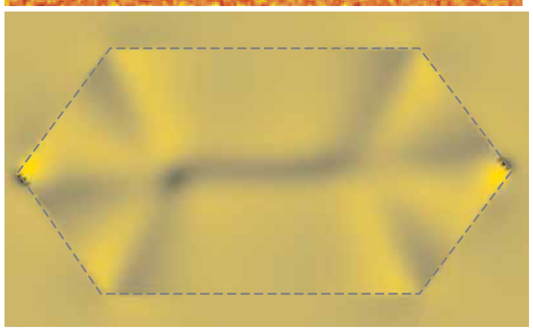
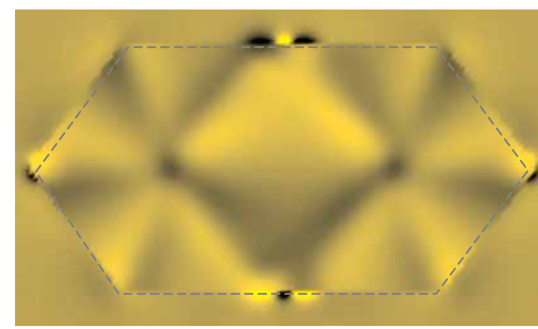
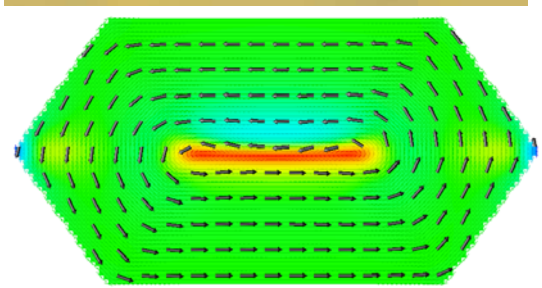
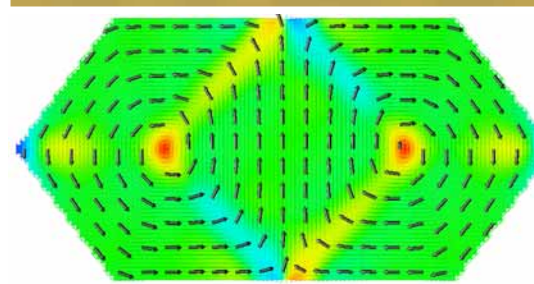


P.O. Jubert et al. EPL 63, 138 (2003)

