e-ESM, an online higher-education Magnetism event

MICROMAGNETISM I

GROUND STATES, HYSTERESIS AND DYNAMICS

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ICMM

CSIC

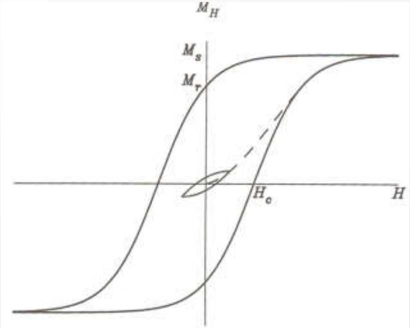
What is micromagnetism?

The aim of micromagnetism is calculation of magnetic states and their dynamics for a given ferromagnetic system, i.e.

<u>magnetic moment configuration</u>
<u>in the classical (semi-classical) approximation</u>

given:

- ➢intrinsic parameters
- ➢microstructure
- ➢morphology (geometry)
- ➢applied field
- ➢temperature
- ➢External stimuli (current, voltage, laser

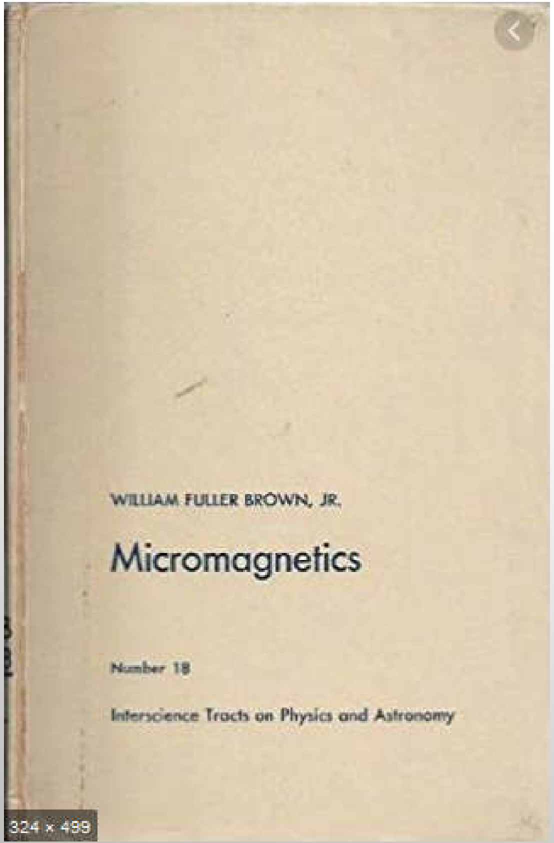


Micromagnetic simulations need as an input experimental information

✓About microstructure
✓About local intrinsic parameters

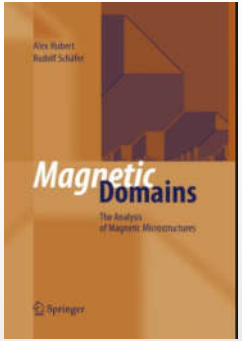
This information does not alway exist with sufficient details

1963



Analytical theory for magnetization reversal

A.Aharoni, A.Hubert, H.Kronmuller D.Givord etc.



Going to numerics

H. Kronmuller, J.Fidler, J.Miltat etc.

Numerical micromagnetics

T.Shrefl (1993), M.Donahue (NIST oomf1998)

Principle lines in micromagnetism:

- **Classical micromagnetism**
  Total energy minimization
  Hysteresis processes:coercivity and remanence.
  Thin films, multilayers, magnetic elements: dots, antidots, stripes, wires etc.

- **Magnetisation dynamics**
  Integration of the LLG equation (up to 100 ns)
  Fast magnetisation switching of thin films and magnetic elements

- **Temperature effects**
  Langevin dynamics simulations (LLG equation + white noise)

- **Spin-torque dynamics**
  current-induce magnetisaiton dynamics, Slonczewki equation

- **Long-time dynamics**
  Magnetic viscocity and thermal stability
  Kinetic Monte Carlo and energy barrier calculations

- **High-temperature dynamics**
  Femto-second dynamics and HAMR
  Landau-Lifshitz-Bloch equation

MICROMAGNETIC PROGRAMS

- **OOMMF (OBJECT-ORIENTED MICROMAGNETIC FRAMEWORK)**

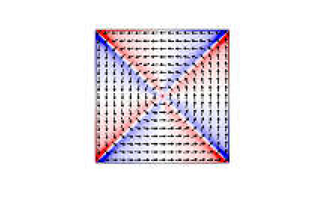
HTTP://MATH.NIST.GOV/OOMMF

- FINITE DIFFERENCES
- FAST FOURIER TRANSFORM FOR MAGNETOSTATIC INTERACTIONS

- **MUMAX3**

HTTP://MUMAX.GITHUB.IO/

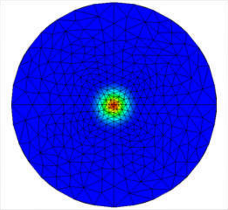
- FINITE DIFFERENCES
- GPU-BASED



- **BORIS**

FOR SPINTRONICS AND ULTRAFAST DYNAMICS

HTTPS://WWW.BORIS-SPINTRONICS.UK/



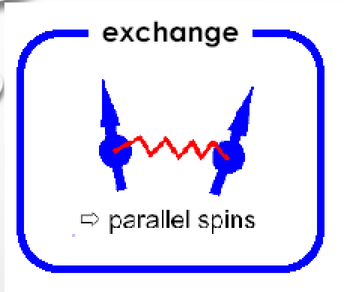
- **NMAG (FIDIMAG FROM THE SAME GROUP), JOOMF**

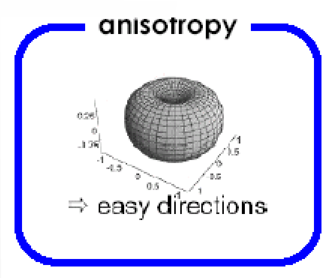
FINITE ELEMENTS (MULTISCALE ATOMISTIC/MICROMAG CODE)

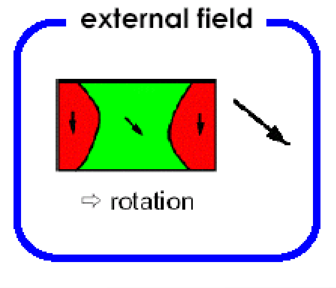
HTTP://NMAG.SOTON.AC.UK/NMAG

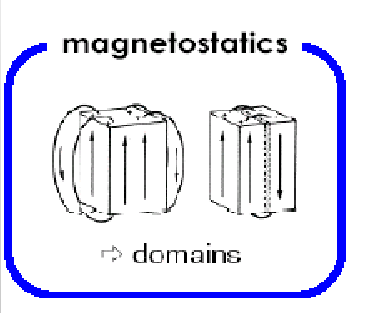
HTTPS://COMPUTATIONALMODELLING.GITHUB.IO/FIDIMAG/

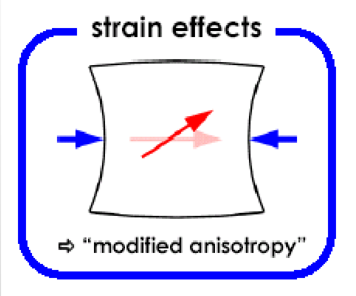
MAGNETIC ENERGIES

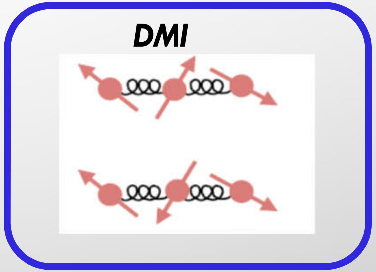


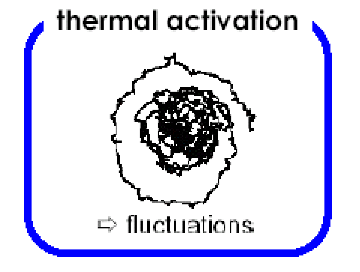












The relevance of different energies depend on the system dimensions

Novel torques and fields

Classical micromagnetic sumulations:

W.F.Brown "Micromagnetics" 1963

Classical approximation of continuous magnetic media

Consists of the minimization of total magnetic energy:

$$E_{ext} = -\int_V \vec{H}_{ext}(\vec{r})\vec{M}(\vec{r})dV$$ External field

$$E_{ani} = -\int_V K_{ani}(\vec{r})\left[\vec{m}(\vec{r})\vec{e}(\vec{r})\right]^2 dV$$ Anisotropy

$$E_{ex} = \int_V A_{ex}(\vec{r})\left[(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2\right]dV$$ Exchange

$$E_{magn} = -\frac{1}{2}\int_V \vec{M}(\vec{r})\vec{H}_{magn}(\vec{r})dV$$ Magnetostatic

Magnetostatic energy:

$$\vec{H}_{magn} = -grad\ U_{magn}$$

$$\Delta U_{magn} = \begin{cases} 4\pi\nabla\vec{M} & inside \\ 0 & outside \end{cases}$$

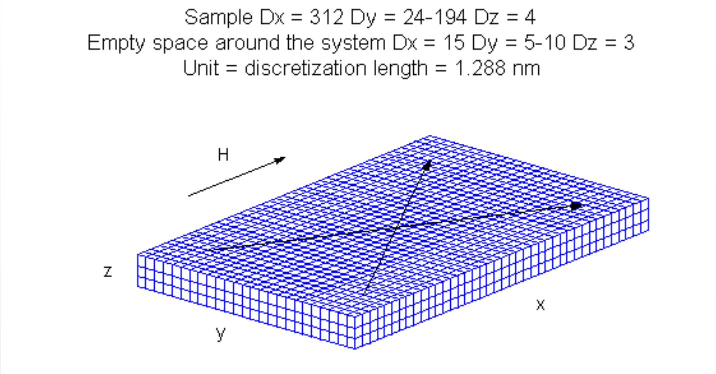
Boundary conditions:

$$U^{outside}_{magn}\Big|_\Sigma = U^{inside}_{magn}\Big|_\Sigma$$

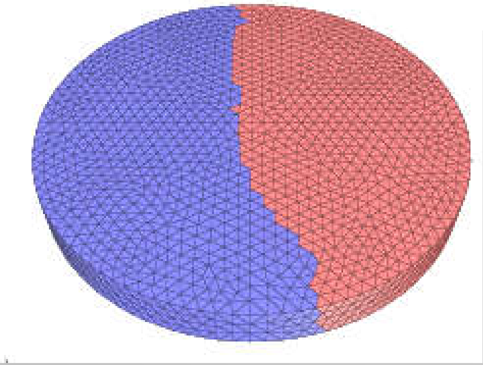
$$\left(\frac{\partial U^{inside}_{magn}}{\partial \vec{n}} - \frac{\partial U^{outside}_{magn}}{\partial \vec{n}}\right)_\Sigma = 4\pi\vec{M}\vec{n}$$

DISCRETIZATION IN FINITE DIFFERENCES:

Finite elements:



System geometry and dimensions

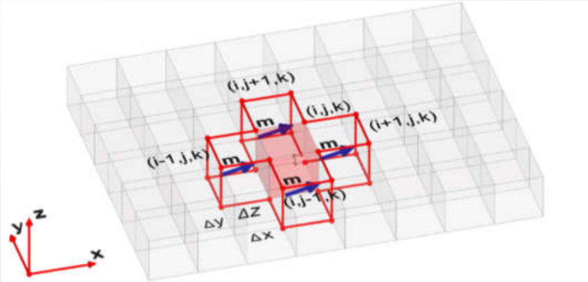


Defines magnetisation, e.g. on nodes, and uses continuous interpolation inside element.

Constant magnetisation inside each cell

$$E_Z = -\int_V \vec{M}\vec{H}dV \rightarrow -H\sum_i \vec{M}_i\Delta^3$$

Exchange field



MAGNETOSTATIC POTENTIAL

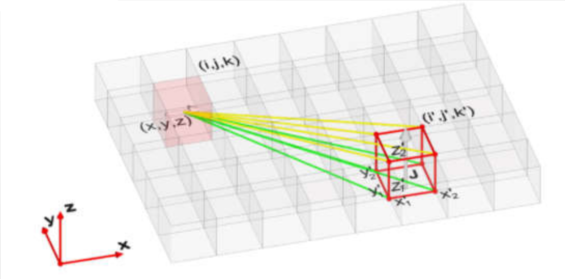
Volume charges

Surface charges

$$u(\boldsymbol{r}) = -\frac{1}{4\pi}\left[\int_{\Omega} \frac{\nabla' \cdot \boldsymbol{M}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}\boldsymbol{r}' - \int_{\partial\Omega} \frac{\boldsymbol{M}(\boldsymbol{r}')\cdot\boldsymbol{n}}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}s'\right].$$

Magnetostatic field

$$u(\boldsymbol{r}) = \frac{1}{4\pi}\int_{\Omega} \boldsymbol{M}(\boldsymbol{r}')\cdot\nabla'\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}\boldsymbol{r}'.$$



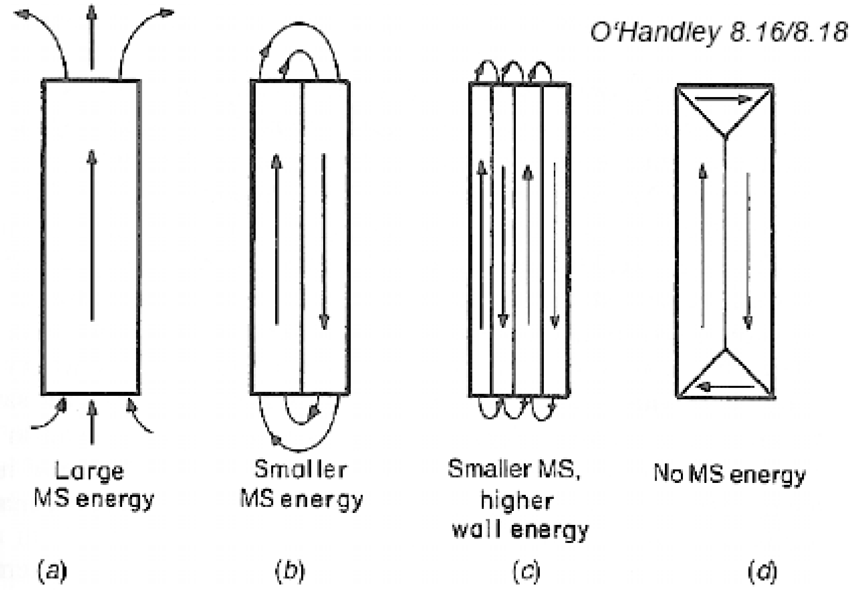
$$\boldsymbol{H}_{\text{demag}}(\boldsymbol{r}) = -\nabla u(\boldsymbol{r}) = \int_{\Omega} \widetilde{\boldsymbol{N}}(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{M}(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'$$

Fast Fourier Transform

(or FEM-BEM method)

Minimization of surface charges

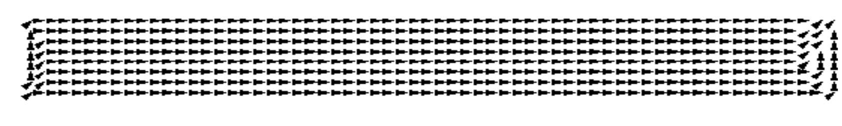
Magnetostatic Energy



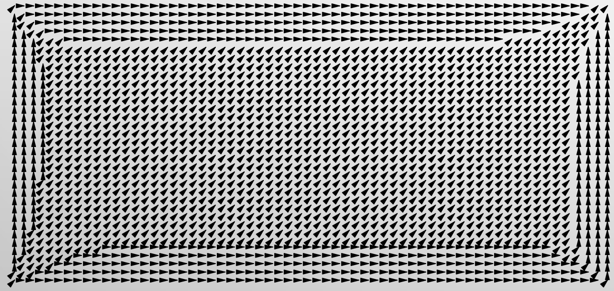
Closure domains: in magnetic hard directions problem: magnetostriction!

