Micromagnetic Simulation of Magnetization Reversal in Small Particles with Surface Anisotropy

W. Scholz, D. Suess, J. Fidler, T. Schrefl

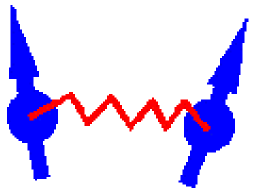
Vienna University of Technology
http://magnet.atp.tuwien.ac.at/

Outline

- Finite element micromagnetics
- Demagnetizing field in FePt nanoparticles
- Magnetocrystalline anisotropy and surface anisotropy in FePt
- Coalesced particles and multiple easy axes
- Coercivity of core/shell particles
- Surface anisotropy
- Summary

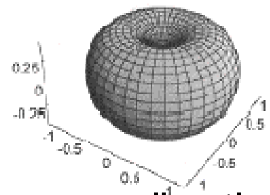
Finite Element Micromagnetics

exchange



⇨ parallel spins

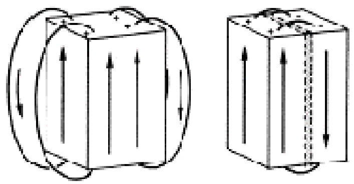
anisotropy



⇨ easy directions

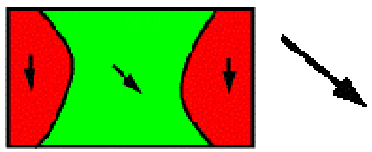
$$E_{tot} = E_{exch} + E_{ani} + E_{mag} + E_{Zee}$$

magnetostatics



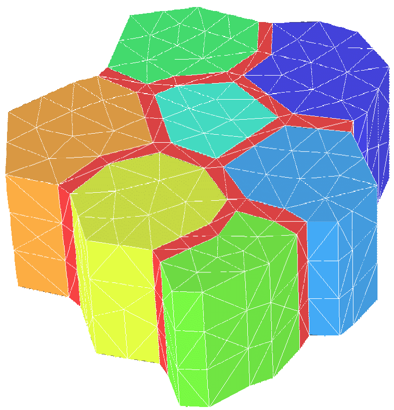
⇨ domains

external field



⇨ rotation

Finite Element Approach

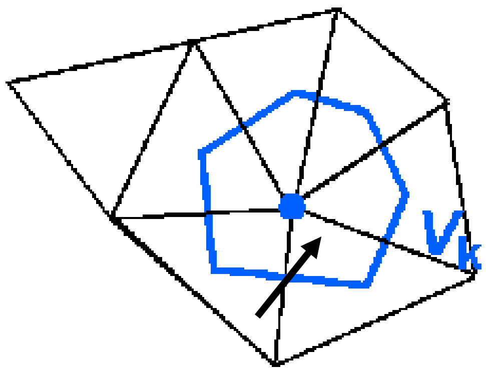


- expand J with basis function φ defined on tetrahedral finite elements

$$\vec{J}(\vec{x}) = \sum_{i=1}^{nodes} \vec{J}_i \varphi_i(\vec{x})$$

- energy as a function of J_1, J_1 … J_N

$$E(\vec{J}_1, \vec{J}_2 .... \vec{J}_N)$$

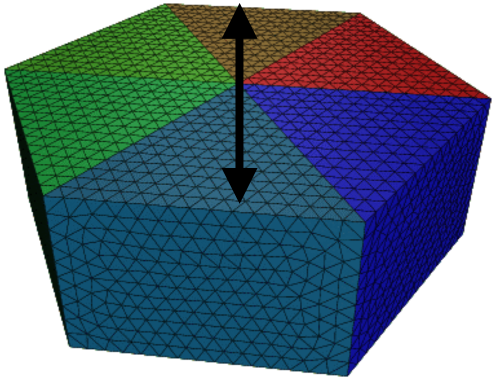


- LMVM (limited memory variable metric) method for energy minimization (only gradient required)