Remanent Configurations

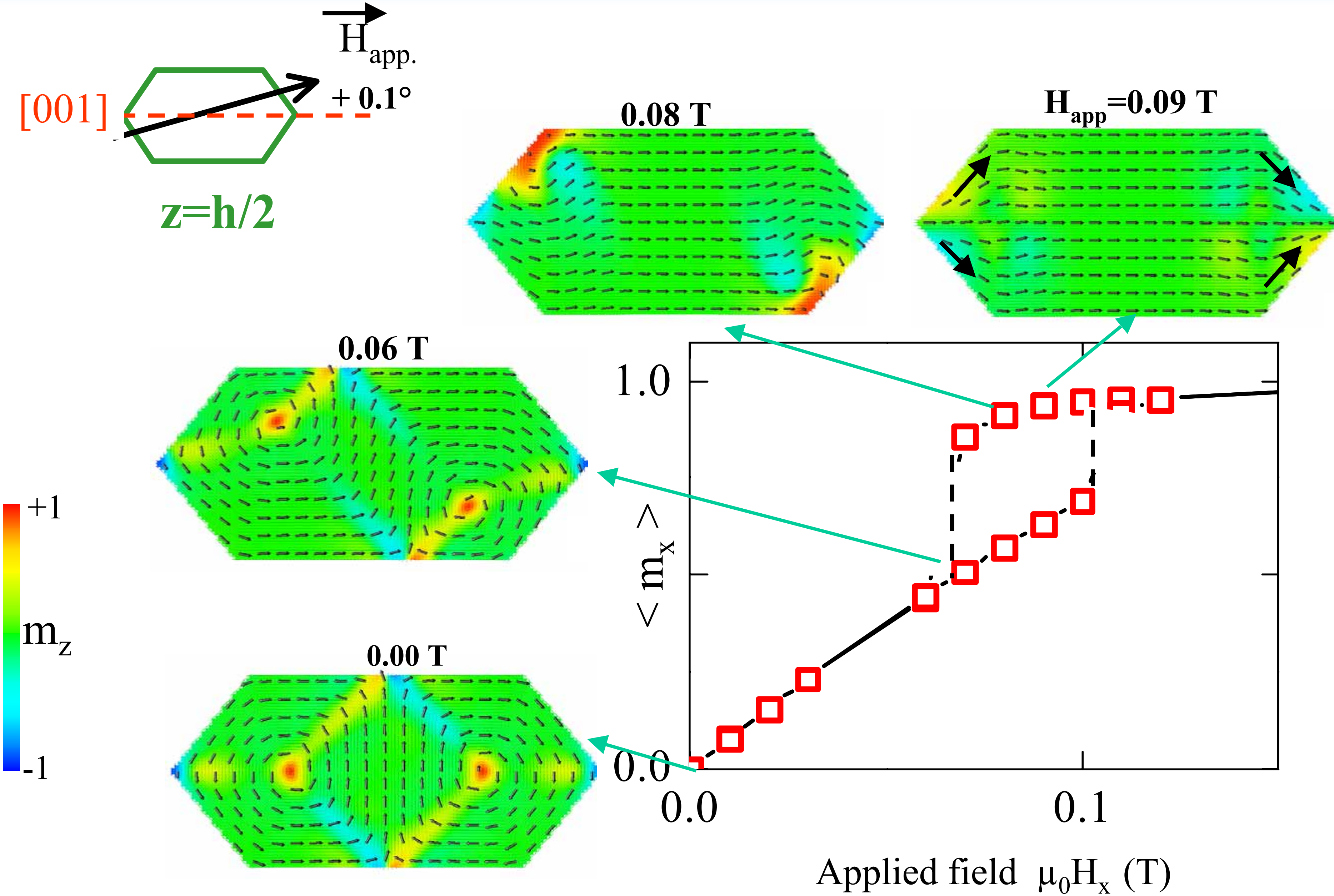


MFM tip ~ monopole ⟹ MFM response ~ $\partial_z H_z$

