Atomistic models of ultrafast spin dynamics

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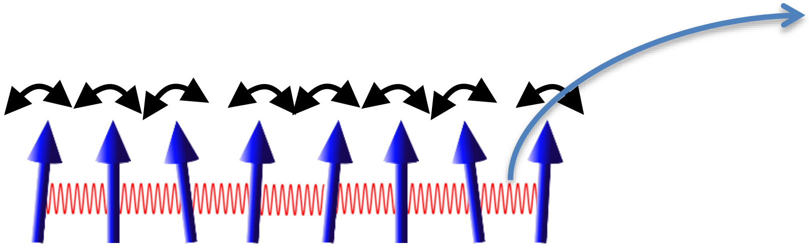
SEVENTH FRAMEWORK PROGRAMME

Towards femtosecond processes

- We will look at magnetic processes at increasing rates.
- Firstly the (nanosecond) processes possible with normal magnetic field processes will be introduced
- Then (picosecond) experiments using the Stanford Linear Accelerator (SLAC) will be described.
- Finally we look at the response to femtosecond lasers (arguably the fastest human-generated events)
- The conclusion is that reversal of the magnetisation is possible in hundreds of fs ***in the absence of an applied field! Thermally Induced Magnetisation Switching (TIMS)***
- TIMS recently demonstrated using current-induced heating (Yang Yang et.al., https://arxiv.org/abs/1609.06392)
- **Possible new recording technology?**

Can we go faster?

- Control of magnetization dynamics in applied field limited by precession time.
- There are a number of other ways to control magnetization:
  - Spin transfer torque
  - Heat assisted magnetic recording
- The exchange interaction gives rise to magnetic order.

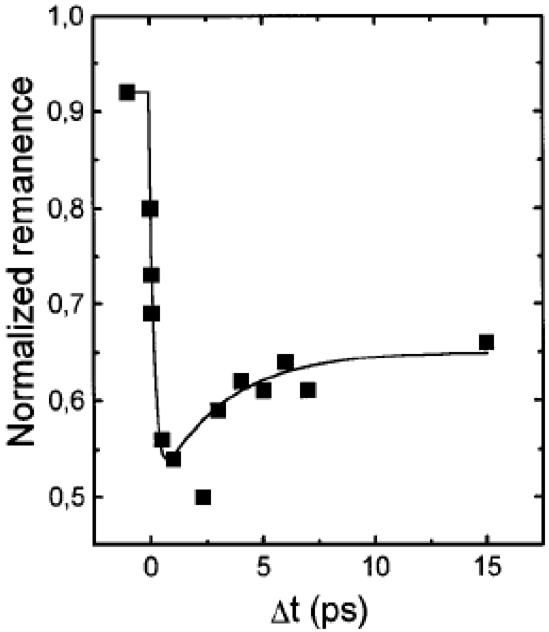


Timescale:

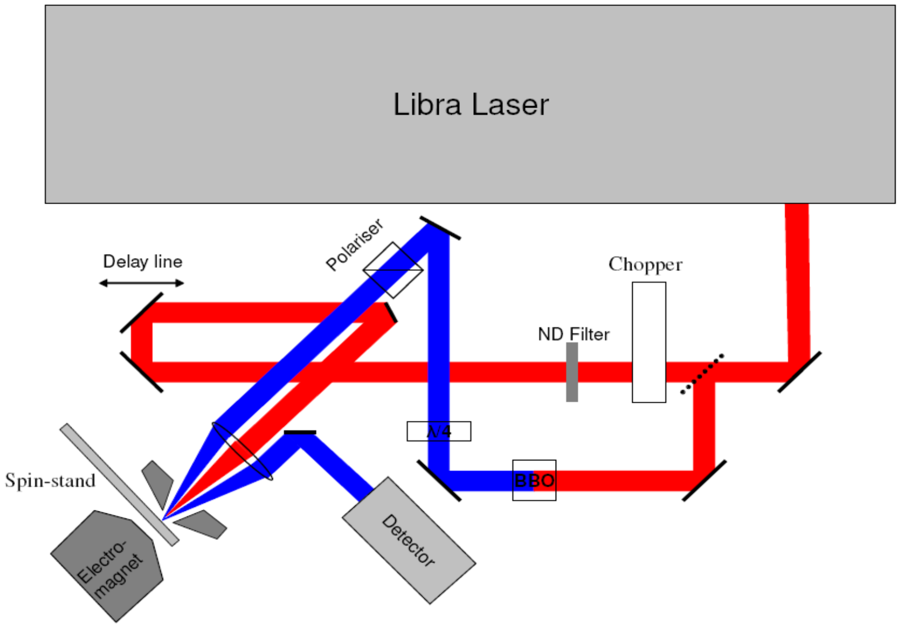
10’s -> 100’s fs

- The strongest force in magnetism. Can we excite processes on this timescale?
- How does this relate to the Quadrilemma?