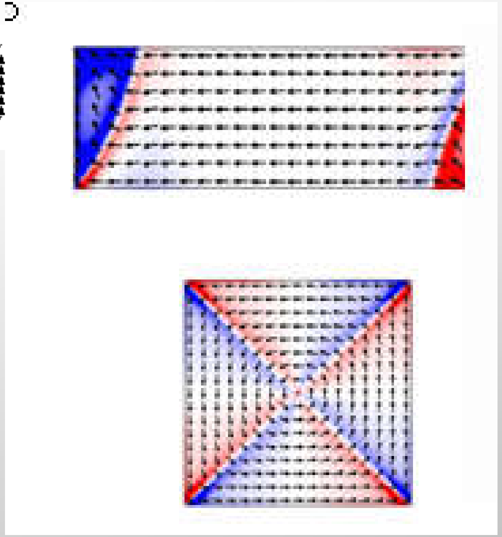
POLE AVOIDANCE PRINCIPLE

The minimization of the magnetostatic energy leads to the “avoidance” of surface charges = Magnetisation parallel to surfaces



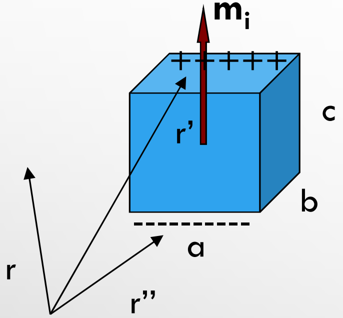
H = 0 T



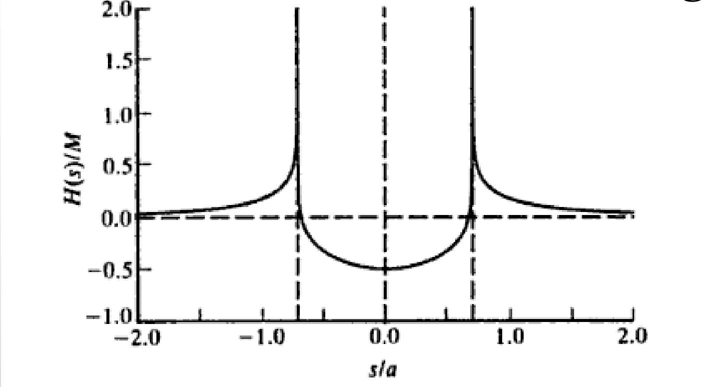


SATURATED CUBE

$$\phi(\vec{r}) \propto \frac{M}{4\pi}\left(\iint_{\Sigma} \frac{dx'dy'}{|\vec{r}-\vec{r}'|} + \iint_{\Sigma'} \frac{dx''dy''}{|\vec{r}-\vec{r}''|}\right)$$



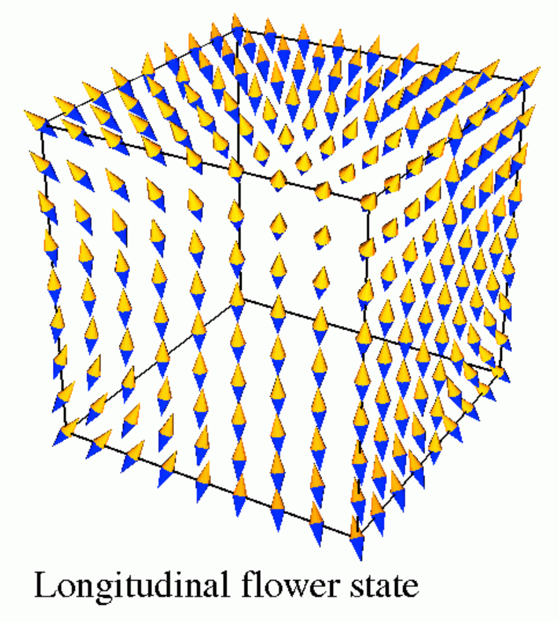
$$\vec{H} = -grad\,\phi$$

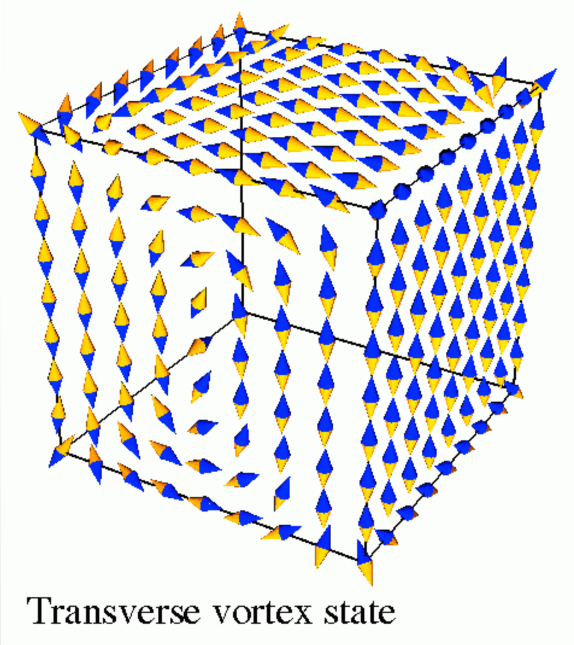


•The magnetostatic fields are stronger at the corners.

•This expression will not be valid if the magnetisation process is not homogeneous

M-MAG STANDARD PROBLEM (FROM OOMMF WEBPAGE)





See also M.A.Schabes abd H.N.Bertram “Magnetisation processes in ferromagnetic cubes”, J.Appl. Phys. 64 (1988) 1347.

Important length scales:

- *Néel Domain wall width (Exchange correlation length)*

$$\delta_o = (A/K_1)^{1/2}$$

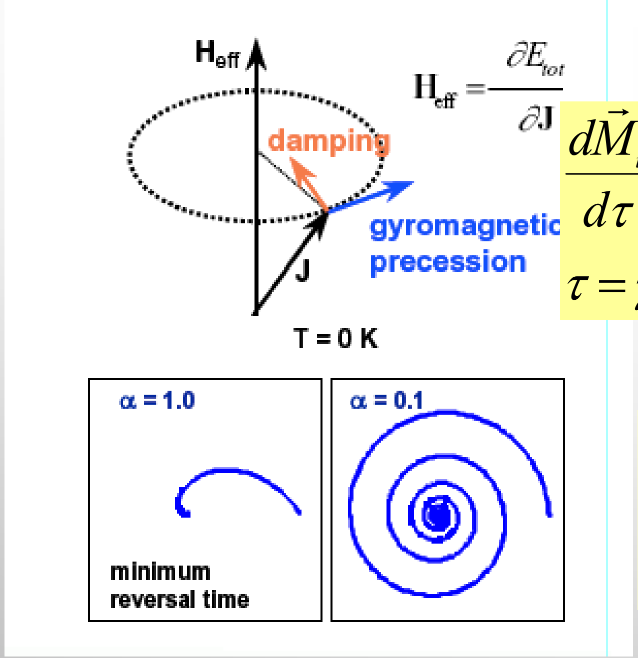
- *Exchange correlation length* ("magnetostatic correlation length")

$$l_o = (A/\mu_o M_s^2)^{1/2}$$

- *Critical domain size*

$$R_{SD} = 36\,(AK_1)^{1/2}/\mu_o M_s^2$$

Dynamics: the Landau-Lifshitz-Gilbert equation of motion



$$\frac{d\vec{M}_i}{d\tau} = -\vec{M}_i \times \vec{H}_i - \alpha \vec{M}_i \times \left(\vec{M}_i \times \vec{H}_i\right)$$

$$\tau = \gamma_0 t/(1+\alpha^2), \quad \vec{H}_i = (-1/M_s V_i)(\delta E/\delta \vec{M}_i)$$

$$\vec{H} = \vec{H}_{\text{int}} + \vec{h}_{therm}$$

$$<h_i> = 0, \qquad <h_i(t) h_j(t+\tau)> = \frac{2\alpha k_B T}{M_s V_i (1+\alpha^2)} \delta(\tau)\delta_{ij}$$

Brown’s condition for equilibrium M | | H_{int}

$$\left[\vec{M} \times \vec{H}_{total}\right] = 0$$

LLG EXTENSIONS

Slonszewski Spin-transfer torque (two ferromagnets, one with fixed polarization p with non-Magnetic spacer)
also for spin-orbit torques (thin film coupled to another layer with high SO coupling)

$$\frac{dm}{dt} = -\frac{\gamma}{1+\alpha^2}([m \times H_{eff}] + \alpha [m \times [m \times H_{eff}]] - \frac{\hbar j}{eM_S d} g(\Theta) (\beta [m \times p] - [m \times [m \times p]])).$$

Zhang-Li model (current through magnetic materials,
For domain walls

$$\frac{\partial \vec{M}}{\partial t} = -\gamma \vec{M} \times H_{eff} + \alpha \vec{M} \times \frac{\partial \vec{M}}{\partial t} + -u \frac{\partial \vec{M}}{\partial x} + \beta u \vec{M} \times \frac{\partial \vec{M}}{\partial x}$$

THERMAL MICROMAGNETICS

Langevin dynamics approach

$$\frac{d\vec{M}}{dt} = -\frac{\gamma}{1+\alpha^2}\vec{M}\times\vec{H} - \frac{\gamma\alpha}{M_s(1+\alpha^2)}\vec{M}\times(\vec{M}\times\vec{H})$$

$$\vec{H} = \vec{H}_{Zeeman} + \vec{H}_{aniso} + \vec{H}_{exch} + \vec{H}_{magnetost} + \vec{H}_{therm}$$

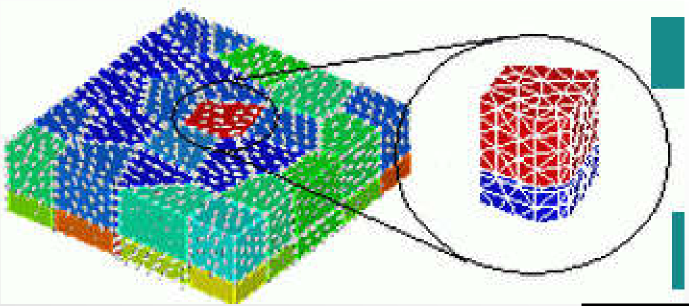
$$< H_{therm,i}(t) >= 0, \quad < H_{therm,i}(t) H_{therm,j}(t') >= \frac{2\alpha k_B T}{\gamma M_s V}\delta_{ij}\delta(t-t')$$

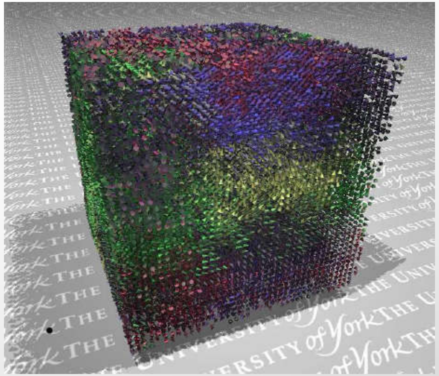
•Initially introduced for nanoparticles
•This was brought to micromagnetics.

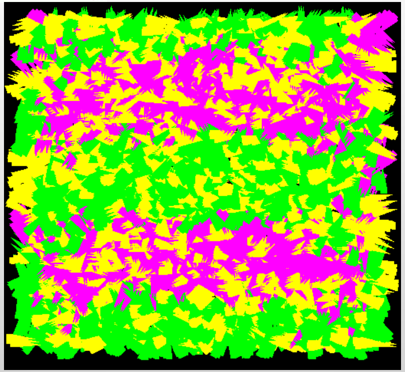
No correlations
In time
and different particles!!

W.F.Brown, Phys Rev 130 (1963) 1677.

MICROMAGNETIC MODELS OF NANOSTRUCTURED MATERIALS



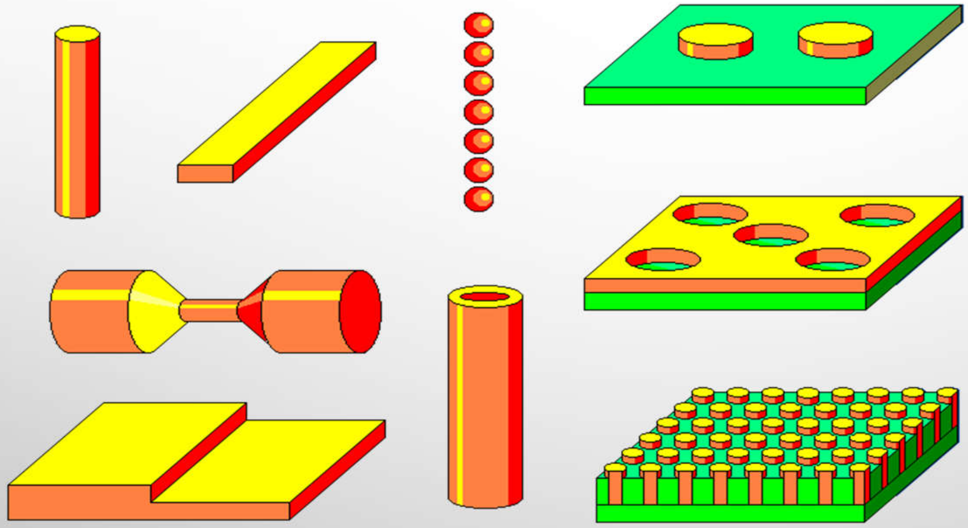




Models need nanostructure and micromagnetic parameters from experiment

Nanotecnology

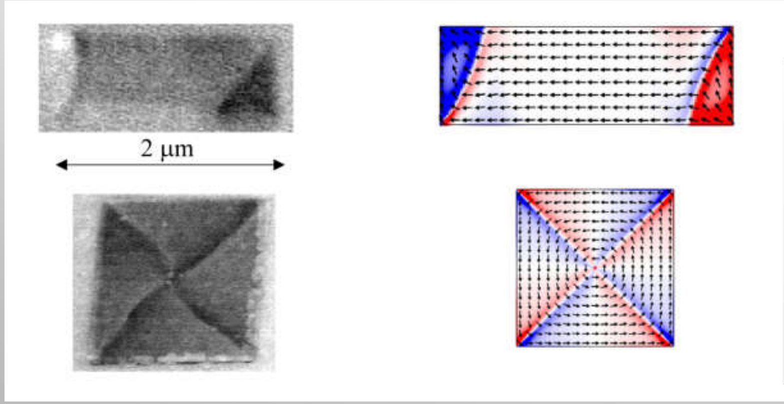
Magnetsotatic fields strongly
depend on the shape of the nanoelement

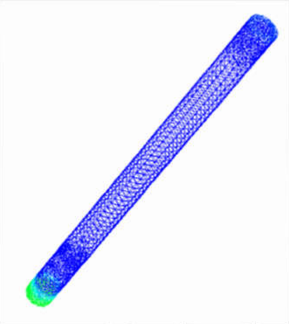


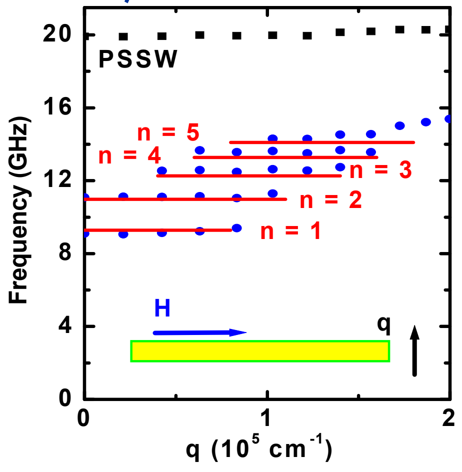
Magnetic nanostructures have at least one of the dimensions comparable to magnetic correlation lengths: D ~ Lex

This leads to new finte-size fenomena related to competition between the exchange and magnetostatic energies

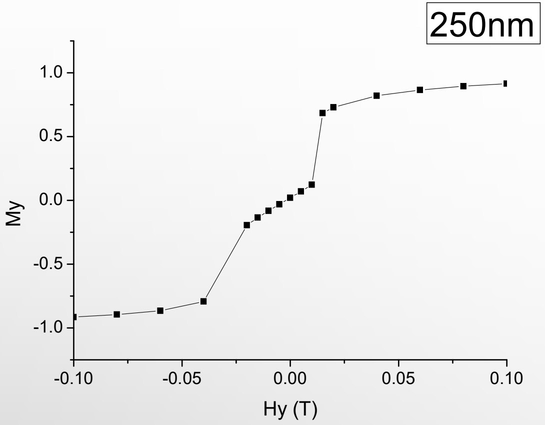
- ✓ Shape anisotropy
- ✓ Configurational anisotropy
- ✓ Magnetisation deviation at the nanostructure boarders
- ✓ Stabilisation of different states (e.g.vortex or skyrmion states)
- ✓ Confinement and quantisation of spinwaves

