ESCUELA POLITÉCNICA NACIONAL

MICROMAGNETIC SIMULATIONS WITH OOMMF

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Outline

- What are micromagnetic simulations?
- What is OOMMF?
- Why use micromagnetic simulations?
- Energetics of a ferromagnet
- How does OOMMF work?
- Run a simple job
- OOMMF simulations and experiments

What are micromagnetic simulations?

- Micromagnetic simulations are based on the theory micromagnetics, which is a continuum theory.
- Well established tools in order to make quantitative predictions of the behaviour of magnetic systems
- In continuum approximation, the magnetization is considered as a continuous vector field, and it is a function of space and time. **M**=**M**(**r**,t)
- Magnetization is represented by a normalized magnetization field **m**(**r**,t)

$$\boldsymbol{m}(r,t) = \frac{\boldsymbol{M}(r,t)}{M_s}$$

What is OOMMF?

- OOMMF stands for Object Oriented MicroMagnetic Framework
- OOMMF is a widely used simulation tool.
- It was developed by Mike Donahue and Don Porter at NIST
- It is a portable, extensible public domain micromagnetic program
- It is written in C++ and Tcl
- There is a Python interface for OOMMF by M. Beg *et al.* AIP Advances **7**, 056025 (2017)
- Windows, Unix, macOs
- Available at nanoHUB
- More than 3253 papers citing OOMMF

Why use micromagnetic simulations?

- Fabricating samples is a time consuming and expensive process. It would be nice to have a way of testing elements before fabrication.

- Explaining experimental results.

- OOMMF (and other packages) allow the user to determine the possible magnetization distributions supported by an element of a particular size and shape.

Energetics of a ferromagnet

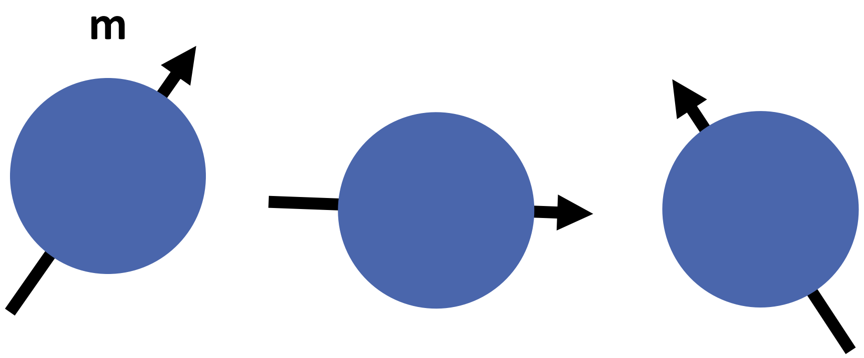
- Ferromagnetic elements can be visualized as a collection of magnetic dipoles that interact like tiny bar magnets.
- The magnetization configurations supported (domain patterns) depend on a balanced of the various energy terms in the system, e.g.

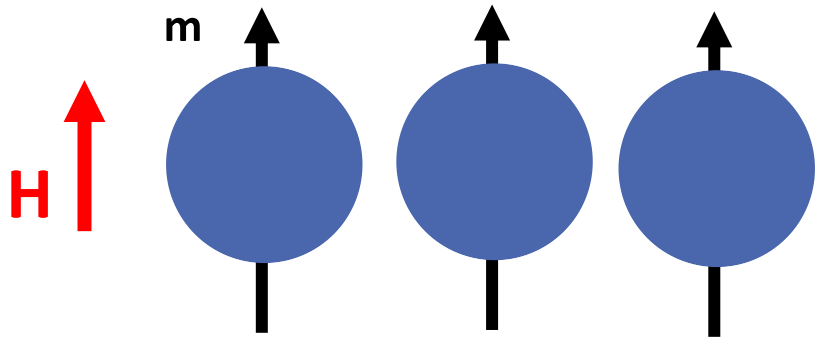
- Zeeman energy
- Exchange energy
- Demagnetization energy
- Crystalline anisotropy energy
- Antisymmetric exchange energy
- Interlayer-exchange energy
- Others

Zeeman energy

An applied field will interact with spins. The dipoles will align with field to reduce energy.

$$E_Z = -\int_V \mu_0 M_s \boldsymbol{m} \cdot \boldsymbol{H} dV$$

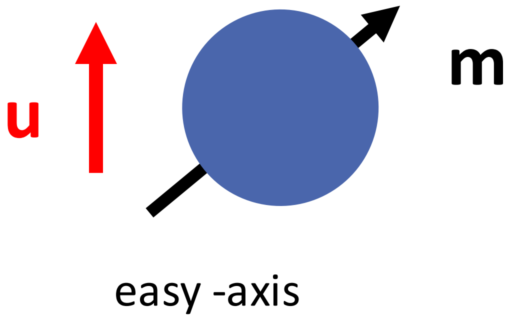


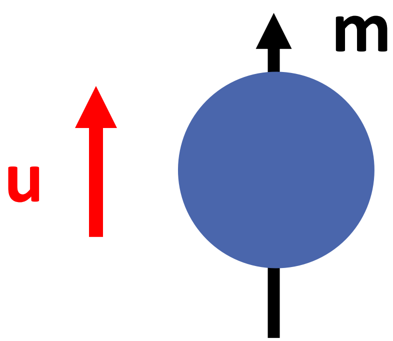


Crystalline anisotropy energy

- Favours the parallel alignment of the magnetization to certain axes referred to as easy axes.
- Parameters: $K\ (J/m^3)$
- Easy axis uniaxial anisotropy

$$E_{ua} = -\int_V K(\boldsymbol{m} \cdot \boldsymbol{u})^2 dV$$

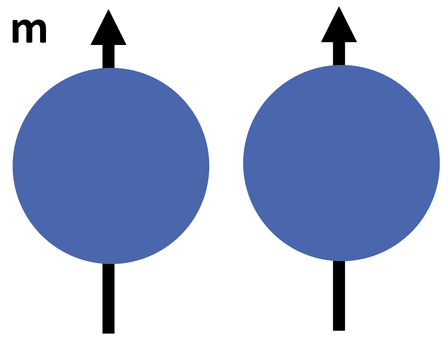




Exchange energy (Ferromagnetic)

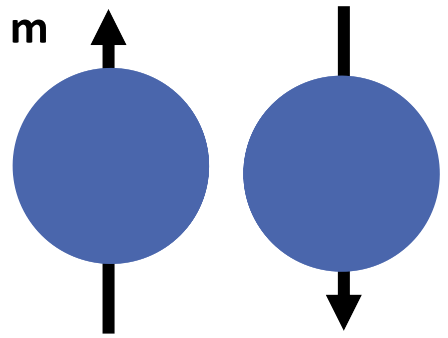
- Parallel magnetic moment alignment.
- Parameter: A (J/m)

$$E_{ex} = \int_V A(\boldsymbol{\nabla m})^2 dV$$



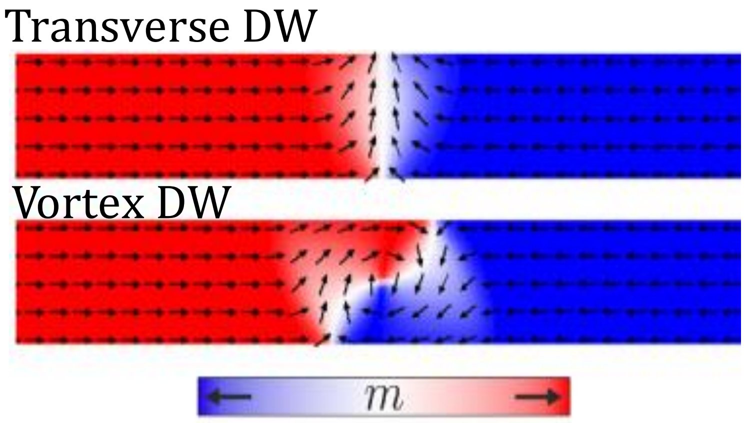
Demagnetization energy

- Long range interaction
- Accounts for the dipole– dipole interaction of a magnetic system.
- Each magnetic moment “feels” the neighbours at the distance.
- Also referred to as magnetostatic energy.