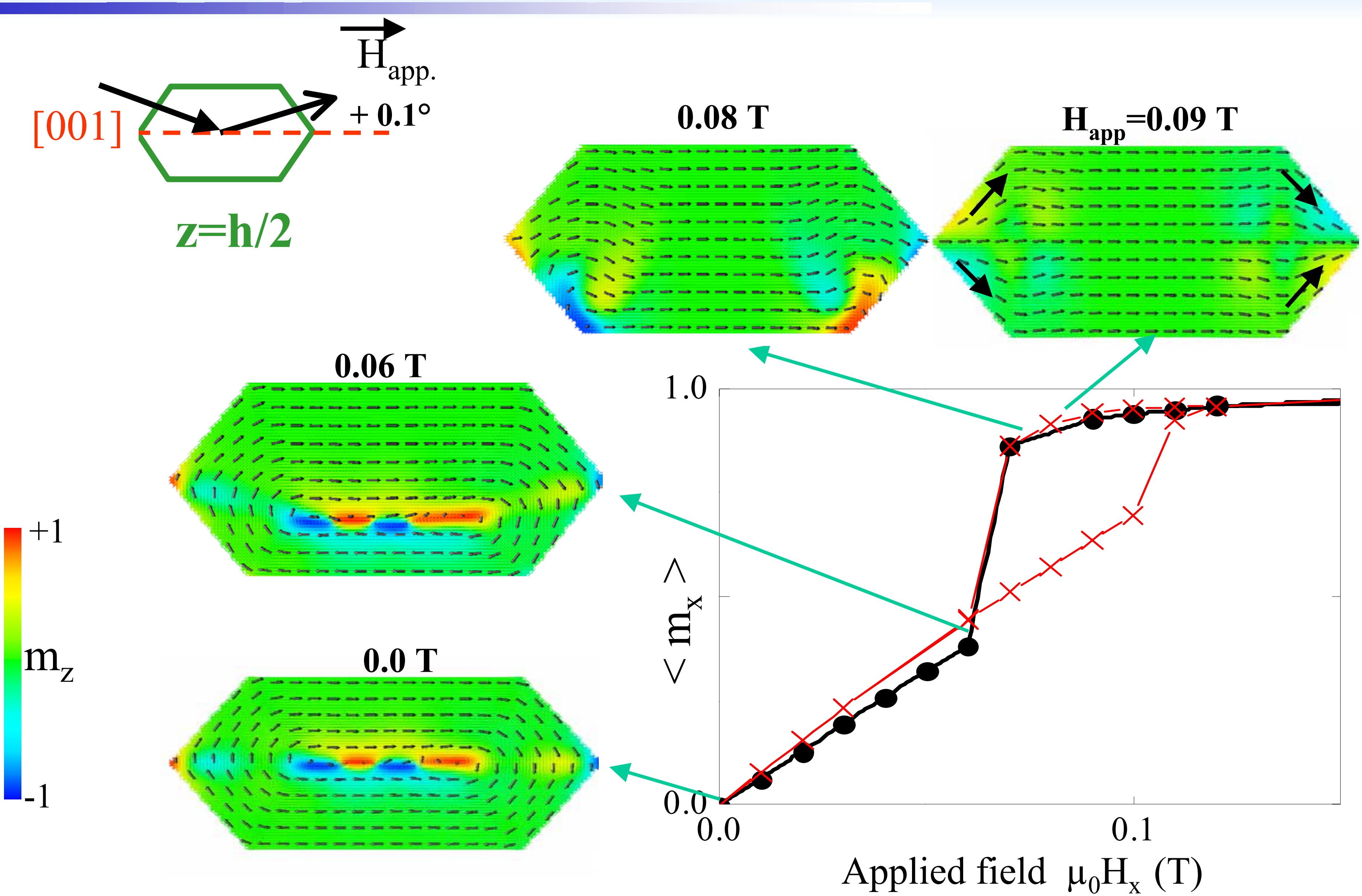
	Landau state	Diamond state
MFM measured		
MFM simulated		
simulated configuration		