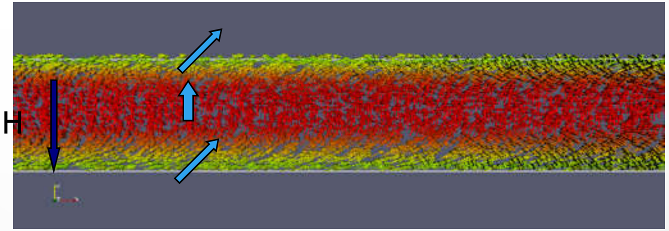


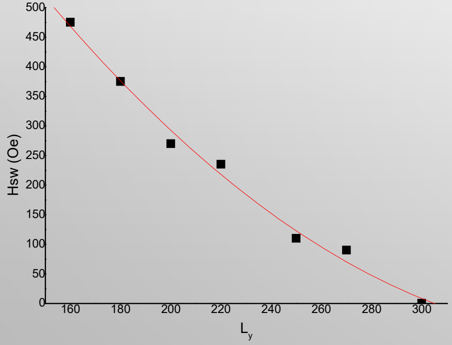


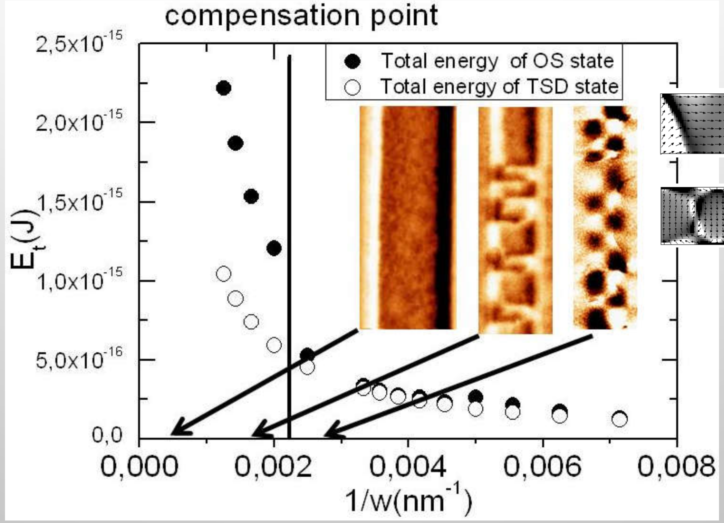


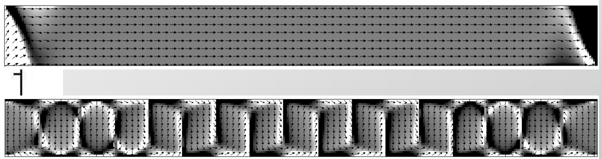
LITOGRAPHED STRIPES WITH PERPENDICULAR ANISOTROPY



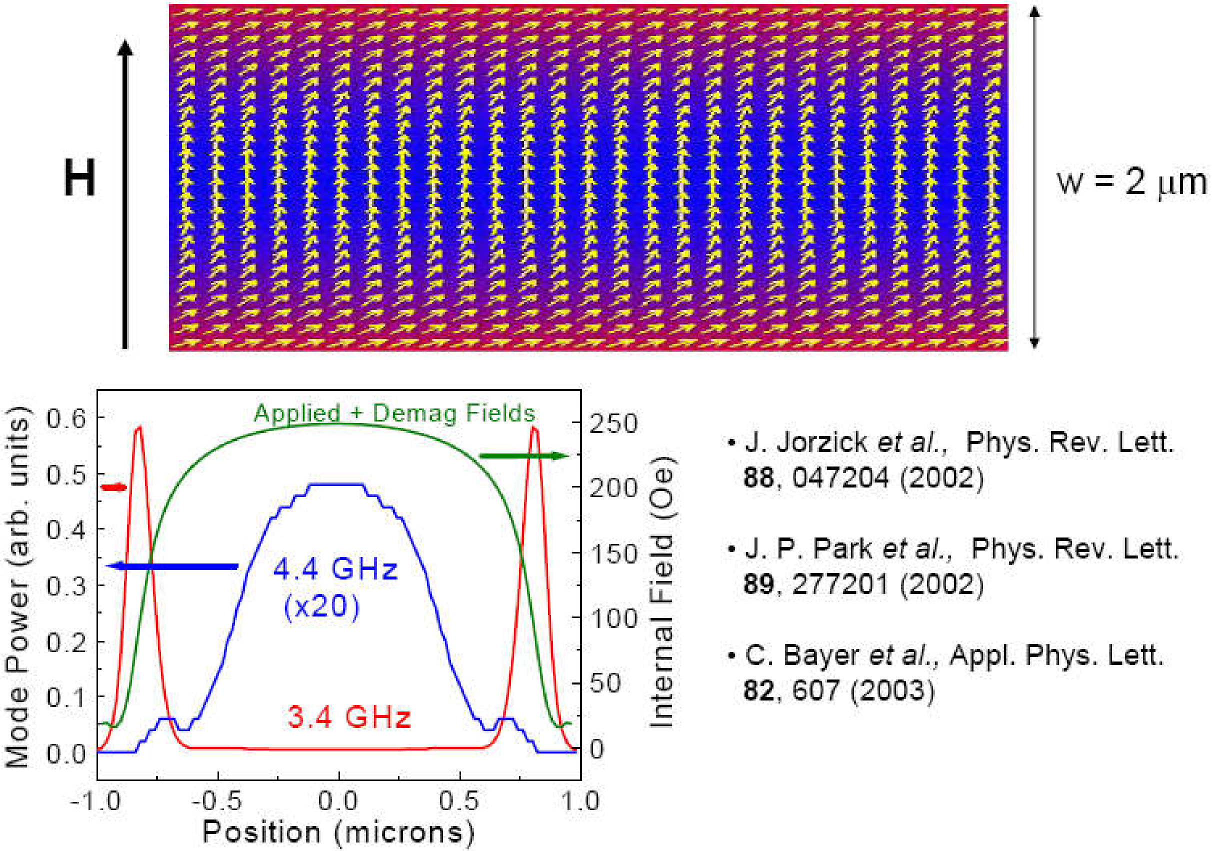






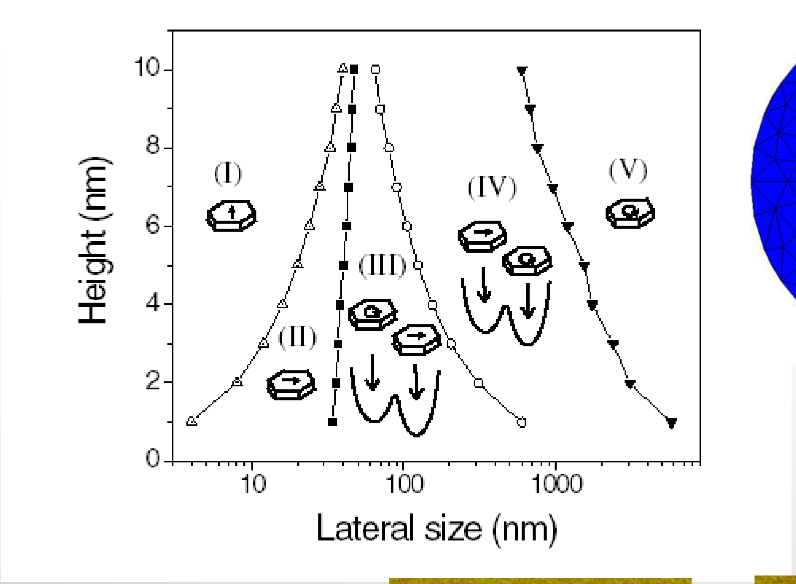


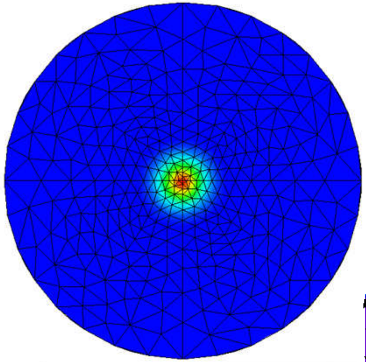
Quasi-One Dimensional Wires: Spin-wave Localization

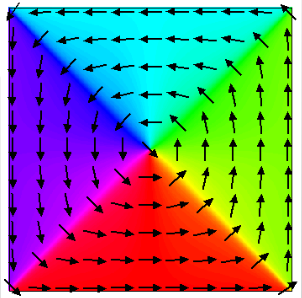


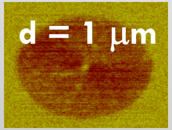
- J. Jorzick *et al.*, Phys. Rev. Lett. **88**, 047204 (2002)
- J. P. Park *et al.*, Phys. Rev. Lett. **89**, 277201 (2002)
- C. Bayer *et al.*, Appl. Phys. Lett. **82**, 607 (2003)

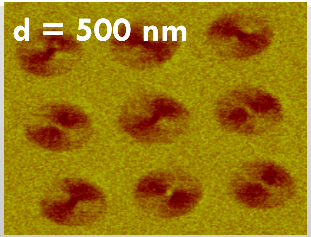
MAGNETIC DOTS

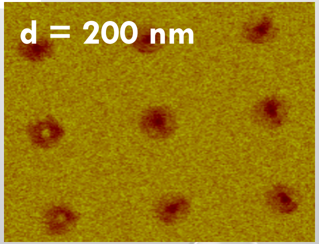


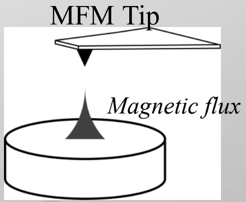








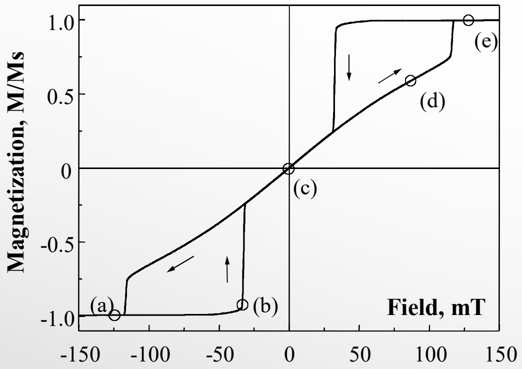


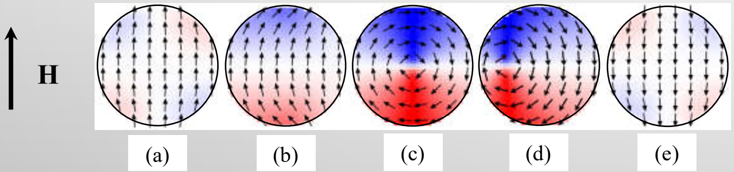


MFM Images:
Thickness = 60 nm
FeNi

Magnetic Vortex State in circular ferromagnetic dot

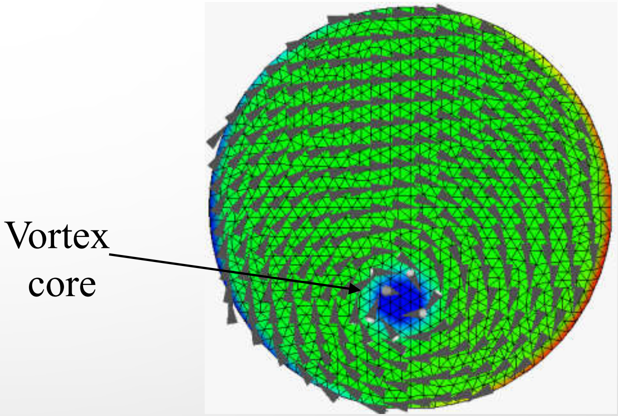
Micromagnetic calculations: hysteresis loop and field-evolution of the vortex spin structure

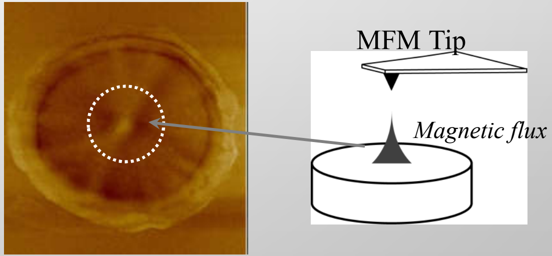




V. Novosad et al. IEEE Trans. Magn., 2001

Experiments: hysteresis loop and MFM observation of the vortex state in remanence

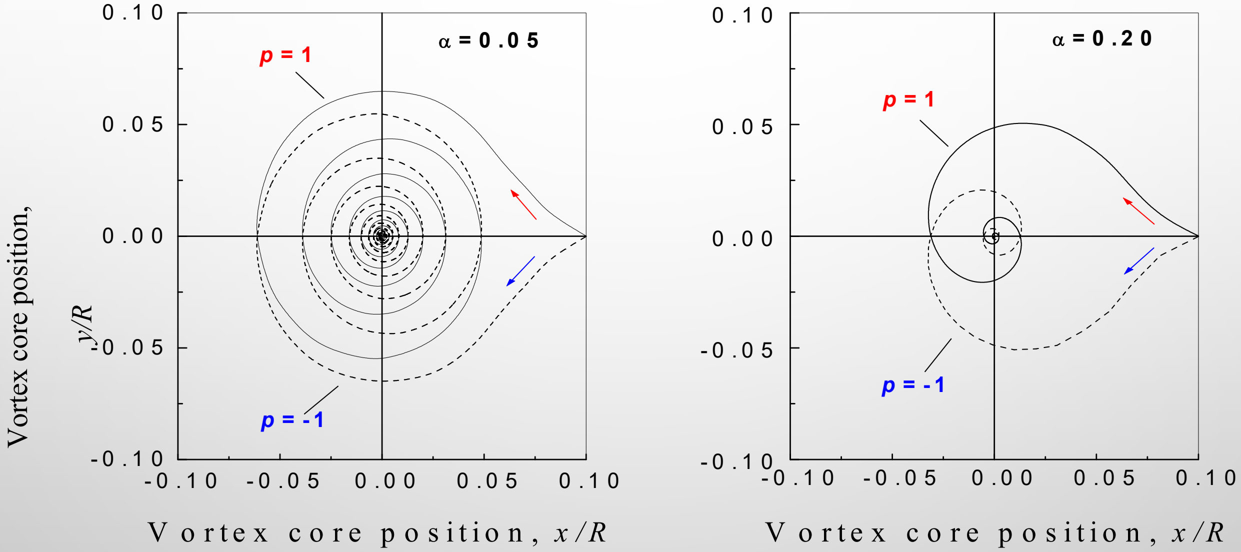




Magnetization reversal due to formation of the magnetic vortex state in circular dot

Vortex translation mode in a circular dot

Vortex core trajectory



The "*translational mode*" of the vortex excitations corresponds to the spiral vortex core rotation around the dot center. Its direction (counter-clockwise or clockwise) is defined by the combination of the vortex polarization and chirality.

VORTEX CORE REVERSAL

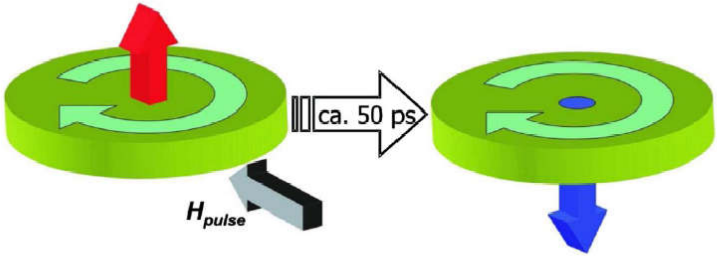
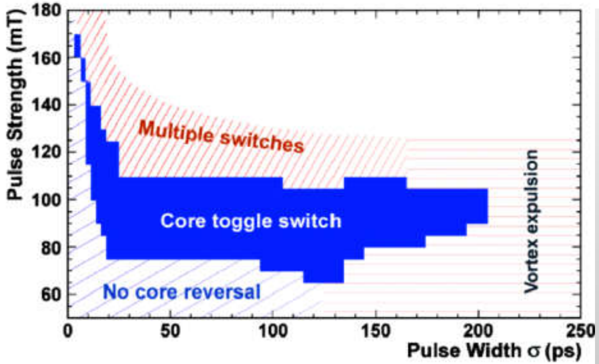
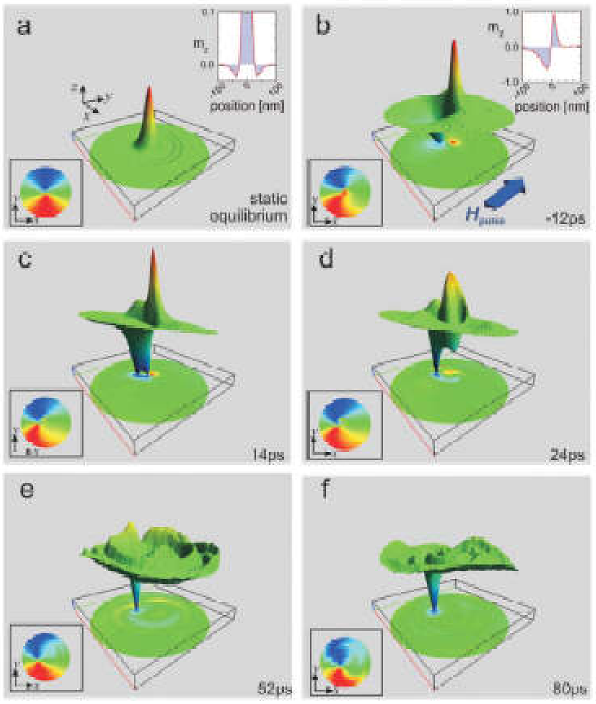


FIG. 1 (color online). Schematics of a field-pulse driven vorte
core switching. The vortex core magnetization can be switchec
by a short magnetic field pulse applied in the film plane. Thi
switching process requires only 40–50 ps.

