Micromagnetics

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Outline



Stoner



Wohlfarth

Brown

Why micromagnetics? Magnetic recording Strong magnets What is micromgnetics? Energy contribution Magnetization dynamics How does it work? Finite element method Can I do it myself? Examples

Why do we need micromagnetics? An introduction

Permanent magnets

700 kg of NdFeB per MW

1.5 kg NdFeB

Ancient magnets (1600)





Armed loadstone

Modern magnets (1984)



Interactions



Electron holography TEM study Reconstructed phase image of magnetization structure



Multiscale simulation



 \rightarrow Design guidelines for magnet development



magnetization, crystalline anisotropy, exchange constant,

. . . .

grain size, boundary phases,

Magnetic recording



1956





Magnetic media account for 92 % of newly stored information



1 Tbit/in² 25 nm periodicity 20 nm islands



10 Tbit/in² 8 nm periodicity 6 nm islands







Bashir, Schrefl et al. JMMM 324 (2012) 269 pole tip

shield



EP Wohlfarth



A MECHANISM OF MAGNETIC HYSTERESIS IN HETEROGENEOUS ALLOYS

BY E. C. STONER, F.R.S. AND E. P. WOHLFARTH Physics Department, University of Leeds

(Received 24 July 1947)

Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences, Vol. 240, No. 826. (May 4, 1948), pp. 599-642.





The size must be below a critical value, depending on shape, such that the particle constitutes a single domain, in which boundary formation is precluded.

20 n 100 Yang, Nanotechnology 22 (2011) 385301



12 nm

exchange spring



At this value, namely

$$H_0 = \frac{1}{2} (d\gamma/dx)_{\rm max.}/I_0,$$

the boundary will move spontaneously

EC Stoner, EP Wohlfarth, Phil. Trans. Roy. Soc. A240 (1948) 599



switching in the write field

$\frac{1+\alpha^2}{|\gamma|} \frac{d\mathbf{M}}{dt} = -\mathbf{M}\mathbf{x}\mathbf{H}_{eff} - \frac{\alpha}{M_s}\mathbf{M}\mathbf{x}\mathbf{M}\mathbf{x}\mathbf{H}_{eff}$





elastic band method

saddle points

Dittrich et al, JMMM 250 (2002) 12 Henkelman et al, J Chem Phys113 (2000) 22



thermal switching

energy barrier: 128 k_BT



pol tip antiferromagnetically coupled

> bit patterned islands soft/hard magnetic

> > soft under layer



pol tip antiferromagnetically coupled

> bit patterned islands soft/hard magnetic

> > soft under layer

Magnetization Dynamics



Gyromagnetic precession M rotates around H_{eff}

Dissipative term "force" proportional to generalized velocity

damping parameter

Micromagnetic basics

Micromagnetic basics



Torque Forces on the magnetic moment

Energies Micromagnetic energy contributions



Deviation from equilibrium Reversal modes
Micromagnetics, Domains, and Resonance

WILLIAM FULLER BROWN, JR.

Department of Electrical Engineering, University of Minnesota, Minneapolis 14, Minnesota

JOURNAL OF APPLIED PHYSICS SUPPLEMENT TO VOL. 30, NO. 4 APRIL, 1959

Search for equilibrium



→ Magnetization can only rotate forces on M are torques



Exchange



Anisotropy



External magnetic forces



 $T_3 = -J_s H_0 \sin\phi.$

Internal magnetic forces



Internal magnetic forces



 \rightarrow non-uniform magnetic states





(a)

MAGNETIC

IHol < Her









(c)



I have always been grateful to the editors for the promptness with which they rejected it that enabled me to send it to the Physical Review

WF Brown, Domains, micromagnetics, and beyond: Reminiscences and assessments, J Appl Phys 49 (1978) 1937 ... numerical integration by use of high-speed computers. This method is laborious, but it needs to be applied ...