Magnetic Domains and Reversal Processes

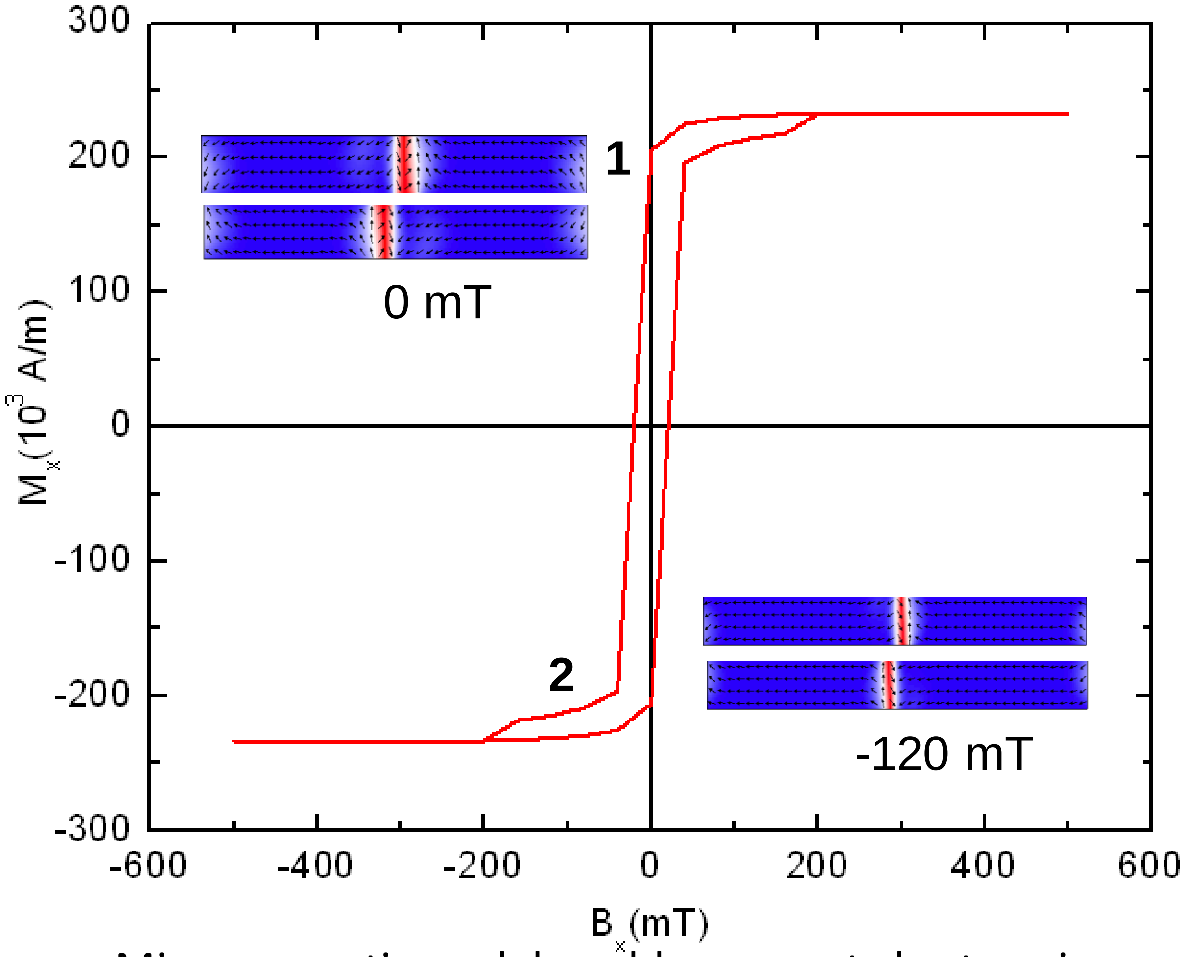
- The ground state of a system is given by the minimization of E_{total}
- The competition between different energy contributions leads to various magnetization configurations in a magnetic systems. For example, formation of magnetic domains, which are separated by domain walls.



Micromagnetic model resolves the structure of magnetic domains and domain walls

Magnetic hysteresis

- Characteristic fingerprint of a system.
- At a high field, all magnetic moments in the sample are aligned within the field direction.
- Reducing the field leads to the nucleation of magnetic domains, whereby the configuration of these domains depends on the competition of the different energy contributions.



Micromagnetic model enables accurate hysteresis computations of macroscopic magnets

How does OOMMF work?

- We need to design an element and then input the dimensions along with appropriate material parameters and applied field values. This defines the magnetic problem.

- OOMMF searches numerically for a magnetization vector field that solves the Landau-Lifshitz-Gilbert (LLG) equation.

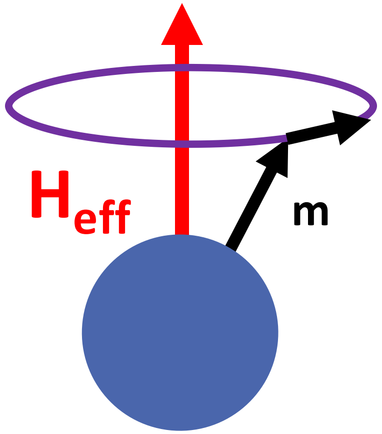
- After each step, the spins are adjusted slightly and the calculation is redone. This process continues until the total system energy of the system is minimized.

- We end up with a relatively realistic result for the micromagnetic state.

Landau-Lifshitz-Gilbert Equation

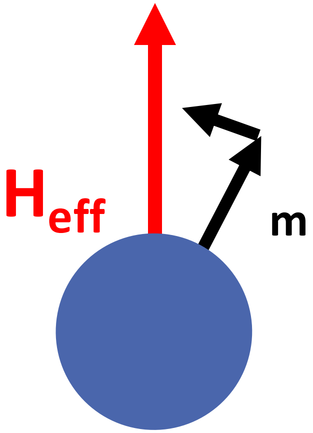
PRECESSION

- **m** precess around $\mathbf{H}_{\mathbf{eff}}$
- γ_0 = gyromagnetic ratio



GILBERT DAMPING

- **m** align with $\mathbf{H}_{\mathbf{eff}}$
- α =damping coefficient



$$\frac{d\boldsymbol{m}}{dt} = -\frac{\gamma_0}{1+\alpha^2}\boldsymbol{m} \times \boldsymbol{H}_{eff} - \frac{\gamma_0 \alpha}{1+\alpha^2}\boldsymbol{m} \times (\boldsymbol{m} \times \boldsymbol{H}_{eff})$$

MIF file

```
# MIF 2.1
# Description: Cobalt stripe
set pi [expr 4*atan(1.0)]
set mu0 [expr 4*$pi*1e-7]


# structure: Cobalt stripe


Specify Oxs_BoxAtlas:a1 {
  xrange {0 1000e-9}
  yrange {0 100e-9}
  zrange {0 5e-9}
  name a1
  }


Specify Oxs_MultiAtlas:atlas {

atlas :a1
}

# Atlas, defines system size and layer structure

Specify Oxs_RectangularMesh:mesh {
  cellsize {5e-9 5e-9 5e-9}
  atlas :atlas
}

# cell size 5nm x 5nm x 5nm
```

Specify simulation volume, Atlas ≥ 1

Specify how to discretize

MIF file

```
Specify Oxs_Exchange6Ngbr:CoFe {
  atlas :atlas

  A {
    a1 a1 30e-12
    }
}


Specify Oxs_UniaxialAnisotropy {
axis { 1 0 0 }
K1 2e3
}

Specify Oxs_Demag {}


Specify Oxs_UZeeman:extfield0 [subst {
  comment {Field values in milli Tesla}
  multiplier 795.77472
  Hrange {
{1000 0 0  -1000 0 0 40}
{-1000 0 0  1000 0 0 40}
  }
}]
```

