

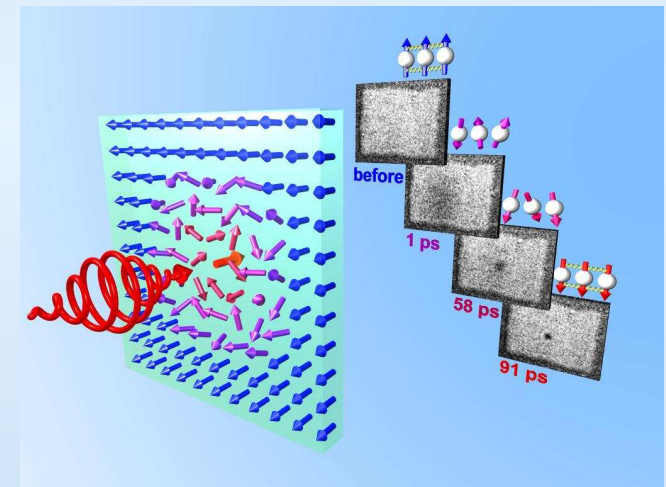
Spin dynamics at finite temperatures

U. Nowak

Universität Konstanz, Germany

Topics:

- Motivation
- Theoretical framework for thermal spin dynamics
- Laser induced spin dynamics and opto-magnetic writing
- Domain wall motion and spin Seebeck effect
- Summary



(<http://www.ultramagnetron.org>)

People involved

In Konstanz:



S. Gerlach



D. Hinzke



N. Kazantseva



F. Schlickeiser



O. Storz



S. Wienholdt



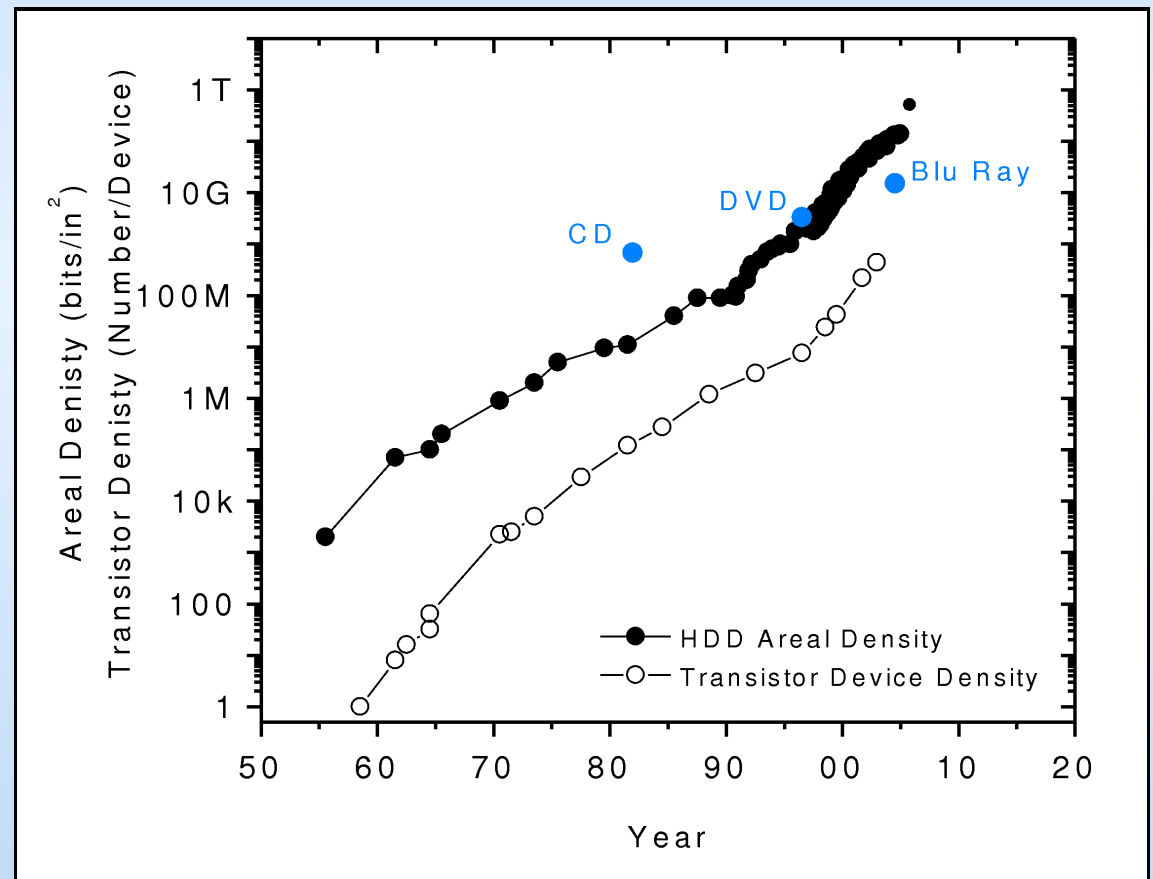
U. Ritzmann

Collaborations:

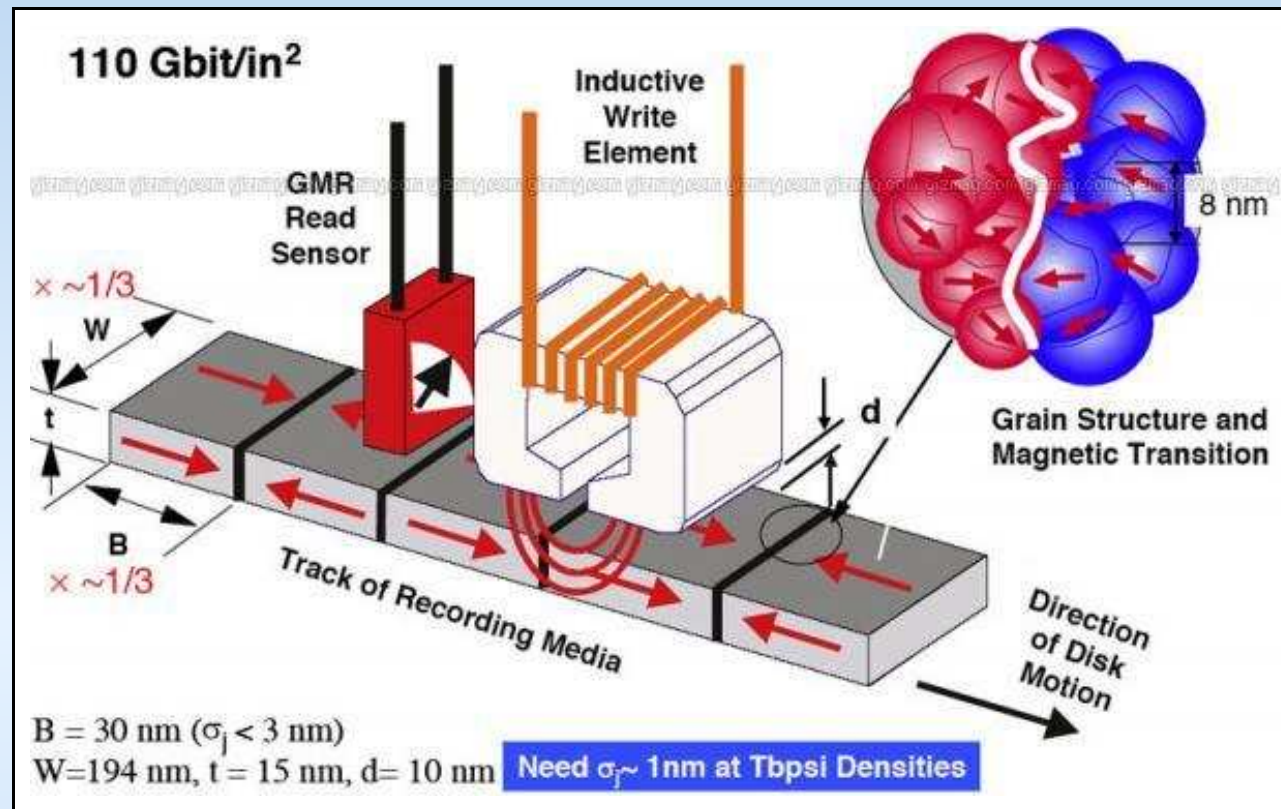
- *T. Ostler, J. Barker, R. Evans, R. W. Chantrell*, University of York, UK
- *U. Atxitia, O. Chubykalo-Fesenko*, CSIC, Madrid, Spain
- *K. Vahaplar, A. Kalashnikova, A. Kimel, A. Kirilyuk, Th. Rasing*, Radboud University Nijmegen, Netherlands

Information storage

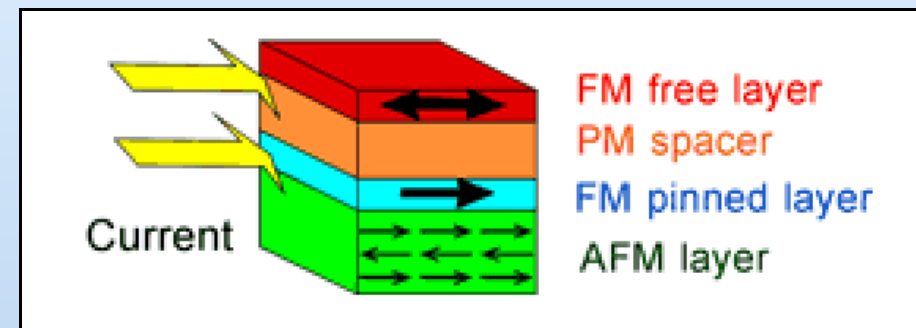
- information storage is a key technology in the modern world
- important criteria for hi-tech storage devices are storage density, speed, stability, and price
- leading storage device is hard disc: 2005 storage density is 245 GBit/in² demonstration in Seagate labs



Hard discs: a nano-technology

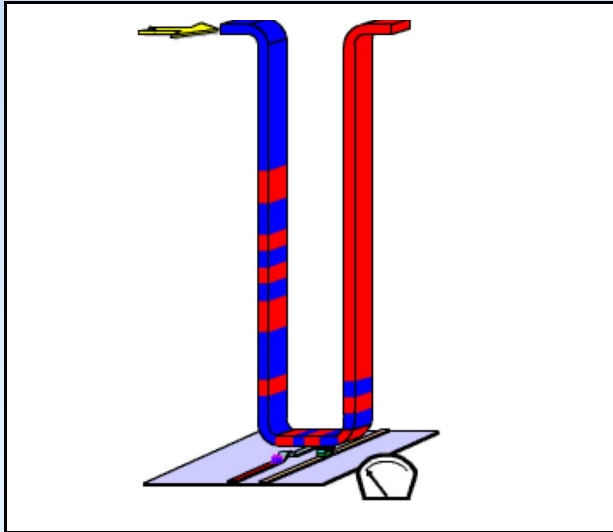


- bit dimension: $\ll 30 \times 200 \text{ nm}$
- read/write head flies $< 10 \text{ nm}$ high
- data rate $> 1 \text{ Gbit/sec}$
- time scale of writing procedure $< 1 \text{ ns}$



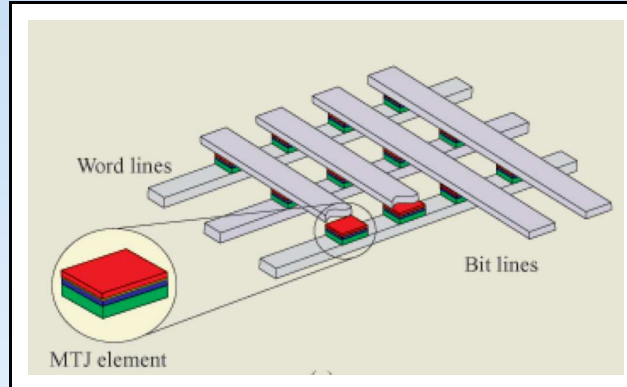
Ideas for future storage devices

Racetrack memory



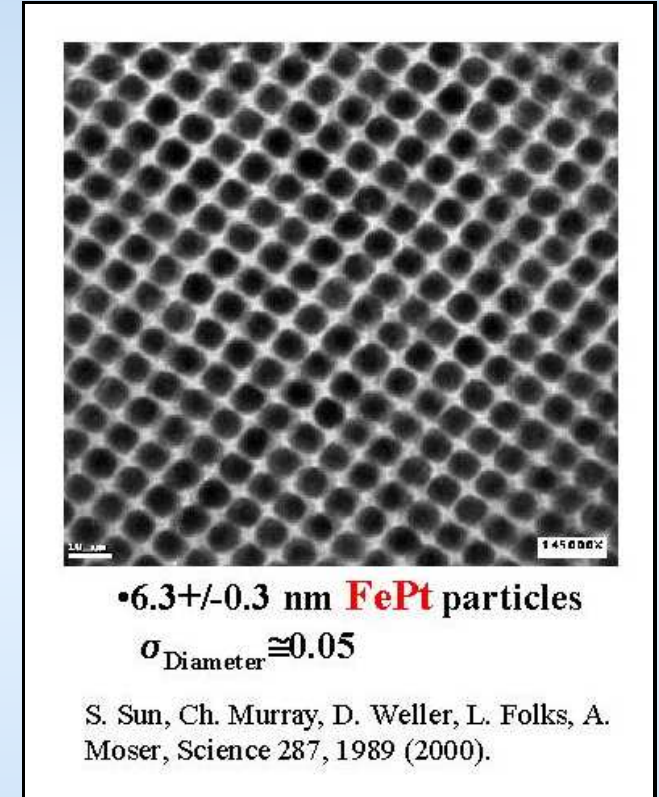
- information stored in domain walls
- domain wall pattern is moved with a current (spin torque effect)