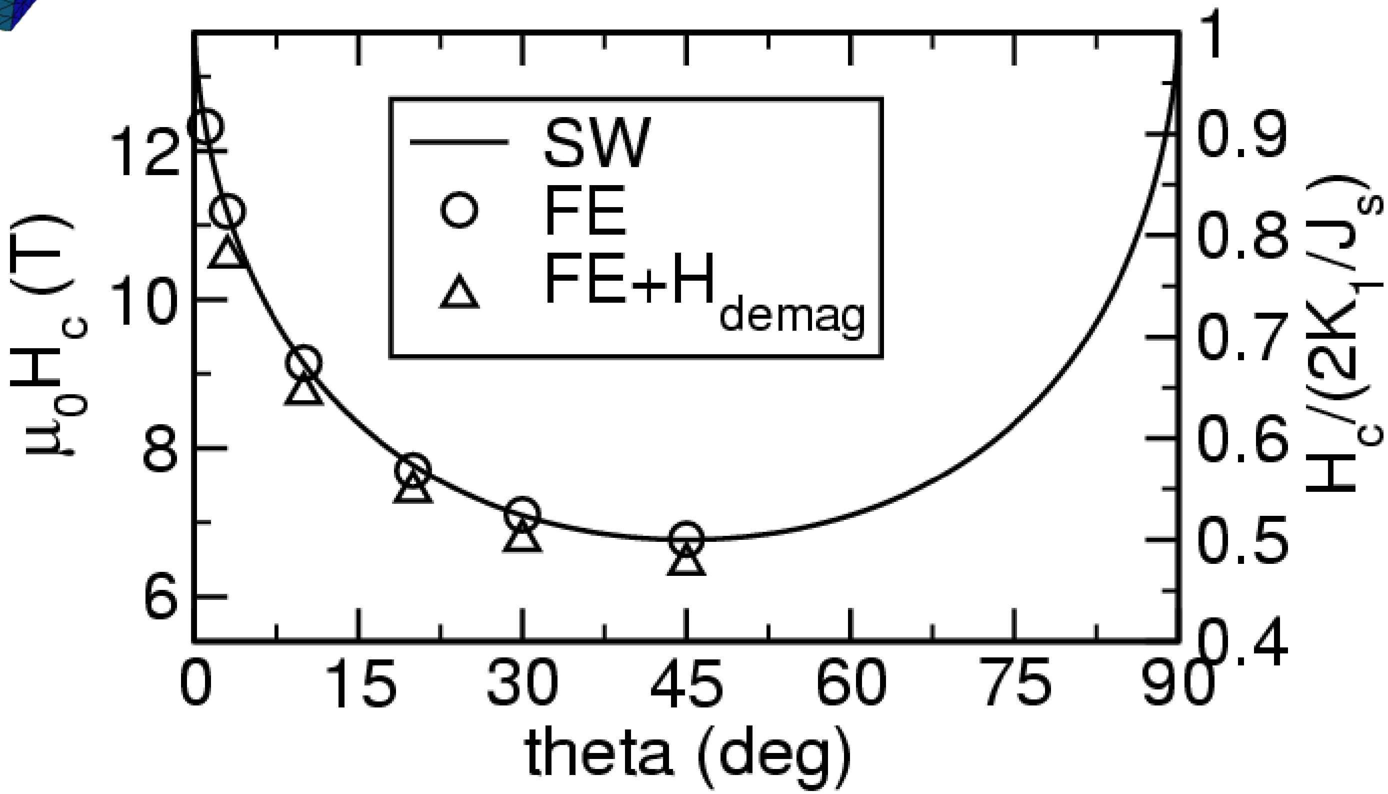
$$\vec{H}_k = -\frac{1}{V_k} \frac{\partial E(\vec{J}_1, \vec{J}_2 .... \vec{J}_N)}{\partial \vec{J}_k}$$

Micromagnetics meeting Wednesday (today!) 7:30pm Salon 4/5
Presentation of the free open source micromagnetics package "magpar", which has been used for these simulations.