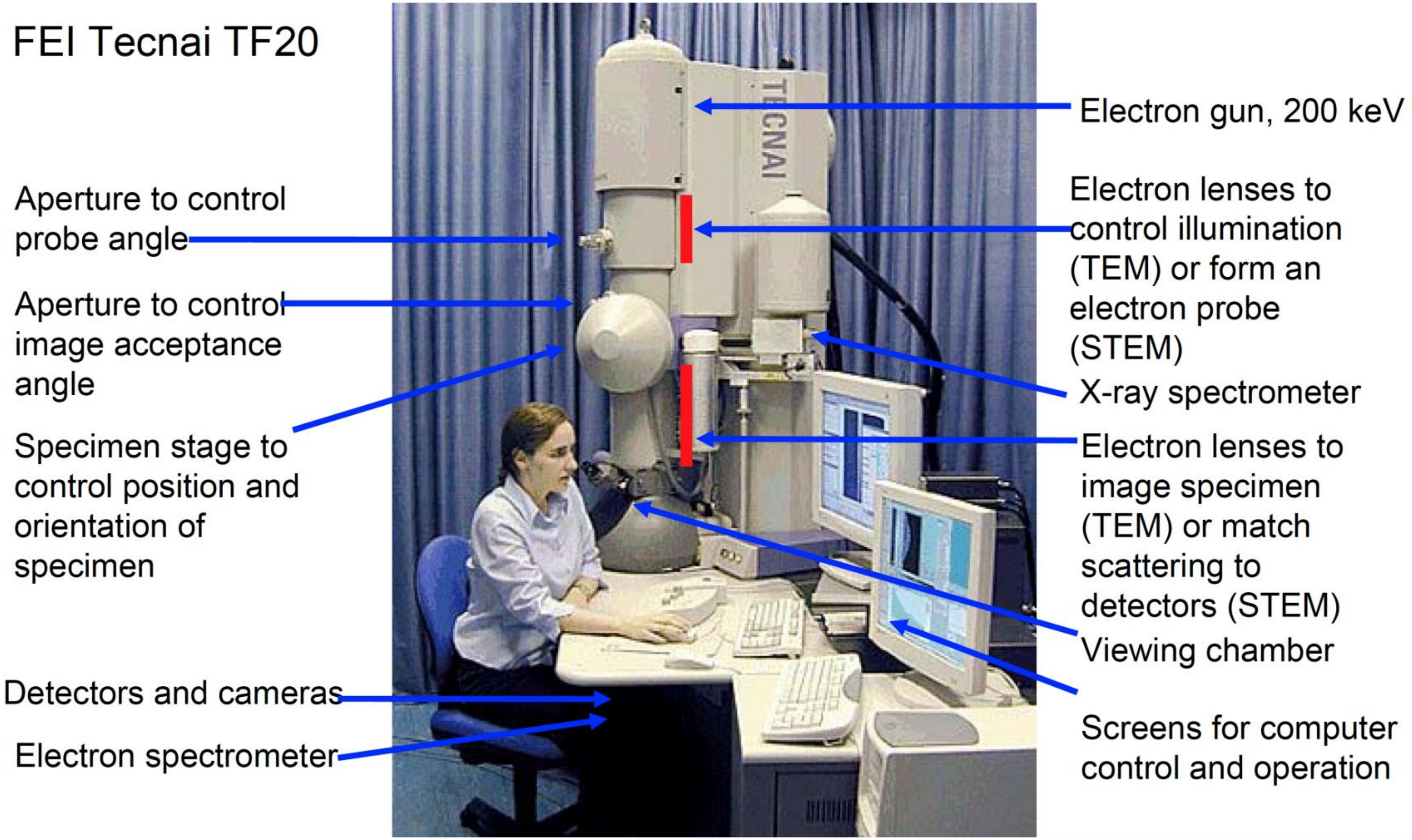
Specify as many energy terms as needed

MIF file

```
Specify Oxs_EulerEvolve {
alpha 0.5
  start_dm 0.01
}

Specify Oxs_AtlasVectorField:init {
atlas :atlas
values {
a1 {1 0 0}
}
}


Specify Oxs_TimeDriver {
 basename Co-stripe
 evolver Oxs_EulerEvolve
 comment {1 deg/ns = 17453293 rad/sec; If Ms=8.6e5, and lambda is small,
         then mxh=1e-6 translates into dm/dt = 2e5 rad/sec = 0.01 deg/ns}
 stopping_dm_dt .01
 mesh :mesh
 Ms  { Oxs_AtlasScalarField {
     atlas :atlas
     default_value 0
     values {
       a1 14e5

     }
 }}
 m0 init
}
```

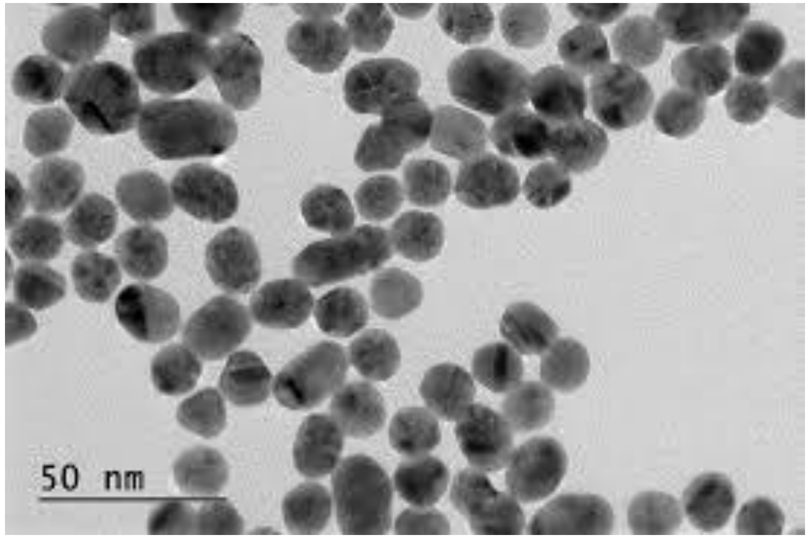
Specify as many vector fields as needed

TEM Schematic



Basic TEM imaging modes: Bright field

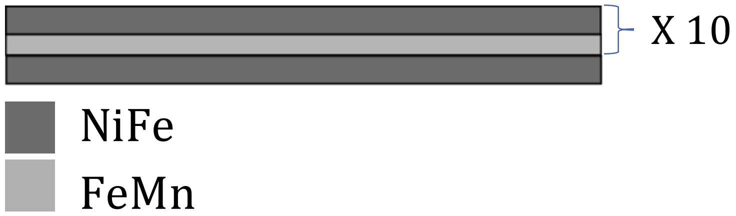
- Most common mode of operation.
- Electrons are reflected, scattered or transmitted when they encounter the sample. The transmitted electrons form the BF image.
- Regions that are thicker, have a higher atomic number, or higher density will appear darker.
- The image is a 2D projection of your sample

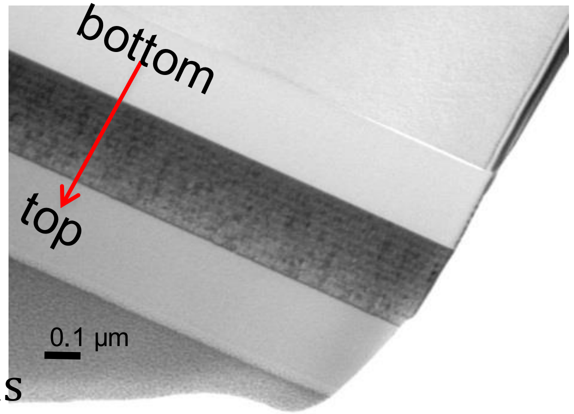


https://wwwf.imperial.ac.uk/blog/fonsmad2015-velox/2015/07/18/tem-of-gold-nanoparticles-results/