(TA-) MRAM



- information stored in array of magnetic tunnel junctions
- some concepts involve spin torque switching and thermal activation

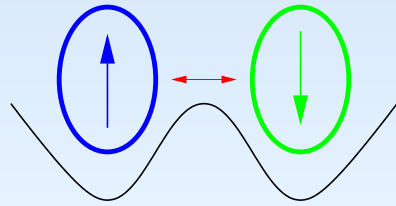
Bit patterned media



- improved hard disc
- information stored in single magnetic nanoparticles

Magnetic data storage: ultimate limits

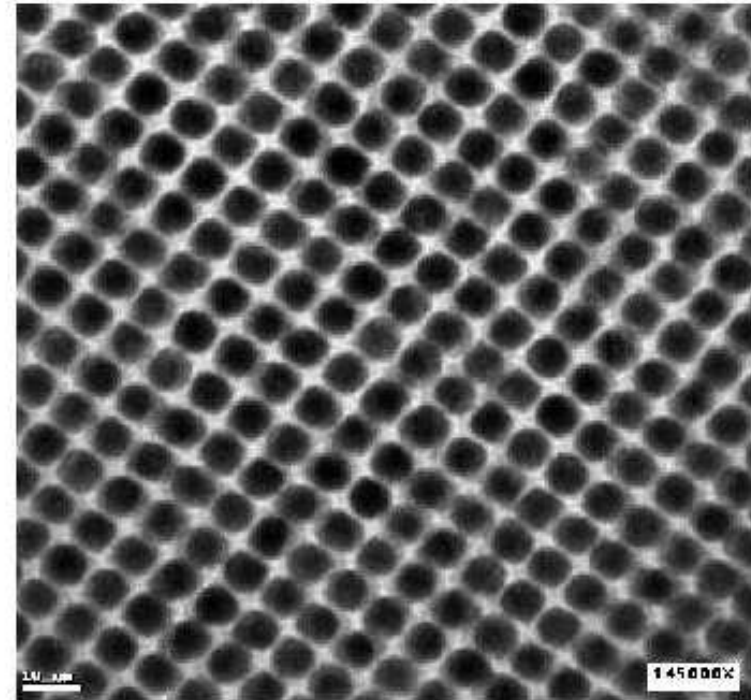
- idea: self-organised magnetic array of nanoparticles as storage media
- problems:
 - super-paramagnetic limit:



$$\Delta E \approx K_1 V$$

small volume $V \rightarrow$ need materials with high anisotropy constant K_1

- large $K_1 \rightarrow$ coercivity is also large (e. g. $\approx 18\text{T}$ for FePt)



• 6.3 ± 0.3 nm **FePt** particles

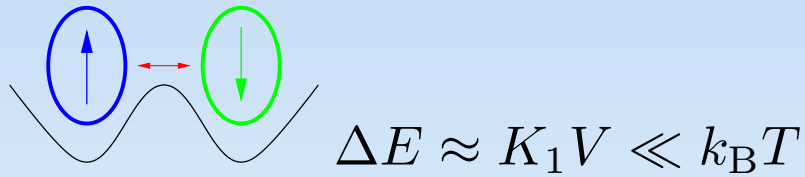
$$\sigma_{\text{Diameter}} \cong 0.05$$

S. Sun, Ch. Murray, D. Weller, L. Folks, A. Moser, *Science* 287, 1989 (2000).



Heat assisted magnetic recording

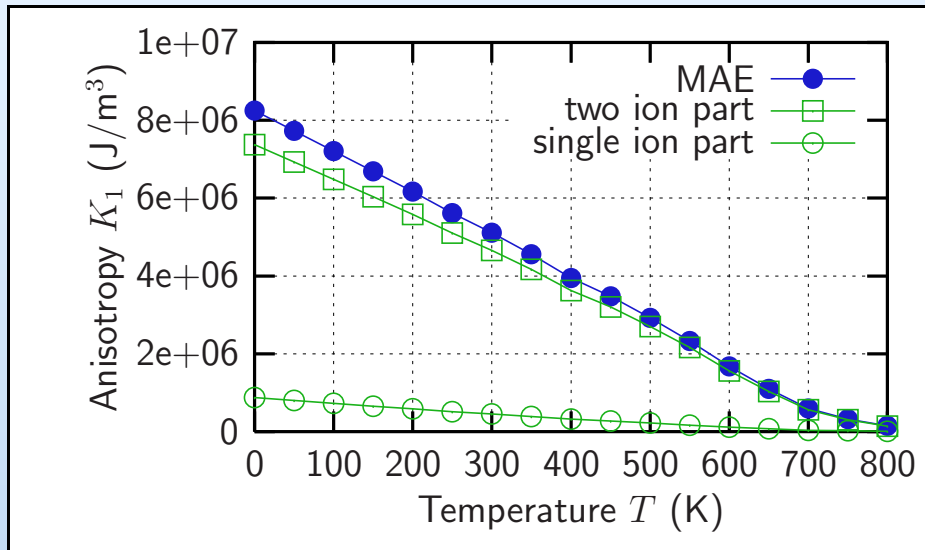
- super-paramagnetic limit:



for nanoparticles in the nanometre regime:

- ⇒ materials with high anisotropy constant K_1
- ⇒ coercivity is also large (e. g. $\approx 18\text{T}$ for FePt)

- HAMR:



(Mryasov et al., *Europhys. Lett.* **69**, 805 (2005))

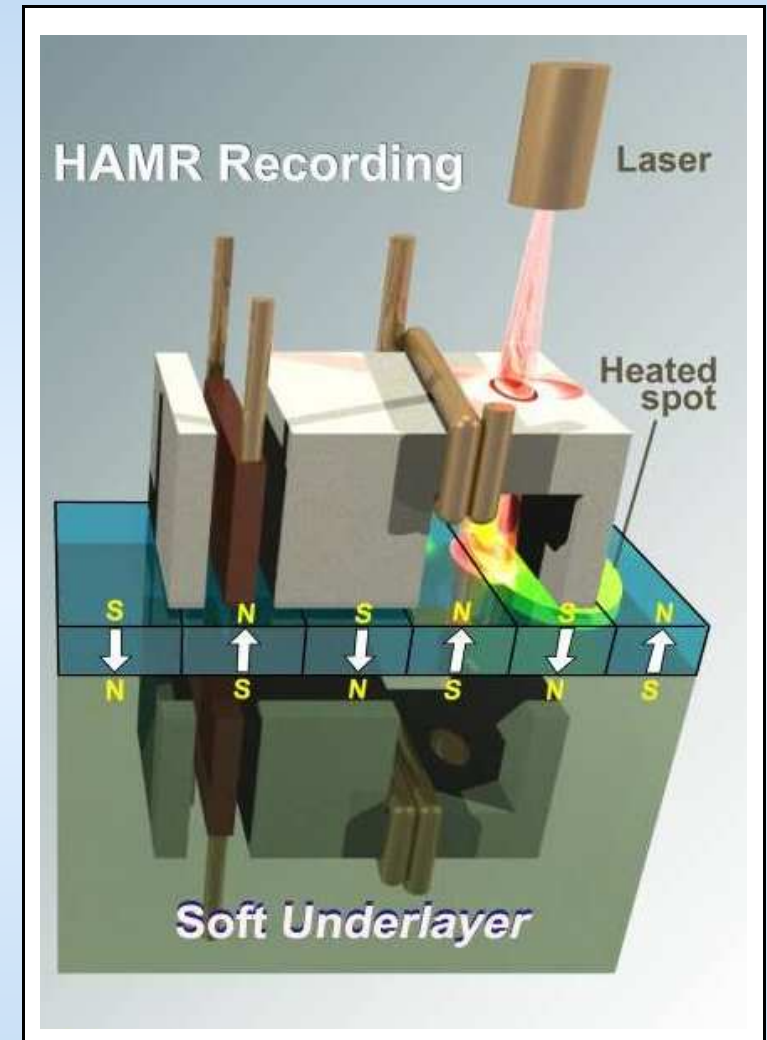
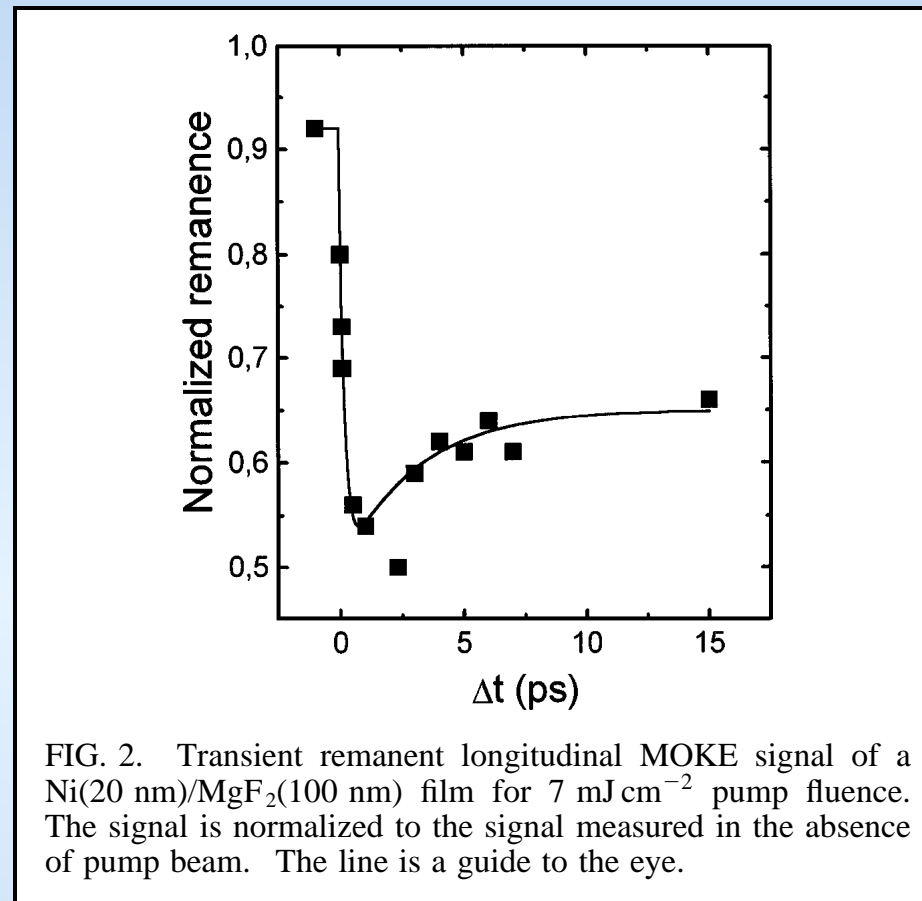


image by Mark Lutwyche, Seagate

Pump probe experiments and HAMR



- magnetisation can break down and recover on ps time scale

(Beaurepaire, Merle, Daunois, Bigot, *Phys. Rev. Lett.* **76**, 4250 (1996))

- ⇒ search for new heat-assisted magnetic recording schemes

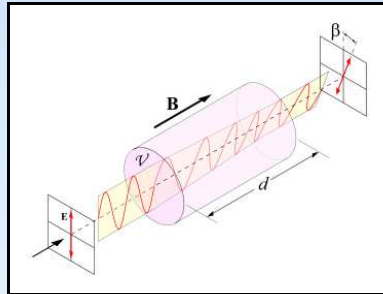
Opto-magnetic writing

- writing information without applying an external magnetic field

- uses circularly polarised light

- field pulse due to inverse Faraday effect:

$$\mathbf{B} \sim \mathbf{E} \times \mathbf{E}^*$$



(http://en.wikipedia.org/wiki/Faraday_effect)

- time scale: some picoseconds
- writing procedure with combined field and temperature pulse

(*Kimel et al. Phys. Rev. Lett.* **99**, 047601 (2007),

Nature **435**, 655 (2005))

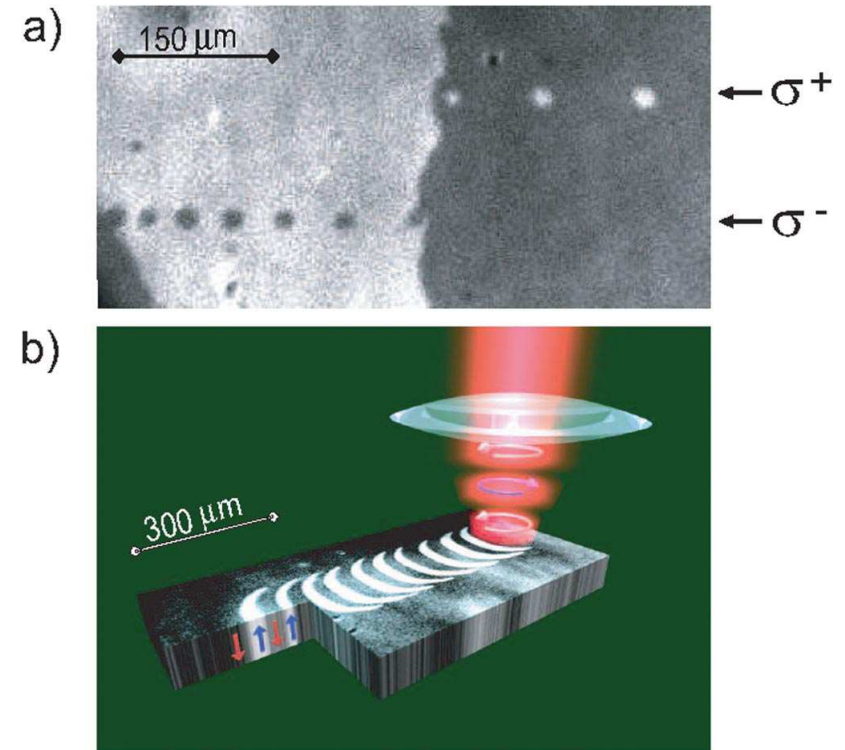


FIG. 4 (color). All-optical magnetic recording by femtosecond laser pulses. (a) The effect of single 40-fs circular polarized laser pulses on the magnetic domains in $\text{Gd}_{22}\text{Fe}_{74.6}\text{Co}_{3.4}$. The domain pattern was obtained by sweeping at high-speed (~ 50 mm/s) circularly polarized beams across the surface so that every single laser pulse landed at a different spot. The laser fluence was about 2.9 mJ/cm². The small size variation of the written domains is caused by the pulse-to-pulse fluctuation of the laser intensity.