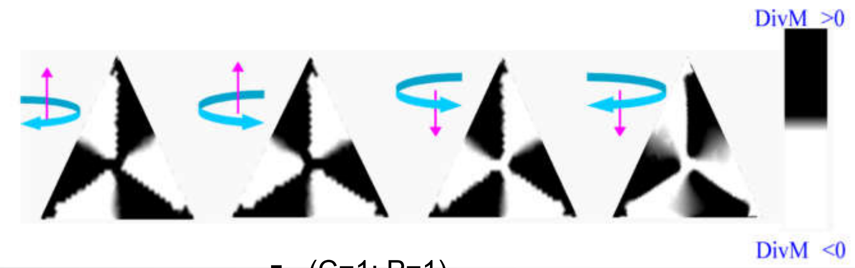


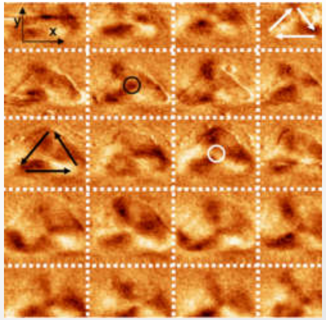
R.Hertel et al PRL <u>98</u> (2007) 117201

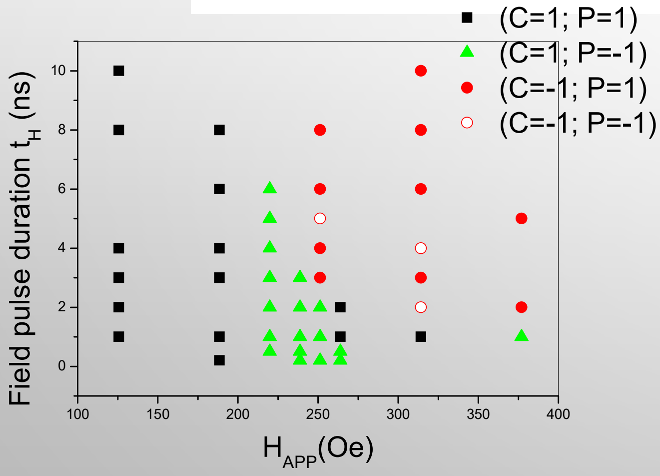


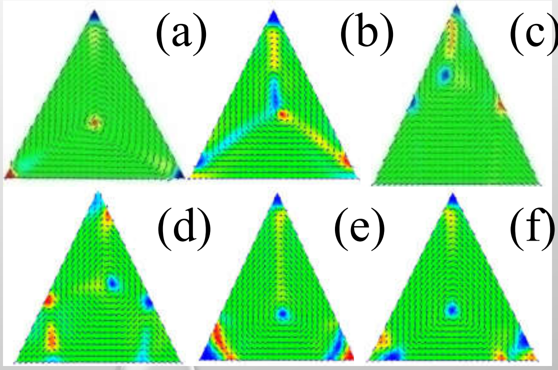
Experimental observation with synchrotron:
B.Van Wayenberge, Nature 444 (2006)

TRIANGULAR DOTS: SIMULTANIOUS CONTROL OF POLARITY AND VORTICITY





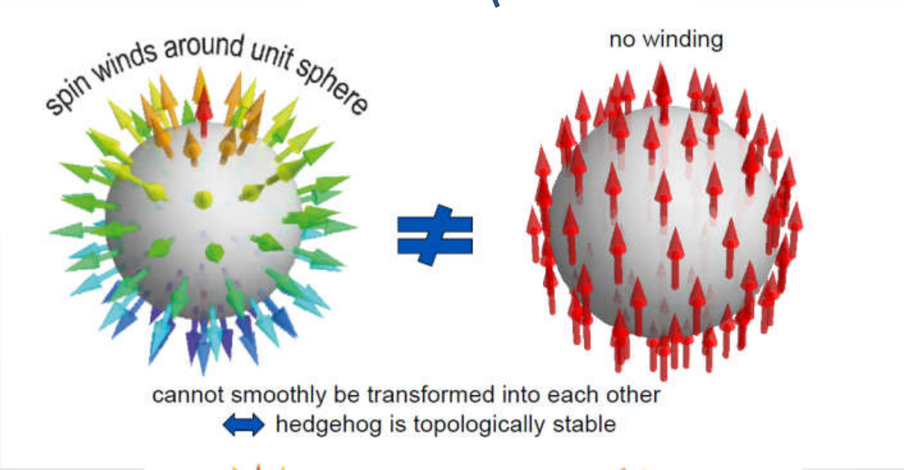




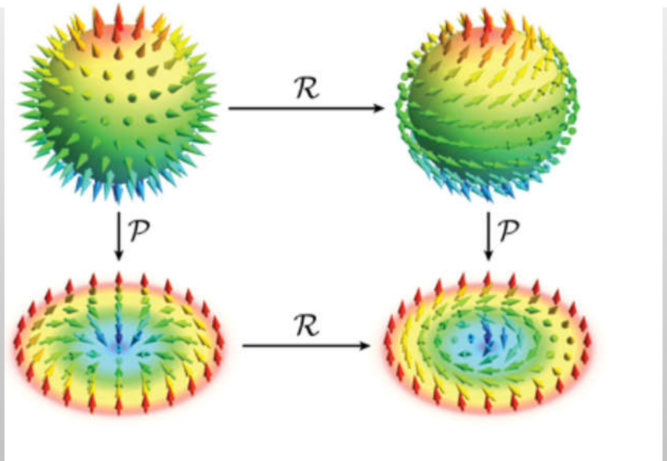
*Small fields + small duration -> core reversal

* Larger fields + larger duration -> chirality reversal

TOPOLOGICALLY NON-TRIVIAL MAGNETIC STRUCTURES (SYSTEMS WITH DMI)

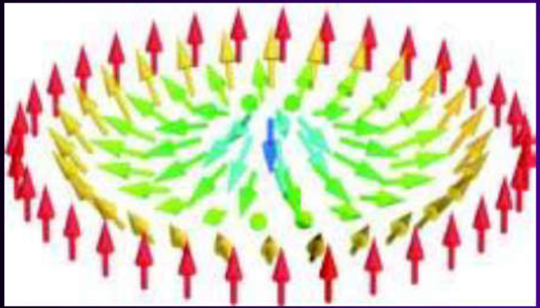


Non-trivial skyrmion

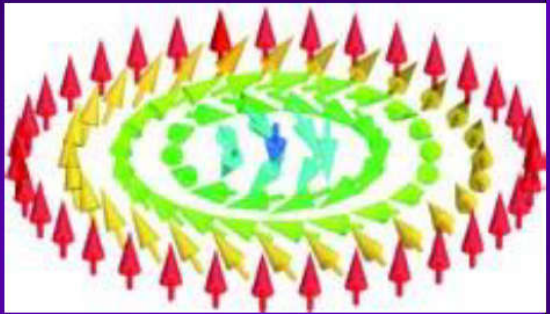


Single magnetic (baby-)skyrmion

"hedgehog" Neel skyrmion



Bloch skyrmion "vortex-like"

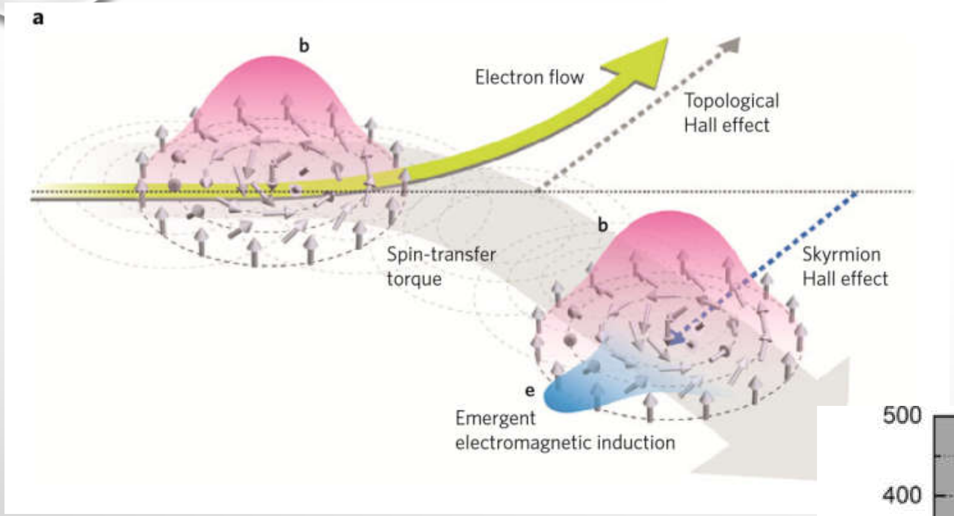


- Spins down at core, up everywhere else, homogeneous in *z*-direction
- Topological excitation,

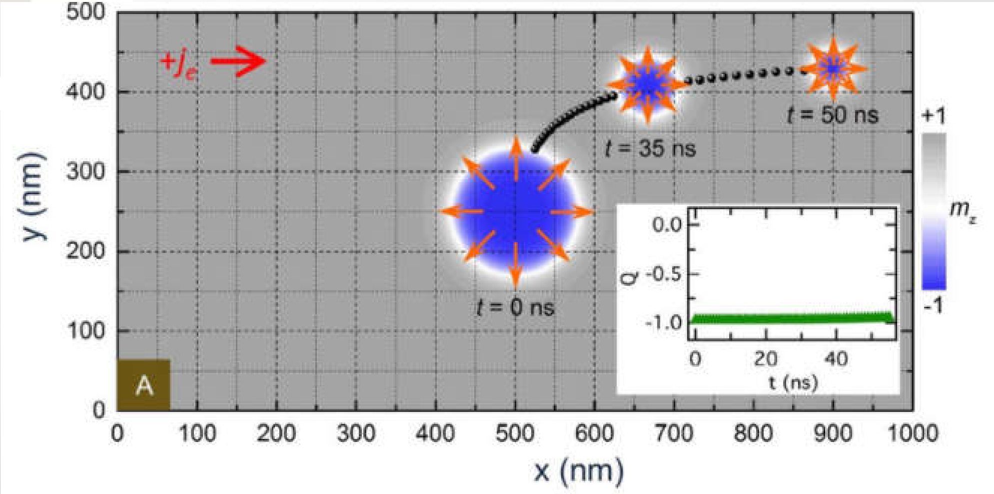
characterized by winding number: $4\pi W = \int d\vec{x}\, \Omega \cdot \frac{\partial \Omega}{\partial x} \times \frac{\partial \Omega}{\partial y}$

Pictures from Fert et al., Nature Nanotechnology (2013)

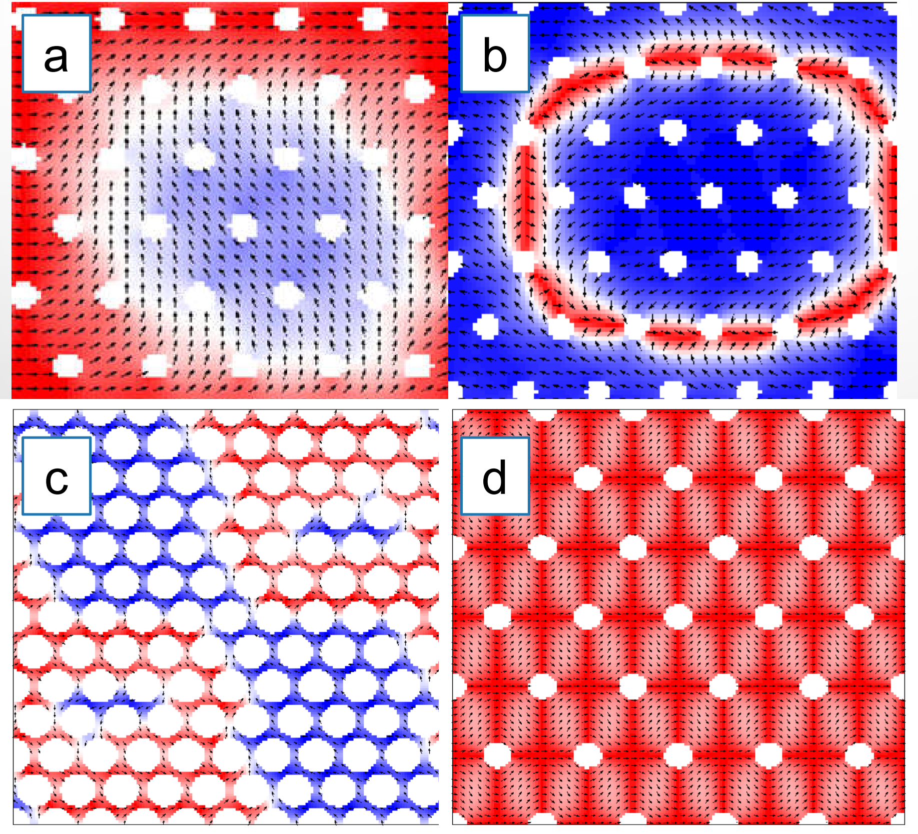
Topological effects in skymions



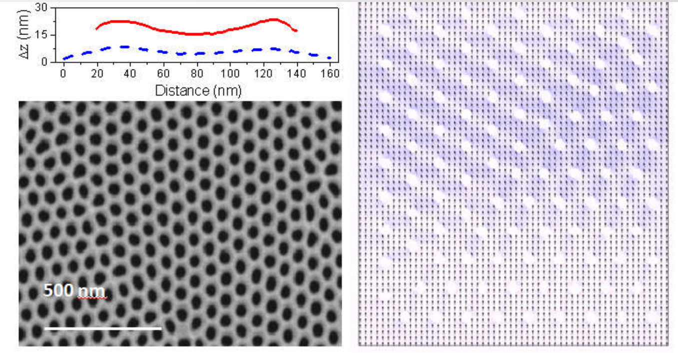
Micromagnetic simulations:
W.Jang et al (2017)



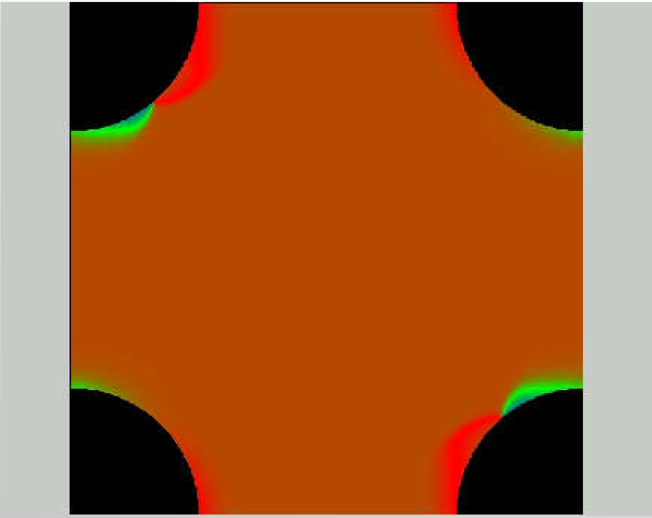
ANTIDOTS

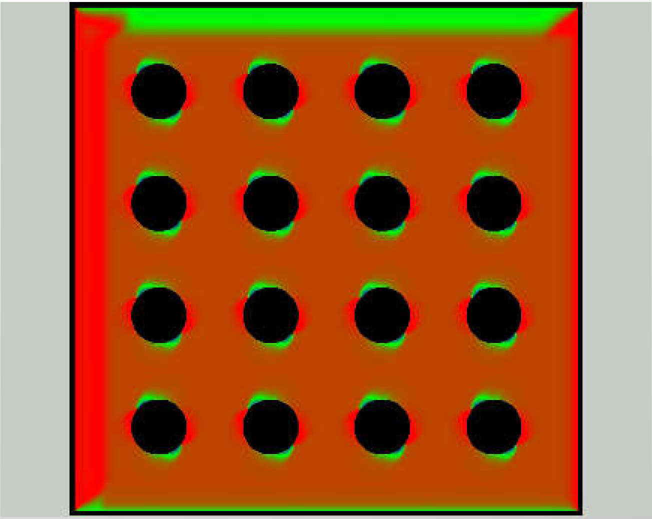


a) Diluted regime D<<L: nucleation
b) Pinned regime (D ~ L) Nucleation +pinning
c) Creap regime (L-D <<D) Multiple nucleation
d) chess-like structure