Analysis

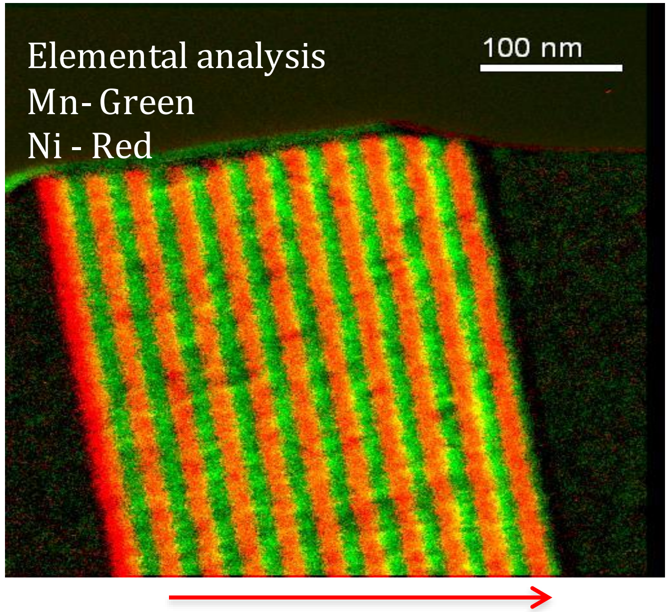
Si/SiO/NiFe(20nm)/[FeMn(15nm)/NiFe(20nm)] X 10/Ta

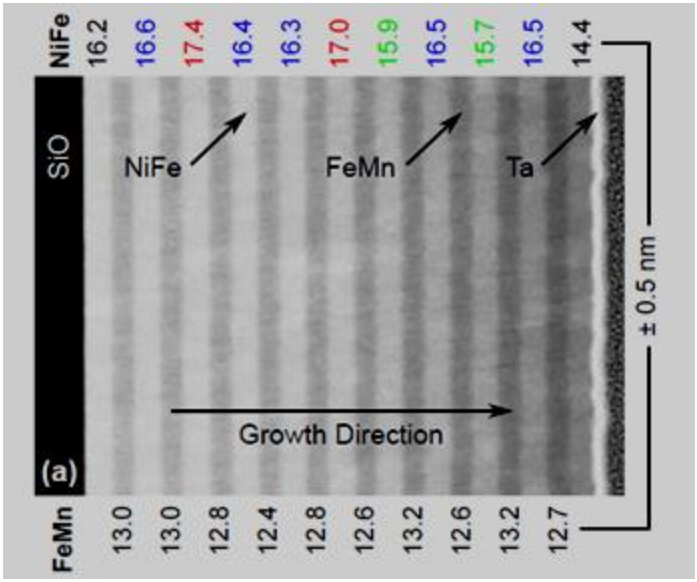




Elemental Analysis

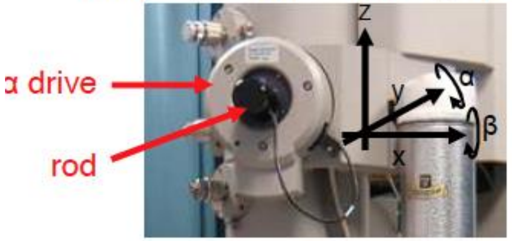
Magentic Analysis

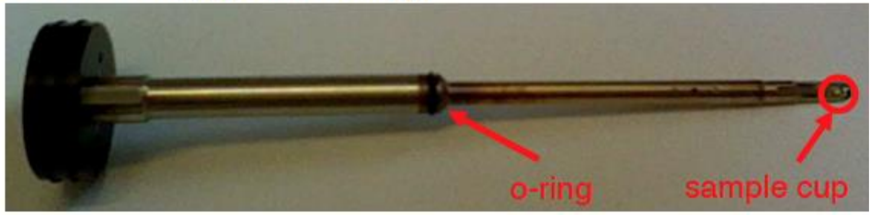




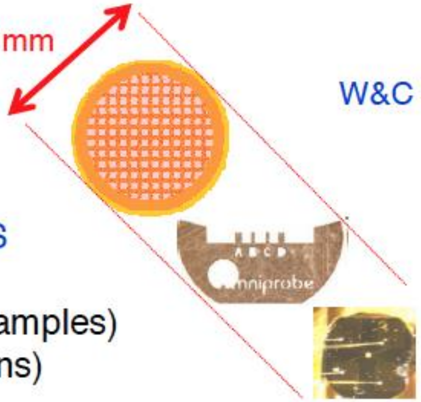
Sample holders

PURPOSE
- Position in *x*, *y* with precision, reproducibility, small step size and stability
- Position in *z* to keep pre- and post-specimen optics fixed
- Keep *x*, *y* and *z* of image point fixed while tilting (eucentricity)

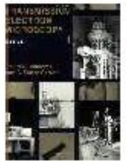




OPTIONS
- heating / cooling
- single tilt / double tilt / rotate
- low background
- electrical connections



W&C Ch. 8,10



CLEAN, ELECTRON TRANSPARENT SAMPLES
- dispersed onto holey-C & grid (nanomaterials)
- mounted onto Omniprobe holder (FIB lift-out samples)
- dimple-ground & ion-milled disk (bulk specimens)
- SiN membrane (thin films)

Sample holders

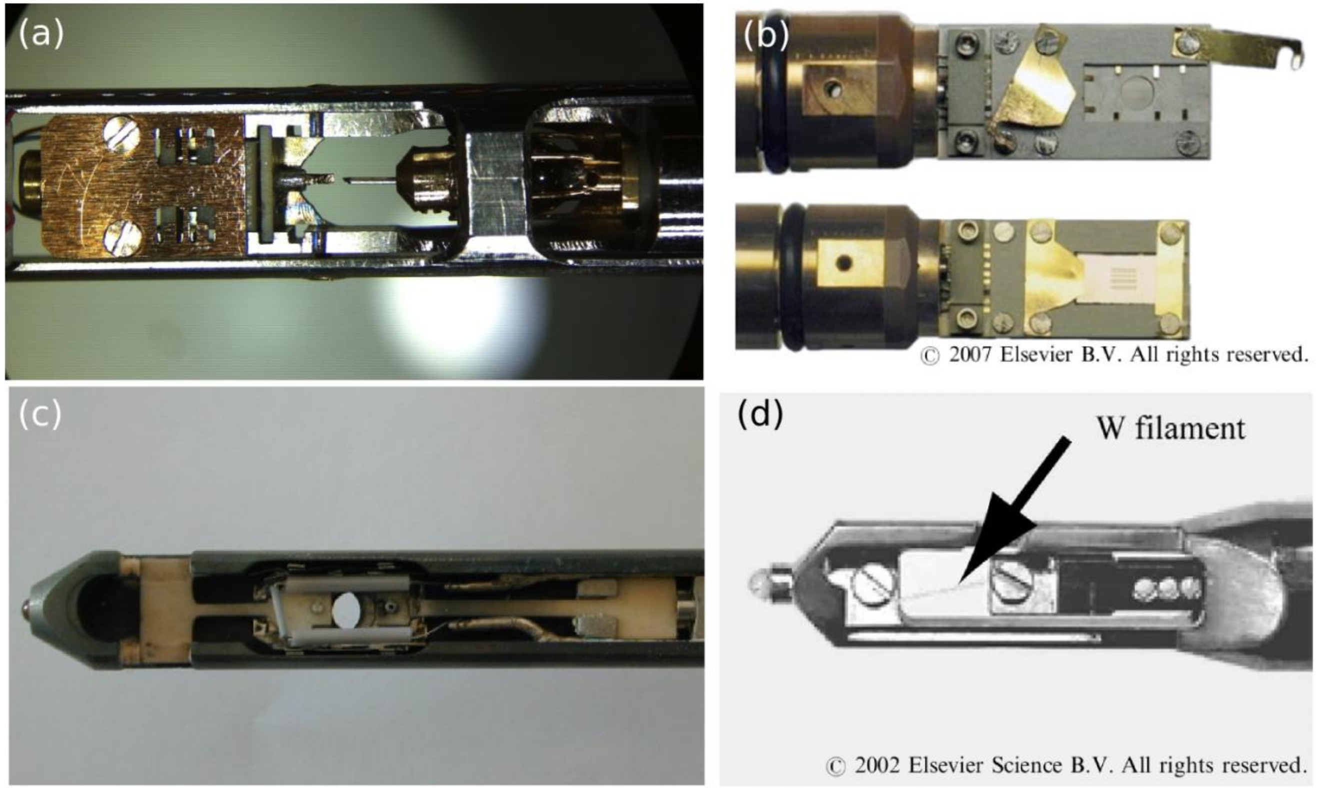
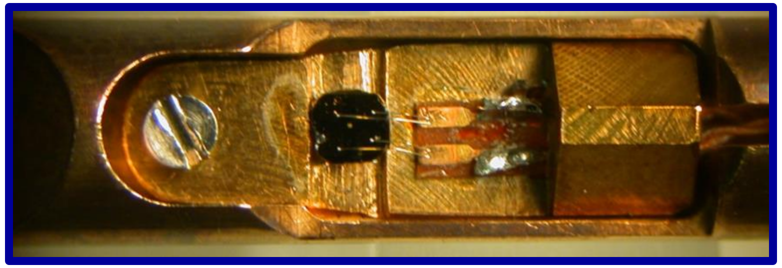
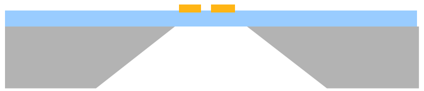