WF Brown, J Appl Phys 30 (1959) S62

Numerical micromagnetics

Numerical micromagnetics

-MxH_{eff}

-MxMxH_{eff}

Basic equations Magnetization dynamics

Demagnetizing field Integral approach Finite elements

Numerics Sparse linear algebra Computer hardware

Computational magnetism



length scales

$\frac{1+\alpha^2}{|\gamma|} \frac{d\mathbf{M}}{dt} = -\mathbf{M}\mathbf{x}\mathbf{H}_{eff} - \frac{\alpha}{M_s}\mathbf{M}\mathbf{x}\mathbf{M}\mathbf{x}\mathbf{H}_{eff}$



Partial differential equations

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

(2)

(3)

$$\mathbf{H}_{eff} = \frac{A}{M_s^2} (\nabla^2 \mathbf{M}) + f(\mathbf{M}) - \nabla U + \mathbf{H}_{ext}$$

$$\nabla^2 U = \nabla \cdot \mathbf{M}$$
 $U \sim \frac{1}{r}$ for $r \to \infty$

Partial differential equations

$$\frac{1+\alpha^{2}}{|\gamma|} \frac{d\mathbf{M}}{dt} = -\mathbf{M}_{\mathbf{X}}\mathbf{H}_{eff} - \frac{\alpha}{M_{s}}\mathbf{M}_{\mathbf{X}}\mathbf{M}_{\mathbf{X}}\mathbf{H}_{eff}$$
(1)

$$\frac{\mathbf{exchange}}{\mathbf{H}_{eff}} = \mathbf{A}(\nabla^{2}\mathbf{M}) - \nabla\mathbf{U} + \mathbf{K}(\mathbf{k}\cdot\mathbf{u})\mathbf{k} + \mathbf{H}_{ext}$$
(2)

external

(3)

$$\nabla^2 U = \nabla \cdot \mathbf{M} \qquad U \stackrel{1}{\sim} r^{-} \quad \text{for } r \to \infty$$

static

Integral approach



divide particles into cubic cells rigid magnetic moment within each cell

sum over charge sheets (FFT) to obtain the **magnetostatic field**

"one" LLG equation per cell

Finite element approach





divide particles into finite elements (tetrahedrons) Interpolate **M**, U within the elements

solve partial differential equation for the magnetic potential

energy as a function of **M**(**r**) ⇒ effective field ⇒ magnetic moment



sparse matrix algebra

sparse matrix







From Uniform to multidomain states Four easy examples

Example 1: Simple particle reversal











Example 1: Simple particle reversal





Very hard material: Neglect thermal activation







Sphere Reversal modes

Cube Size dependence of coercive field



R Skomski, Simple models of magnetism, Oxford University Press, 2008





Reversal by curling





Switching of a cube



Demagnetizing field















Soft magnet: no cyrstalline anisotropy







Soft magnet: no cyrstalline anisotropy



No external field

Permalloy (NiFe) 100 x 100 x 5 nm³

If uniformly magnetized all directions have the same energy



R Dittrich et al, J Appl Phys, 93 (2003) 7891. R Cowburn, et al. J Appl Phys, 87 (2000) 7067.














Anisotropy field larger than magnetostatic field







Anisotropy field larger than magnetostatic field

No external field

Domain walls and grains

thin Nd₂Fe₁₄B specimen

P Thompson et al. J. Phys. D 30 (1997) 1854





What is the energy of the domain wall ?





 $\gamma = 4 \cdot \sqrt{A \cdot K_1}$ domain wall energy

Some numbers

Material	$\mu_0 M_s$ (T)	$A \text{ (pJ m}^{-1}\text{)}$	$K_1 ({\rm MJ} {\rm m}^{-3})$	δ (nm)
Fe	2.15	8.3	0.05	40
Co	1.76	10.3	0.53	14
Ni	0.61	3.4	-0.005	82
BaFe ₁₂ O ₁₉	0.47	6.1	0.33	14
SmCo ₅	1.07	22.0	17	3.6
$Nd_2Fe_{14}B$	1.61	7.7	4.9	3.9

Skomski, Nanomagnetics, J. Phys.: Condens. Matter 15 (2003) R841–R896

Domain wall width is characteristic length scales

Characteristic length scales

Non-uniform magnetization

confined in regions smaller than the domain wall width $\pi\delta_0$

Effective pinning if

defect size = domain wall width $\pi\delta_0$

Characteristic length scales

Characteristic length

interplay between the two most important micromagnetic energy contributions



Pinning type permanent magnets



if domain walls cannot move

magnet remains stable

Example 4: Magnetic domains



No magnetocrystalline anisotropy



No external field

Element size



closure domains



RD Gomez et al

0 Oe 40 80 120

-120 -80

-40

Nano elements (L < 1µm)

> one domain + end domains

Thin film elements

Large elements $>1 \mu m$





Hext

Magnetic force microscopy Gomez et al.