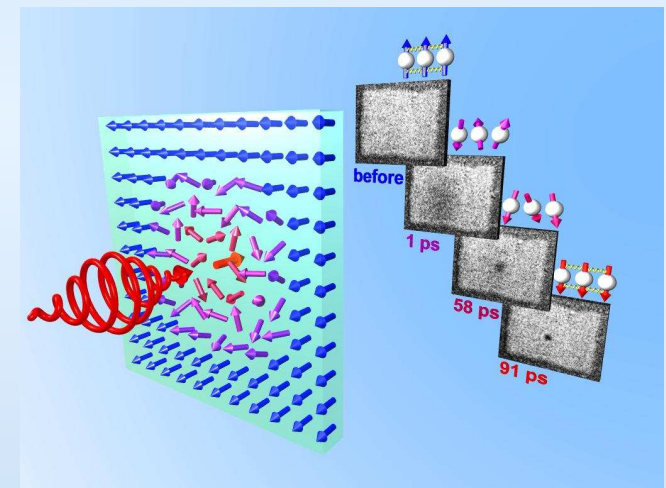
Modeling of light-induced reversal mechanisms

U. Nowak

Universität Konstanz, Germany

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(<http://www.ultramagnetron.org>)

Goals and concepts

- **goals:** understanding of spin structures and dynamics, involving
 - time scales from femtoseconds to years
 - length scales from electronic to sample size
 - temperatures from zero up to the Curie temperature
- **concepts:** multi-scale modelling

electronic structure:

- e.g. SDFT theory
- periodic structures, layers or small clusters
- ☺ many material properties from first principles
- ☹ mainly ground state calculations



atomic spin model:

- e.g. stochastic Landau - Lifshitz equation, Monte Carlo methods
- up to 10^7 spins
- ☺ finite temperatures, dynamic properties
- ☹ some phenomenological modelling needed



continuum theory:





- Landau-Lifshitz-Bloch equation of motion
- up to some μm^3
- ☺ non-equilibrium thermodynamics for realistic sample size
- ☹ more phenomenological modelling needed



Atomic spin model

- model of localised spins $\underline{S}_i = \underline{\mu}_i / \mu_s$ on a given lattice

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \underline{S}_i \cdot \underline{S}_j - d_z \sum_i (S_i^z)^2 - \mu_s \underline{B} \cdot \sum_i \underline{S}_i - w \sum_{i < j} \frac{3(\underline{S}_i \cdot \underline{e}_{ij})(\underline{e}_{ij} \cdot \underline{S}_j) - \underline{S}_i \cdot \underline{S}_j}{r_{ij}^3}$$

exchange  anisotropy  external field  magneto-static 

- parameters (Heisenberg exchange, anisotropy constants, atomic magnetic moment):

- phenomenological: fit experimental values
- derived from first principles

(Mryasov et al., *Europhys. Lett.* **69**, 805 (2005))

(Szunyogh et al., *Phys. Rev. B* **79**, 020403(R) (2009))

- dipolar interaction with $w = \mu_0 \mu_s^2 / 4\pi$ leads to:





- shape anisotropy
- non-trivial domain configurations
- large numerical effort



Atomic spin model

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exchange  anisotropy  external field  magneto-static 

- aims:

- ground states → energy minimisation
- zero temperature dynamics → Landau-Lifshitz-Gilbert equation of motion
- equilibrium thermodynamics → Monte Carlo, mean-field, spin wave theory, random phase approximation, Langevin dynamics

☞ non-equilibrium thermodynamics →

- Langevin dynamics

(Brown, *Phys. Rev.* **130**, 1677 (1963))

- time-quantified Monte Carlo

(Nowak et al. *Phys. Rev. Lett.* **84**, 163 (2000))



Stochastic Landau-Lifshitz-Gilbert equation

- Landau-Lifshitz-Gilbert equation with thermal noise:

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

precession



$$t_{\text{prec}} \approx 1/\gamma B$$

$$- \frac{\alpha\gamma}{(1+\alpha^2)\mu_s} \underline{S}_i \times (\underline{S}_i \times \underline{H}_i(t))$$

relaxation



$$t_{\text{relax}} \approx t_{\text{prec}}/\alpha$$

with $\underline{H}_i(t) = -\frac{\partial \mathcal{H}}{\partial \underline{S}_i} + \underline{\zeta}_i(t)$

fluctuations



and $\langle \underline{\zeta}_i(t) \rangle = 0$, $\langle \zeta_{i\eta}(0) \zeta_{j\theta}(t) \rangle = \delta_{ij} \delta_{\eta\theta} \delta(t) 2\alpha k_B T \mu_s / \gamma$.

α : describes coupling to the heat bath (\rightarrow damping constant)

- minimal time scales:

- for the demagnetisation

$$\tau_{\text{dis}} \approx \frac{\mu_s}{2\alpha\gamma k_B T} \approx 300\text{fs}$$

- for the reordering process

$$\tau_{\text{re}} \approx \frac{\mu_s}{\alpha\gamma J} \approx 1\text{ps}$$



Stochastic Landau-Lifshitz-Gilbert equation

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- Langevin dynamics simulation:

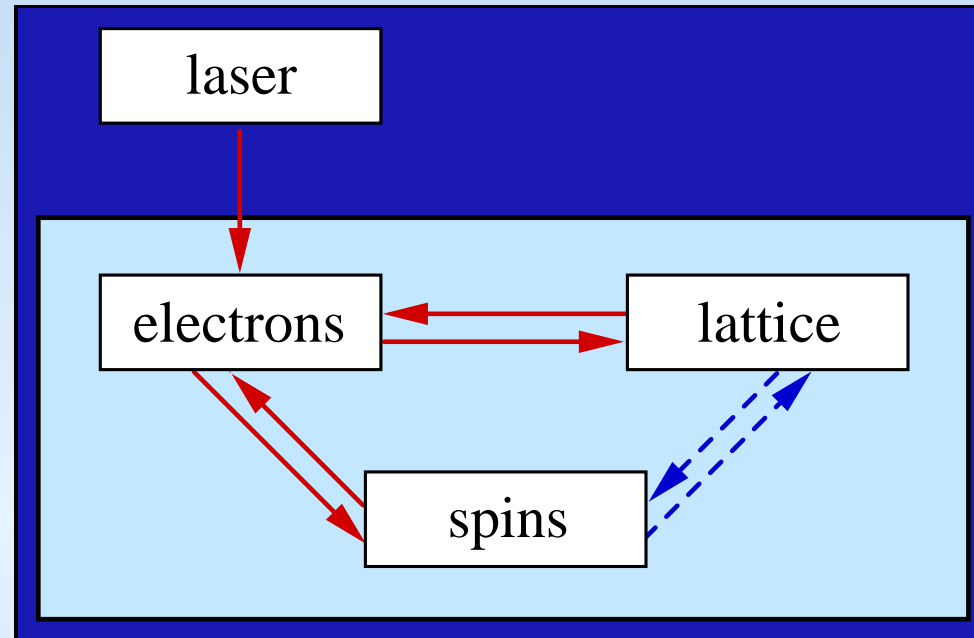
numerical integration of the LLG equation

(see e. g. Nowak, *Ann. Rev. of Comp. Phys.* **9**, 105 (2001))

- Heun-method \Rightarrow Stratonovich integral
- simulation of 10^7 spins possible with FFT methods
($\approx 40\text{nm}$)³



Simulating the magnetic response to the heat pulse



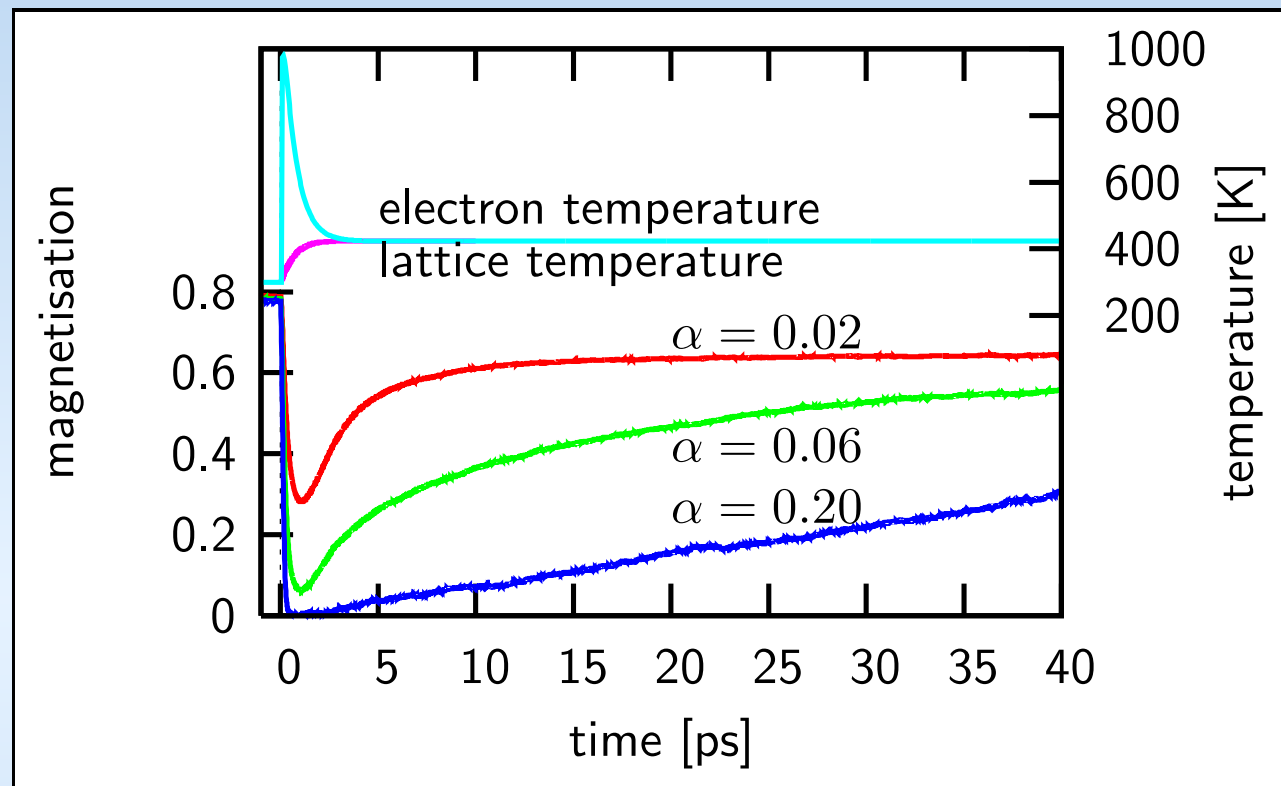
- two temperature model: *(Kaganov, Lifshitz, Tanatarov, Sov. Phys. JETP 4, 173 (1957))*

$$\text{electrons: } C_e \frac{dT_e}{dt} = -G_{el}(T_e - T_l) + P(t)$$

$$\text{lattice: } C_l \frac{dT_l}{dt} = G_{el}(T_e - T_l)$$

- perform thermodynamic spin model simulations with $T_e(t)$ as temperature of the heat bath