Demagnetizing field

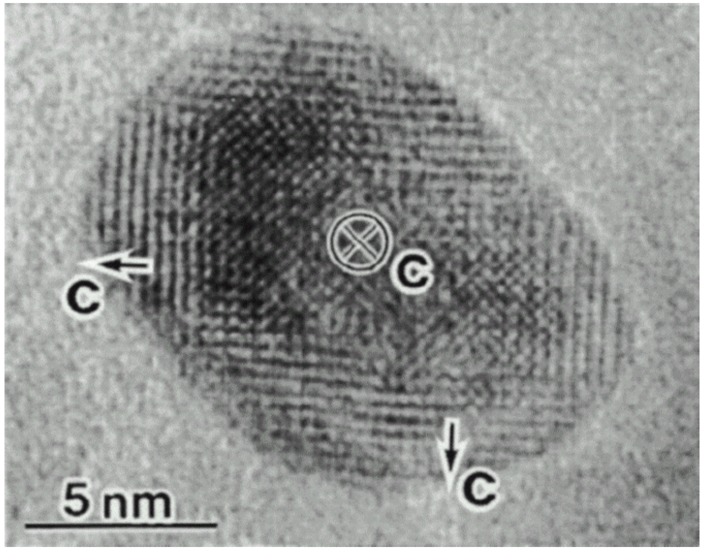


FePt material parameters:
K_V = 7.7 MJ/m^3
J_s = 1.43 T
A = 10^{-11} J/m
uniaxial anisotropy