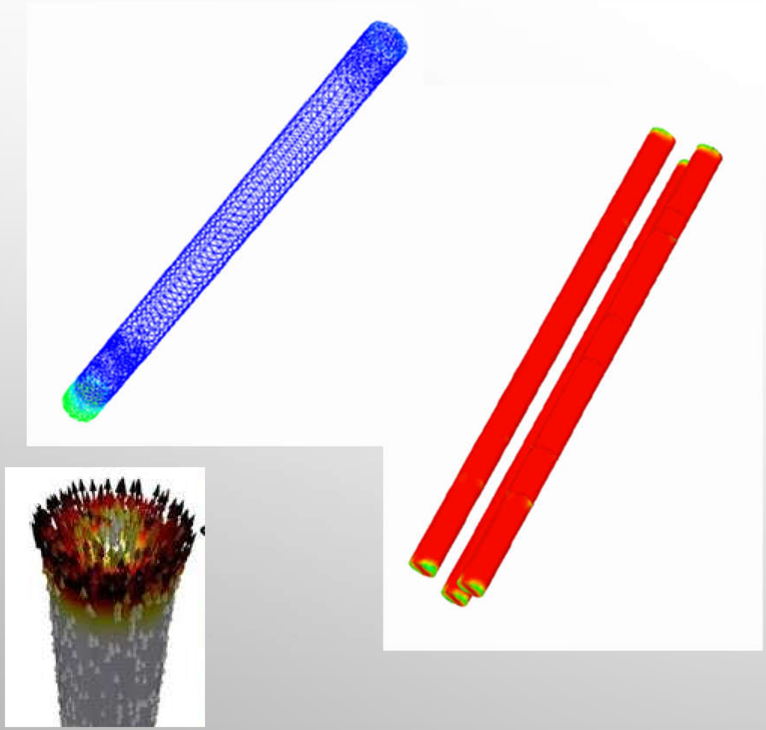


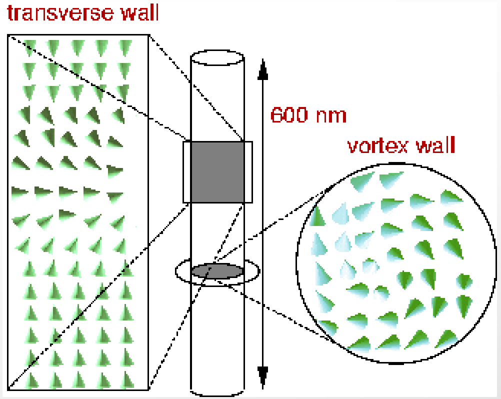
TWO MAIN PROPAGATION MECHANISMS





MAGNETIC CYLINDRICAL NANOWIRES



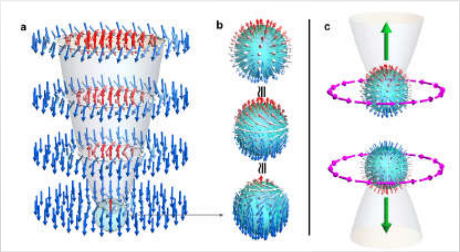


Naturally perpendicular anisotropy

Naturally chiral systems

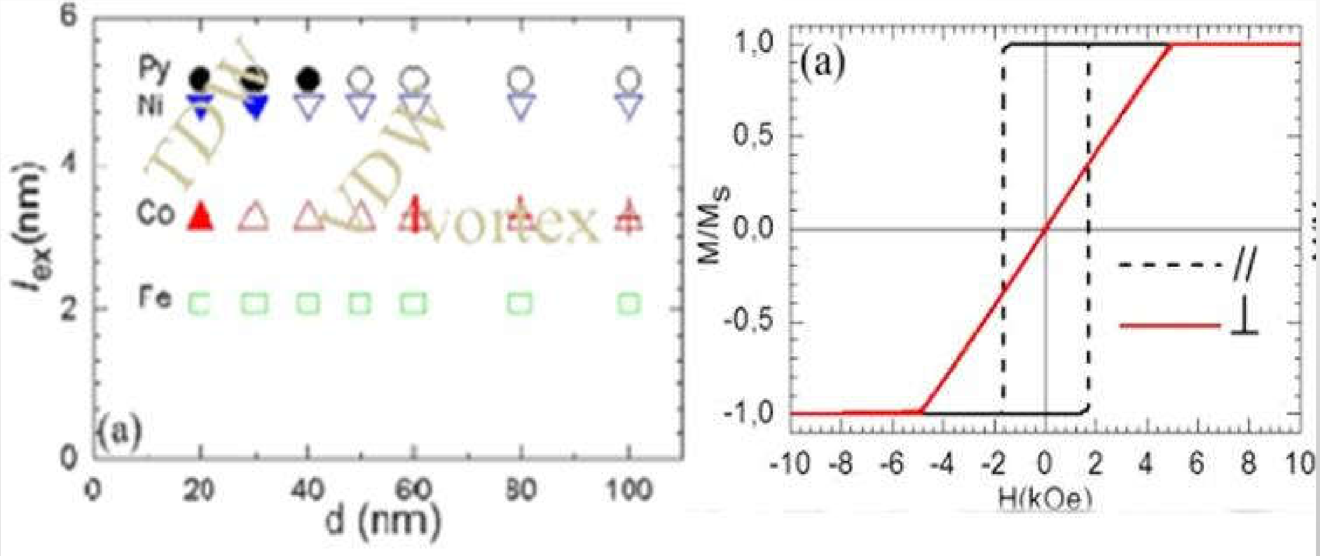
No Walker breakdown

Velocities up to



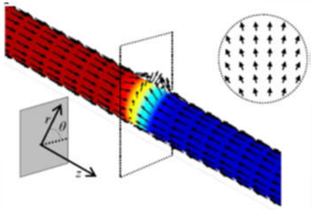
Charolou et al PRL(2019)

DIFFERENT REVERSAL MODES IN NANOWIRES

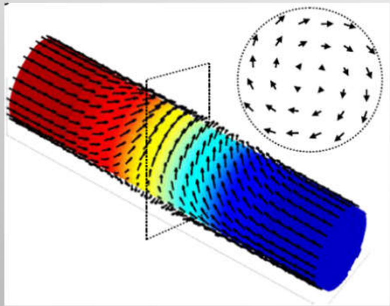


REMANENT STATES AND REVERSAL MODES

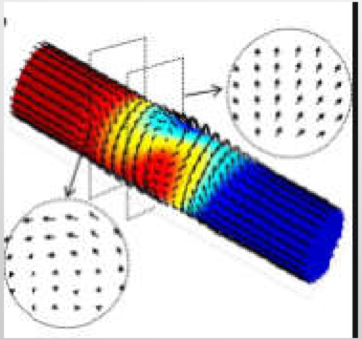
Small diameters <40nm
Single domain state
Transverse domain wall



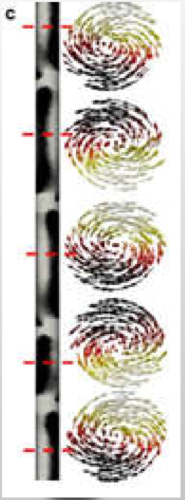
The MOST typical situation
Intermediate diameters:
Single domain state
Vortex (BLOCH-point) domain Wall

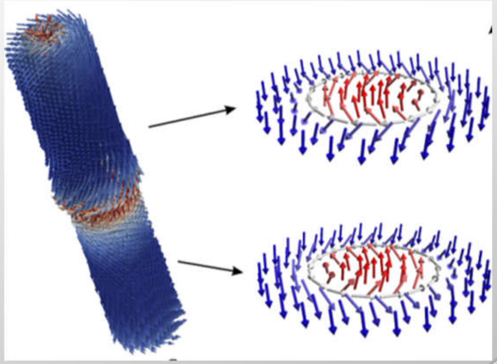


Vortex (vortex-antivortex) DW



Large diameters >100nm or large Ms :
Vortex (skyrmions) tube dynamical or at the remamence

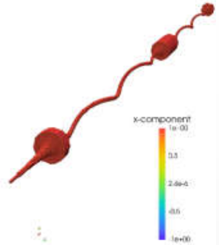




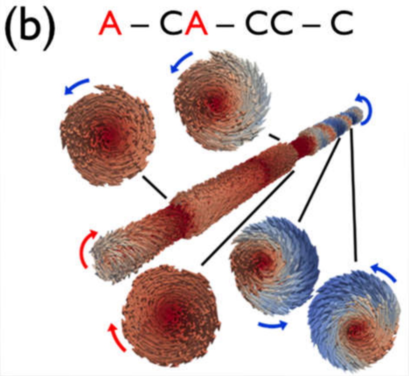
Co hcp
With perpend anisotropy

C.A. Ferguson *et al.* , J. Magn. Magn. Mater. 381 (2015) 457–462

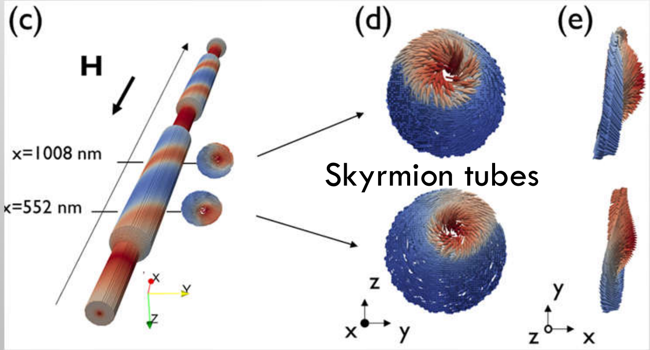
DEMAGNETISATION PROCESES



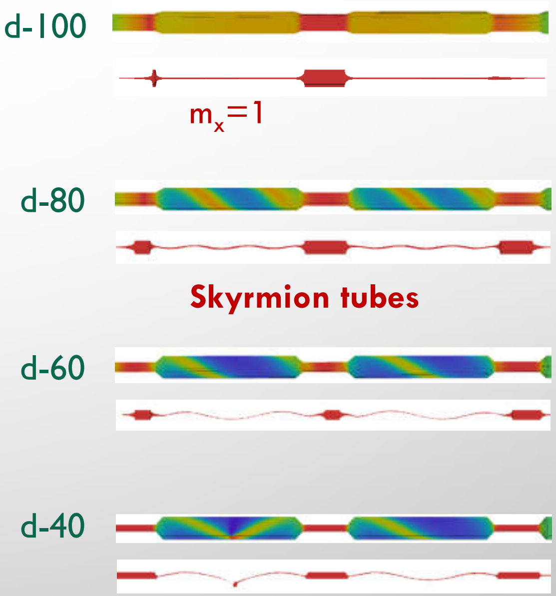
Remanence: Open vortex structures with arbitrary chirality



State before switching



Minor diameter



SOME ADVICES

- ✓ Use always small discretization length (1-2 nm), vortices or Bloch points may be there
- ✓ Remember that this is a continuous approximation (not valid at atomic scale or rapidly varying parameters)
- ✓ Magnetic systems can have many metastable states (different programs not always give the same result)
- ✓ Dynamic integration may be better than direct energy minimization (takes the system our of plane)
- ✓ Temperature fluctuations are only valid for low temperatures only, they are good as a mean to “shake” the system
- ✓ Do no expect coincidence with the experiment, especially in the value of the coercive field
- ✓ Be critical and check against analytical calculations

MICROMAGNETISM II

(NON-STANDARD),

TEMPERATURE, MULTISCALE DESCRIPTION AND ULTRAFAST DYNAMICS

O.CHUBYKALO-FESENKO

INSTITUTO DE CIENCIA DE MATERIALES DE MADRID,

CSIC, SPAIN

THERMAL FLUCTUATIONS PLAY VERY IMPORTANT ROLE IN MAGNETISATION DYNAMICS:

At the microscopic level:

- At the equilibrium they are responsible for thermally excited spinwaves.
- Spinwaves are responsible for temperature-dependence of macroscopic properties and for thermal magnetisation reversal via the spinwave instabilities and energy transfer to main reversal mode.

At more macroscopic level

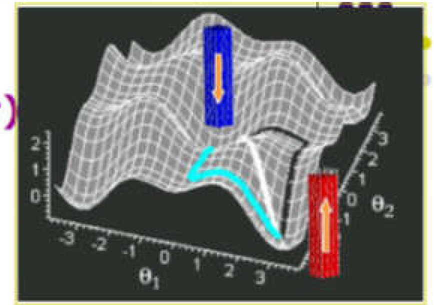
- Thermal fluctuations are responsible for random walk in a complex energy landscape
- Eventually energy barriers could be overcome with the help of thermal fluctuations leading to magnetisation decay.

LONG-TIME DYNAMICS: ENERGY BARRIER EVALUATION

Slow processes:

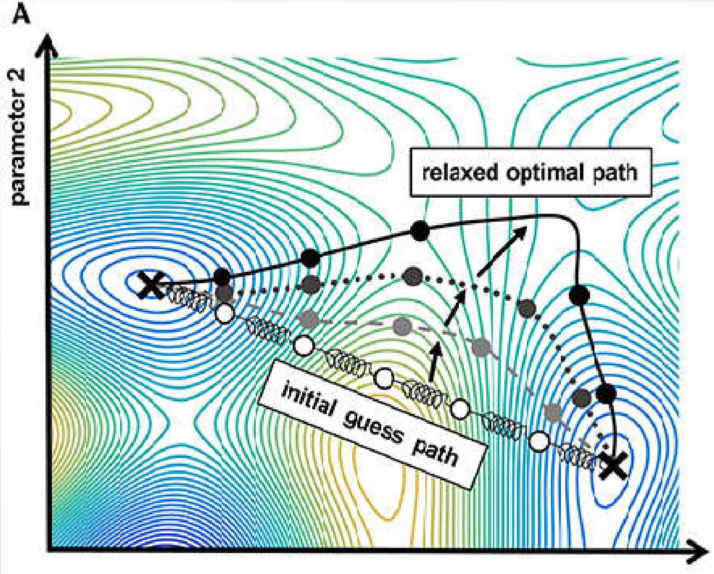
$k_B T << \Delta E$ (Energy barrier)

$$t_i = t_0 \exp(\Delta E / k_B T)$$

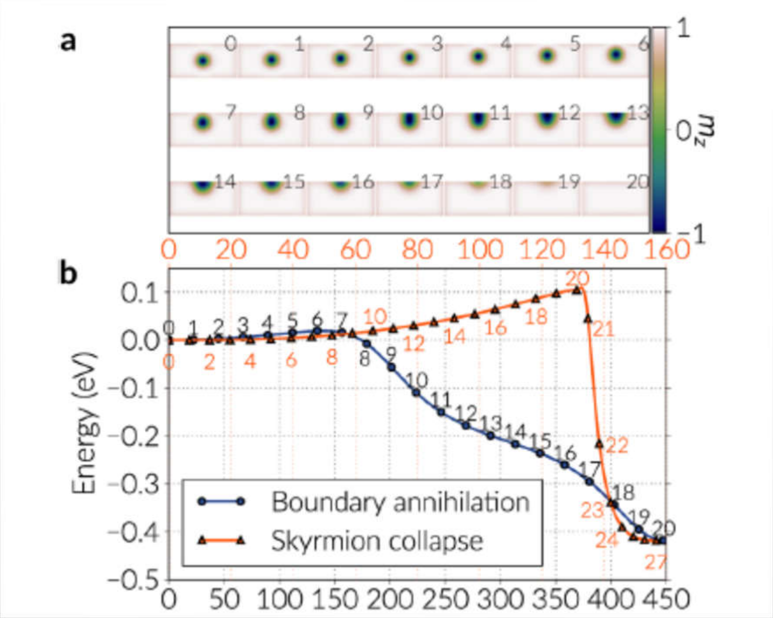


- Energy barrier calculation is essential part for determination of long-time thermal stability and slow thermal relaxation
- This is important from the point of view of magnetic recording applications.
- Evalulation of energy barriers should be done in a multidimensional space and is a difficult problem
- **In systems with many minima, the energy barriers should be constantly re-evaluated**
- **The result may depend on the initial guess due to the motion on a sphere**