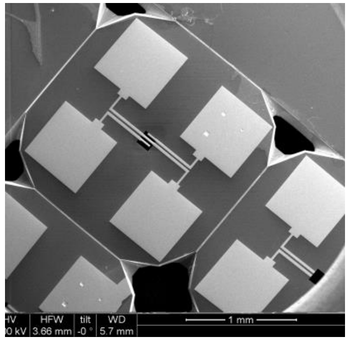
Figure 1: Sample holders for in situ a) Holder with a scanning probe for indentation, biasing or field emission measurement. b) Custom made sample holder for multi-contacted sample (8 contact pads – courtesy of (Kim, Kim, et al., 2008)). c) Sample holder for strain (traction) experiments. d) Sample holder for high temperature observations (courtesy of (Nishizawa et al., 2002)).

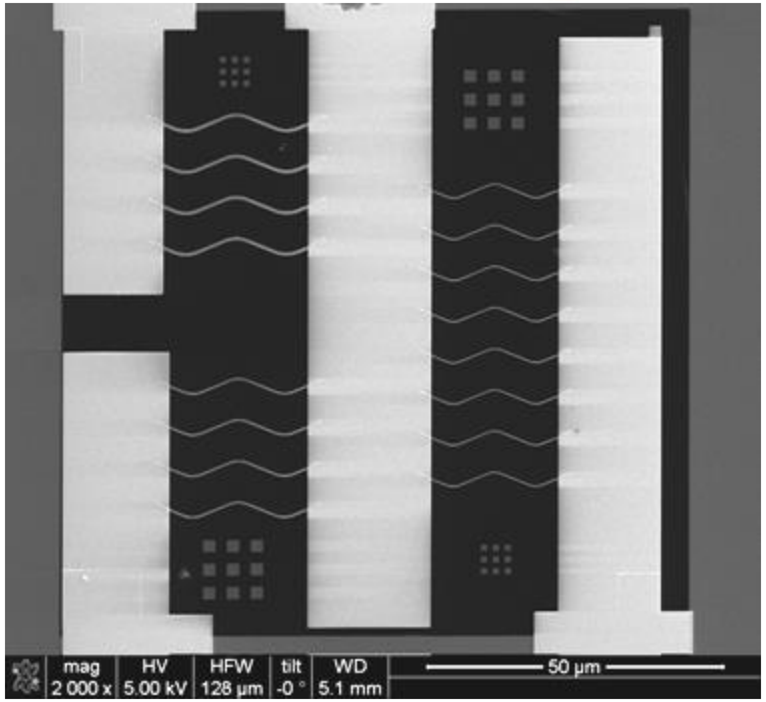
Aurélien Masseboeuf. In Situ Characterization Methods in Transmission Electron Microscopy. Alain Claverie and Mireille Mouis. Transmission Electron Microscopy in Micro-Nanoelectronics , John Wiley & Sons, Inc., pp.199-218, 2013, 9781118579022. ff10.1002/9781118579022.ch8ff. ffhal-01430590f