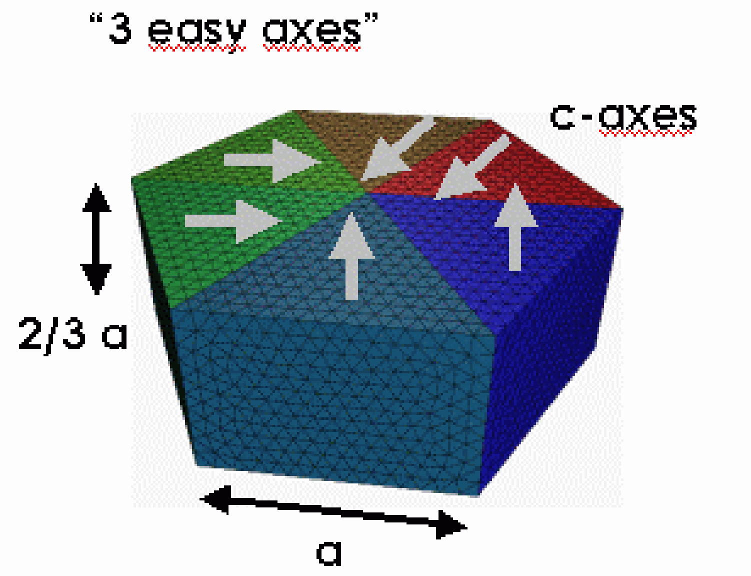


Model of FePt nanoparticles

thin film of FePt particles embedded in an Al_2O_3 matrix



B. Bian, D. Laughlin, K. Sato, Y. Hirotsu, J. Appl. Phys. 87, 2000, 6962

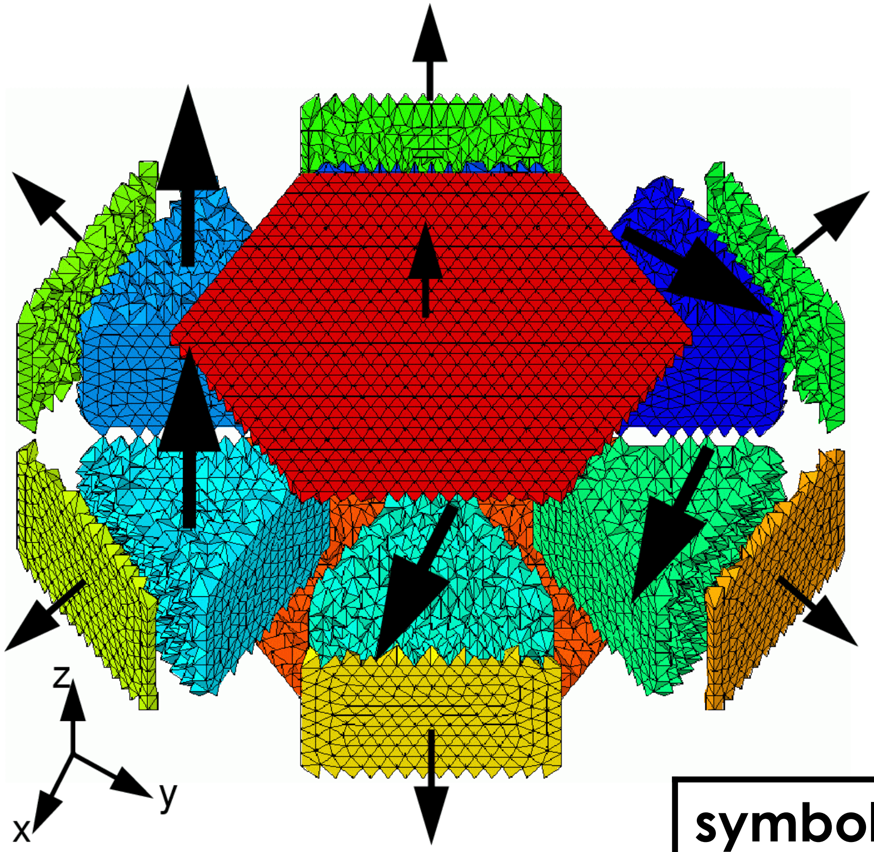


↑:→:↗	H_c (kA/m)
5:1:0	3330
4:2:0	3140
4:1:1	3310
3:3:0	3630
3:2:1	3420
2:2:2	3430

Surface Anisotropy

- **Surface oxidation**
  Xray absorption fine structure spectroscopy indicates oxide shell of 0.4 nm around 4-6 nm FePt particles γ-Fe_3O_4 have been assumed for the surface shell surrounding the FePt core: K_s = -0.011 MJ/m^3, J_s = 0.5 T, A = 1.32e-11 J/m.
  - S. Anders, S. Sun, C. B. Murray, C. T. Rettner, M. E. Best, T. Thomson, M. Albrecht, J. U. Thiele, E. E. Fullerton, and B. D. Terris, Microelectronic Engineering 61-62, 569 (2002).
  - S. Anders, M. F. Toney, T. Thomson, R. F. C. Farrow, J.-U. Thiele, and B. D. Terris, Tech. Rep. SLAC-PUB-9989, SLAC - Stanford Linear Accelerator Center (2003).
  - S. Anders, M. F. Toney, T. Thomson, and J.-U. T. B. D. Terris, Tech. Rep. SLAC-PUB-9994, SLAC - Stanford Linear Accelerator Center (2003).
- **Instrinsic surface anisotropy**
  K_s = 46 MJ/m^3 ; K_s/K_v=6
  - Y. Labaye, O. Crisan, L. Berger, J. M. Greneche, and J. M. D. Coey, J. Appl. Phys. 91, 8715 (2002).

Particle geometry



Core/shell configuration:

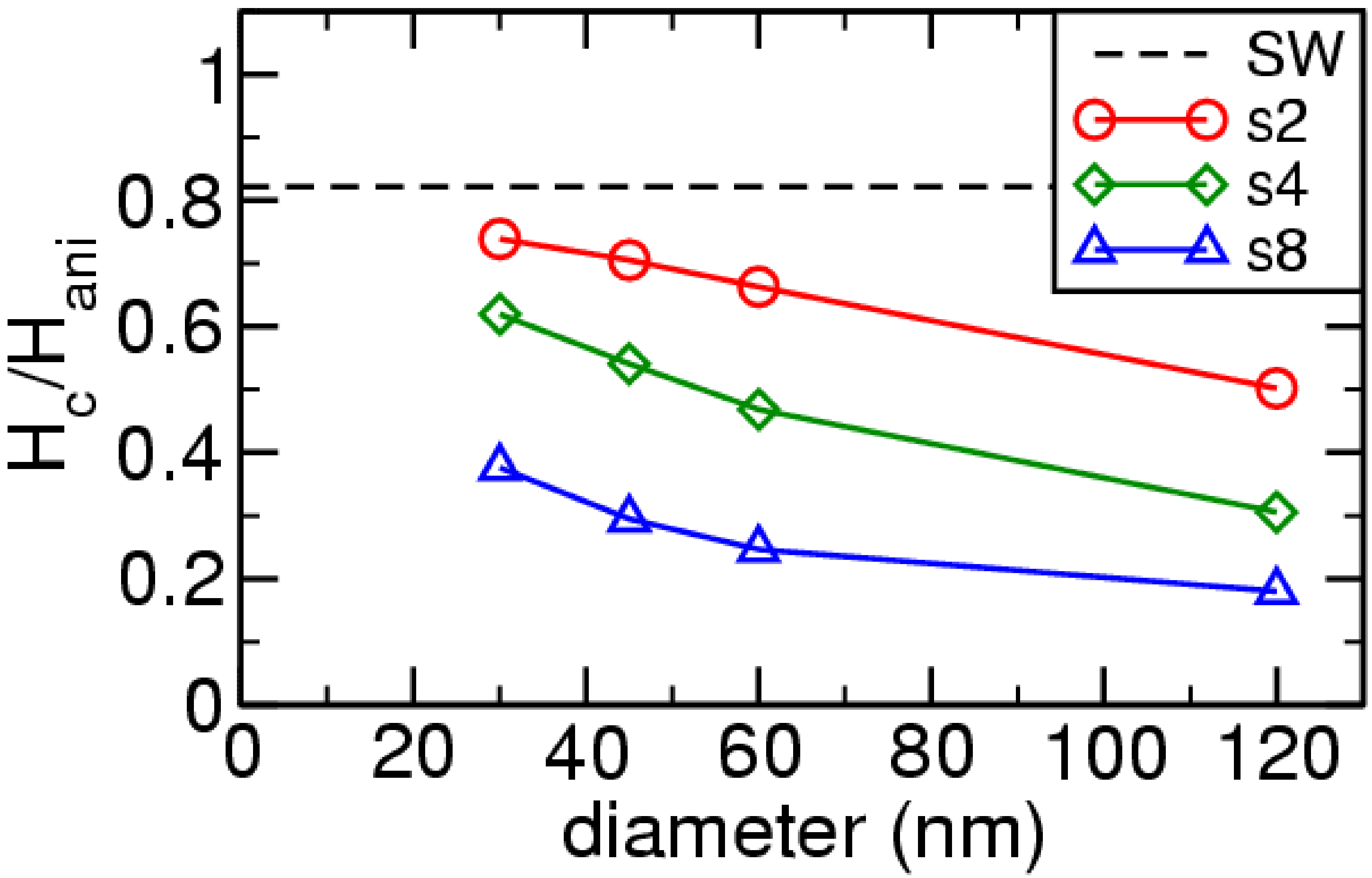
Core: FePt material parameters

Shell: modified material parameters and anisotropy (perpendicular/ in-plane of surface)

