ESCUELA
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OOMMF MICROMAGNETIC SIMULATIONS: AN IMPORTANT TOOL TO UNDERSTAND DOMAIN WALL BEHAVIOR OBTAINED BY LORENTZ TRANSMISSION ELECTRON MICROSCOPY

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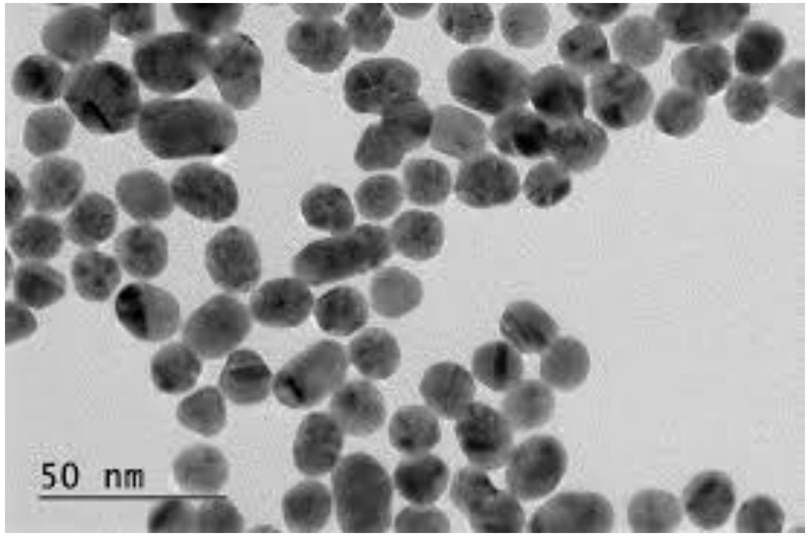
14 October 2022

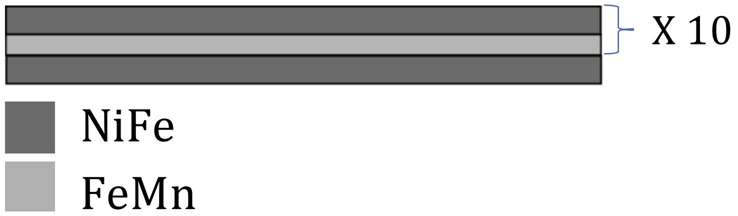
TEM Instrument

TEM: Image mode/Analysis

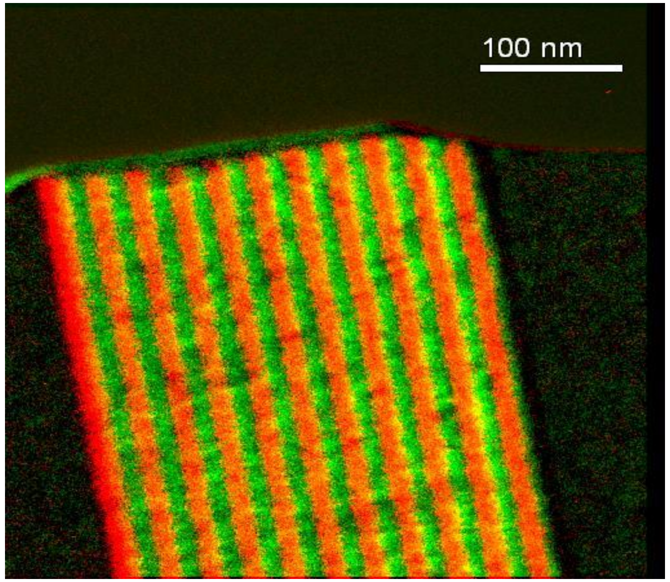


https://wwwf.imperial.ac.uk/blog/fonsmad2015-velox/2015/07/18/tem-of-gold-nanoparticles-results/

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



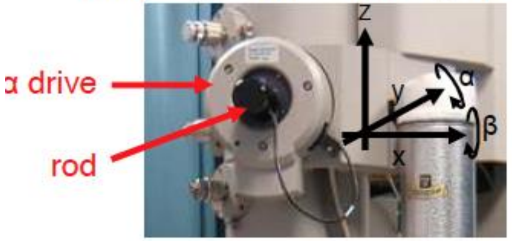
Elemental Analysis

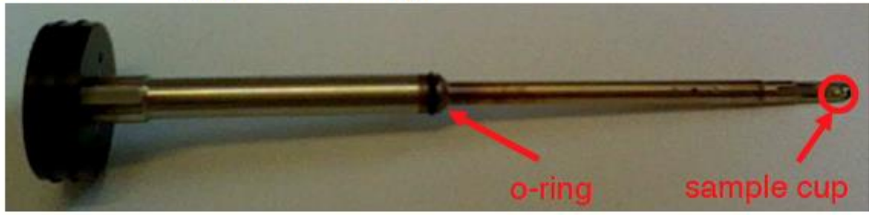


Sample holders

PURPOSE

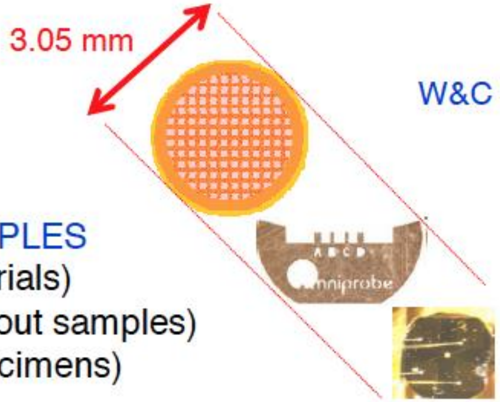
- Position in *x*, *y* with precision, reproducibility, small step size and stability
- Position in *z* to keep pre- and post-specimen optics fixed
- Keep *x*, *y* and *z* of image point fixed while tilting (eucentricity)