Magnetisation dynamics for different α



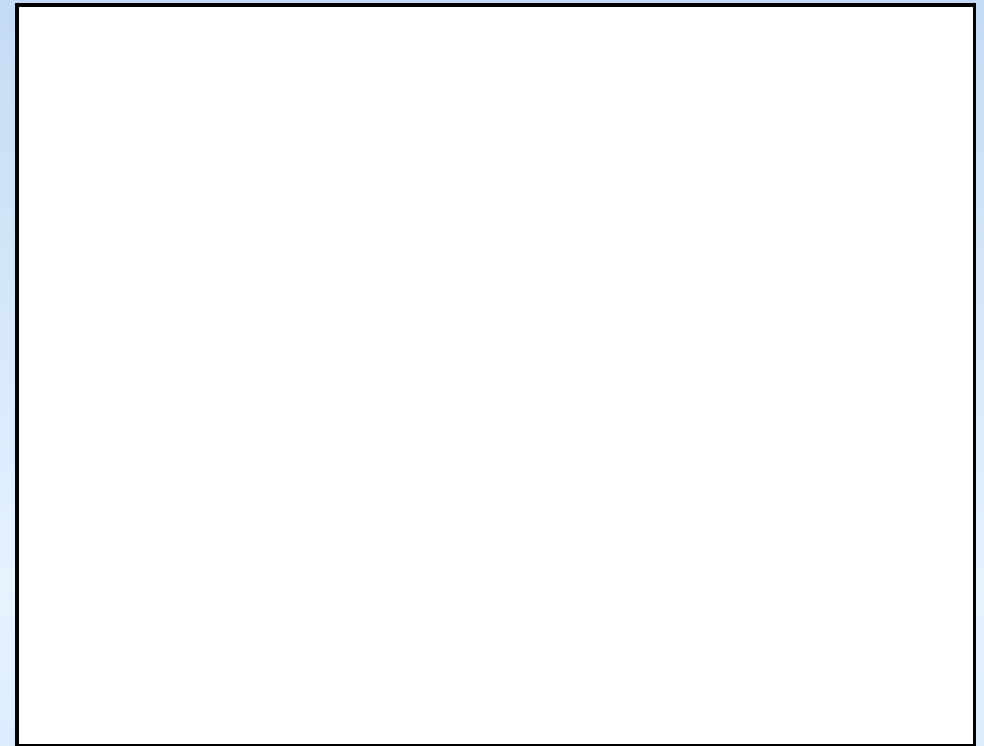
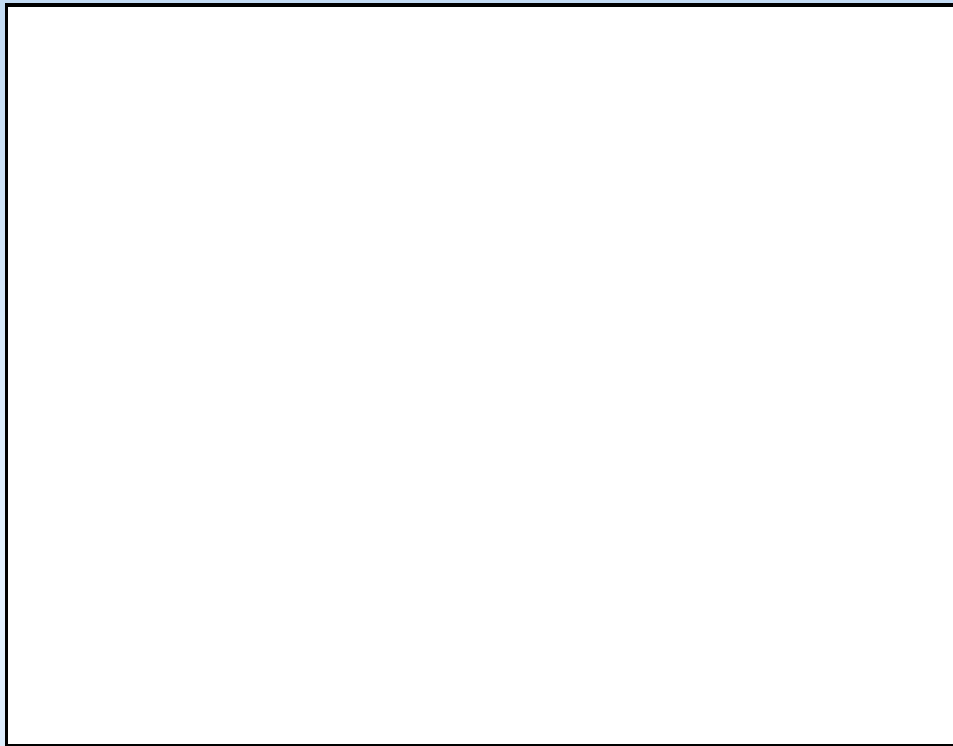
(Kazantseva et al., *Europhys. Lett.* **90**, 247201 (2003))

- electron (and lattice) temperature from two-temperature model, material parameters for Ni, realistic assumptions for laser power and duration

(Rieh, Dürr, Eberhardt, *Phys. Rev. Lett.* **81**, 27004 (2008))

- Langevin dynamics simulations for model with 80^3 spins and periodic boundary conditions

Magnetic states after 19ps



- $\alpha = 0.02$: faster recovery due to non-zero initial magnetisation

- $\alpha = 0.2$: slow recovery due to zero initial magnetisation

Micromagnetic continuum theory

- description on a length scale \gg lattice constant a :

magnetisation assumed as smooth vector field $\underline{S}(\underline{r})$ with constant length

$$E = \frac{J}{2a} \int_V (\nabla \underline{S})^2 dV - \frac{d_z}{a^3} \int_V S_z^2 dV - M_s \int_V \underline{S} \cdot \underline{B} dV - \frac{\mu_0}{2} \int_V \underline{S} \cdot \underline{H}_s dV$$

exchange

anisotropy

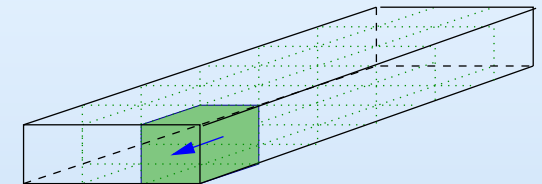
external field

magneto-static

- Landau-Lifshitz-Gilbert equation is standard equation of motion
- for a micromagnetic theory at elevated temperatures:

☹ LLG equation with Langevin dynamics will fail:

thermally excited spin wave spectrum is limited by cell size



☺ alternative approach must include thermodynamics of the cell (macro-spin) itself

⇒ Landau-Lifshitz-Bloch equation

(Garanin, *Phys. Rev. B* **55**, 3050 (1997))

(Garanin and Chubykalo-Fesenko, *Phys. Rev. B* **70**, 212409 (2004))

Magnetisation relaxation close to Curie temperature

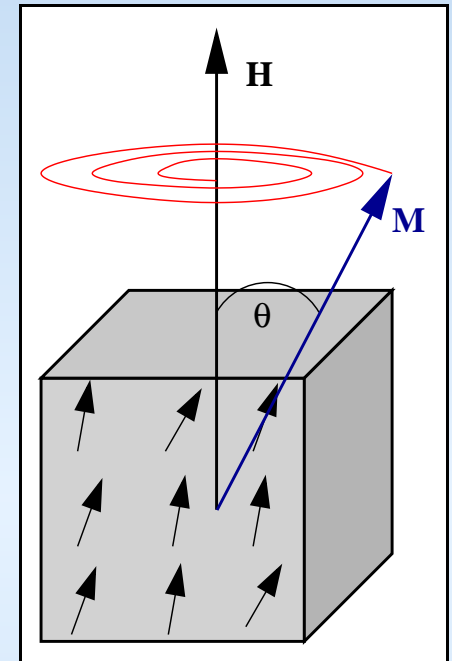
Consider relaxation of magnetisation which is initially tilted by an angle θ with respect to an external field

- at zero temperature:

$$m_x(t) = m_0 e^{-t/\tau_{\perp}} \cos(t/\tau_p)$$

with transverse relaxation time $\tau_{\perp} = 1/\alpha\gamma H$

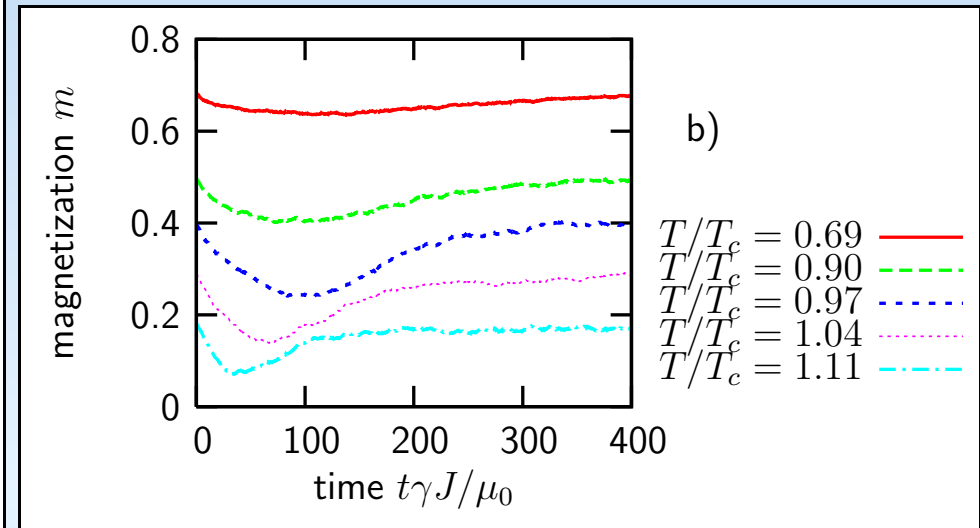
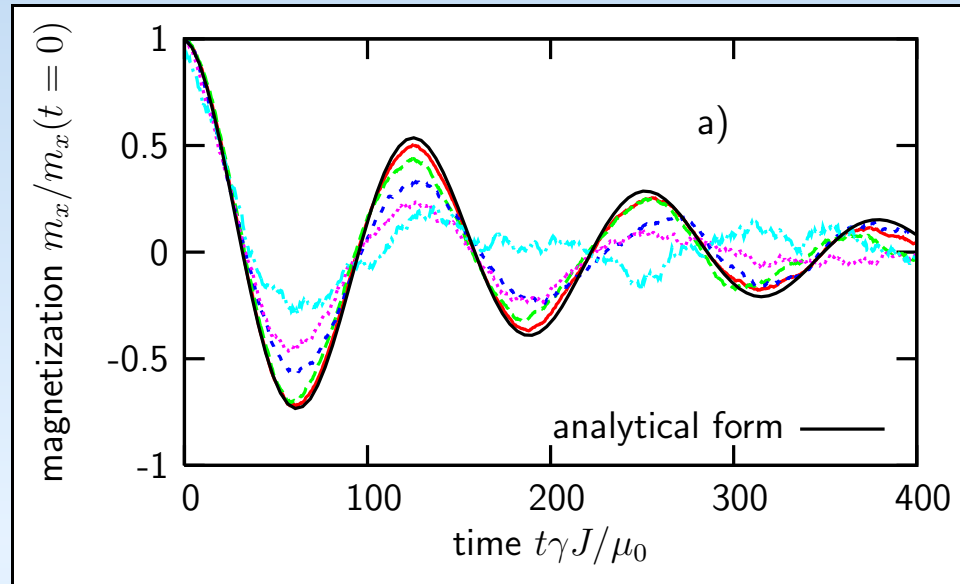
- for finite temperature:
 - simulation of spin model (48^3 spins) with LLG equation
 - simulation of single macro-spin with LLB equation