Sample holders



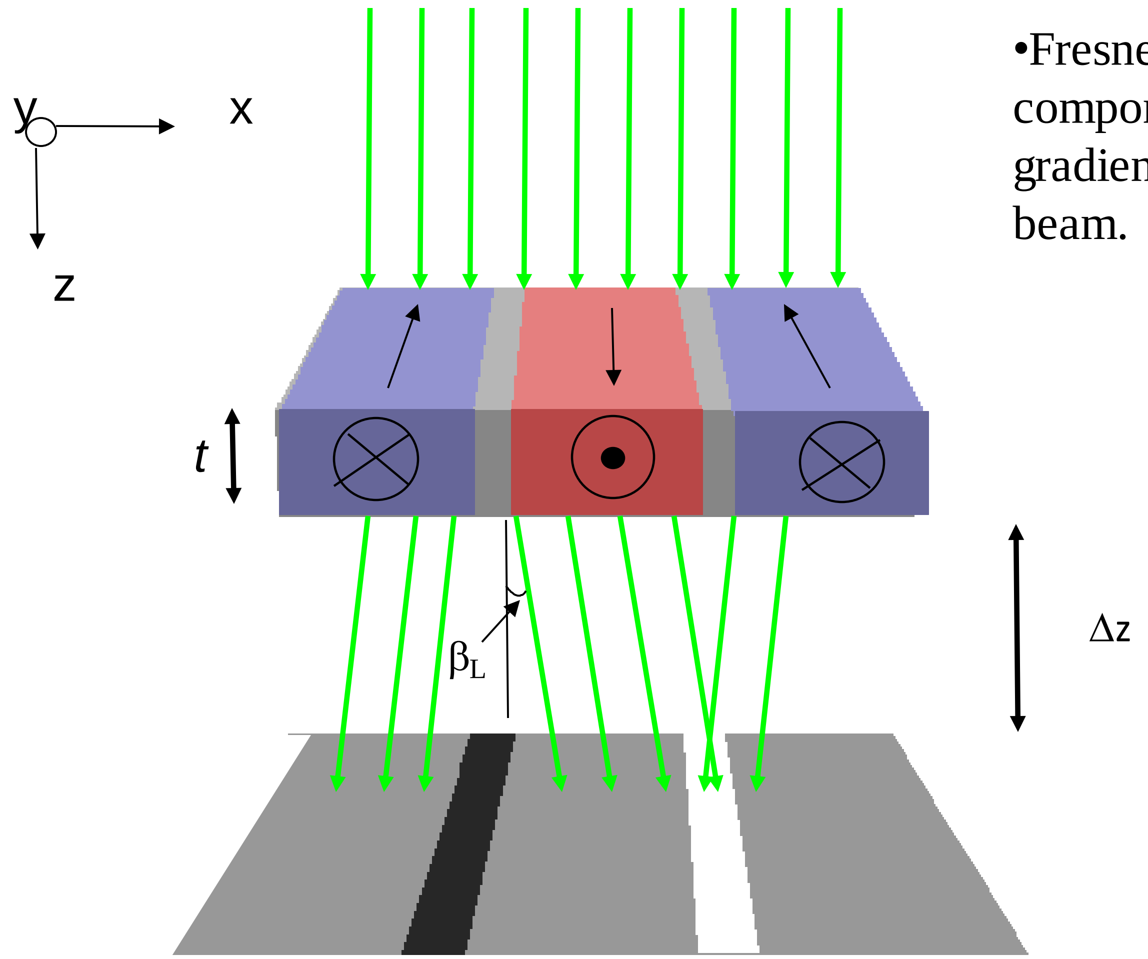




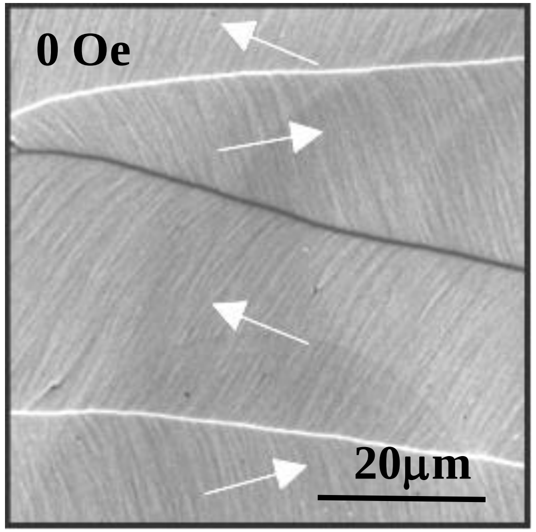


- Specimen in field free space in TEM
- TEM rod with 4 electrical contacts
- Fabrication: 2 step EBL “lift-off” process
- Substrate: supported 50 nm thick Si_3N_4 membrane
- NiFe film deposition by UHV evaporation

Fresnel Microscopy

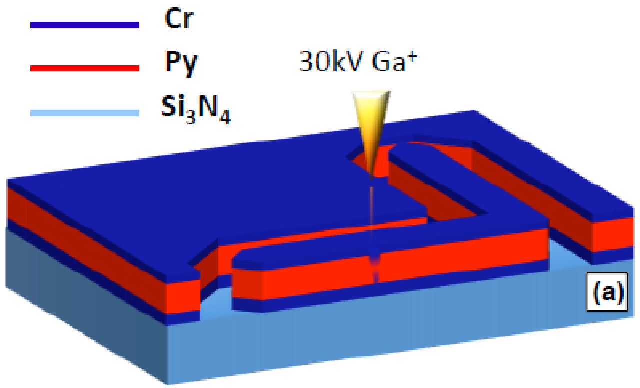


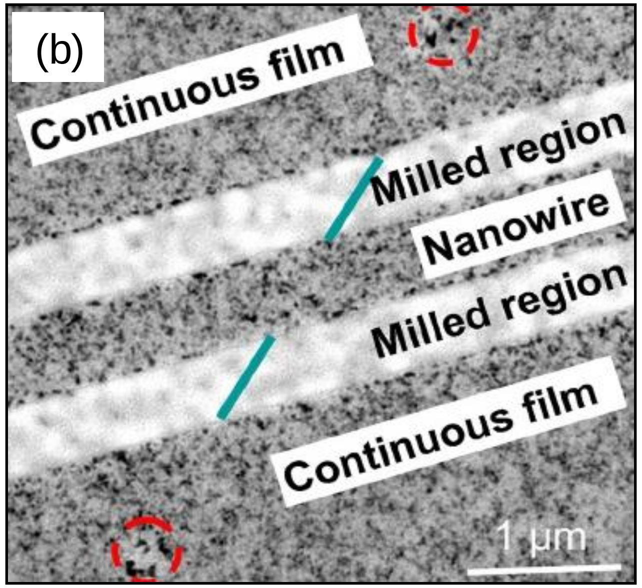
•Fresnel mode contrast arises due to components of magnetic induction gradient perpendicular to the electron beam.

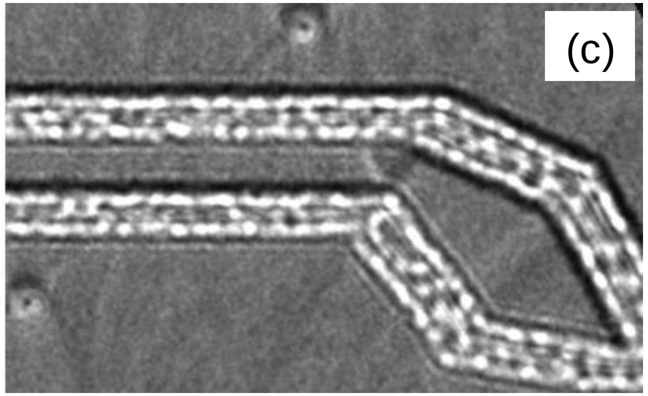


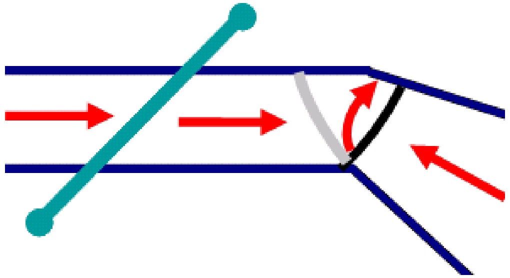
Domain-Wall Engineering

Use irradiation to locally alloy (change magnetic properties)









Domain-Wall Engineering

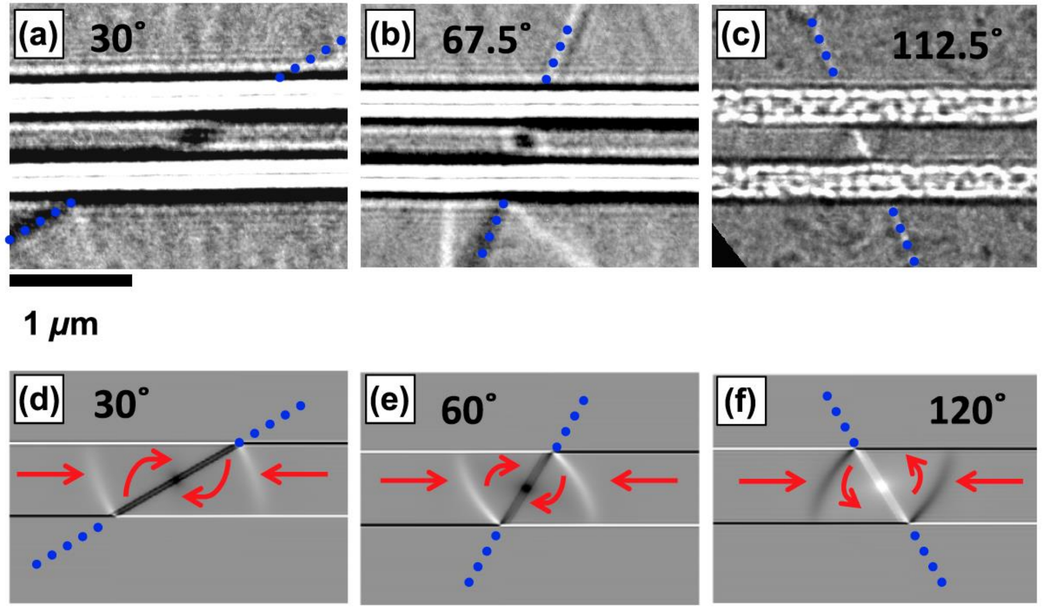


FIG. 6. (a)–(c) Fresnel images of Cr/Py/Cr nanowires showing DWs pinned at the linear irradiated sites written with a dose of 16×10^{15} ions/cm^2. (d)–(f) Corresponding calculated Fresnel images from simulations.