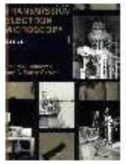


OPTIONS

- 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

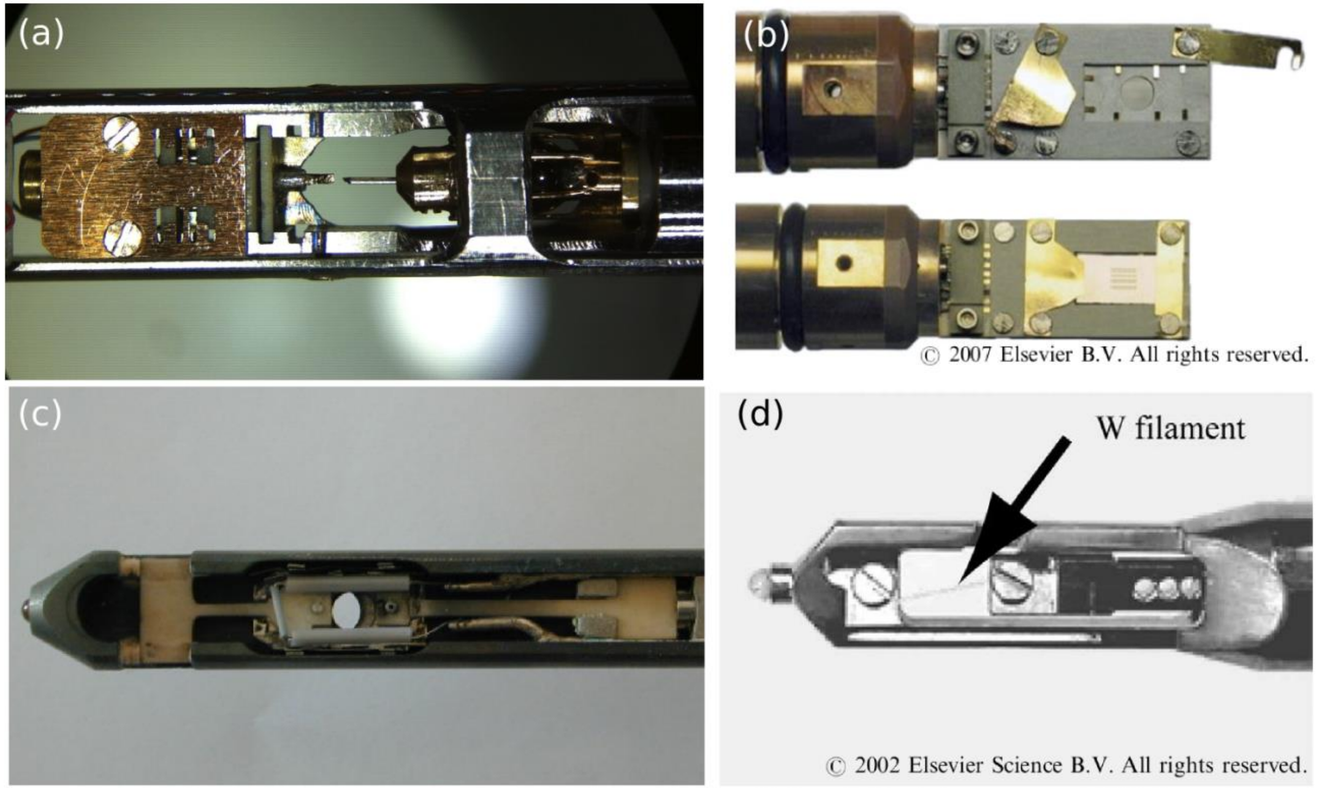
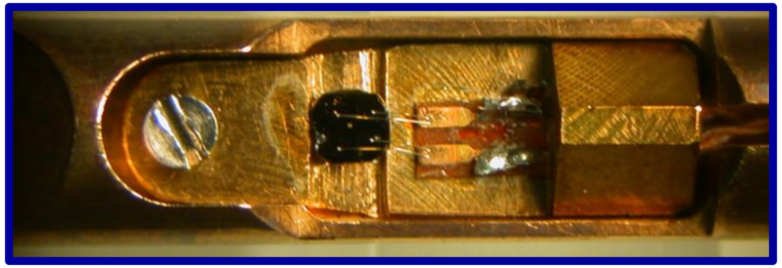
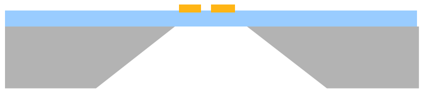


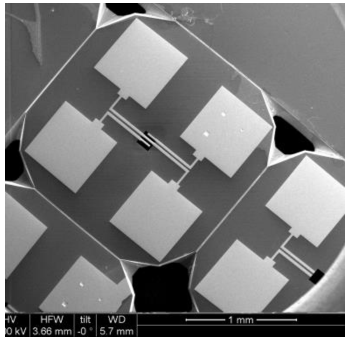
Figure 1: Sample holders for in situ a) Holder with a scanning probe for indentation, biasing or field emission measurement. b) Custom made sample holder for multi-contacted sample (8 contact pads – courtesy of (Kim, Kim, et al., 2008)). c) Sample holder for strain (traction) experiments. d) Sample holder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

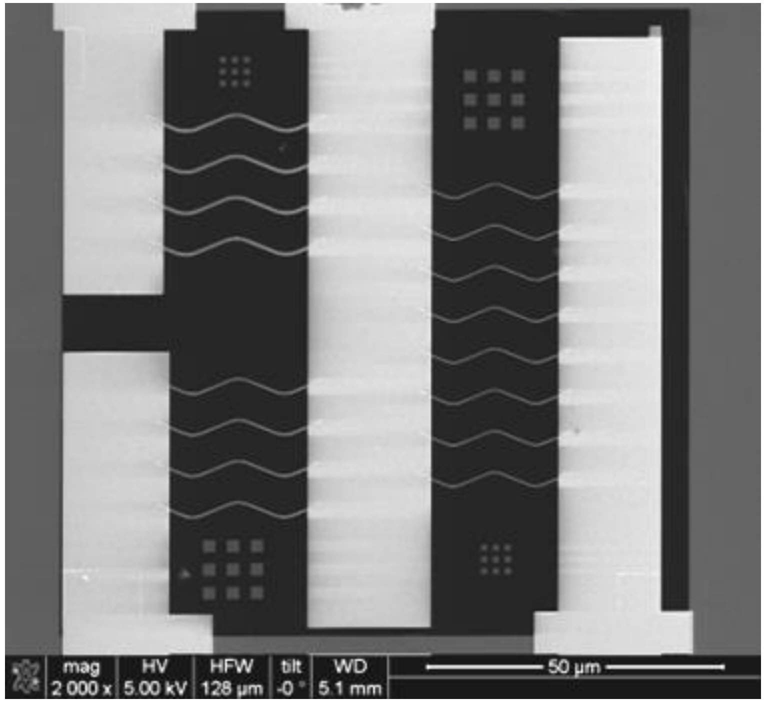
Aurélien Masseboeuf. In Situ Characterization Methods in Transmission Electron Microscopy. Alain Claverie and Mireille Mouis. Transmission Electron Microscopy in Micro-Nanoelectronics , John Wiley & Sons, Inc., pp.199-218, 2013, 9781118579022. ff10.1002/9781118579022.ch8ff. ffhal-01430590f

Sample holders







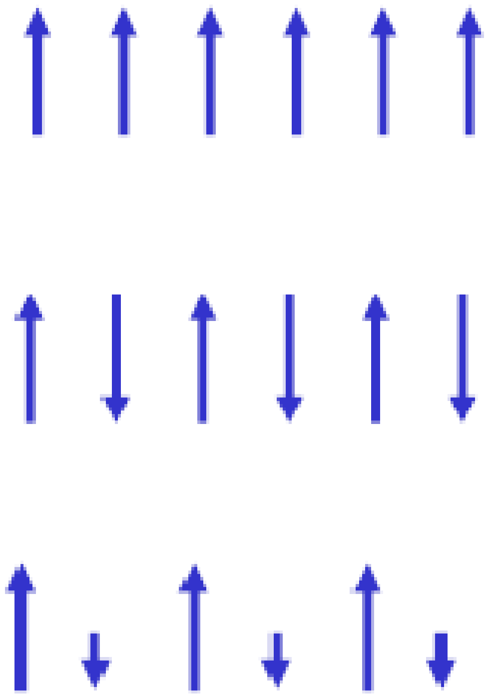


- Specimen in field free space in TEM
- TEM rod with 4 electrical contacts
- Fabrication: 2 step EBL “lift-off” process
- Substrate: supported 50 nm thick Si_3N_4 membrane
- NiFe film deposition by UHV evaporation

Magnetic order

Exchange Interaction

$$\hat{\mathrm{H}} = -\sum_{<i,j>} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$