Simulation of spin model with LLG equation

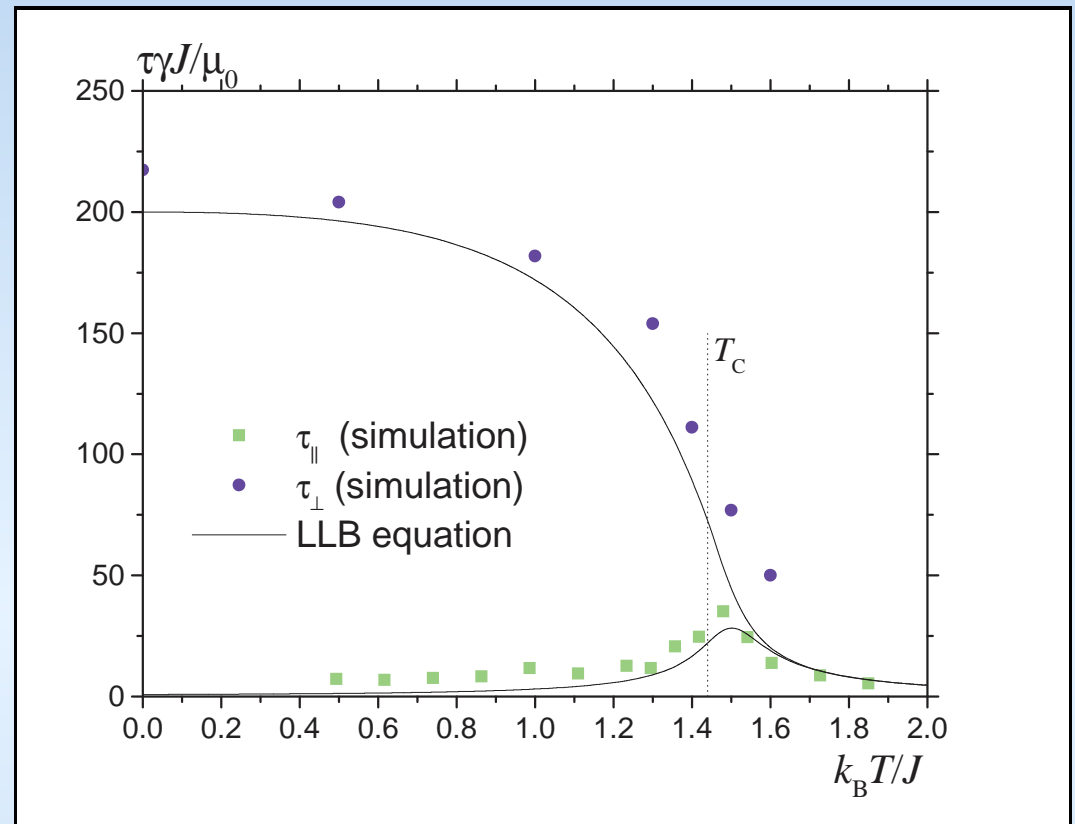
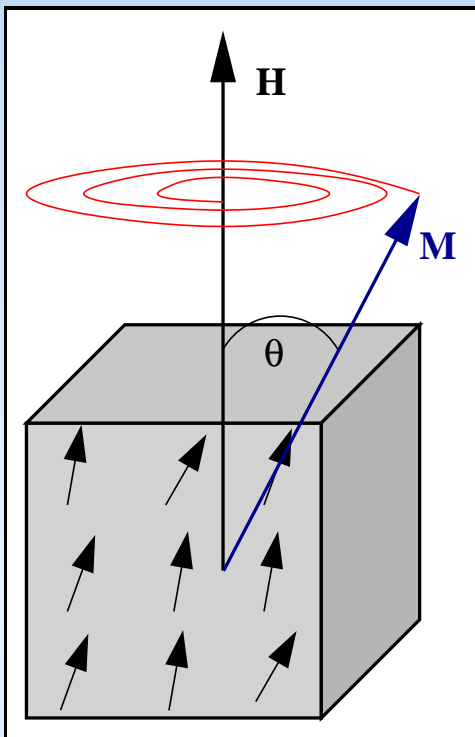
$\theta = 30^\circ$

$\theta = 135^\circ$



- $\theta = 30^\circ$: transverse relaxation faster approaching $T_c \rightarrow \tau_\perp$ decreases
- $\theta = 135^\circ$: magnetisation shows dip during reversal

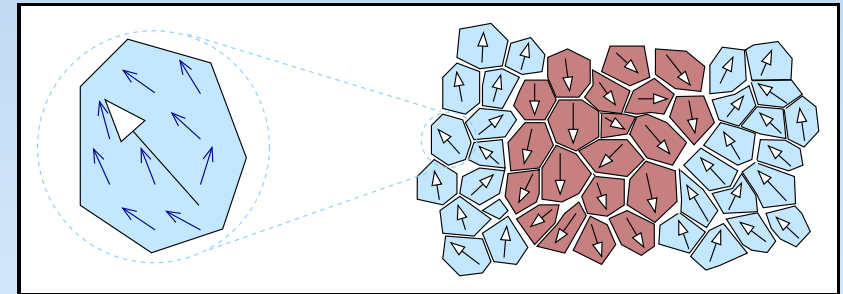
Longitudinal and transverse relaxation time



- longitudinal relaxation time shows critical slowing down
- transverse relaxation time breaks down close to Curie temperature
- magnitude of magnetisation not constant in time (and space)
- ☺ all these effects well described by LLB equation

Landau-Lifshitz-Bloch equation of motion

- atomistic simulations only possible up to $(20\text{nm})^3$ system size; for larger samples macro-spin models are necessary



- new, alternative approach is **Landau-Lifshitz Bloch equation** for the macroscopic thermodynamic magnetisation $\underline{m} = \langle \underline{S} \rangle$:

(Garanin, PRB 55, 3050 (1997)), Garanin and Chubykalo-Fesenko, PRB 70, 212409 (2004)

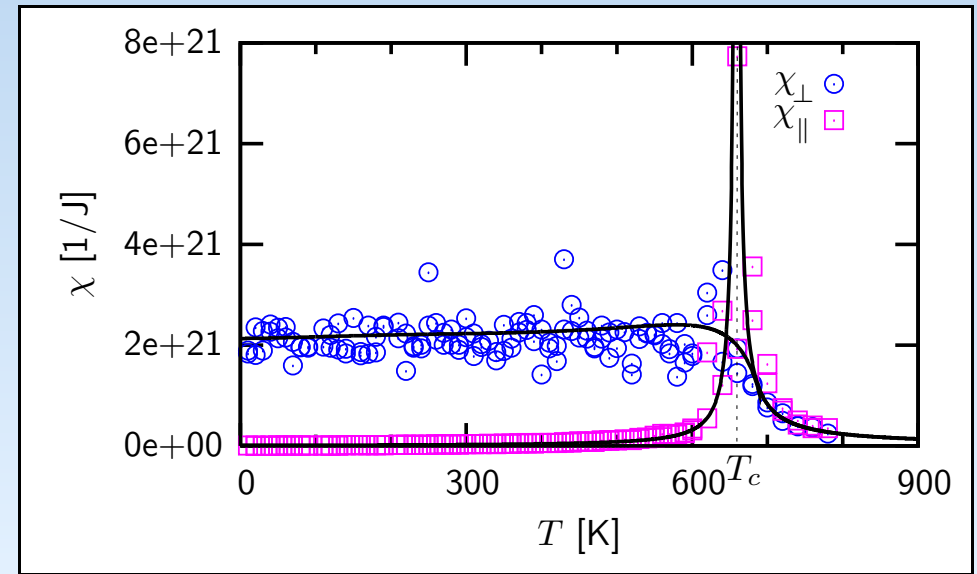
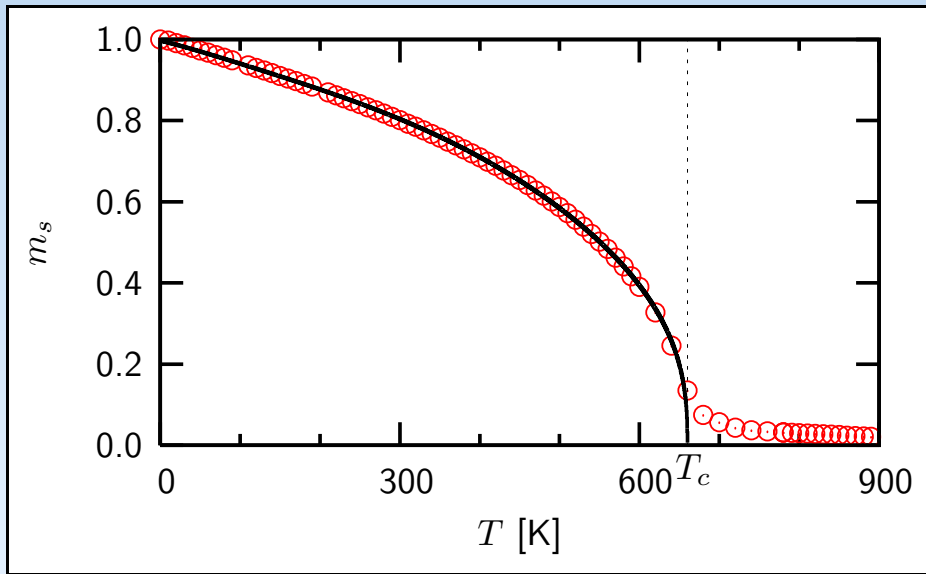
$$\dot{\mathbf{m}}_i = -\gamma \mathbf{m}_i \times \mathbf{H}_{\text{eff}}^i + \frac{\gamma \alpha_{\parallel}}{m_i^2} \left(\mathbf{m}_i \cdot (\mathbf{H}_{\text{eff}}^i + \zeta_{\parallel}^i) \right) \mathbf{m}_i - \frac{\gamma \alpha_{\perp}}{m_i^2} \mathbf{m}_i \times \left(\mathbf{m}_i \times (\mathbf{H}_{\text{eff}}^i + \zeta_{\perp}^i) \right)$$

$$\alpha_{\parallel} = \frac{2\lambda T}{3T_c} \text{ and } \alpha_{\perp} = \lambda \left(1 - \frac{T}{3T_c} \right) \text{ for } T < T_c \text{ and } \alpha_{\perp} = \alpha_{\parallel} \text{ for } T \geq T_c$$

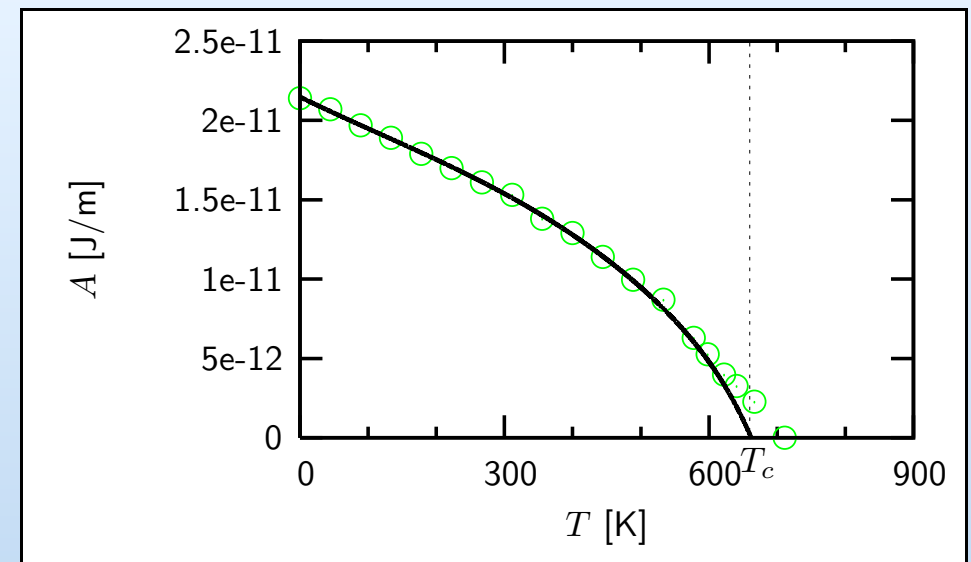
$$\mathbf{H}_{\text{eff}}^i = \mathbf{H} - \frac{m_x^i \mathbf{e}_x + m_y^i \mathbf{e}_y}{\tilde{\chi}_{\perp}} - \frac{2A(T)}{m_e^2 M_s^0 \Delta^2} \sum_j (\mathbf{m}_j - \mathbf{m}_i) - \begin{cases} -\frac{1}{2\tilde{\chi}_{\parallel}} \left(1 - \frac{m_i^2}{m_e^2} \right) \mathbf{m}_i & T \leq T_c \\ \frac{1}{\tilde{\chi}_{\parallel}} \left(1 - \frac{3T_c m_i^2}{5(T - T_c)} \right) \mathbf{m}_i & T \geq T_c \end{cases}$$

- one needs $m_e(T)$, $A(T)$, $\tilde{\chi}_{\perp}(T)$, $\tilde{\chi}_{\parallel}(T)$