Phys. Rev. Applied 3, 034008 (2015)

Domain-Wall Engineering

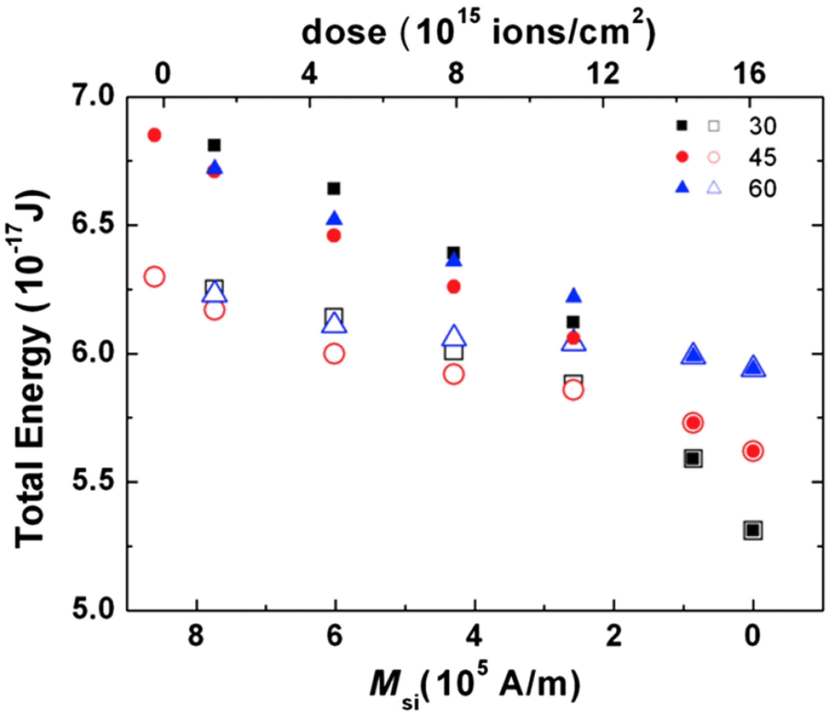


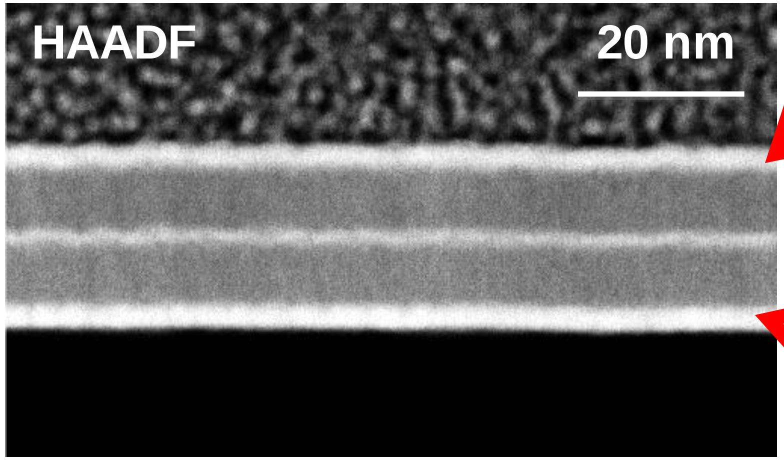
FIG. 7. Calculated total energy vs M_{si} for different orientations of the modified region, for VW (open symbols), and TW (closed symbols) domain walls in the 500-nm-wide, 10-nm-thick wire.

Phys. Rev. Applied 3, 034008 (2015)

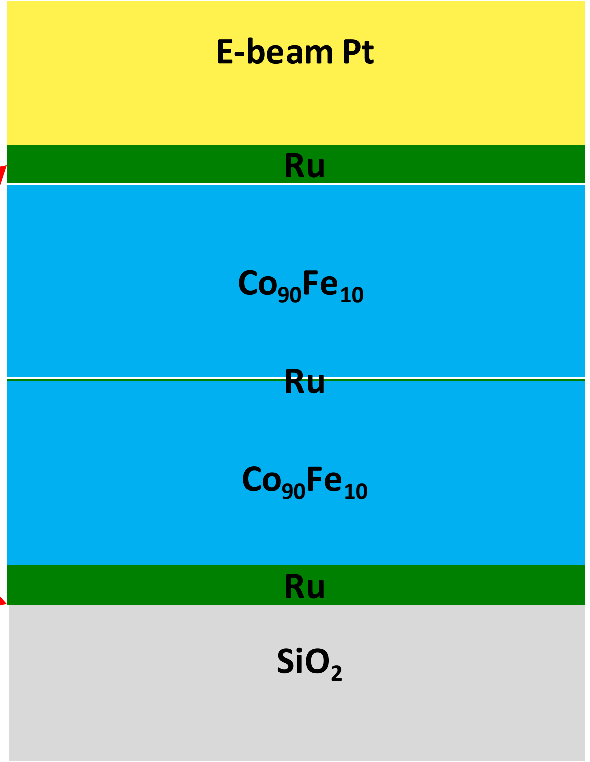
Multicapa sección transversal

Investigated Ru(2)\CoFe(10)\Ru(0.7)\CoFe(10)\Ru(2) [nm] wires.

TEM cross-section image

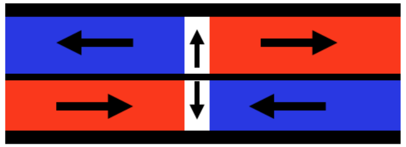


Camera length 8 cm; C1 aperture 40µm

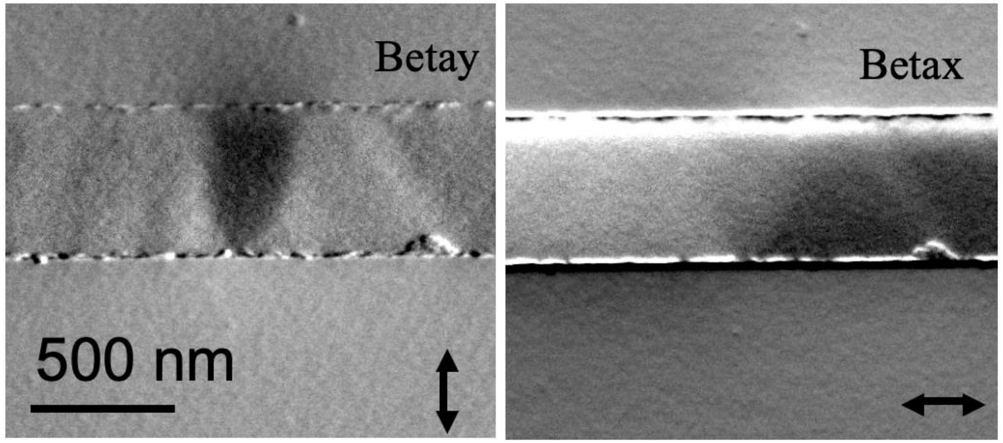


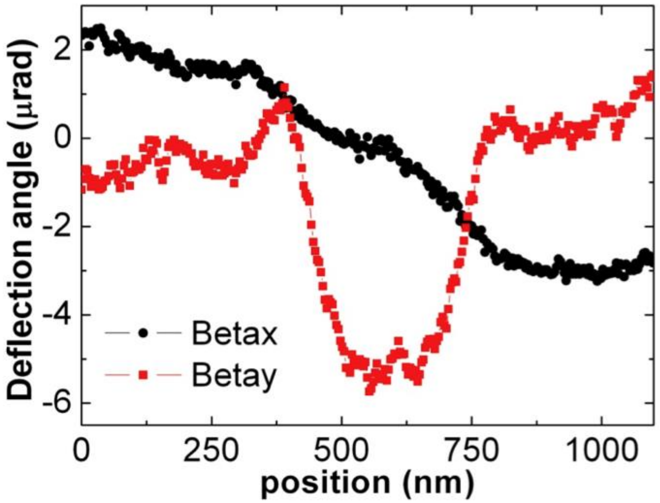
Schematic representation of the multilayer system