Micromagnetic simulation

Thermal effects Stochastic dynamics and energy barriers

Example 5: End domains



No magnetocrystalline anisotropy





No external field

Example 5: End domains

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210Saddle 208energy (k_BT) 206 5 k_bT 204 S-State 202 C-State 200^L 0.25 0.50.75arc length (a.u.)

150 nm

End domain configurations

C-state to S-state transition

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Mag Noise Switching of end domains

Relaxation time about 5 ns $\tau = (1/f_0) \exp(E_b/k_BT)$

Thermal effects

Equation of motion

- Gyromagnetic precession
- Damping
- Stochastic field



M = M(time, temperature)

nanoseconds

Path finding method

- Energy landscape
- Find a path between two local minima



 $\tau = f_0^{-1} \exp(E_{\text{barrier}}/k_B T)$

years

Elastic band method



Initial guess Straight line in configuration space

Minimum energy path Highest transition probability at zero temperature

Energy barrier MEP connects two minima over the lowest saddle point

- minima
- maxima
- saddle points

R Dittrich, T Schrefl, D Suess, W Scholz, H Forster, J Fidler, J. Magn. Mater. 250 (2002) 12. G Henkelman, BP Uberuaga, H Jonsson, J. Chem. Phys.113 (2000) 22.

Elastic band method



Images intermediate states between A and B

Springs between subsequent images to enforce continuity

Force on each image due to potential energy and spring

Minimum energy path Components of the force that is normal to the path are zero **Open source micromagnetics** An example using MAGPAR

Integral approach





 rigid magnetic moment within each cell



• "one" LLG equation per cell



Magnetostatics (Integral)

Field sources

$$\rho(\mathbf{r}) = -\operatorname{div} \mathbf{M} \ (\mathbf{r})$$
$$\sigma(\mathbf{r}) = \mathbf{M} \ (\mathbf{r}) \cdot \mathbf{n}$$

volume charges surface charges

Magnetic field

$$U(\mathbf{r}) = \frac{1}{4\pi} \int_{V_0} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' + \frac{1}{4\pi} \int_{S} \frac{\sigma(\mathbf{r}') \cdot df'}{|\mathbf{r} - \mathbf{r}'|}$$
$$H_{d}(\mathbf{r}) = -\nabla U(\mathbf{r})$$

Magnetostatics (FEM)

(1)

(2)

Partial differential equation $\nabla^2 U(r) = \nabla \cdot M(r)$ for $r \in \Omega_{in}$ $\nabla^2 U(r) = 0$ for $r \in \Omega_{ext}$

Boundary condition normal component of *B* field is continuous $B = \mu_0 (H + M)$ $\mu_0 (-\nabla U^{\text{in}} + M) \cdot \mathbf{n} = \mu_0 (-\nabla U^{\text{ext}} + 0) \cdot \mathbf{n}$ $M \cdot \mathbf{n} = (\nabla U^{\text{in}} - \nabla U^{\text{ext}}) \cdot \mathbf{n}$

 $(\nabla U^{\rm in} - \nabla U^{\rm ext}) \cdot \boldsymbol{n} = \boldsymbol{\sigma} \tag{3}$

→ Solve (1), (2), and (3) using standard numerical methods (finite elements, finite differences)

Finite element micromagnetics



subdivide grains into tetrahedrons

Interpolate magnetization and the magnetic scalar potential

calculate Gibbs free energy for each element

define a magnetic moment and a effective field at each node

solve a system of ordinary differential equations

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$$\frac{1+\alpha^2}{|\gamma|}\frac{d\mathbf{M}}{dt} = -\mathbf{M}\mathbf{x}\mathbf{H}_{eff} - \frac{\alpha}{M_s}\mathbf{M}\mathbf{x}\mathbf{M}\mathbf{x}\mathbf{H}_{eff}$$