Equilibrium properties for LLB approach

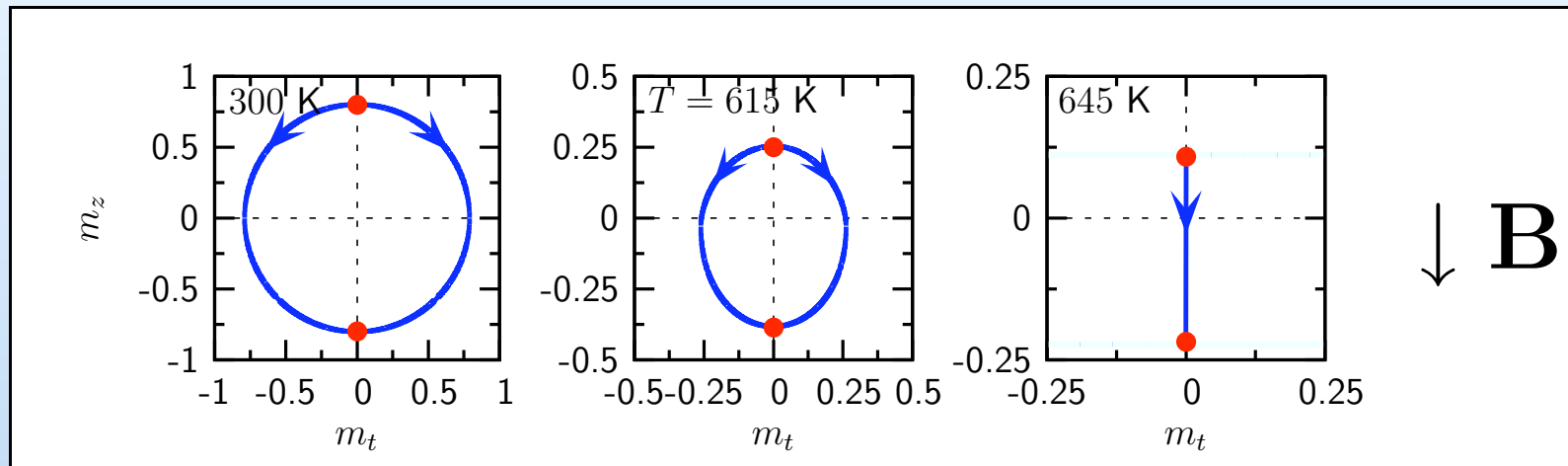
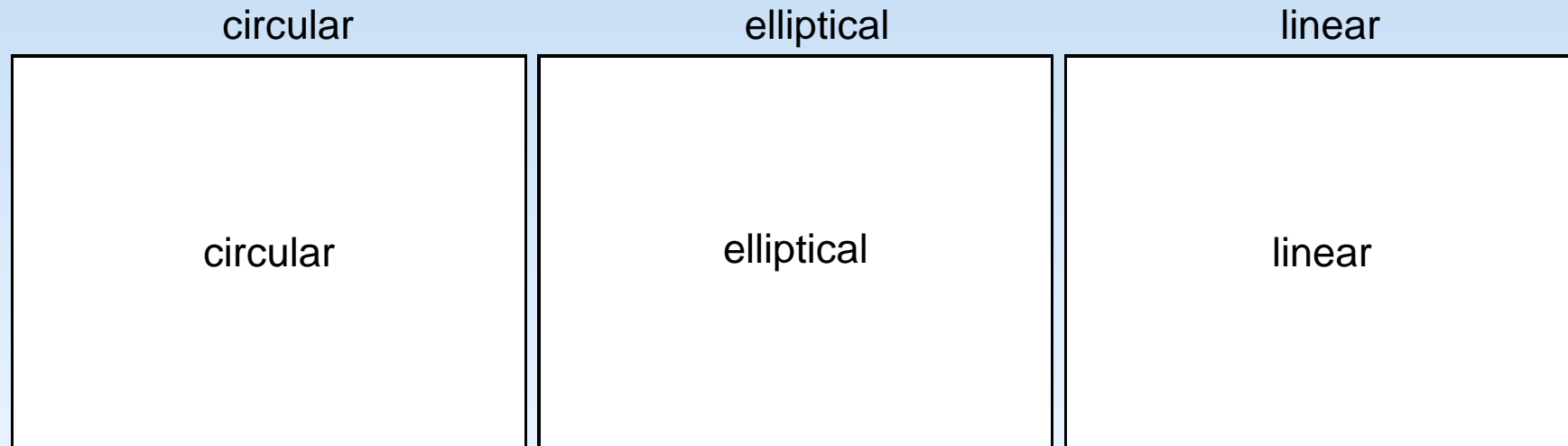


- zero field magnetisation $m_s(T)$
- susceptibilities $\chi_{\parallel}(T)$ and $\chi_{\perp}(T)$
- exchange stiffness $A(T)$
- here from Langevin dynamics simulations of the FePt model
- alternatively from other methods (MFA, MC, RPA) or from experiment



Single LLB macro-spin: reversal paths

- different reversal paths possible, depending on temperature:



(Kazantseva et al., *Europhys. Lett.* **86**, 27006 (2009))

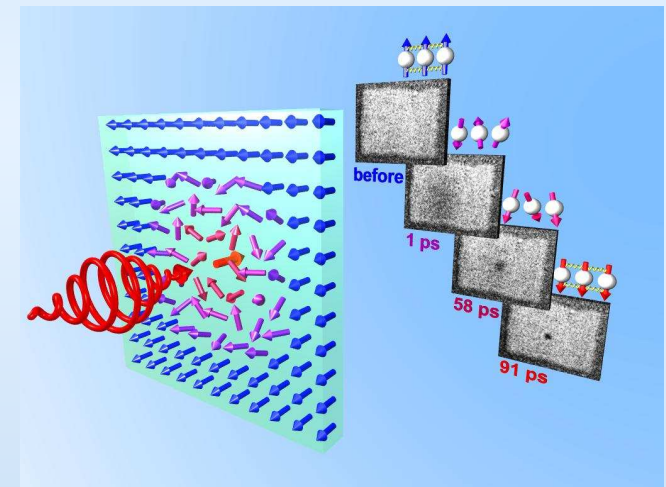
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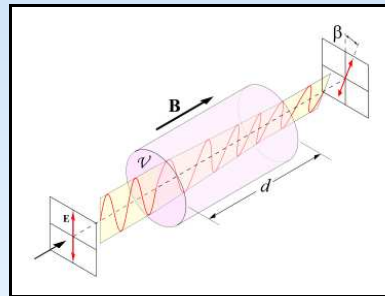
Opto-magnetic writing

- writing information without applying an external magnetic field

- uses circularly polarised light

- field pulse due to inverse Faraday effect:

$$\mathbf{B} \sim \mathbf{E} \times \mathbf{E}^*$$



(http://en.wikipedia.org/wiki/Faraday_effect)

- time scale: some picoseconds
- writing procedure with combined field and temperature pulse

(*Kimel et al. Phys. Rev. Lett.* **99**, 047601 (2007),

Nature **435**, 655 (2005))

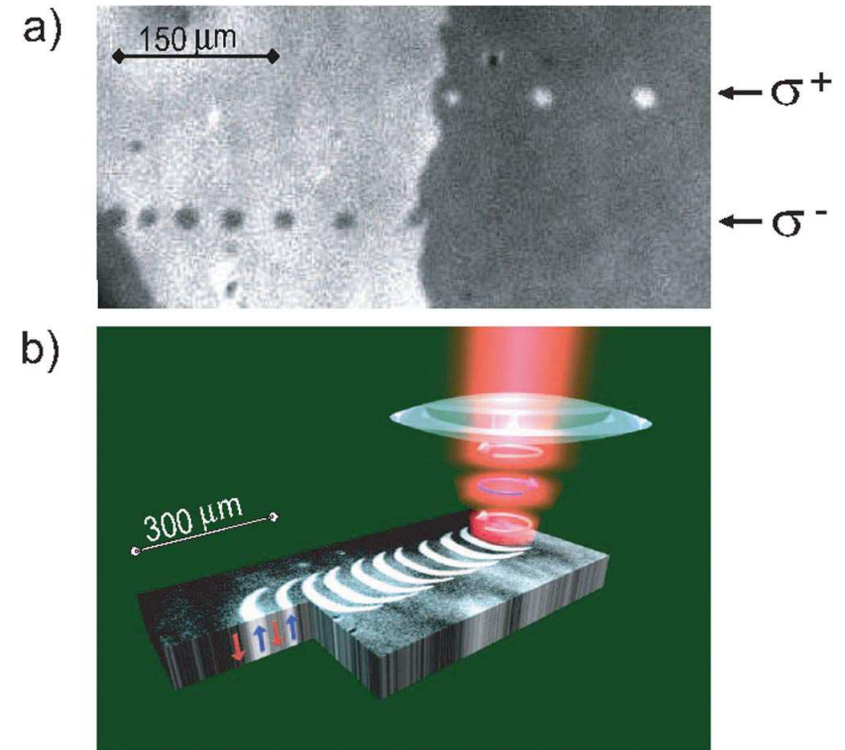
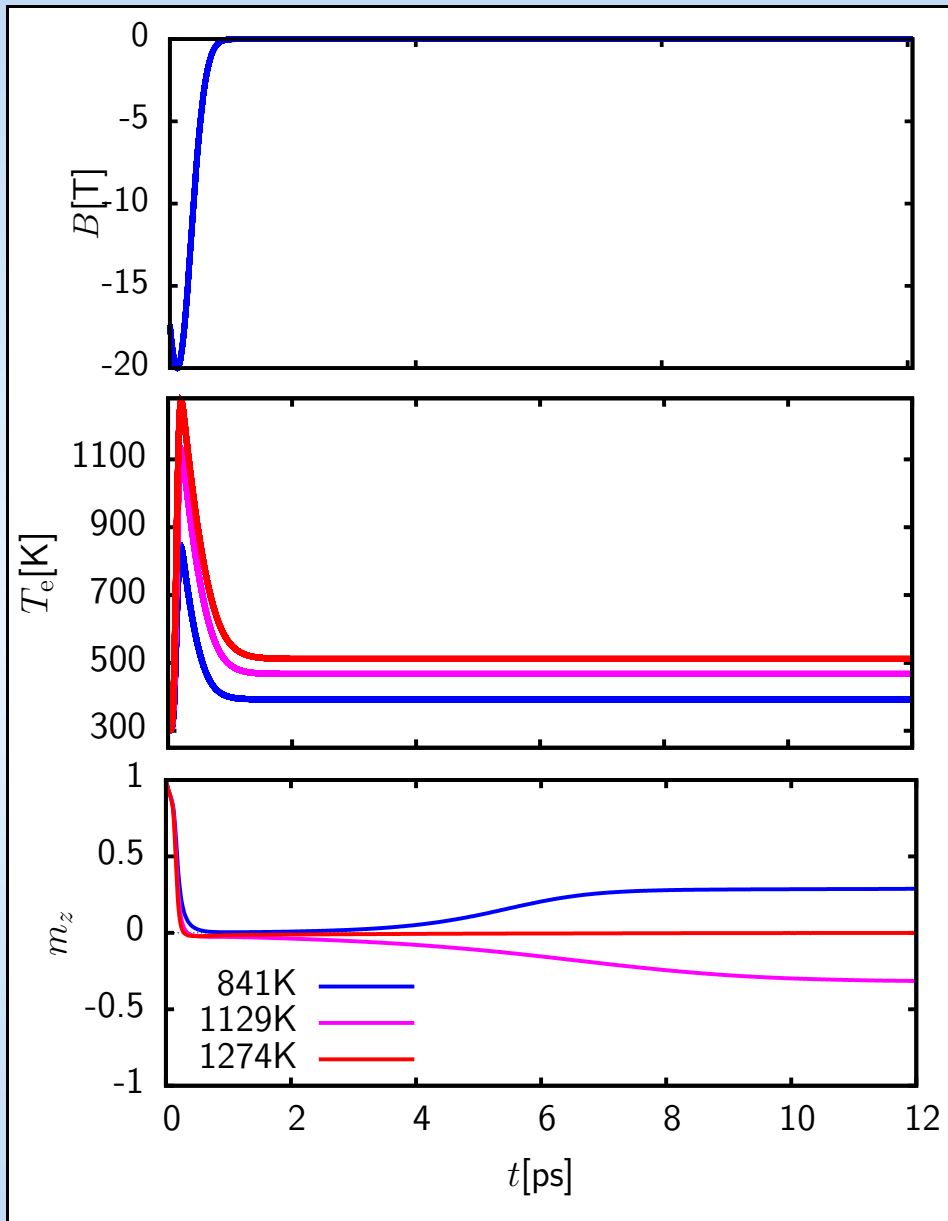