(a) $J_{ij} > 0$

Ferromagnetism (FM)
Fe, Co, Ni

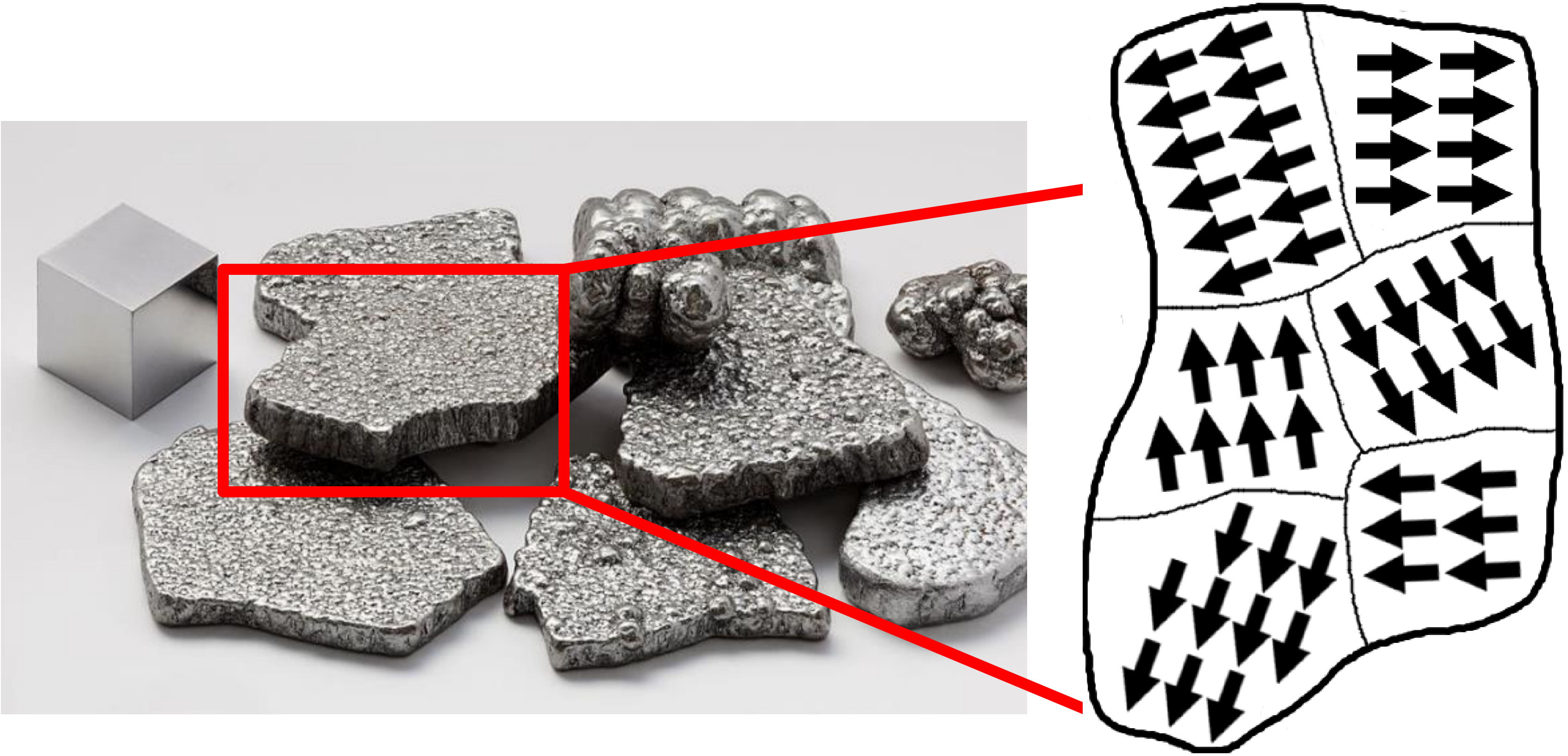
(b) $J_{ij} < 0$

Antiferromagnetism (AFM)
FeO, Co_3O_4, MnO, $BiFeO_3$

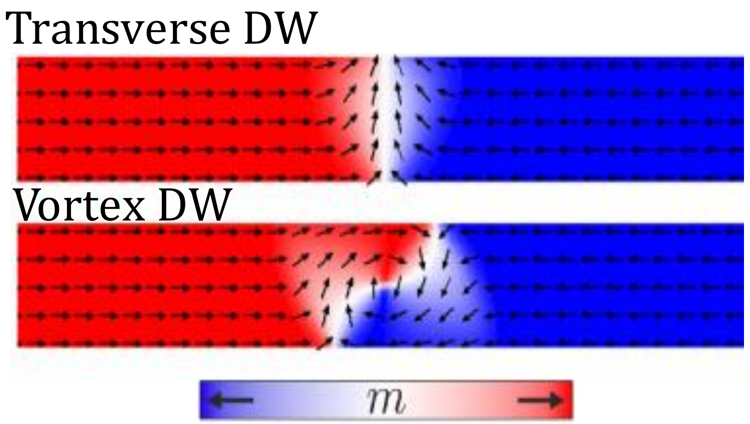
(c) more J's

Ferrimagnetism (FiM)
Fe_3O_4, $CoFe_2O_4$, $NiFe_2O_4$

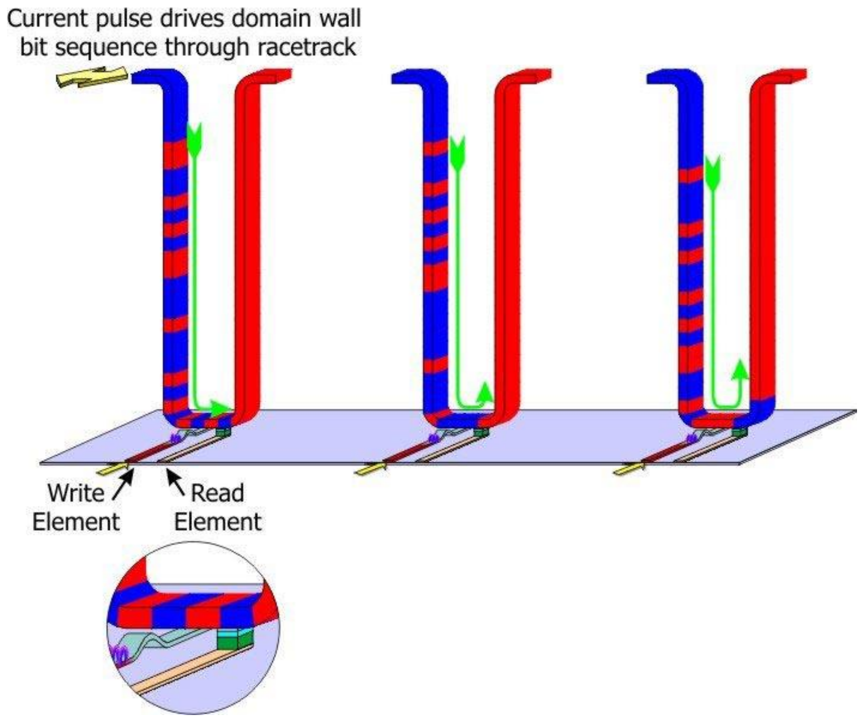
Magnetic domains



Magnetic domain walls



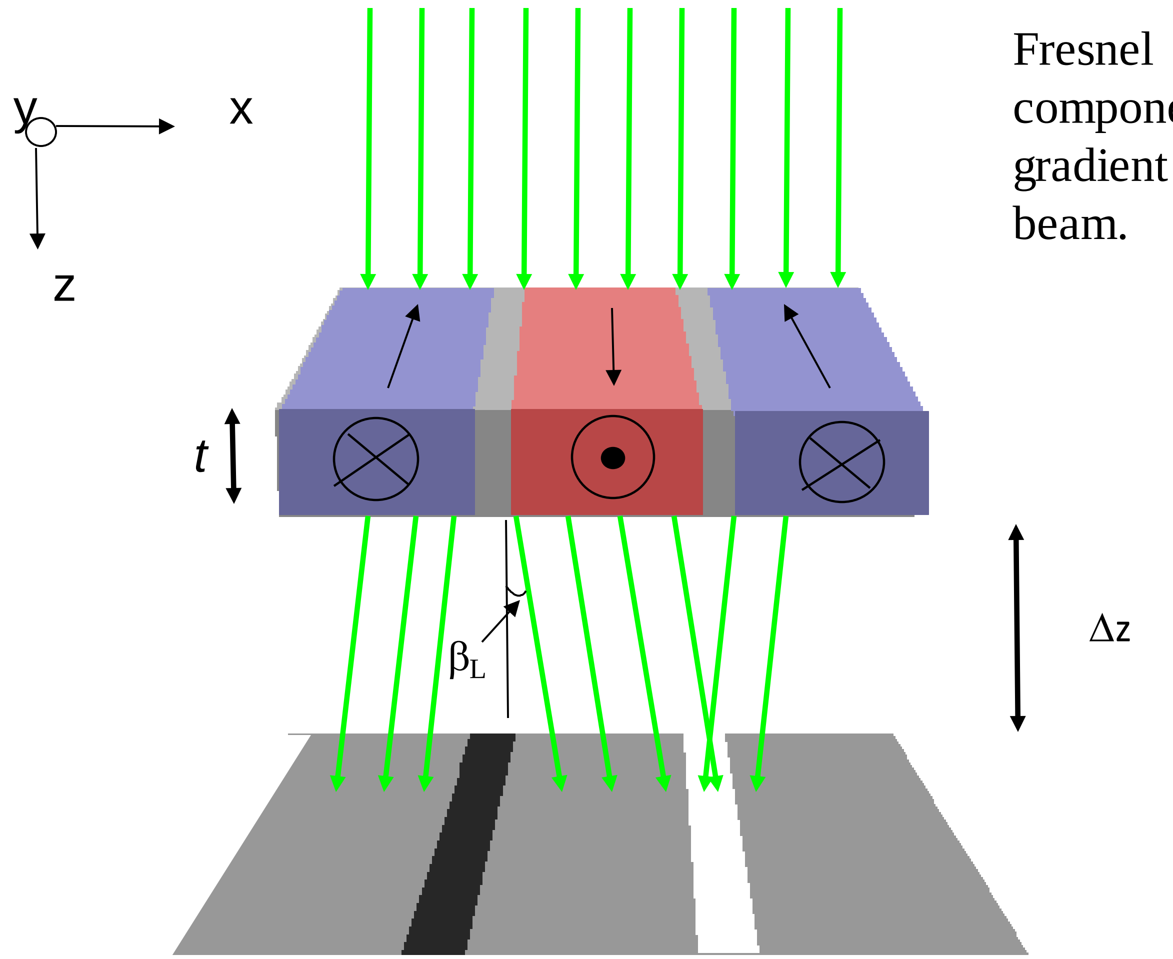
Data Storage



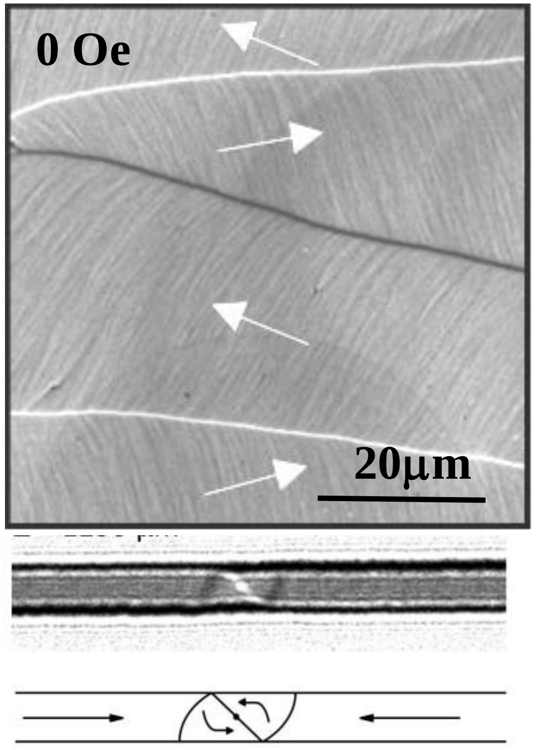
Magnetic Domain-Wall Racetrack Memory

S. Parkin, M. Hayashi, L. Thomas, Science 320, 190 (2008)

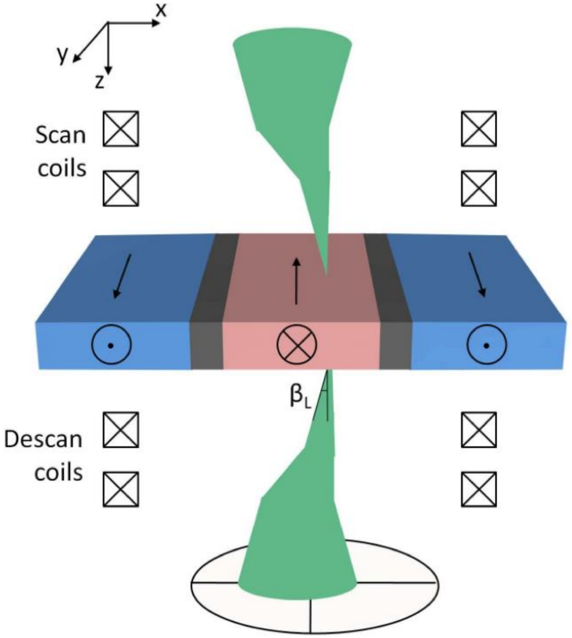
Lorentz Microscopy: Fresnel Mode