Open source micromagnetics

Software	Developer	method	download
OMMF	NIST	Finite difference	math.nist.gov/oommf/
MAGPAR	TU Vienna	Finite elements	http://www.magpar.net/
NMAG	University of Southampton	Finite elements	nmag.soton.ac.uk/nmag/

Open source package "magpar"

magpar is a finite element micromagnetics package which combines several unique features:

Applicability to a variety of static and dynamic micromagnetic problems including uniaxial/cubic anisotropy, exchange, magnetostatic interactions and external fields

Flexibility of the finite element method concerning the geometry and accuracy by using unstructured graded meshes

Availability due to its design based on free, open source software packages

Portability to different hardware platforms, which range from simple PCs to massively parallel supercomputers

Scalability due to its highly optimized design and efficient libraries

magpar is distributed under the terms of the GNU General Public License Website: http://http://www.magpar.net/





MAGPAR input files (1)

Geometry (finite element mesh)

- Mesh import (see Preprocessing)
 - MSC.Patran neutral file
 - AVS project.inp, project.out: finite element mesh file
 - Gmsh , GiD meshes



Mesh of the magpar thin film example

MAGPAR input files (2)

Magnetic material parameters

project.krn: material properties

For each grain (or part of the model with distinct property id) this file contains a line defining its material properties:

theta phi	K1	K2	Js	A	alpha psi	# parameter
(rad) (rad)	(J/m^3)	(J/m^3)	(T)	(J/m)	(1) (rad)	# units

- theta and phi: direction of the uniaxial magnetocrystalline anisotropy axis in spherical coordinates (rad); theta measured from the z-axis, phi measured from the x-axis in the x-y-plane
- K1: first magnetocrystalline anisotropy constant (J/m³)
- K2: second magnetocrystalline anisotropy constant (J/m³)
- Js: saturation polarization (Tesla)
- A: exchange constant (J/m)
- alpha: Gilbert damping constant (dimensionless)
- psi: third <u>Euler angle</u> for cubic anisotropy (assume cubic anisotropy if defined; i.e. valid floating point value). For uniaxial anisotropy set to "uni" (or some other string, which does not represent a valid floating point number).

The grain with property id 1 is assigned the properties in line 1, the grain with property id 2 is assigned the properties in line 2, etc.

MAGPAR input files (3)

Simulation parameters

allopt.txt: simulation parameters

All simulation parameters can be set in the configuration file **allopt.txt**. The example files and the default configuration file **allopt.txt** in the \$MAGPAR_HOME/src/cube subdirectory are thoroughly documented. Any option defined in this file can be overridden by an environment variable or command line option (cf. <u>PETSc manual</u> chapter 14 - Other PETSc Features). This useful feature is used in example **mumag3: mumag standard problem #3**.

Additional PETSc internal logging/info/diagnostic options, which may slow down the simulations (!), are given in allopt_log.txt.

Output files Simulation time External field Solver parameters

• • • •

MAGPAR Thin film example

Calculate equilibrium magnetic state of a thin film

- download magpar and thin film example
- copy everything into one directory
- edit the simulation parameters (allopt.txt)
- start the simulations
- look at the results

MAG program parameters

allopt.txt particle size

```
##### scaling parameters
# size scaling of finite element mesh (unit: m)
-size 1e-6
```

dimensionless Landau-Lifshitz-Gilbert damping constant # define for every grain together with material parameters in *.krn

change to 100 nm

Initial magnetization

allopt.txt particle size

```
###### initial magnetization
   negative values: select abs(init mag), but reverse the magnetization
#
  O: magnetization from inp (set file number by -inp below)
#
#
   1: Mx=1
  2: My=1
#
#
  3: Mz=1
#
  4: Mx=My=Mz=sqrt(1/3)=0.57735027
#
  5: artificial flower state, center: x=y=z=init magparm
#
  6: set magnetization in x-z plane to theta=init magpar (from z-axis)
# 7: vortex state: core radius = init magparm, center in (x=0,y=0)
# 8: random magnetization
#
  9: Bloch wall: center at x = init magparm, width=x/10
#
  10: M // anisotropy axes
-init mag 3
```