Lift scan height 30nm

In plane hysteresis curve

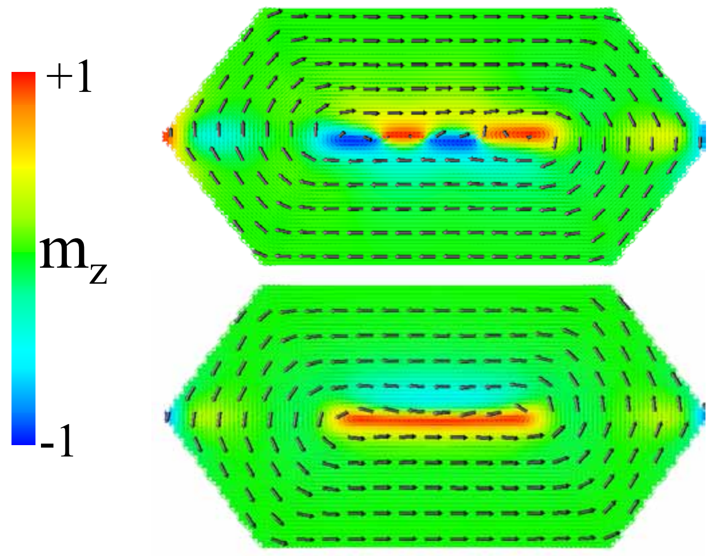


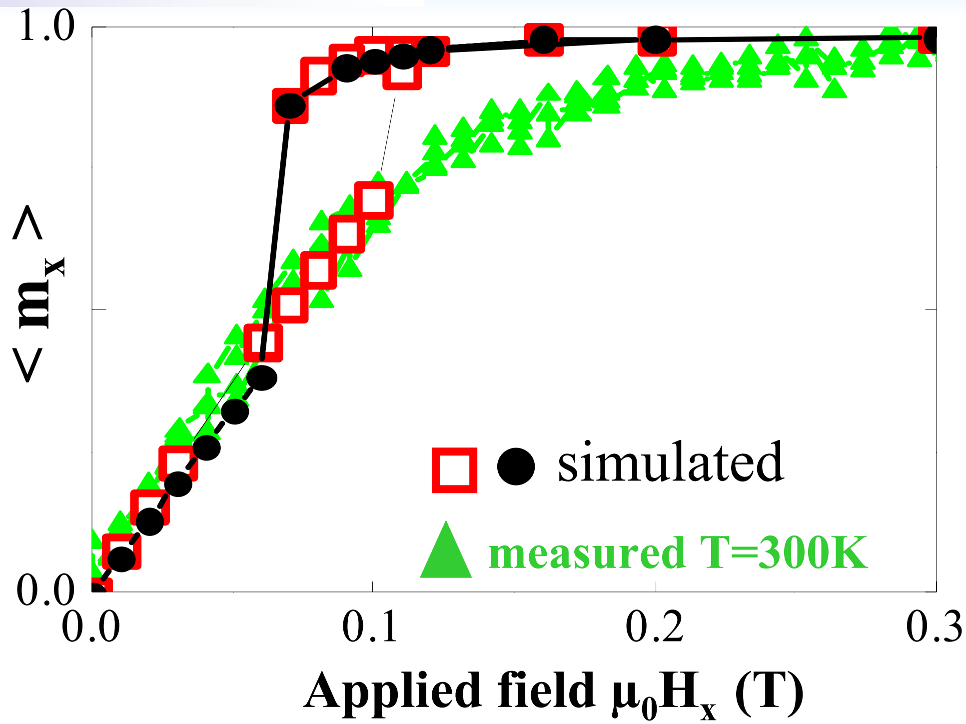
In plane hysteresis curve & distortion



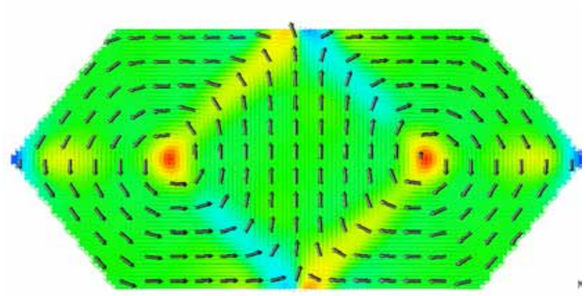
Simulation & Experience

Landau states





Diamant state



- Simulation → remanent state is controlled by small external perturbation.
- MFM resolution is too low to distinguish between the two Landau states.
- Thermal fluctuation effect.

Selected bibliography - books

Basic book on micromagnetics

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  Academic Press, (1998)
- **A. Hubert, R. Schäfer** : *Magnetic Domains*
  Springer (1998)

Selected bibliography - articles

Articles on numerical aspects of micromagetics

- **W.F. Brown Jr., A.E. LaBonte**: J. Appl. Phys. **36**, 1380 (1965)
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- **J. Fidler, T. Schrefl** : Journal of Physics D: Applied Physics, **33** R135-R156 (2000)
- **D. Fredkin , T.R. Koehler**: IEEE Trans. Mag. **26**, 415 (1990)
- **R. Cowburn:** J. Phys. D: Appl. Phys. **33**, R1 (2000)