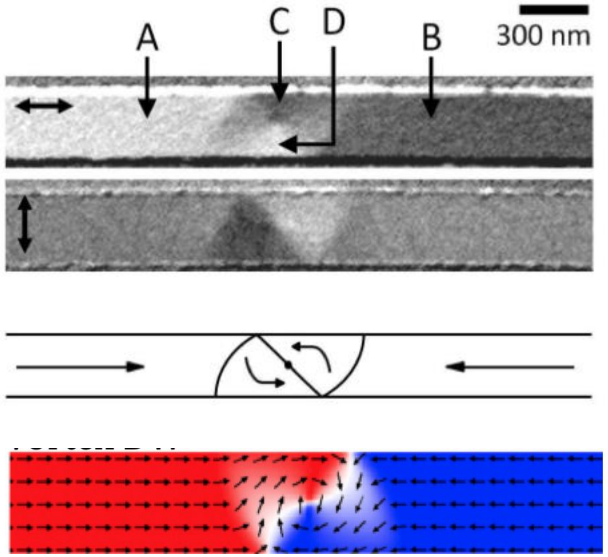
Fresnel mode contrast arises due to components of magnetic induction gradient perpendicular to the electron beam.



Lorentz Microscopy: Differential Phase Contrast imaging (DPC)



$$\beta_L = (e\lambda B_s t)/h$$



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

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)

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

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.

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.

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

- 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.