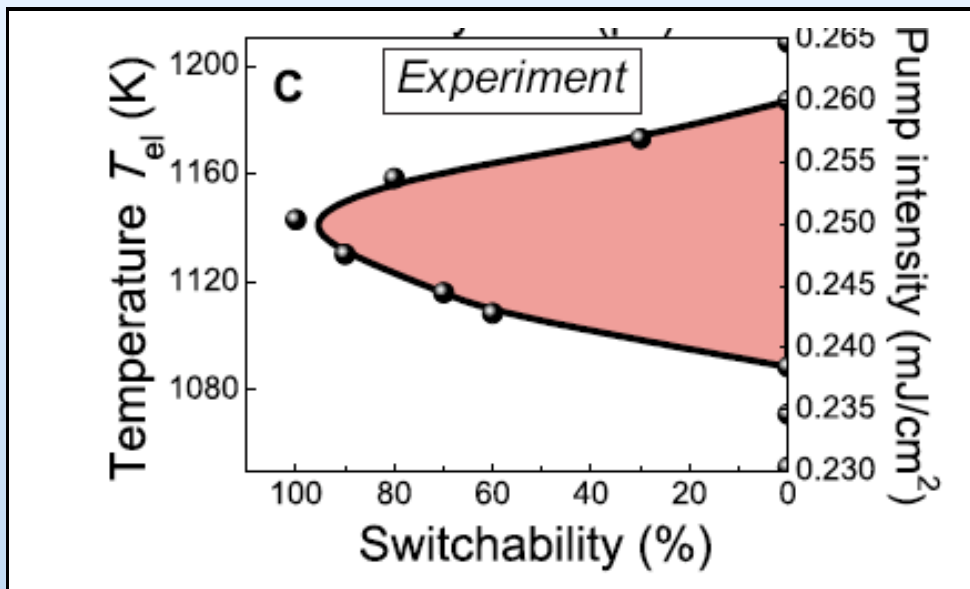
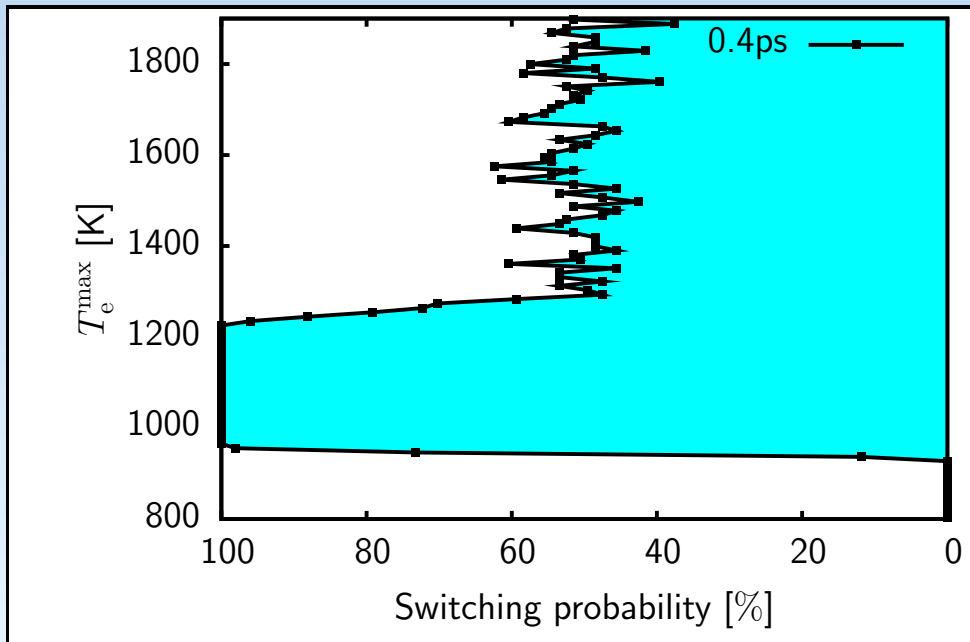
FIG. 4 (color). All-optical magnetic recording by femtosecond laser pulses. (a) The effect of single 40-fs circular polarized laser pulses on the magnetic domains in $\text{Gd}_{22}\text{Fe}_{74.6}\text{Co}_{3.4}$. The domain pattern was obtained by sweeping at high-speed (~ 50 mm/s) circularly polarized beams across the surface so that every single laser pulse landed at a different spot. The laser fluence was about 2.9 mJ/cm². The small size variation of the written domains is caused by the pulse-to-pulse fluctuation of the laser intensity.

Single LLB macro-spin: Opto-magnetic reversal



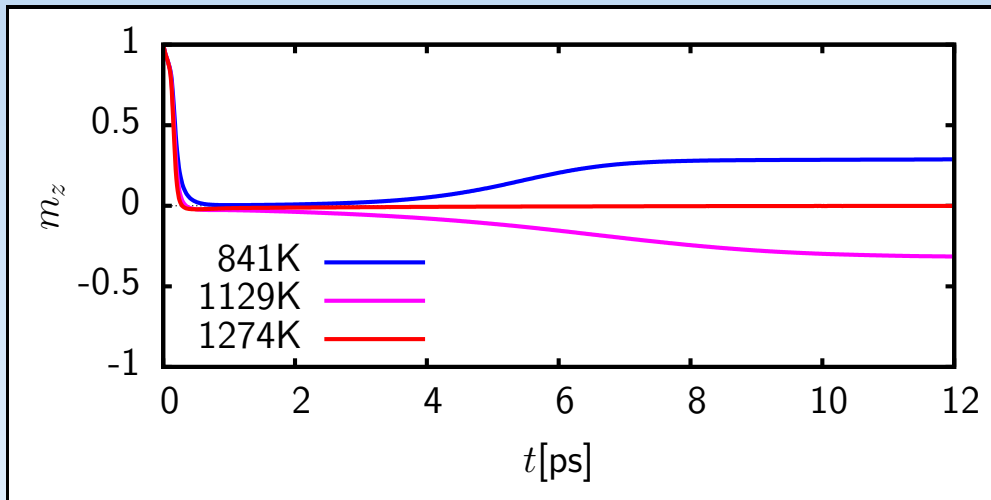
- magnetic field \mathbf{B} in z direction
 - $\mathbf{B} \sim \mathbf{E} \times \mathbf{E}^*$ (inverse Faraday effect)
 - $B_{\max} = 20$ T
 - field pulse duration time $\Delta t = 0.4$ ps
- electron temperature T_e
 - calculated from two-temperature model
- simulation parameters for GdFeCo:
 - $T_c = 500$ K, Anisotropy $K = 6.05 \times 10^5 \text{ Jm}^{-3}$
 - cell size $\Delta = 30$ nm
 - magnetization averaged over 100 simulation runs

Opto-magnetic reversal window



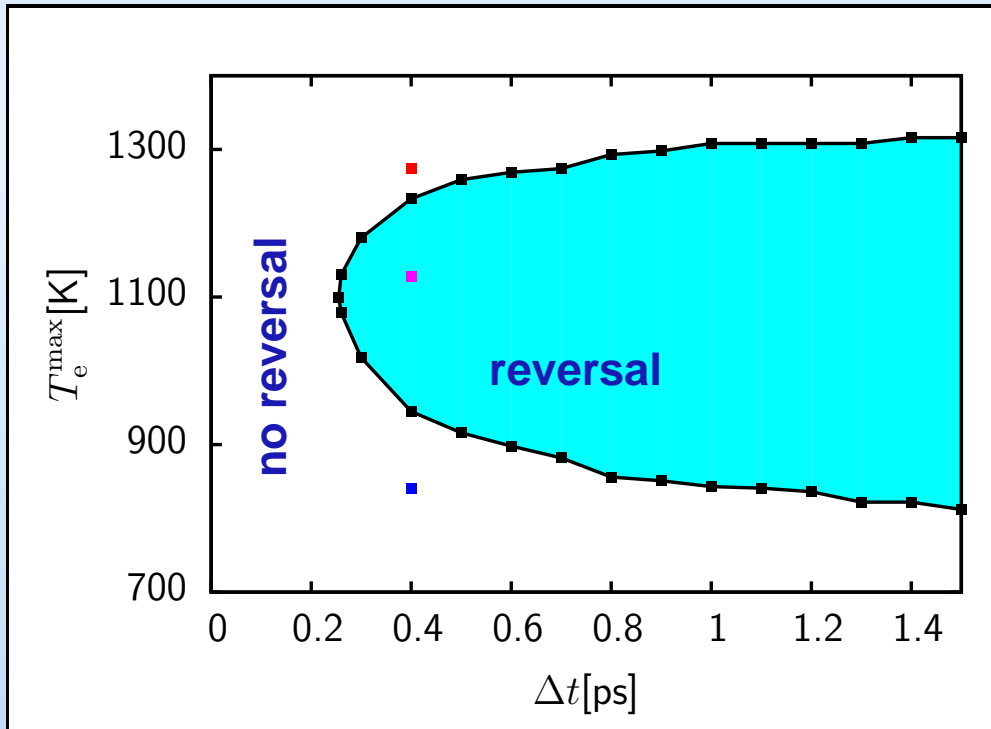
- "reversal window" found numerically as well as experimentally (*Vahaplar et al., Phys. Rev. Lett* **103**, 117201 (2009))
- opening of "reversal window" depends on the field pulse duration as well as the maximum electron temperature
- for high temperature pulses:
 - numerically: sample demagnetised
 - ▶ $P_{SW} = 50\%$
 - experimentally: sample reverts to initial state (independent of helicity)
 - ▶ $P_{SW} = 0\%$

Opto-magnetic reversal window

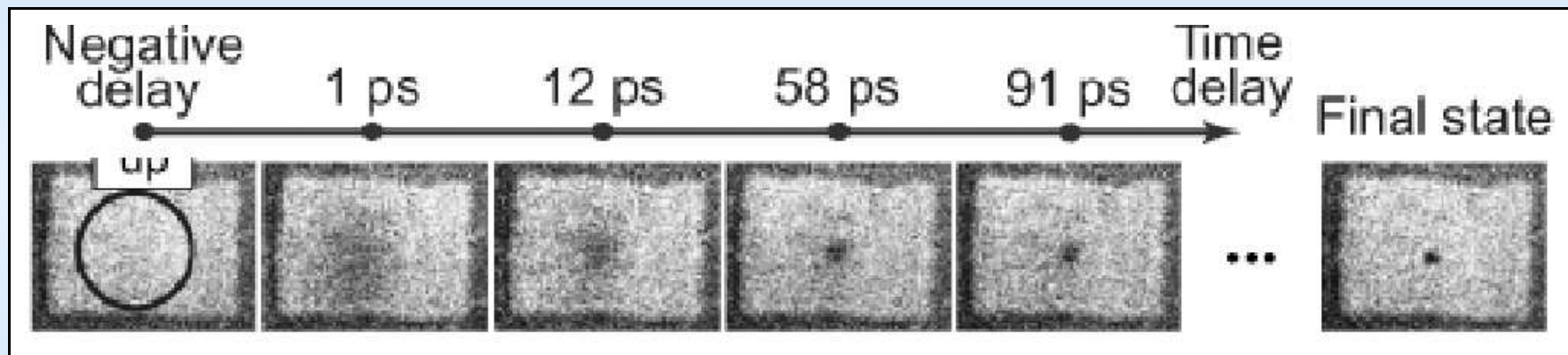
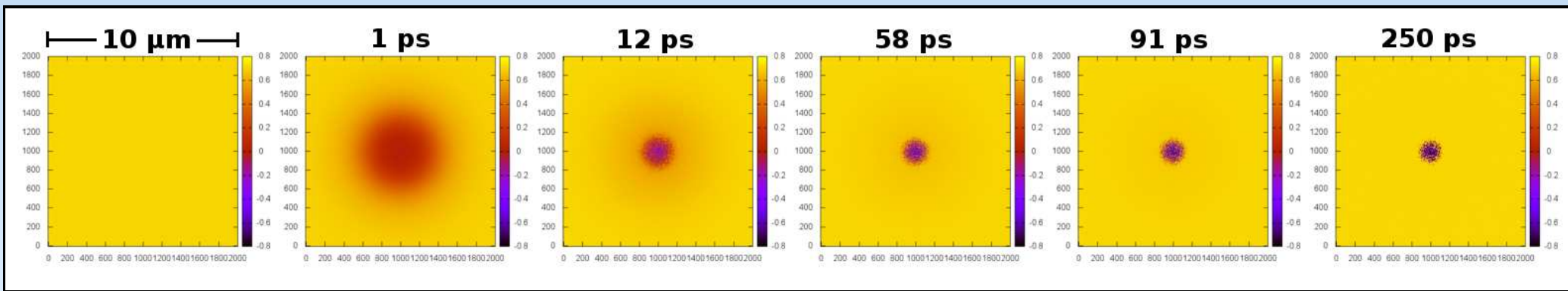


- ▶ T_e^{\max} **too low!**
- ▶ T_e^{\max} **too high!**
- ▶ T_e^{\max} ✓

- "reversal window" depending on peak electron temperature and length of field pulse
- window depends also on:
 - electron-phonon coupling
 - electron and phonon specific heats
 - material parameters of the spin model: damping constant, susceptibility and anisotropy
 - temperature



Opto-magnetic reversal in extended systems



(Vahaplar et al. *Phys. Rev. Lett.* **103**, 117201 (2007))

- simulation of an extended films of size $10 \times 10 \mu\text{m}^2$ possible including dipole-dipole interaction
- laser power assumed to have a gaussian shape

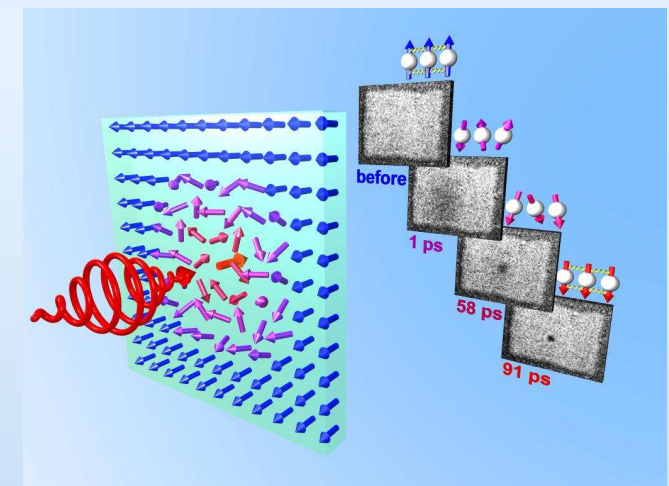
Modeling of light-induced reversal mechanisms

U. Nowak

Universität Konstanz, Germany

Topics:

- Motivation
- Theoretical framework for thermal spin dynamics
- Laser induced spin dynamics and opto-magnetic writing
- **Domain wall motion and spin Seebeck effect**
- Summary