Domain Wall in SAF

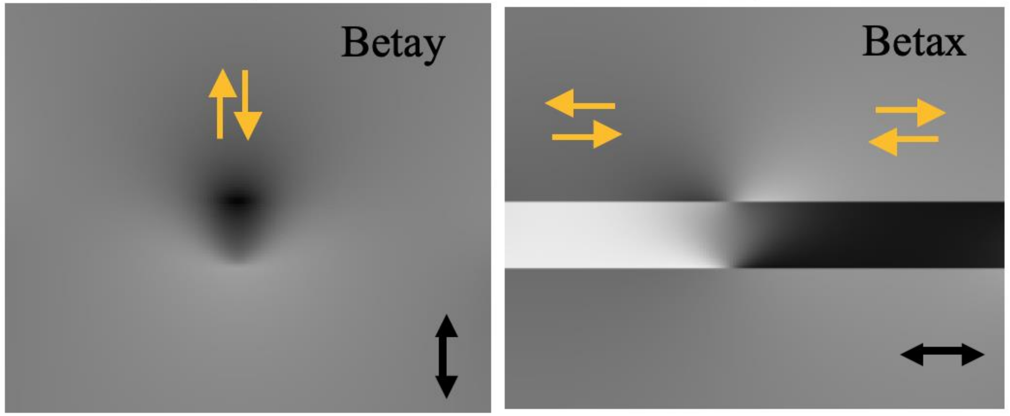


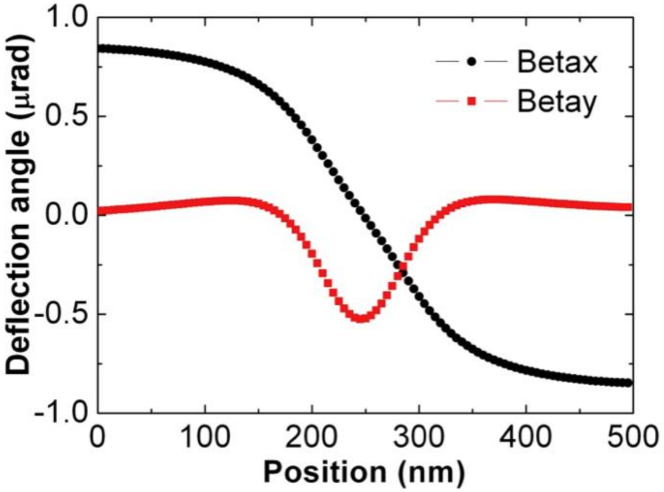
SAF layers (7.2 nm and 12.7 nm-experimental)



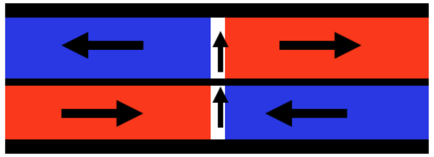


SAF layers (5 nm and 6 nm-simulation)

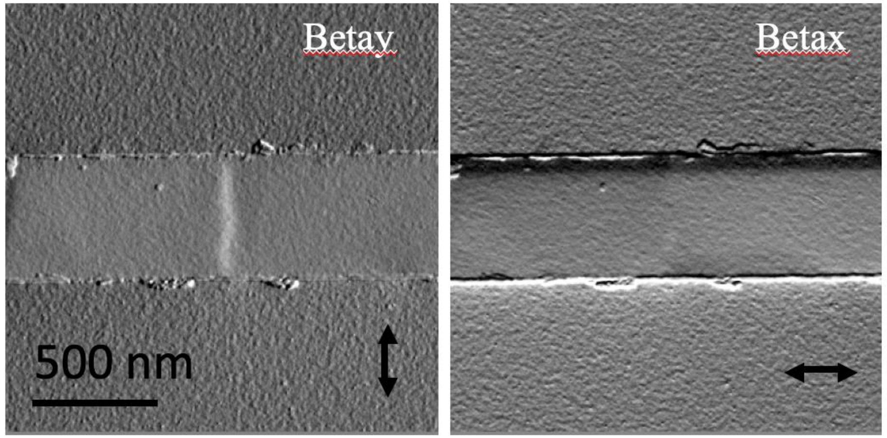


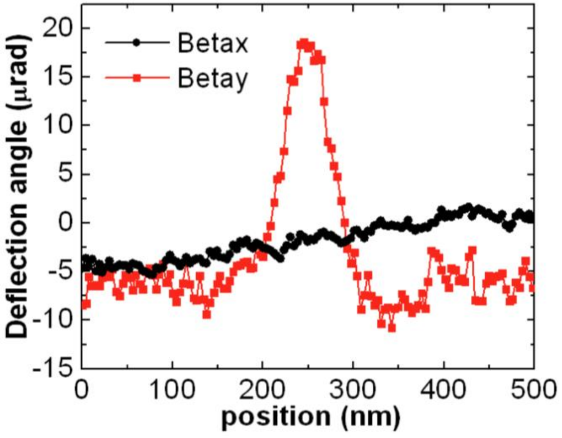


Domain Wall in SAF



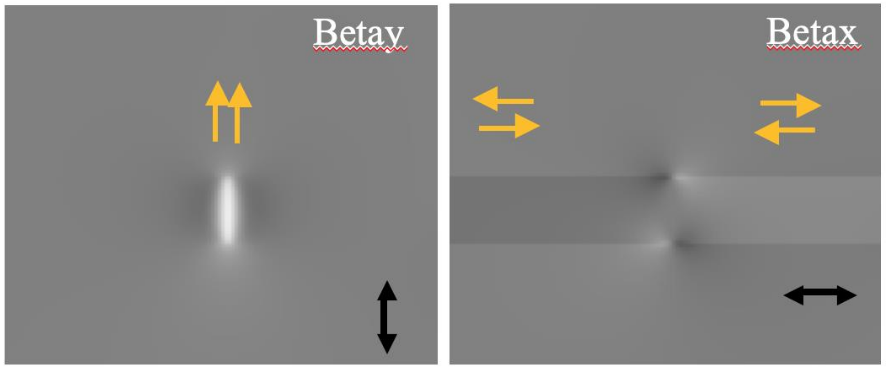
SAF layers (8.9 nm and 11.1 nm-experimental)

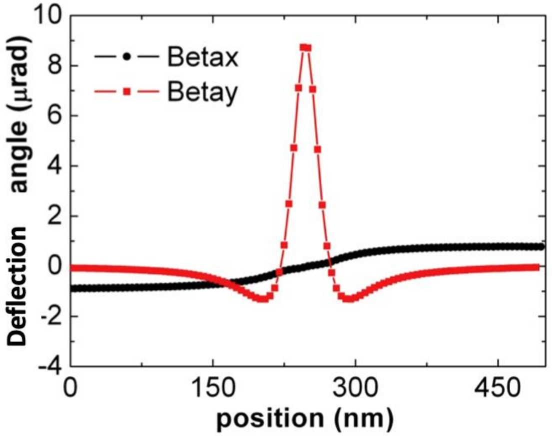




Wall width 80 nm

SAF layers (5 nm and 6 nm-simulation)





Limitations of OOMMF

- Not possible to simulate every magnetic moment in a material. Typically simulate 3D cells with 5 nm sides.
- Simulations use perfect structures with no imperfections. In reality, nanowires have a degree of roughness.
- Simulations are carried out at 0 K, experiments are carried out at room temperature.
- Magnetic fields are applied stepwise in OOMMF; in a TEM magnetic fields are increased continuously.

References

- https://www.tcl-lang.org/
- https://math.nist.gov/oommf/
- https://nanohub.org/
- https://nanohub.org/resources/33609/download/OOMMF_on_nanoHUB_FirstTimeUsersGuide_5.2020.pdf