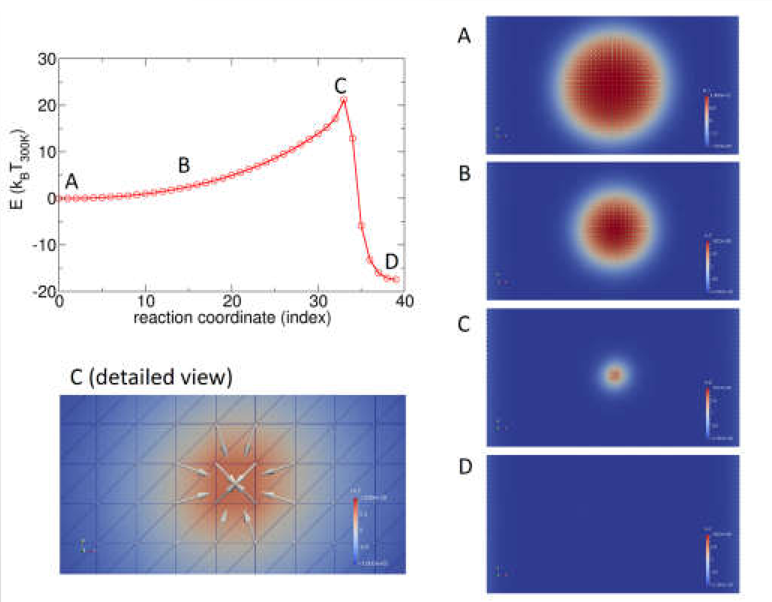
Elastic nudged band method



ENERGY BARRIERS FOR SKYRMIONS

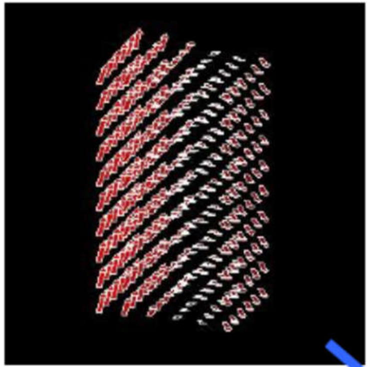


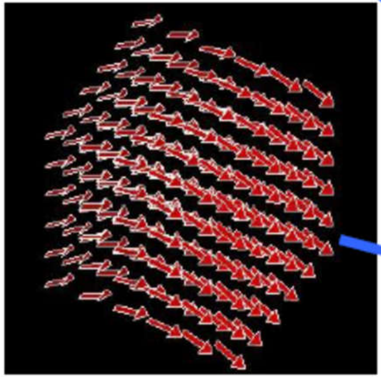
D.Cortes-Ortuño et al SREP 7 (2017)

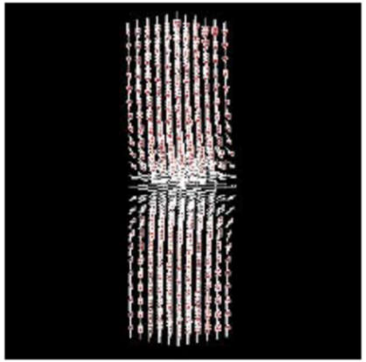


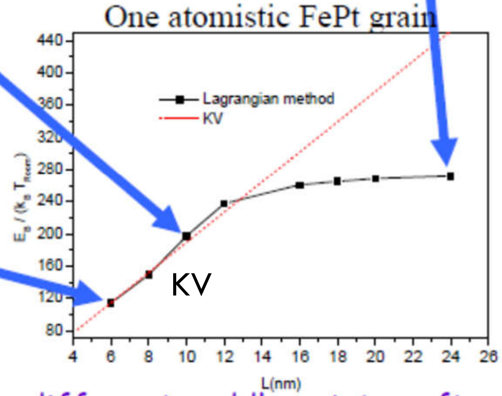
D.Suess et al

Energy barriers in a single FePt grain







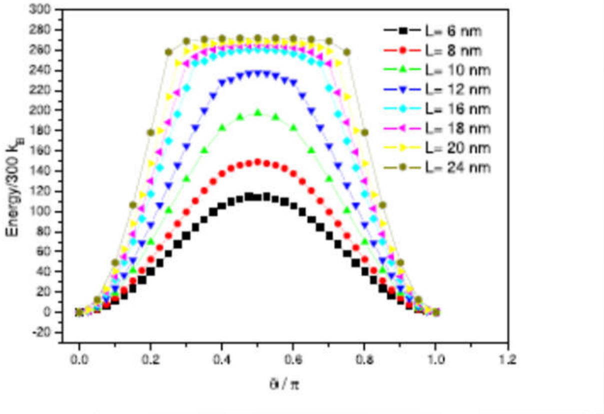


Varying the length-> different saddle point configurations corresponding to different reversal mechanism

Simpler method: constrained minimization

With Lagrange multiplier

$$E = E_0 - \lambda(< m > - m_z^0)$$



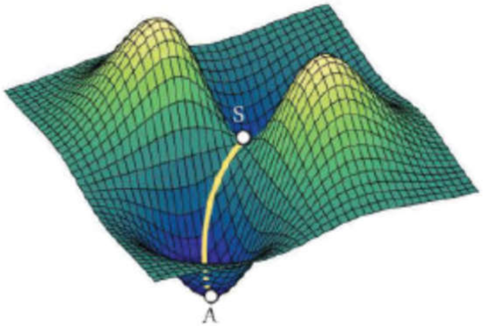
E.Paz et al Physica B 403 (2008)

Transition state theory

J S Langer, *Ann Phys* **54**, 258 (1969)

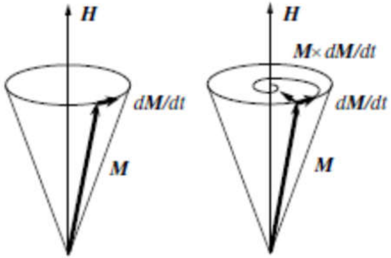
- Connection to (higher-frequency) modes through the Arrhenius prefactor (attempt frequency)
- <u>Example</u>: *Langer's theory of transition rates*

$$\Gamma \equiv \frac{1}{\tau} = \boxed{\frac{\lambda_+}{2\pi}\Omega_0} \exp\left(-\frac{E_a}{k_B T}\right)$$



Dynamical prefactor

Linearised dynamics at *S*,
rate of growth of unstable mode



λ_+

Ratio of curvatures

$$H = \left\{ \frac{\partial^2 E}{\partial \eta_i \partial \eta_j} \right\}$$

Hessian matrix

$$\Omega_0 = \sqrt{\frac{\det H^A}{|\det H^S|}} = \sqrt{\frac{\Pi_i \lambda_i^A}{\Pi_j |\lambda_j^S|}}$$

Ratio of products of eigenvalues of H

From Joo-Von Kim

KINETIC MONTE CARLO

- Evaluate all energy barriers in multidimensional space
- Evaluate all transition rates, according to the Arrhenius law

$$f_i = f_0 \exp(-\Delta E / k_B T) \qquad f = \sum f_i$$

- Choose a particle (cluster) with the probability proportional to its transition rate and invert it
- Approximate the waiting time from the exponential distribution
- Recalculate all the energy barriers $\qquad D(t)dt = f\exp(-ft)dt$

Solution of the Master equations (not too many barriers)

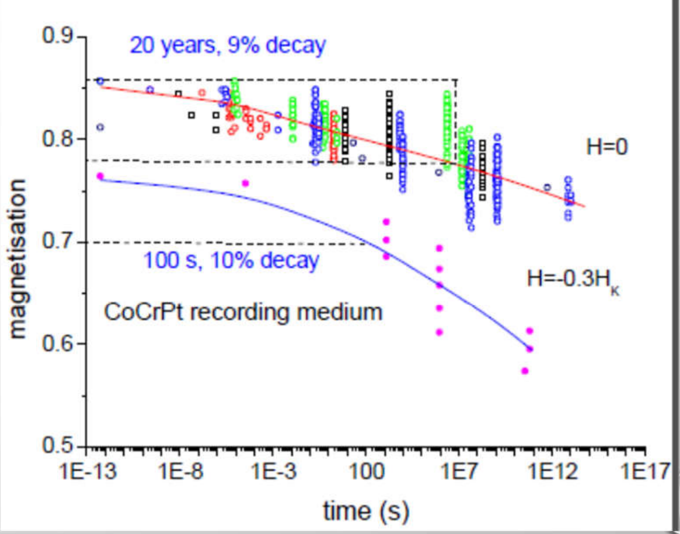
$$\frac{dm_i}{dt} = -\sum_j p_{ij} m_i + \sum_j (1 - p_{ji}) m_j$$

Leaving well

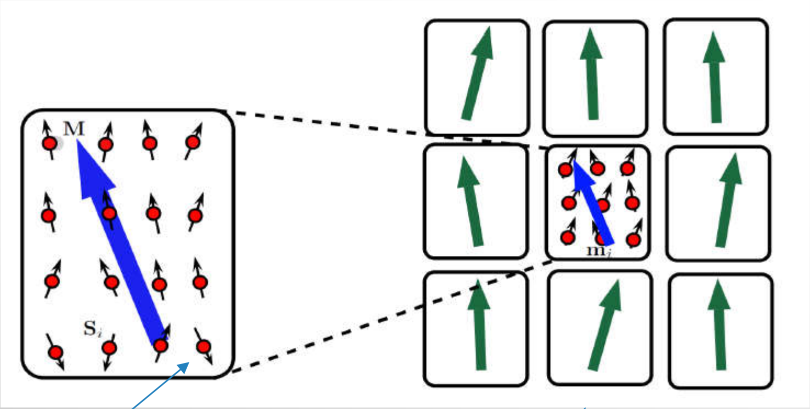
Returning to well

CoCrPt magnetic recording media

<D>=6.5 nm, K=2.4 10^6 erg/cm^3 M=442em/cm^3



DYNAMICS: ATOMISTIC VS MICROMAGNETIC APPROACH



Atomic Spins, S

Micromagnetic units (macrospins), m

Generalized Heisenberg

$$H = -\frac{1}{2}\sum_{ij} J_{ij}^{\alpha\beta} S_i^{\alpha} S_j^{\beta} \rightarrow$$

Takes into account crystal structure

Can be long-range

Micromagnetic exchange

$$E = A\int_V \left[\left(\frac{\partial m_x}{\partial x}\right)^2 + \left(\frac{\partial m_y}{\partial y}\right)^2 + \left(\frac{\partial m_z}{\partial x}\right)^2\right] dV$$

$$A_\nu(0\,K) = \frac{1}{V_{at}}\sum_j J_{0j}^{\nu}\left(a_{0j}^{\nu}\right)^2$$

The theory of thermal magnetization fluctuations of single domain, non-interacting particles was introduced by W.F.Brown
(W.F.Brown Phys Rev **130** (1963) 1677)

"We now suppose that in the presence of thermal agitation, the dissipative "the effective field" describes only statistical (ensemble) average of rapidly fluctuating random forces, and that for individual particle this expression must be augmented by a term h(t) whose statistical average is zero"

$<h_i(t)>=0, \quad <h_i(t)h_j(t+\tau)>=\mu\delta_{ij}\delta(\tau), \quad i,j=x,y,z$

"The random-field components are formal concepts, introduced for convenience, to produce the fluctuations δM"

W.F.Brown outlined two methods:

-Based on the fluctuation-dissipation theorem

-Imposing the condition that the equilibrium solution of the Fokker-Plank equation is the Boltzman distribution

$$\mu = \frac{2\alpha k_B T}{M_s V_i (1+\alpha^2)}$$

O.Chubykalo et al JMMM 272 (2004) 251
For colored noise see U.Atxitia, O.C.-F. PRL 102 (2009) 057203

DYNAMICS: ATOMISTIC/MICROMAGNETIC APPROACH:

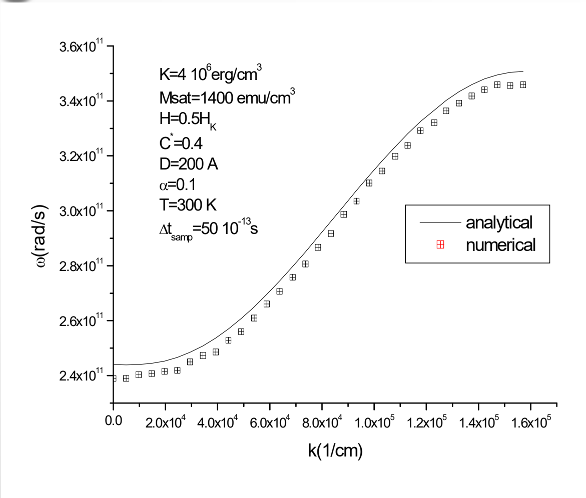
- Dynamic behaviour of the magnetisation is based on the Landau-Lifshitz-Gilbert equation

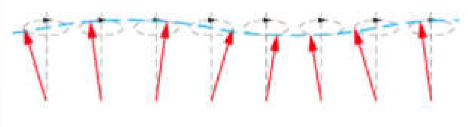
$$\dot{\vec{S}}_i = -\frac{\gamma}{1+\alpha^2}\vec{S}_i \times H_i(t) - \frac{\alpha\gamma}{1+\alpha^2}\vec{S}_i \times (\vec{S}_i \times \vec{H}_i(t))$$

- where γ_0 is the gyromagnetic ratio and α is a intrinsic damping (not to be confused with atomistic coupling-to-the bath parameter damping)
- additional thermal field converts it to stochastic differential equation (Stratonovich sense)-> Langevin dyanmics

$$< h_j(t) >= 0 \qquad < h_i(0)h_j(t) >= \delta(t)\delta_{ij} 2\alpha k_b T / \gamma$$

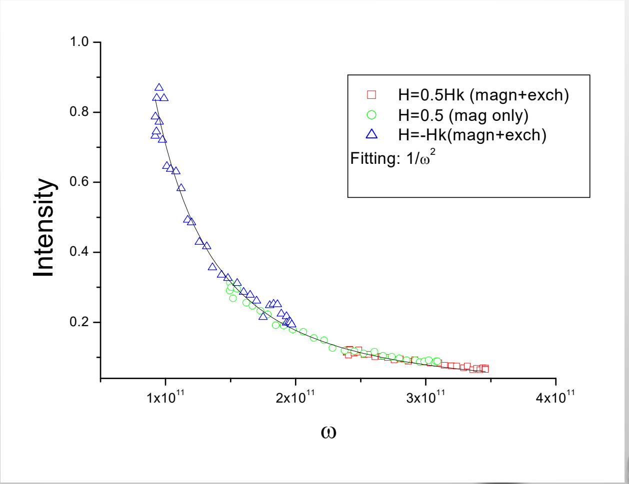
THERMAL SPIN WAVES FROM MAGNETIZATION FLUCTUATIONS

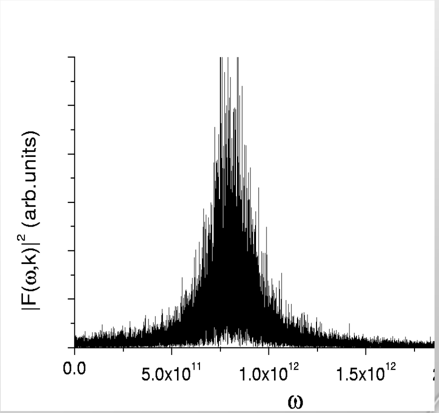




Fluctuation-dissipation theorem

$$Max\ I(\omega,k)=\frac{\gamma k_B T(1+\alpha^2)}{\alpha V_0 M_s}\frac{1}{\omega_k^2}$$

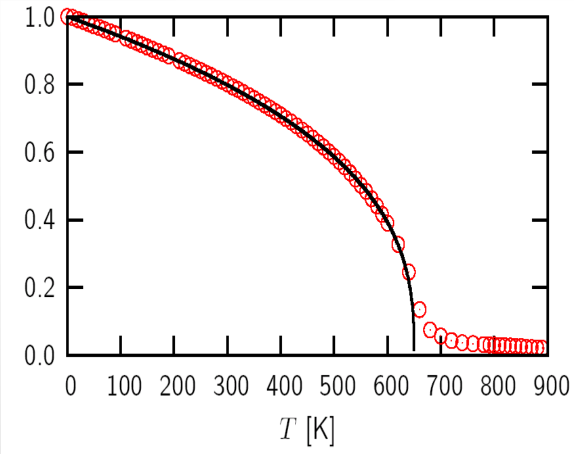




K.Yu Guslienko et al JMMM 272 (2004)

THERMAL LANGEVIN DYNAMICS:
ATOMISTIC VERSUS MICROMAGNETICS APPROACH

G.Grinstein and R.H.Koch PRL 90 (2003) 207201



N.Kazantseva et al PRB 77 (2008)

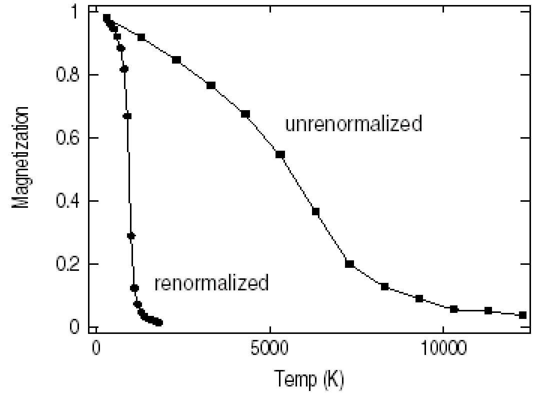


FIG. 1. M vs $\tilde{T}$ curves for the model Permalloy cube, from LLG Eq. (6), with parameters as given in text, and unrenormalized (square symbols) and renormalized (oval symbols) values of the exchange constant.