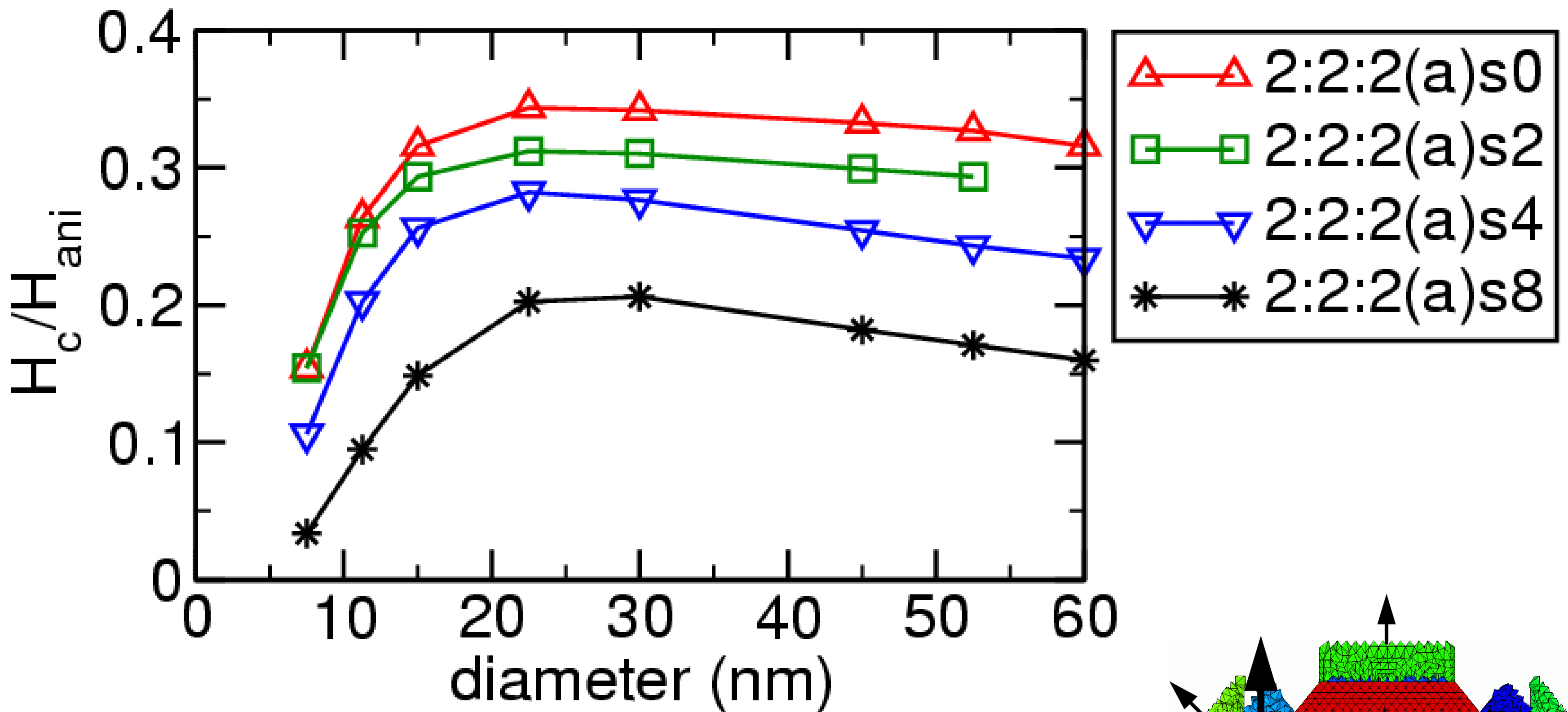
symbol	t_s (nm)	V_{core} (nm^3)	V_{shell} (nm^3)	V_{core}/V_{shell}
s2	1	38000	8000	0.21
s4	2	30000	16000	0.53
s8	4	17000	29000	1.71