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

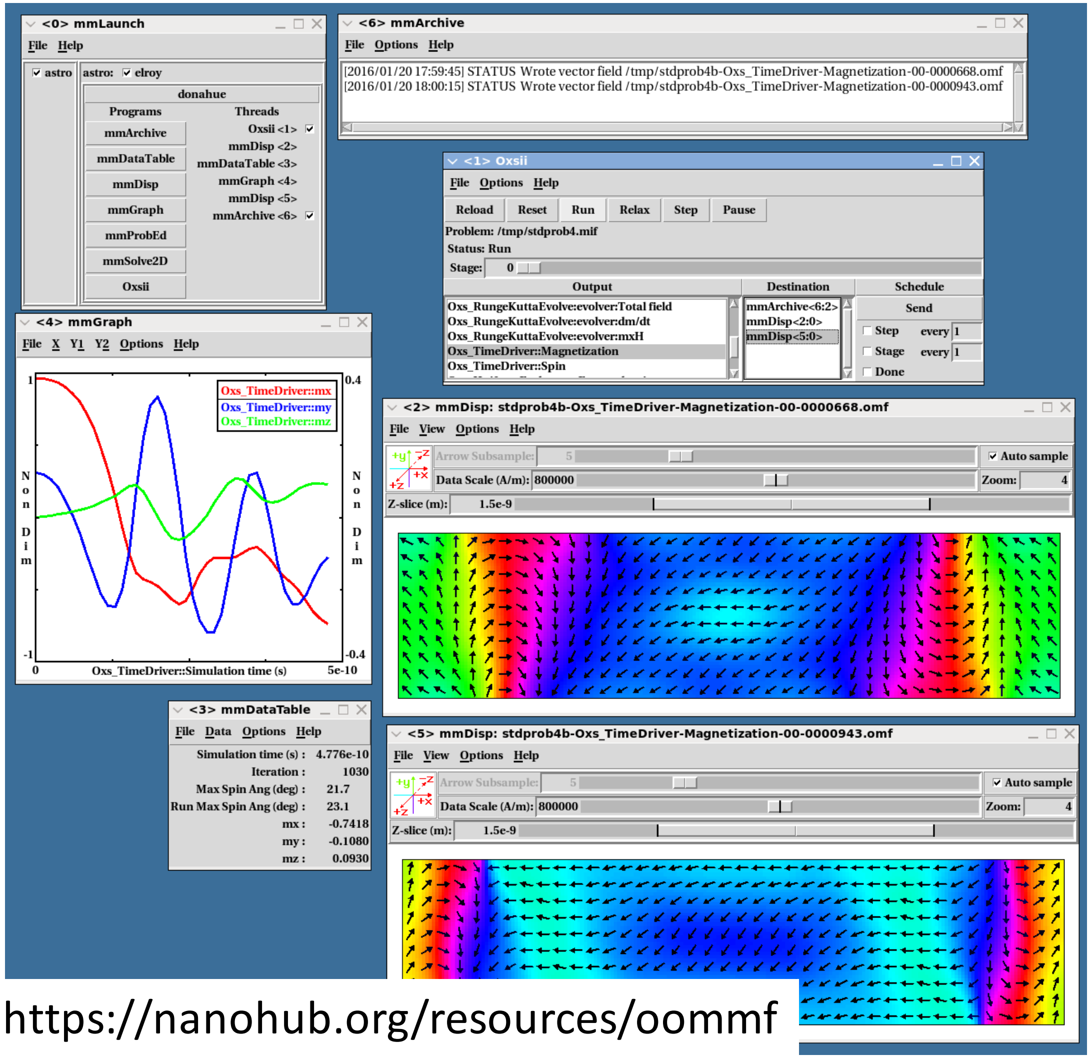
```
Specify Oxs_Exchange6Ngbr:CoFe {
  atlas :atlas

  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

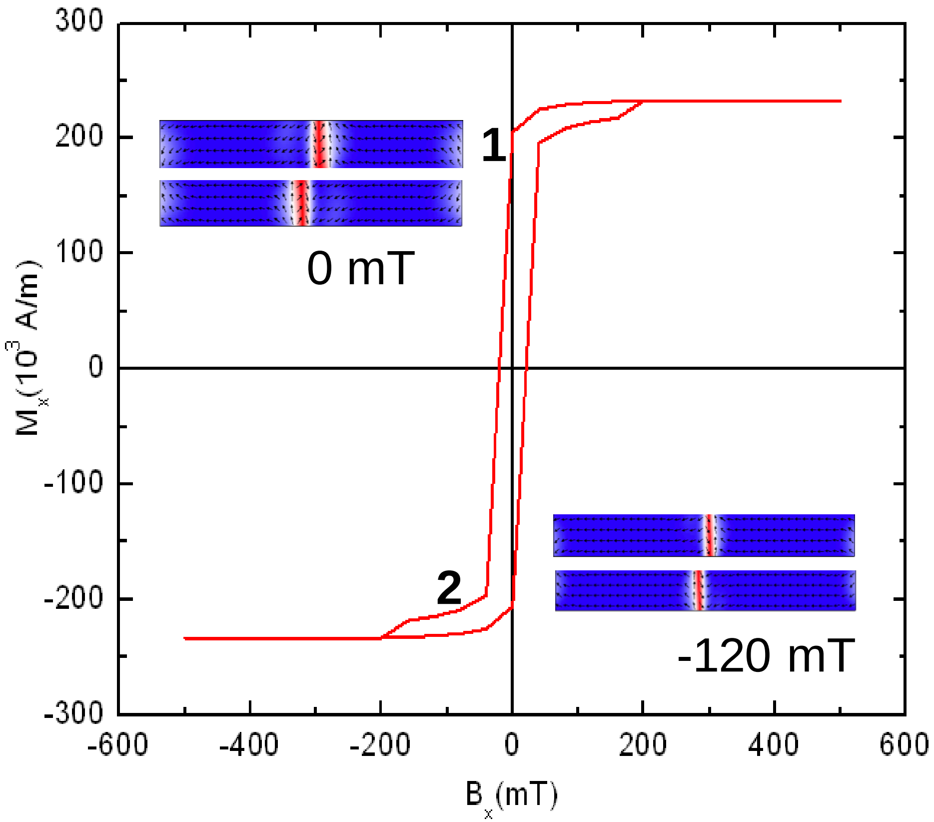
MIF file

```
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

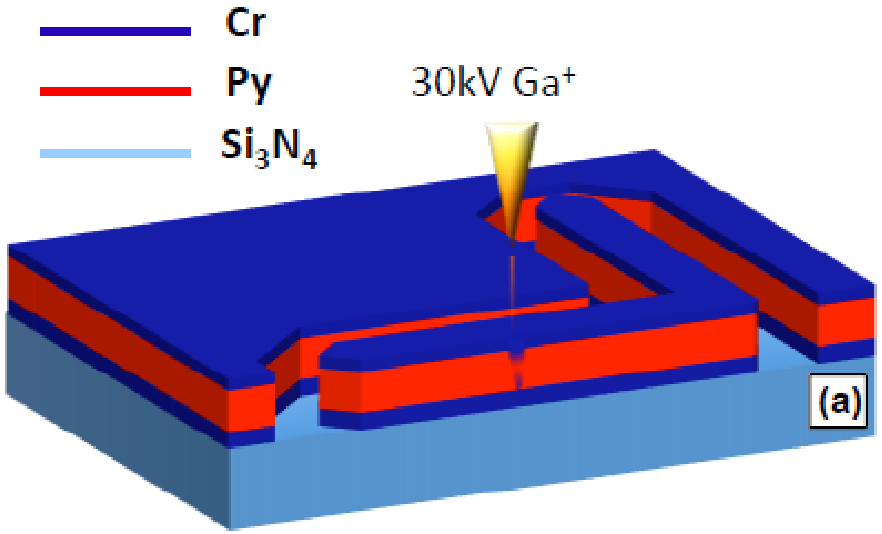


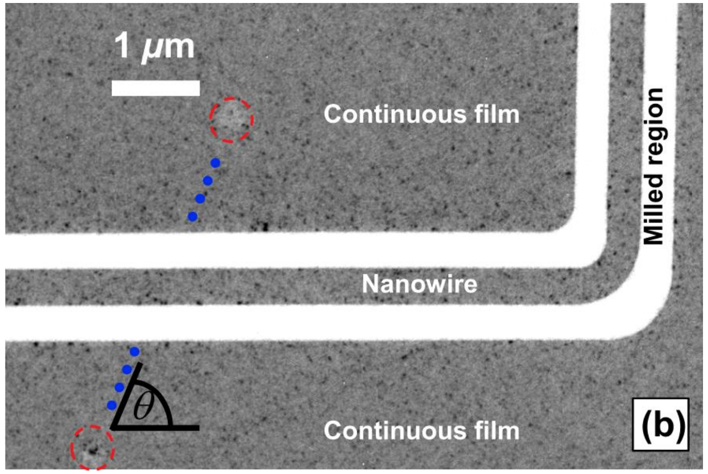
https://nanohub.org/resources/oommf



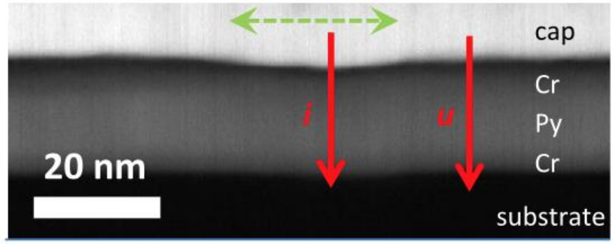
Domain-Wall Engineering

Use irradiation to locally alloy (change magnetic properties)