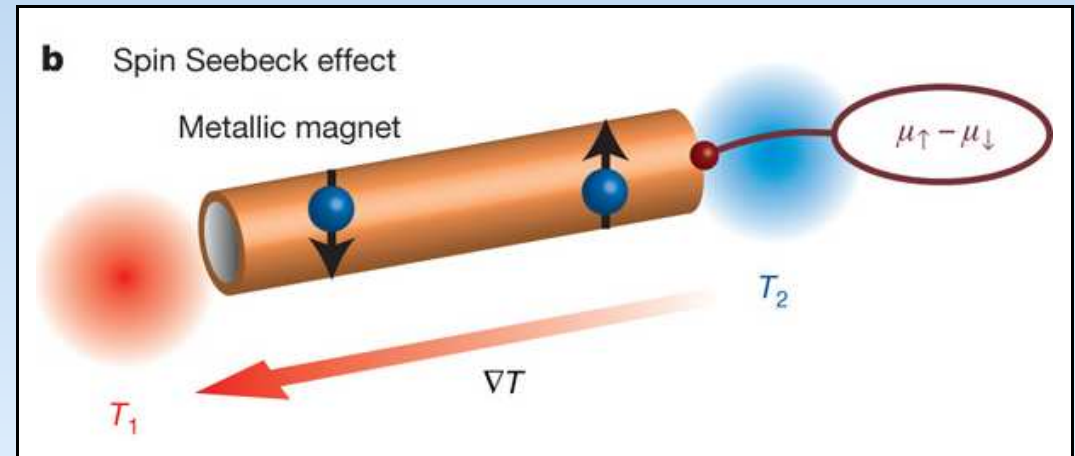
(<http://www.ultramagnetron.org>)



Spin Seebeck effect

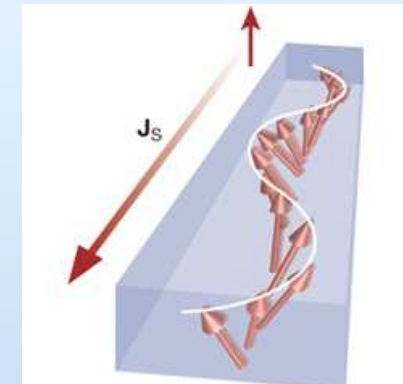
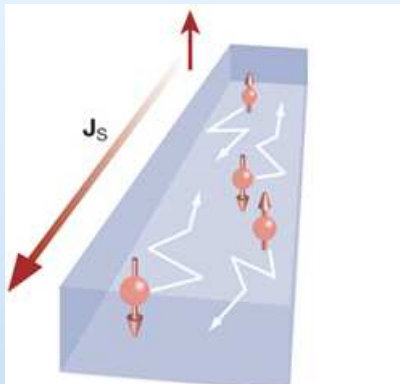
Spin Seebeck effect:

generation a spin voltage through a temperature gradient in a ferromagnet
(K. Uchida et al., *Nature* **455**, 778 (2008))



Spin current:

flow of angular momentum \Rightarrow two possible types of carriers (Y. Kajiwara et al., *Nature* **464**, 262 (2010))

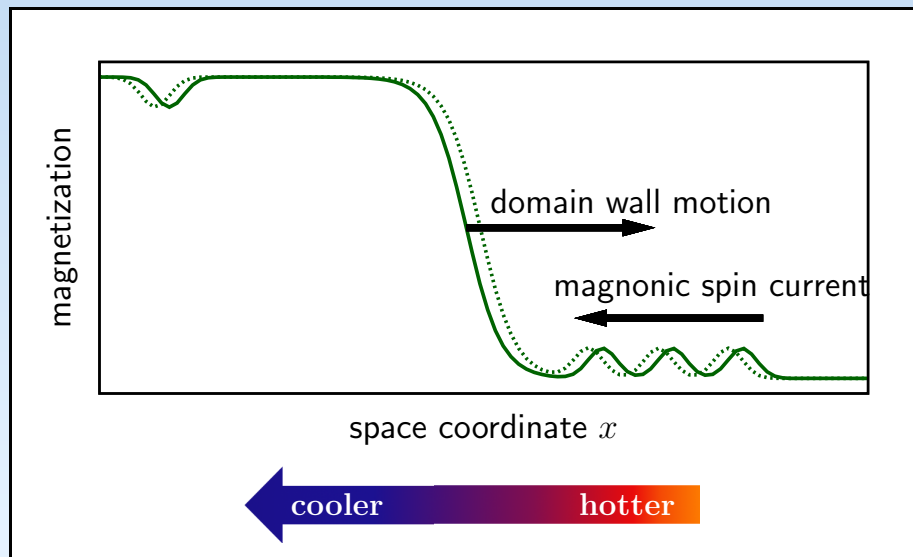


- spin current via polarized electrons

- chargeless spin current via magnons

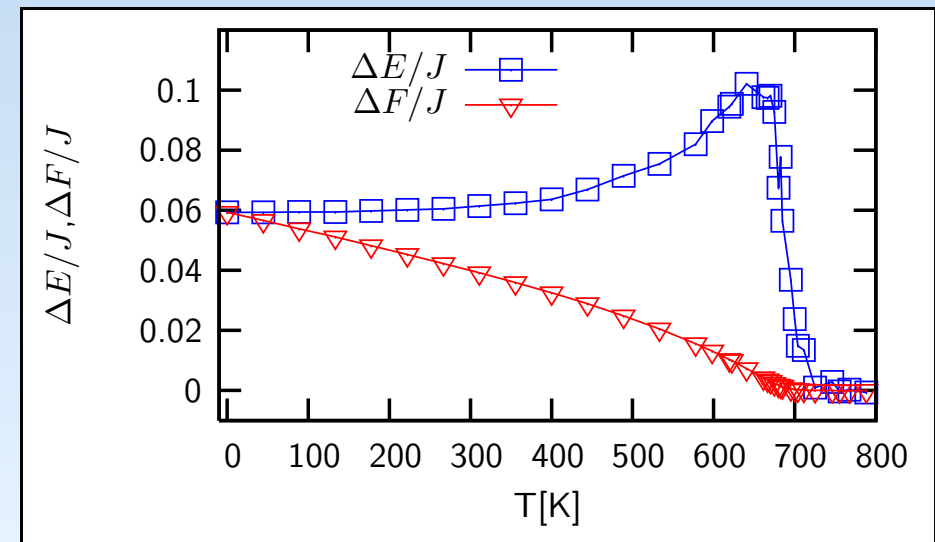
Domain wall in a temperature gradient

Microscopic view:



- magnons from the hotter region enter the colder region changing their sign in the wall
- by conservation of angular momentum the domain wall is pushed towards the hotter region

Thermodynamic view:



(D. Hinzke et al., *PRB* **77**, 094407 (2008))

- free energy $F = E - TS$ of a domain wall is a monotonous decaying function of temperature
- in a temperature gradient the free energy of the domain wall is minimized by moving towards the hotter region

Domain wall motion in a temperature gradients

Microscopic view:

stochastic LLG equation

- spin model simulation of the LLG equation
- magnon current created by hot boundary
- domain wall is attracted by hot boundary

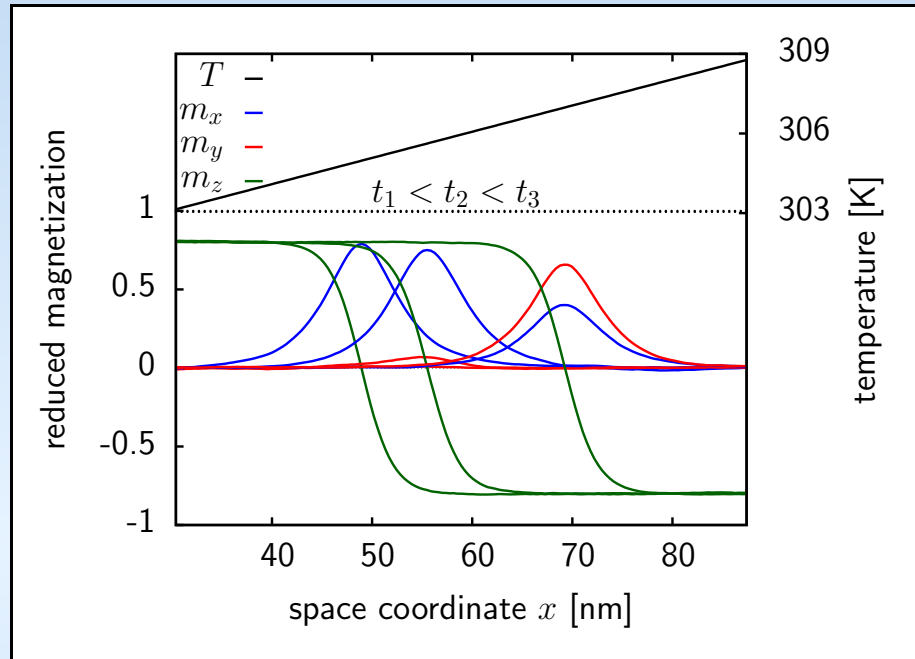
Thermodynamic view:

LLB equation

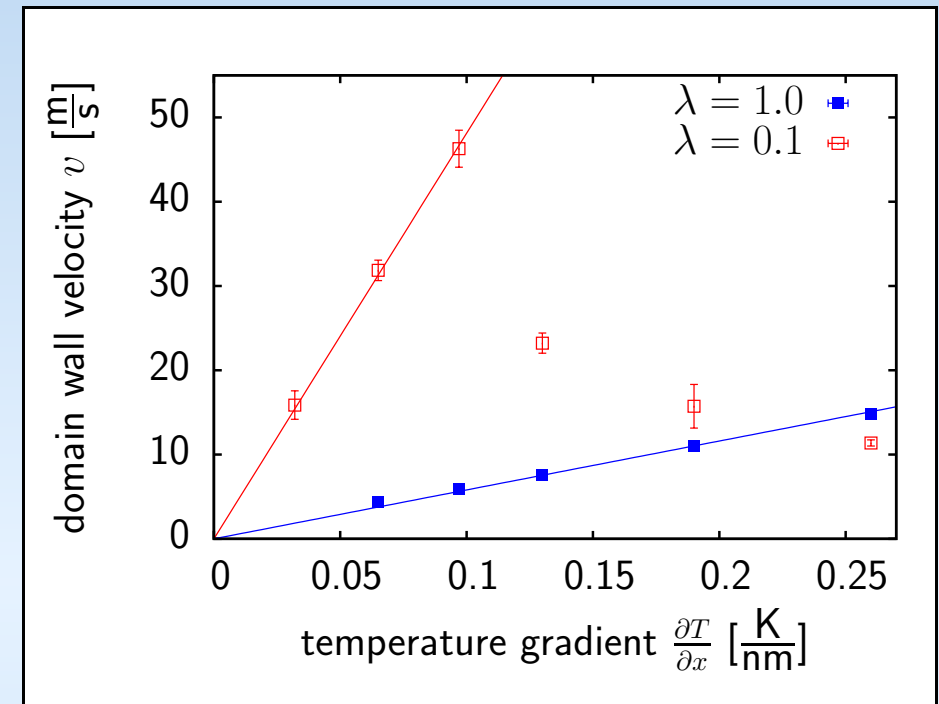
- micromagnetic simulation of the LLB equation
- domain wall moves into the hotter region
- domain wall motion is accompanied by precession (above Walker breakdown)



Domain wall motion in a temperature gradient



- simulation of the Landau-Lifshitz-Gilbert equation of motion
- domain wall moves towards hotter region
- shape and orientation of the domain wall changes



- simulation of the Landau-Lifshitz-Bloch equation of motion
- $v \approx 50$ m/s for $\frac{\partial T}{\partial x} \approx 0.1$ K/nm
 → should be measurable
- Walker breakdown

Final remarks

Summary:

- multiscale modelling:
 - spinmodel for FePt from first principles *Europhys. Lett.* **69**, 805 (2005)
 - from first principles to macro-spins *Phys. Rev. B*, **77**, 184428 (2008)
 - exchange stiffness at finite temperatures *Phys. Rev. B*, **82**, 134440 (2010)
- high temperature spin dynamics:
 - rapid heating dynamics with LLB equation *Appl. Phys. Lett.* **91**, 232507 (2007)
 - LLG equation describes ps spin dynamics *Europhys. Lett.* **81**, 27004 (2008)
 - linear vs. elliptical reversal: analytical results *Europhys. Lett.* **86**, 27006 (2009)
 - ultra-fast spin dynamics: the effect of colored noise *Phys. Rev. Lett.* **102**, 057203 (2009)
 - opto-magnetic writing *Phys. Rev. Lett.* **103**, 117201 (2009)
- domain wall motion by spin currents:
 - current induced domain wall motion *Phys. Rev. B* **91**, 232507 (2010)
 - non-adiabatic spin torque *Phys. Rev. Lett.* **105**, 056601 (2010)
 - domain wall motion in temperature gradients *in preparation*

Acknowledgment:

- EU: FP7 Research Project UltraMagnetron
- CAP: center for applied photonics
- DFG: SFB 767