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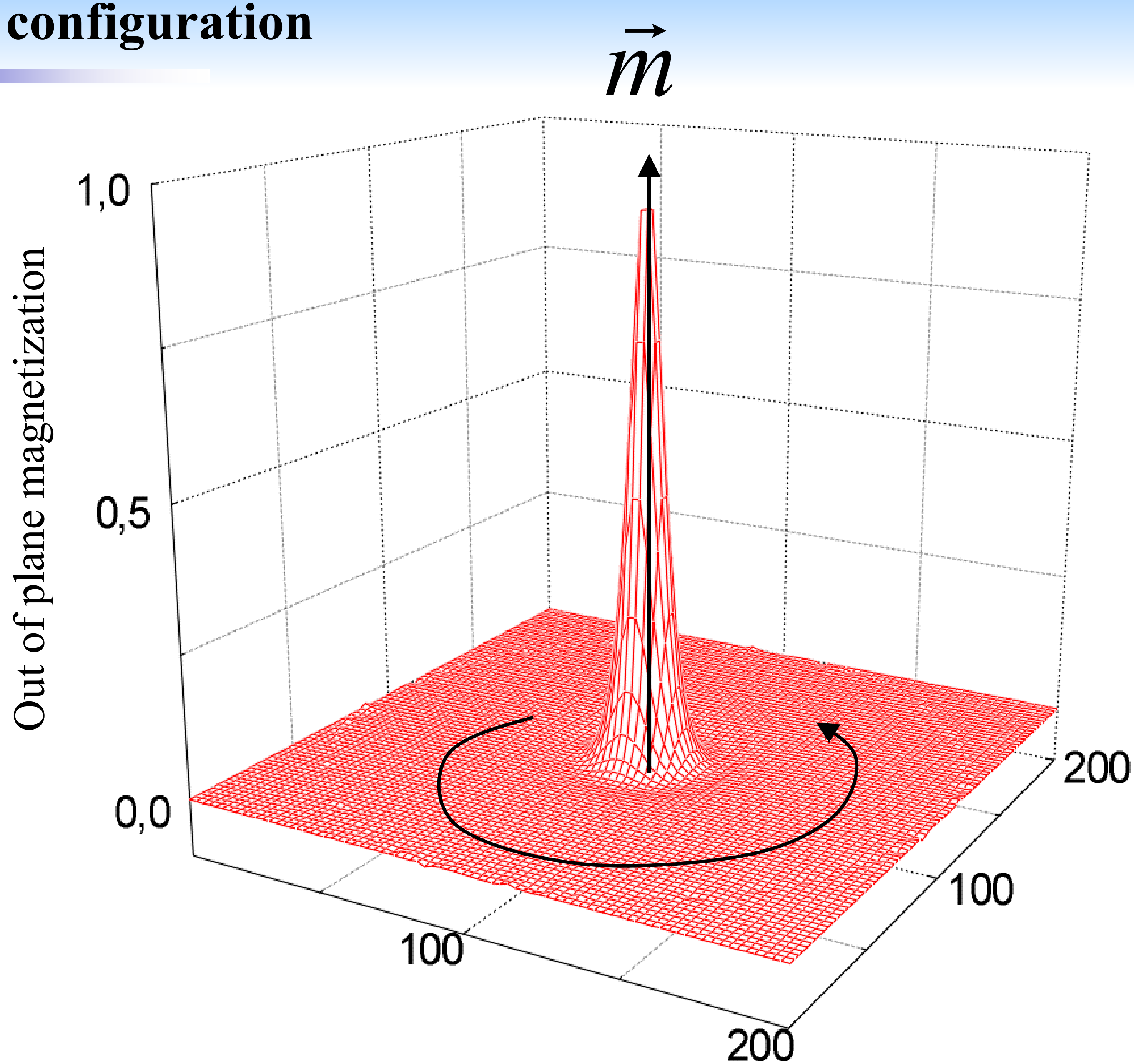
Mulțumesc!
Merci!
Thank you!

Vortex configuration



In-plane single domain state