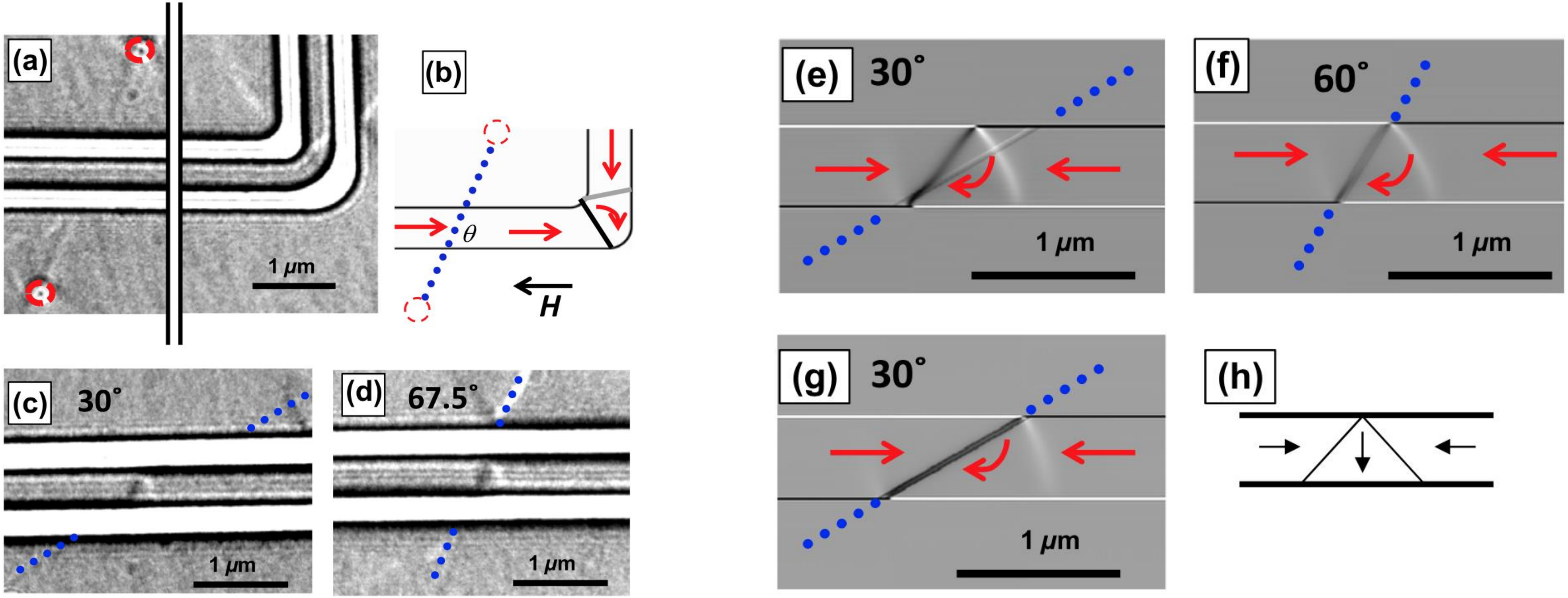


Cr(3nm)/Py(10nm)Cr(5nm)



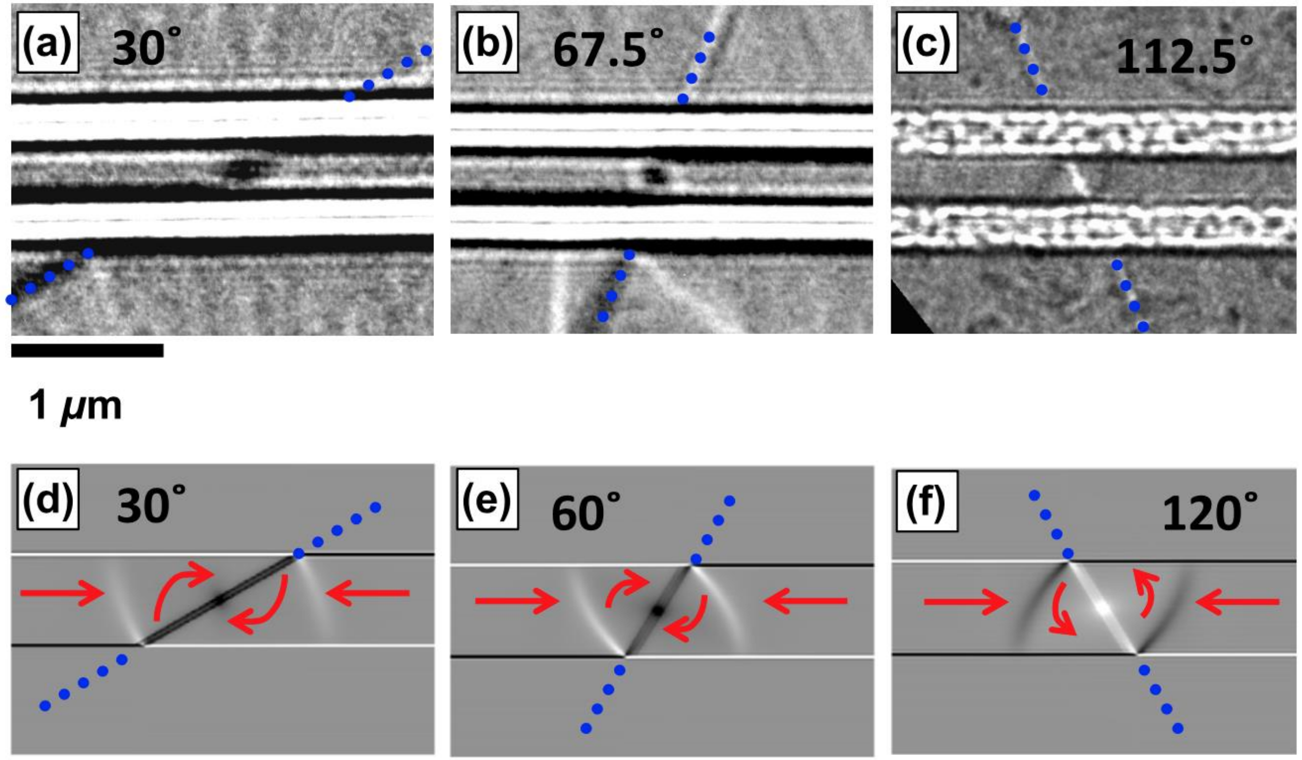
(c)