Change to 1 (parallel x axis)
Time integration

allopt.txt minimization method

minimization method
0: PVODE (LLG time integration) or
1: TAO (energy minimization)
-mode 0

set to time integration

Check mesh size

Finite element size

should be smaller than the exchange length

Exhange length

5 nm for NiFe (permalloy)



100 nm / 20 = 5 nm OK

Refine the mesh

If initial mesh size > exchange length allopt.txt Refine the finite element mesh

regular mesh refinement # number of regular refinement steps # (every step generates 8x as many elements and about 8x as many nodes!!!) -refine 0

Give the number of refinement steps

MAG program parameters

allopt.txt simulation time

#Time step options -----# -ts_max_steps <5000>: Maximum number of time steps (TSSetDuration)
#ignored
-ts_init_time <0>: Initial time (TSSetInitialTime) (unit: ns)
-ts_init_time 0.0
-ts_max_time <5>: Time to run to (TSSetDuration) (unit: ns)
-ts_max_time (-1e99)
-ts_dt <0.020944>: Initial time step (TSSetInitialTimeStep)

change to 5 ns

MAGPAR program parameters

allopt.txt magpar 0.7 parameters

-simName thinfilm



set length scaling factor to microns
initial magnetization in x-direction
solve LLG equation
run problem for 5 ns

slice plane for png files: x-y-plane

You need to add these 4 parameters

Run the program



Start magpar.exe from a DOS command line

Look at the results

Time			Total energy			
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#.date:	Fri d	Jul 🗸 17:27:32	2006			1
#1:	2:	3:	4:	5:	6:	
#eq	inp	time	Hext	Etot	J//Hext	
#	—	(ns)	(kA∕m)	(J/m^3)	[J/Javg]	
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Ø	2	2.381619e-05	0.00000e+00	2.046449e+04	-8.411796e-07	1.000
Ø	0	4.763237e-05	0.00000e+00	2.046421e+04	-1.681367e-06	1.000
Ø	0	7.144856e-05	0.00000e+00	2.046389e+04	-2.520441e-06	1.000
Ø	0	1.391119e-04	0.00000e+00	2.046294e+04	-4.897194e-06	1.000
Ø	0	2.067753e-04	0.00000e+00	2.046198e+04	-7.265673e-06	9.999
Ø	0	2.744386e-04	0.00000e+00	2.046096e+04	-9.626448e-06	9.999
Ø	0	3.832901e-04	0.00000e+00	2.045966e+04	-1.340042e-05	9.999
Ø	0	4.921416e-04	0.00000e+00	2.045816e+04	-1.714958e-05	9.999
Ø	6	6.009931e-04	0.00000e+00	2.045655e+04	-2.087791e-05	9.999
Ø	0	7.098446e-04	0.00000e+00	2.045542e+04	-2.457509e-05	9.999
Ø	0	8.186961e-04	0.00000e+00	2.045396e+04	-2.824701e-05	9.999
Ø	0	9.275476e-04	0.00000e+00	2.045239e+04	-3.189804e-05	9.999
Ø	0	1.036399e-03	0.00000e+00	2.045129e+04	-3.551832e-05	9.999
Ø	0	1.145251e-03	0.00000e+00	2.044986e+04	-3.911392e-05	9.999
Ø	0	1.254102e-03	0.00000e+00	2.044831e+04	-4.268914e-05	9.999
Ø	0	1.423896e-03	0.00000e+00	2.044649e+04	-4.820602e-05	9.999
Ø	0	1.593690e-03	0.00000e+00	2.044429e+04	-5.366641e-05	9.999
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Magnetization patterns



Summary

Micromagnetics

Effects of size, shape, granular structure Dynamics and reversal modes

Energy contributions

From Stoner-Wohlfarth theory to multi-domain magnetization dynamics

Thermal effects

Stochastic dynmmics (short times) Energy barriers (long times)

Solution techniques

Integral approach (regular structures) Finite element approach (irregular structures)

Literature

- G. Bertotti, Hystersis in Magnetism: For Physicists, Materials Scientists, And Engineers, Academic Press, 1998.
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- D. Suess, J. Fidler and T. Schrefl, Micromagnetic simulation of magnetic materials, in Handbook of Magnetic Materials, edited by K.H.J. Buschow, (2006), Elsevier Vol. 16, pp. 41-125
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