Langevin dynamics for the micromagnetics does not correctly describe spinwaves spectrum (high k are cut):

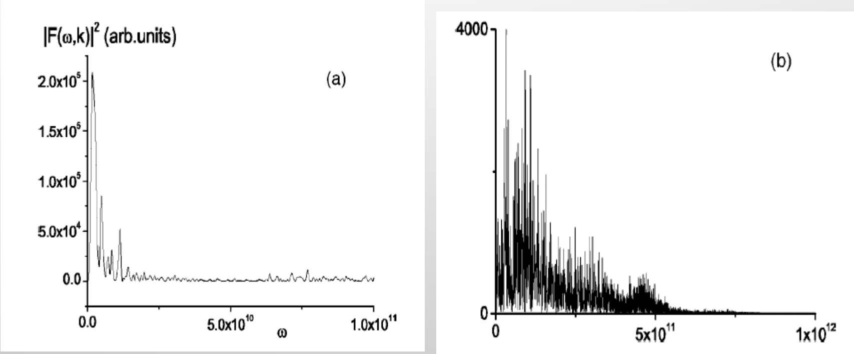
The spectrum is cut, DOS is not correct and Tc is largely over estimated

SPINWAVE ROLE DURING THE MAGNETISATION REVERSAL

- In the vicinity of the nucleation the spinwave instabilities occur.
- Spinwaves generation becomes chaotic and the system thermalizes through the distribution of energy over all degrees of freedom

- At the nucleation reversal the chaos is suppressed and the energy is transferred to the main eigenmode

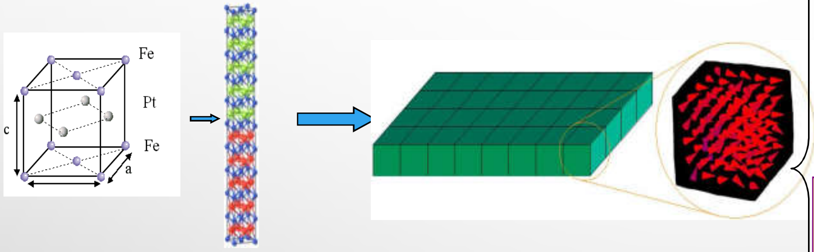
k=0 k=6



O.Chubykalo et al
Phys Rev B 65 (2002) 184428.

$H = -0.99\ H_K$

HIERARCHICAL MULTI-SCALE APPROACH



Ab-initio calculations
μ, J, k, d

atomic cells

Parametrised Hamiltonian

Discrete (atomistic)models
Ms(T), K(T), A(T), D(T), α(T)

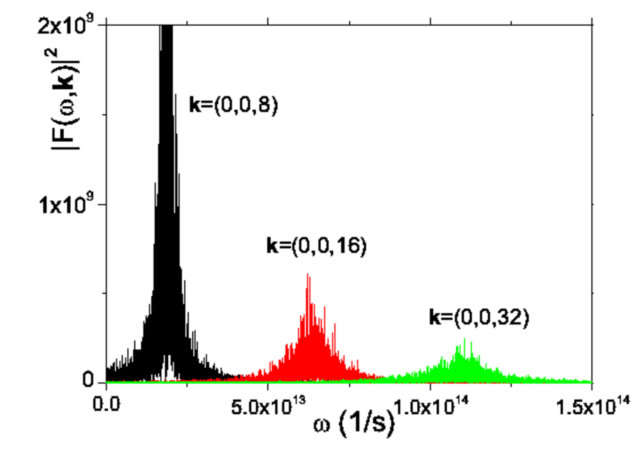
Micromagnetic models

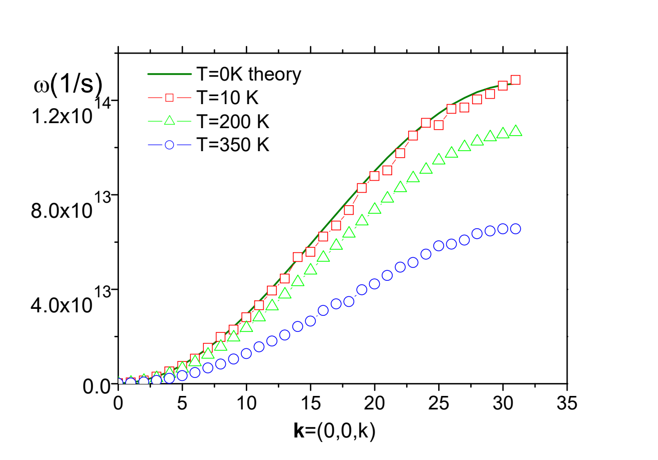
DFT → atomistic(Heisenberg) Hamiltonian → micromagnetics (LLB)

N. Kazatseva et al Phys. Rev. B 77 (2008) 184428

TEMPERATURE-DEPENDENT SPIN WAVE SPECTRUM

Exchange stiffness calculation





$$\omega \propto A(T)k^2$$

$$A(T) = A(0)m^{2-\varepsilon}$$

due to spin-spin correlations

U.Atxitia. … O.C.-F… PRB 82 (2010) 054415

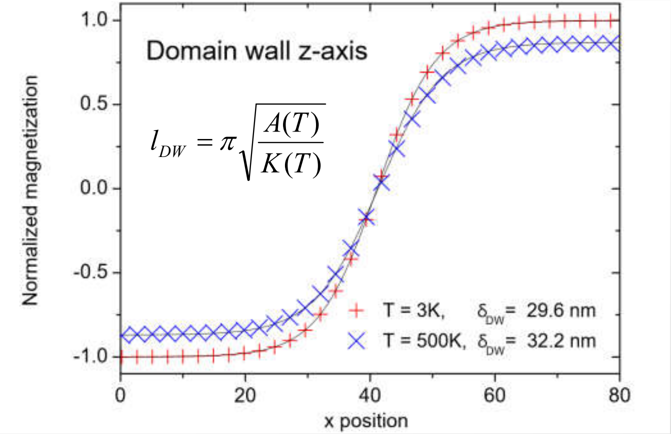
Material-specific, depends on number of neighbors, cristal structure etc.

TEMPERATURE-DEPENDENT DOMAIN WALL WIDTH (HCP CO)

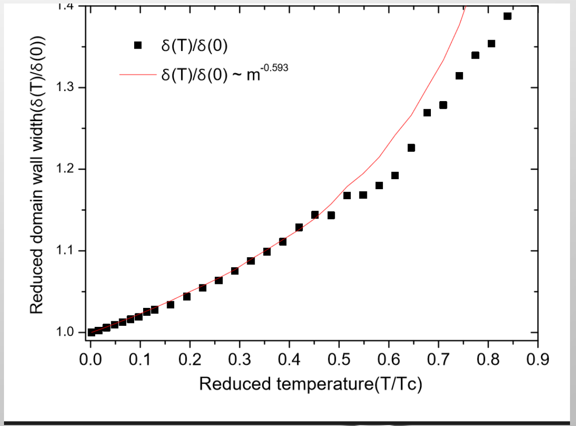
- Domain wall width increases with Temperature

- Slightly different width in x and z directions (< 1 nm difference)
  24-25nm

$$A(T) \propto m^{1.8}$$



- Independently evaluated from the Classical spectral density method (CSDM)



Moreno et al PRB 94 (2016)

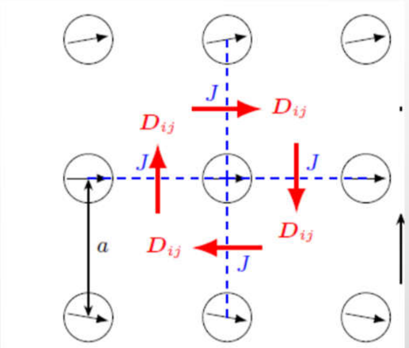
DZYALOSHINSKI-MORIYA INTERACTION

$$E_{DMI} = -\frac{1}{2}\sum_{i,j}\mathbf{D}_{ij}\left[\mathbf{S}_i \times \mathbf{S}_j\right]$$

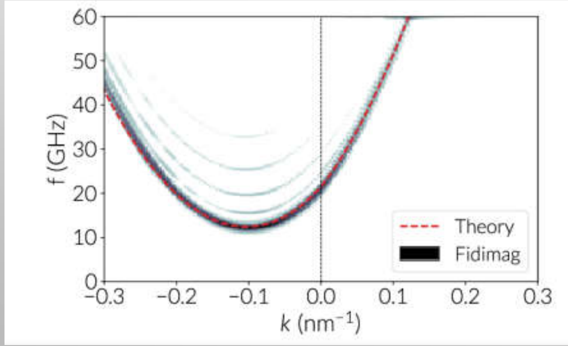
$$\mathbf{D}_{ij} = d\left[\mathbf{u}_{ij} \times \mathbf{z}\right]$$

$$E_{DMI} = 2\hat{D}\int \left[m_z \nabla \mathbf{m} - (\mathbf{m}\cdot\nabla)m_z\right]dS$$

Interfacial FMI



$$\hat{D}(T) = \hat{D}_0 m^{\beta}$$



D.Cortés-Ortuño New J.Phys.(2018)

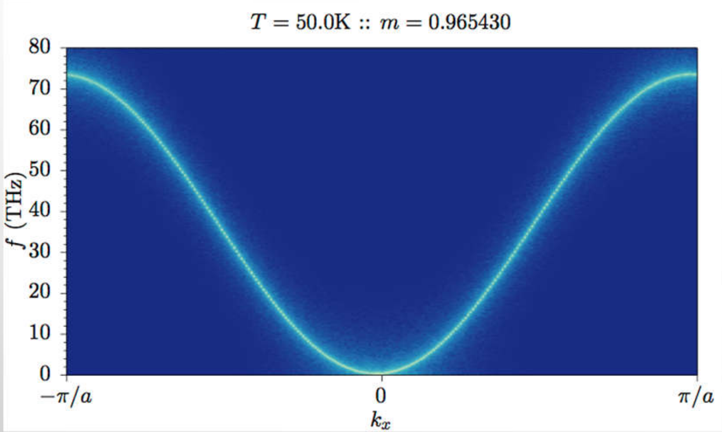
$$\omega(k) = \gamma_0\left(H + \frac{D}{M}k\cos(ak) + \frac{2A}{M}\sin^2(ak)\right)$$

Long wave part:

asymmetric in k part gives DMI,

Symmetric in k part gives exchange

TEMPERATURE-DEPENDENT DMI FROM THE SW SPECTRUM



$$A(T) \propto m^{1.5}; \quad D(T) \propto m^{1.5}$$

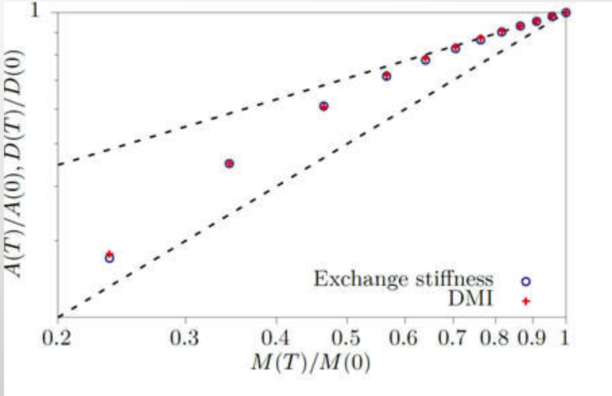
Not universal; simple cubic lattice!

R.Tomasello et al PRB 97 (2018)

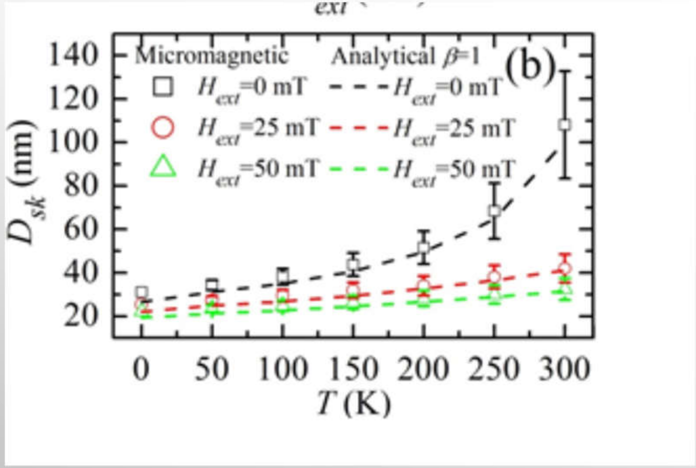
D/J=0.1

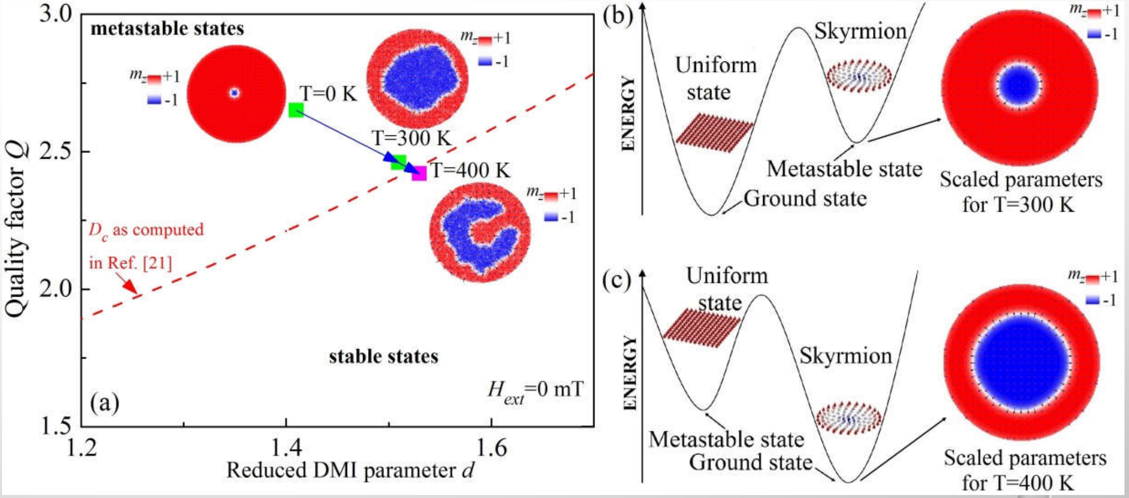
Simple cubic lattice

$$\mathbf{D}_{ij} = d\left[\mathbf{u}_{ij} \times \mathbf{z}\right]$$



SKYRMIONS IN CO/Pt DOT: MOVING IN THE PARAMETER SPACE WITH TEMPERATURE



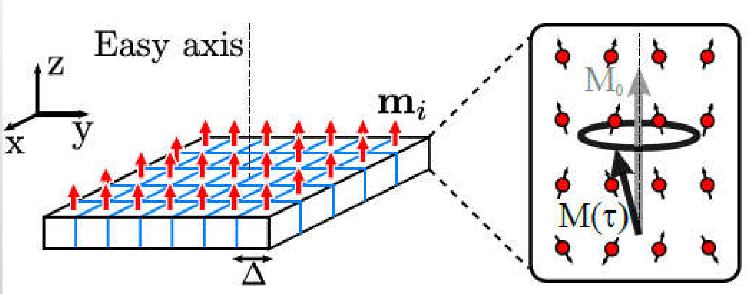


Temperature-dependent skyrmion radius
R.Tomasello, --O.C.F. et al PRB 97 (2018)

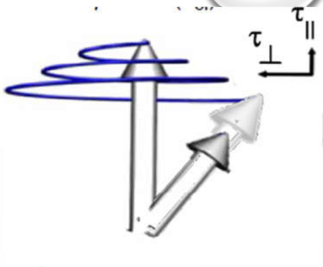
MICROMAGNETIC MODELING AT HIGH TEMPERATURES:

T$\neq 0 \Rightarrow |\mathrm{M}| \neq$ const   LLG micromagnetics is not valid

Landau-Lifshitz-Bloch micromagnetic equation

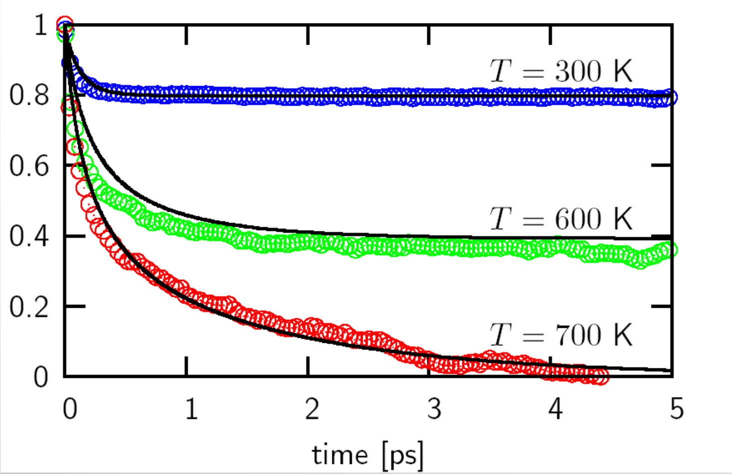


COMPARISON: ATOMISTIC VS MACROSCPIN



solid line – one spin LLB

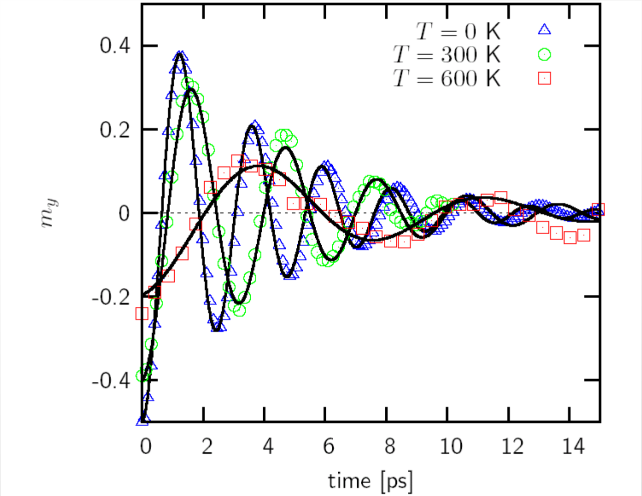
Longitudinal relaxation



Timescale is defined by exchange interactions

Critical slowing down phenomena near phase transition

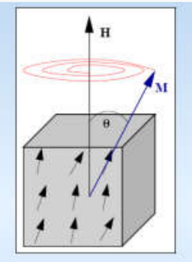
Transverse relaxation



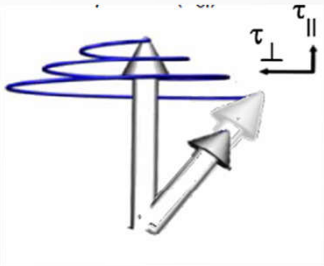
Tmescale is defined by external field

O.Chubykalo-Fesenko et al PRB 74 (2006)

THE LANDAU-LIFHITZ-BLOCH (LLB) EQUATION



$$\frac{d\vec{m}}{dt} = \gamma[\vec{m}\times\vec{H}] + \gamma\alpha_{\parallel}\frac{(\vec{m}\vec{H}_{eff})}{m^2} - \gamma\alpha_{\perp}\frac{[\vec{m}\times[\vec{m}\times\vec{H}_{eff}]]}{m^2}$$



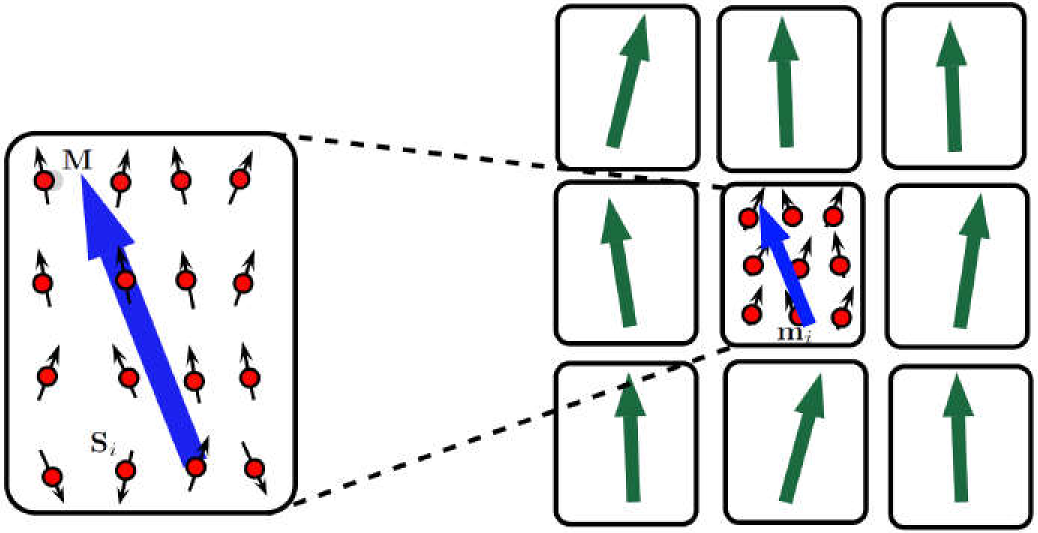
$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \mathbf{H}_A + \begin{cases} \frac{1}{2\tilde{\chi}_{\parallel}}\left(1 - \frac{m^2}{m_e^2}\right)\mathbf{m} & T \lesssim T_C \\ -\frac{J_0}{\mu_0}\left(\frac{T}{T_C} - 1 + \frac{3}{5}m^2\right)\mathbf{m} & T \gtrsim T_C \end{cases}$$

$$\alpha_{\perp} = \lambda\left(1 - \frac{T}{3T_C}\right)$$

$$\alpha_{\parallel} = \frac{2}{3}\frac{T}{T_C}\lambda$$

D.Garanin PRB 55 (1997)

MICROMAGNETIC MODELING BASED ON THE LANDAU-LIFSHITZ-BLOCH EQUATION



Exchange-coupled macrospins

Thermal fields can be included

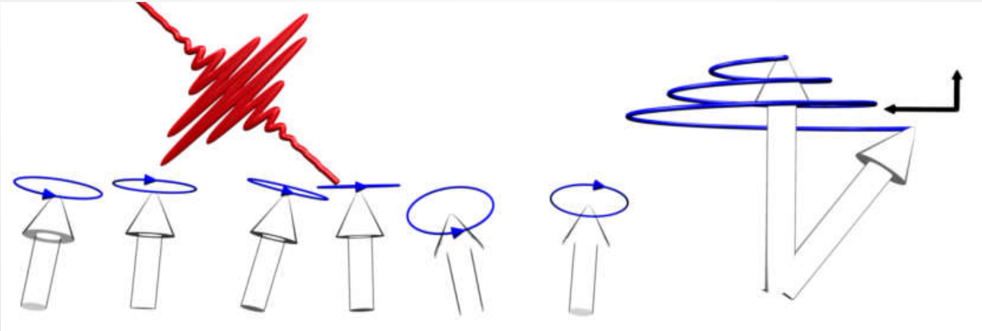
Large scale modeling

U. Atxitia *et al.* Applied Physics Letters **91**, 232507 (2007)

MODELING OF LASER-INDUCED DEMAGNETISATION WITHIN THE LLB APPROACH:

COMPARISON WITH EXPERIMENTS

Schematics: Laser excitation.. in a thermal macrospin model

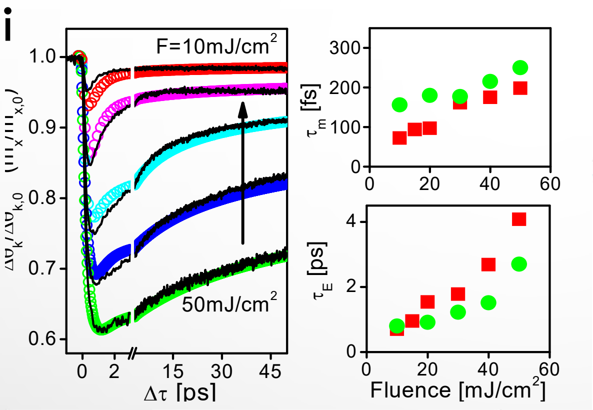


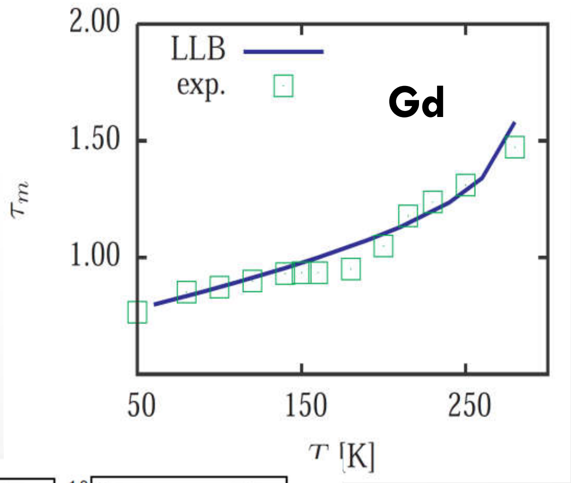
LLB micromagnetics is coupled to electronic temperature from laser heat

Multiple comparison with experiments confirm heat mechanism

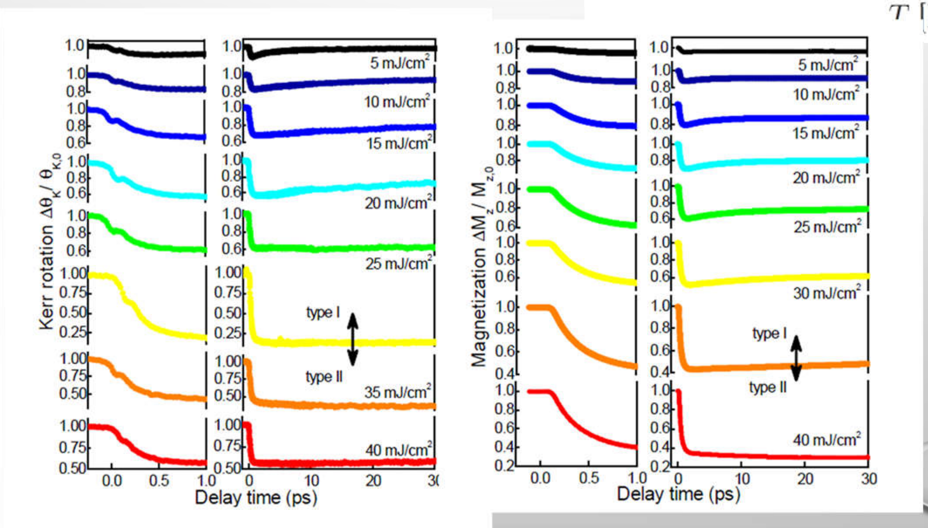
U.Atxitia et al
PRB 81 (2010)

Ni





M.Sultan et al
PRB 85 (2012)

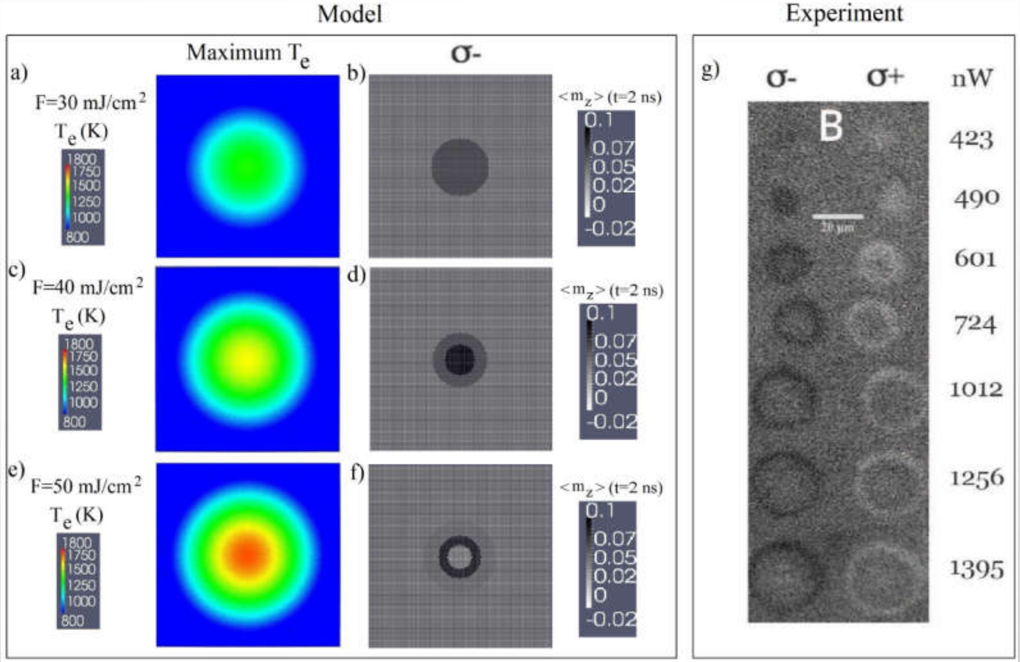


J.Mendil et al
Sci.Reports, 4 (2014)

FePt

MICROMAGNETIC MODELING OF FEPT DYNAMICS UNDER CIRCULARLY POLARISED LASER PULSE :

P.Nieves, O.C.-F. Phys Rev Appl 5 (2016) 014006



Inverse Faraday effect+

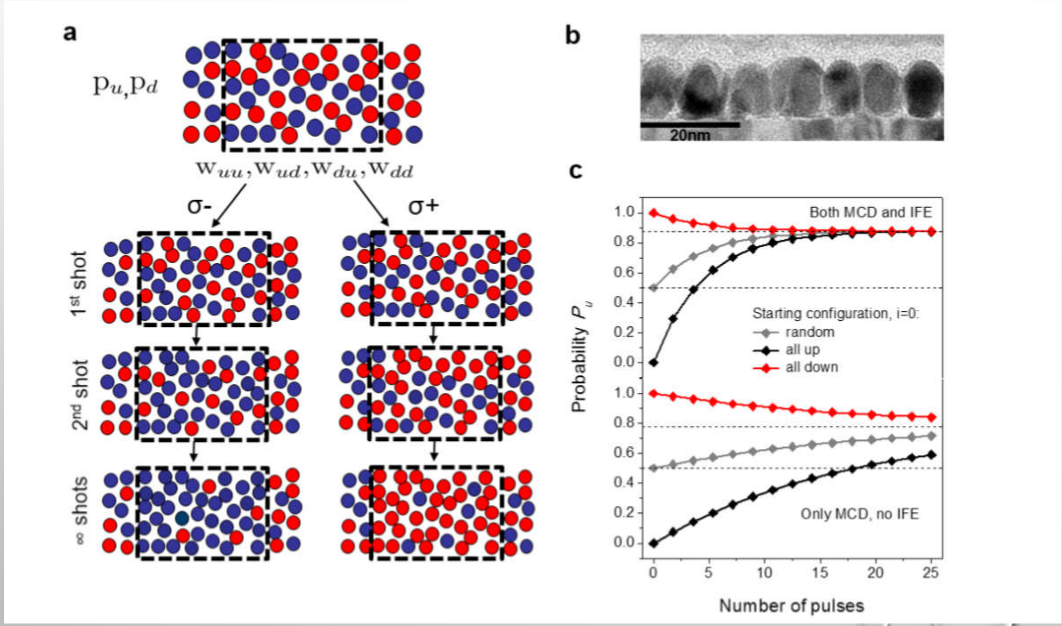
heat

There is an optimum T_e dynamics where the IFE is more efficient

MODELING OF LASER-INDUCED DYNAMICS IN FEPT

ACCUMULATIVE SUPER-PARAMAGNETIC EFFECT

Ab-initio effect -> LLB for siwtching probability -> rate equations



- Inverse Faraday effect:

ΔM=-7.1% Ms (σ+)

-3.5% (Ms) (σ -)

- MCD effect

Δ T=32 K(for Tmax=1100K)

for spin up and spin down

R.John et al
Sci. Rep.. 7 (2017) 4114.

MESSAGES:

- Necessity to include temperature unto modelling in many cases
- Atomistic Langevin dynamics simulations are consistent with thermal spinwave theory
- Micromagnetic Lngevin dynamics simulations can be used in the range T<Tc/3
- Thermal spin wave spectrum –softening with tempeture
- Allows to evaluate Exchange stiffness and DMI parameters, They scale equally with temperature as m^{2-e}
- The scaling relation K(m), A(m), D(m) provides the tool to evaluate many important characteristics
- The example: skyrmion radius increases with temperature
- Importance of spinwaves during laser-induced magnetization dynamics:: excitation of two spinwave modes at percolation length as a criterion for switching