Domain-Wall Engineering
Transverse wall



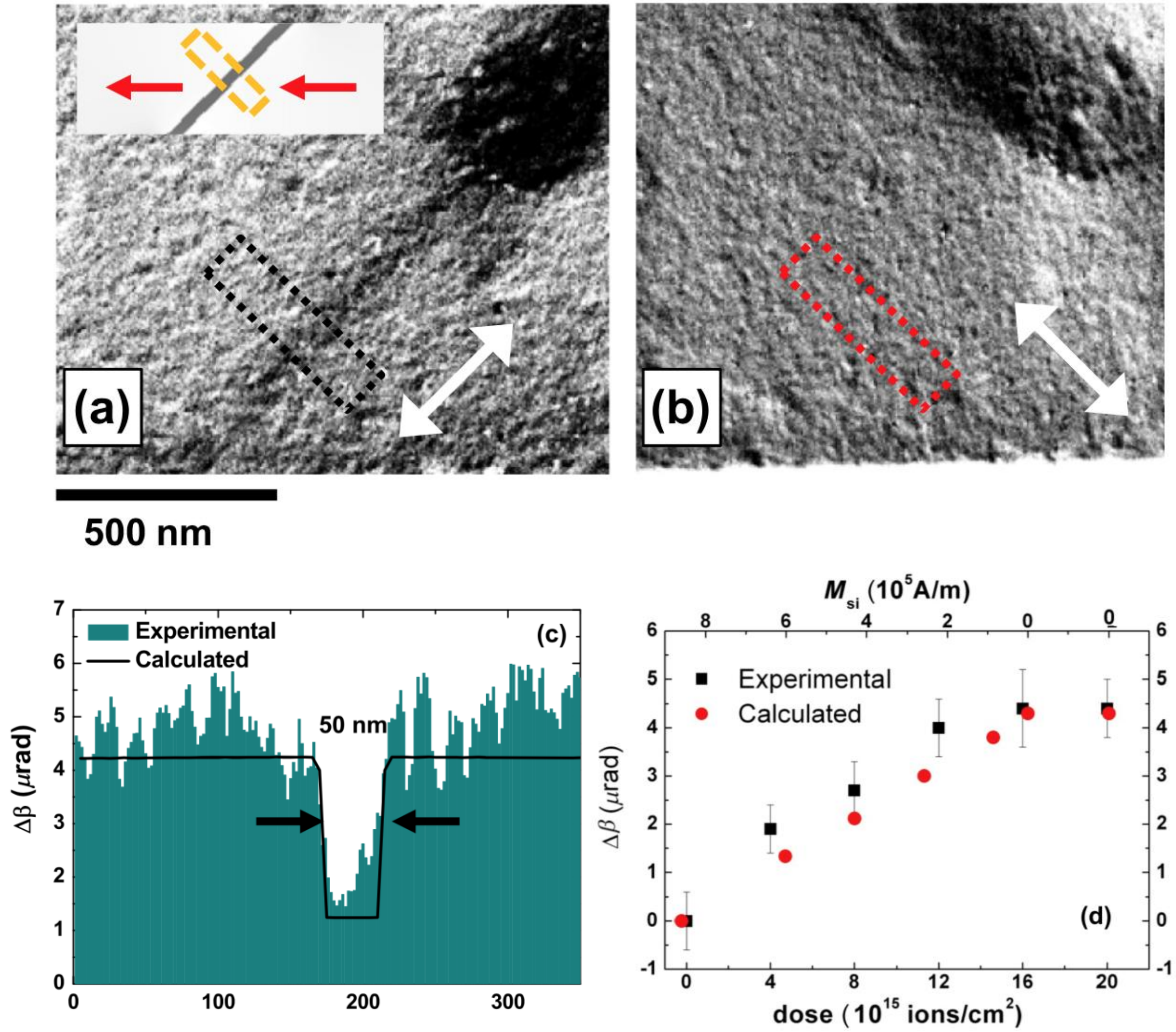
Phys. Rev. Applied 3, 034008 (2015)

Domain-Wall Engineering
Vortex wall



Phys. Rev. Applied 3, 034008 (2015)

Domain-Wall Engineering

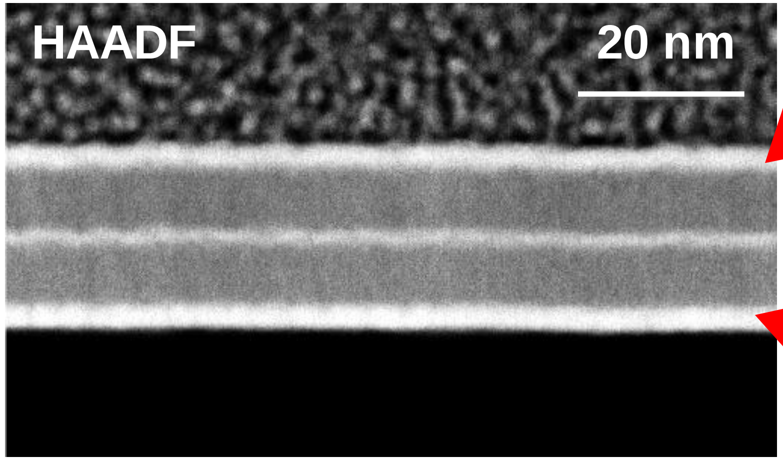


Phys. Rev. Applied 3, 034008 (2015)

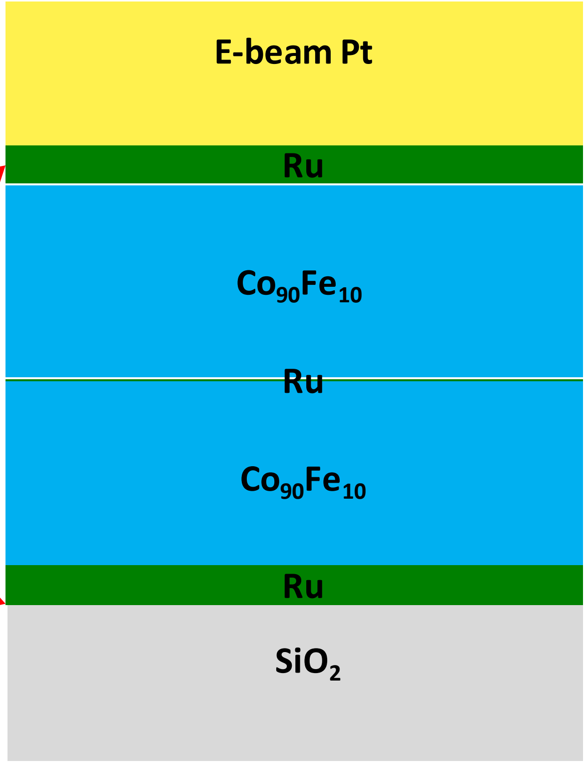
Cross-section multilayer

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

TEM cross-section image

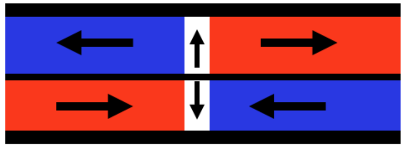


Camera length 8 cm; C1 aperture 40µm

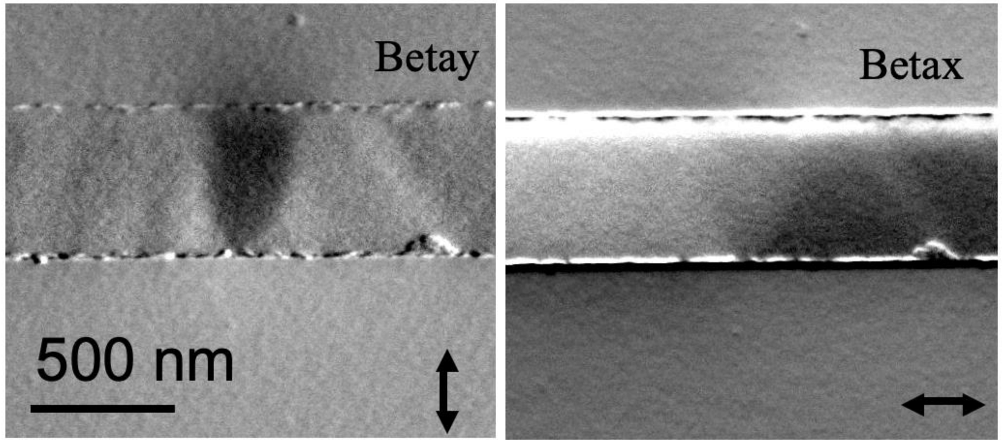


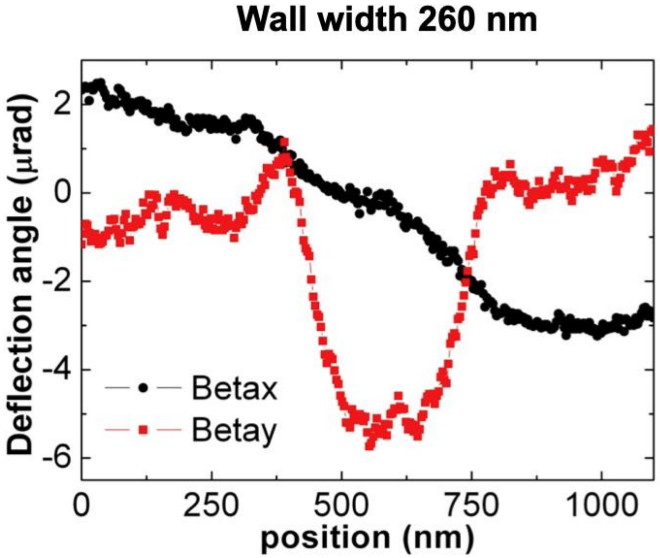
Schematic representation of the multilayer system