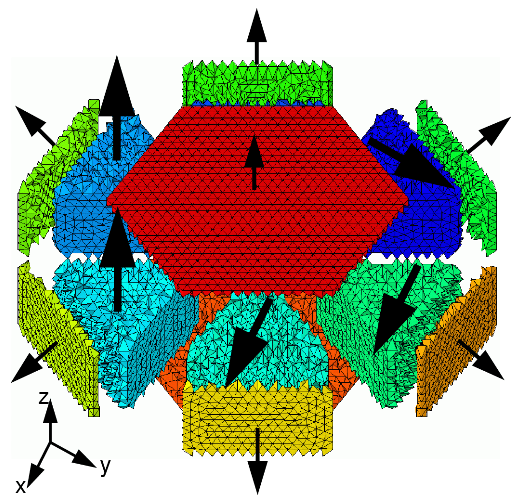
Dependence on shell thickness

Uniaxial core with Fe_2O_3 shell and in-plane anisotropy



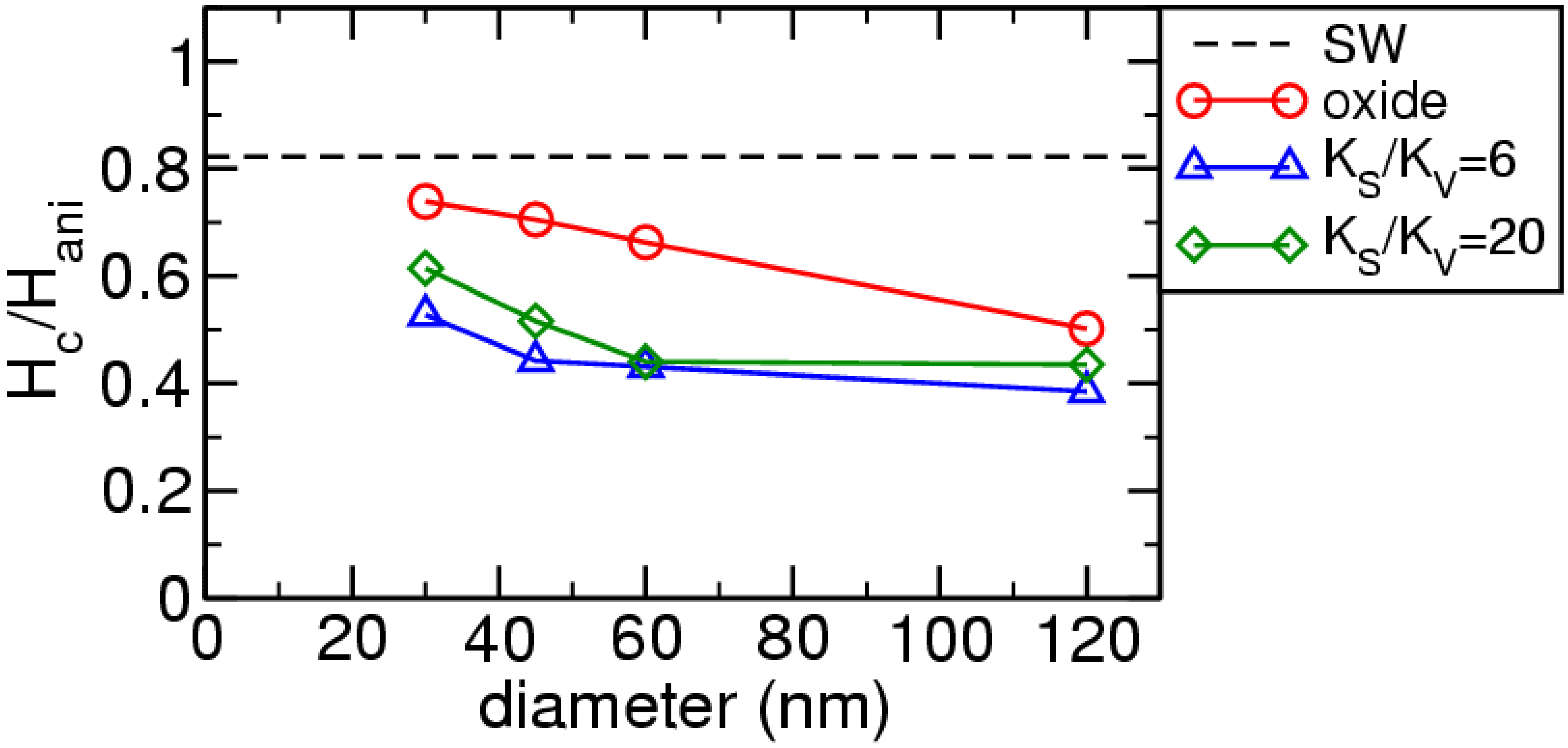
Polycrystalline FePt





Strong/weak surface anisotropy

FePt material parameters
only anisotropy on surface (thin shell: s2) modified



Summary

- Finite element micromagnetics to model nucelation processes in FePt nanoparticles
- Multiple perpendicular easy axes introduce domain walls which lower coercivity significantly
- Distribution of easy axes is of minor importance
- Modified surface properties (oxidation/surface anisotropy) facilitates nucleation and reduces coercivity

Acknowledgement

- Josef Fidler
- Thomas Schrefl
- Dieter Suess, Rok Dittrich, Vassilios Tsiantos, Hermann Forster, Markus Kirschner

Work supported by Austrian Science Fund Y-132 PHY

http://magnet.atp.tuwien.ac.at/