Domain Wall in SAF

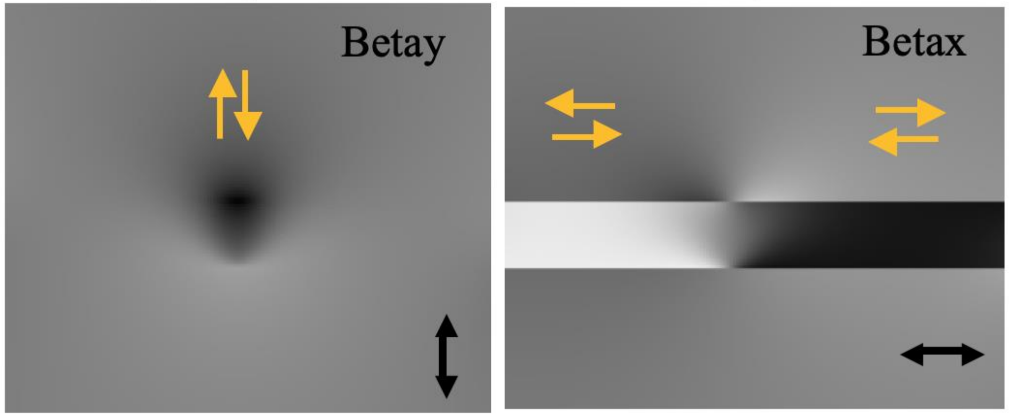


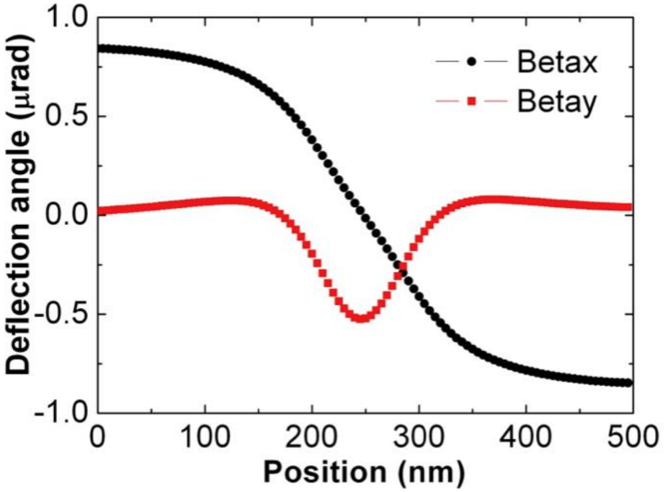
SAF layers (7.2 nm and 12.7 nm-experimental)



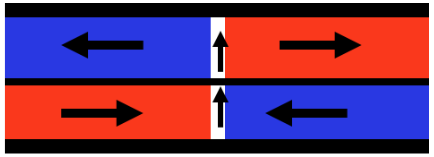


SAF layers (5 nm and 6 nm-simulation)

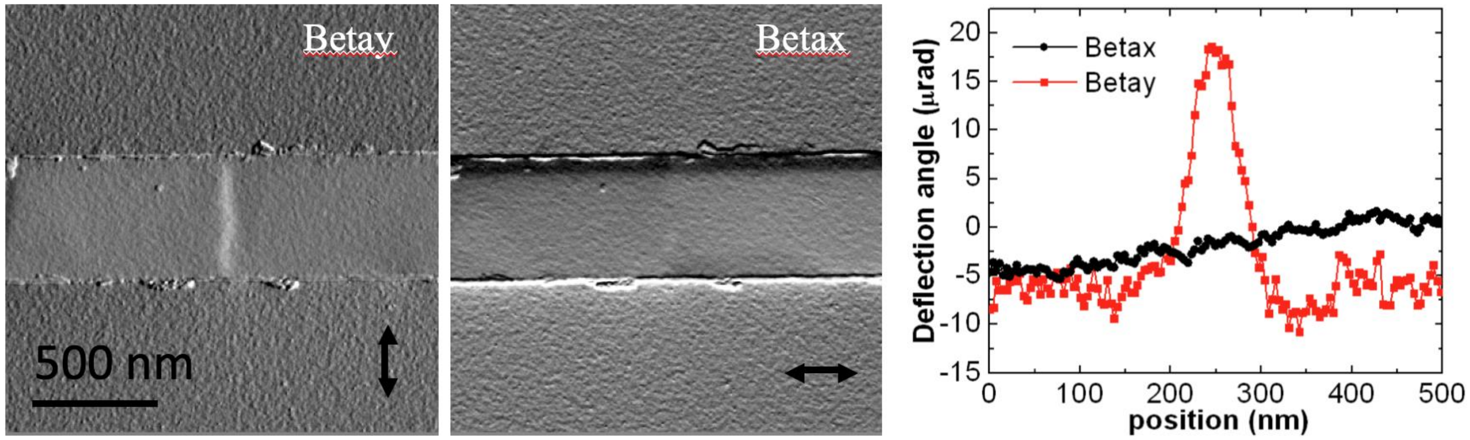




Domain Wall in SAF

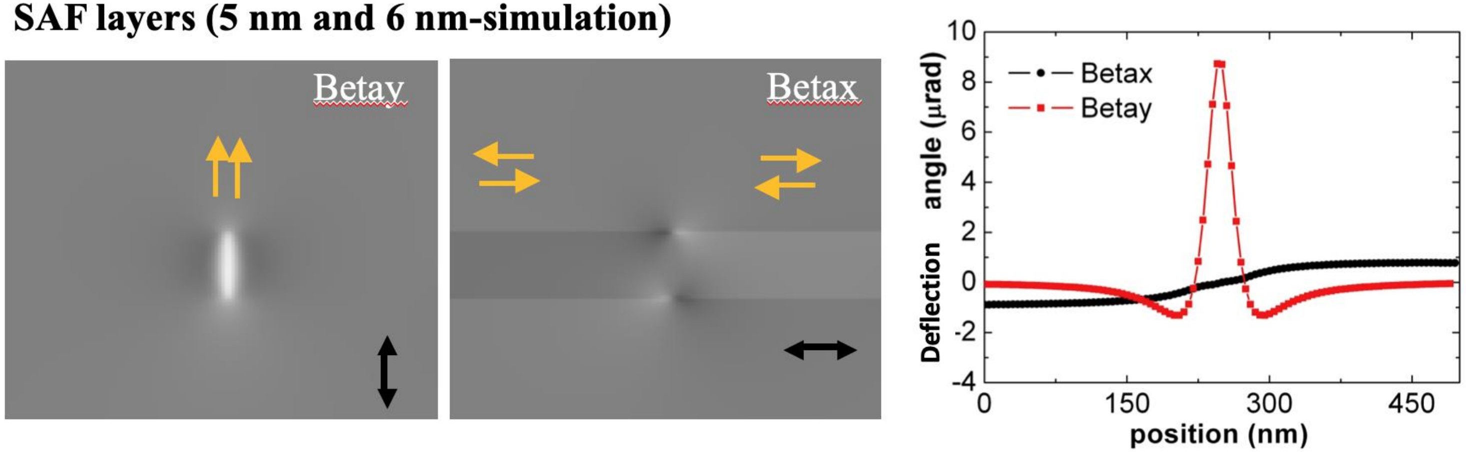


SAF layers (8.9 nm and 11.1 nm-experimental)



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.

Acknowledgements

Materials and Condensed Matter Physics Group, University of Glasgow
The Condensed Matter Physics Group, University of Leeds

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