Fast heating using pulsed fs laser



Fast demagnetisation of Ni (Beaurepaire et al PRL 76 4250 (1996)). Experiments in zero field.



Typical pump-probe set up

Physics of fast magnetisation processes using an atomistic model

- Magnetic properties arise because of the quantum mechanical ‘exchange interaction’ which favours parallel alignment of the atomic spins
- The atomistic approach developed here is based on the construction of a physically reasonable classical spin Hamiltonian based on ab-initio information.
- Atomistic approach is necessary in order to reproduce phase transitions, but we need also a dynamic model
- How is this constructed?

Atomistic model

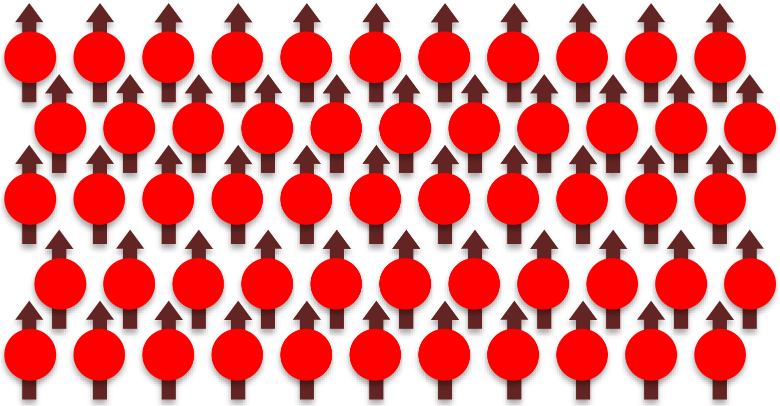
- Uses the Heisenberg form of exchange

$$E_i^{exch} = \sum_{j \neq i} J_{ij} \vec{S}_i . \vec{S}_j$$

- Spin magnitudes and J values can be obtained from ab-initio calculations.
- We also have to deal with the magnetostatic term.
- 3 lengthscales – electronic, atomic and micromagnetic – Multiscale modelling.

The spin dynamics model

$$\dot{\mathbf{S}}_i = -\frac{\gamma_i}{(1+\lambda_i^2)\mu_{i,s}}\mathbf{S}_i \times \mathbf{H}_i - \frac{\lambda_i \gamma_i}{(1+\lambda_i^2)\mu_{i,s}}\mathbf{S}_i \times \mathbf{S}_i \times \mathbf{H}_i$$



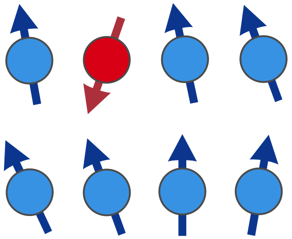
- Assume fixed atomic positions
- Processes such as e-e, e-p and p-p scattering are treated phenomenologically (λ).
- At each timestep we calculate a field acting on each spin and solve using numerical integration.
- To calculate the fields we consider a Hamiltonian (below).

$$x_{n+1} = x_n + \frac{1}{2}[f(x_n, t_n) + f(\bar{x}_{n+1}, t_{n+1})]\Delta t + \frac{1}{2}[g(x_n, t_n) + g(\bar{x}_{n+1}, t_{n+1})]\tilde{\zeta}_n$$

Extended Heisenberg Hamiltonian

$$\mathcal{H} = \underbrace{-\sum_{\langle ij \rangle} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j}_{\text{Exchange}} \underbrace{- \sum_{i=1} D(\mathbf{S_i} \cdot \mathbf{n_i})}_{\text{Anisotropy}} \underbrace{- \sum_i \boldsymbol{\mu}_{s,i} \cdot \mathbf{B}}_{\text{Zeeman}} \underbrace{- \frac{\mu_0}{4\pi}\sum_{i \neq j}\frac{3(\boldsymbol{\mu}_i \cdot \hat{e}_{ij})(\boldsymbol{\mu}_j \cdot \hat{e}_{ij}) - \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j}{r_{ij}^3}}_{\text{Dipole-Dipole}}$$

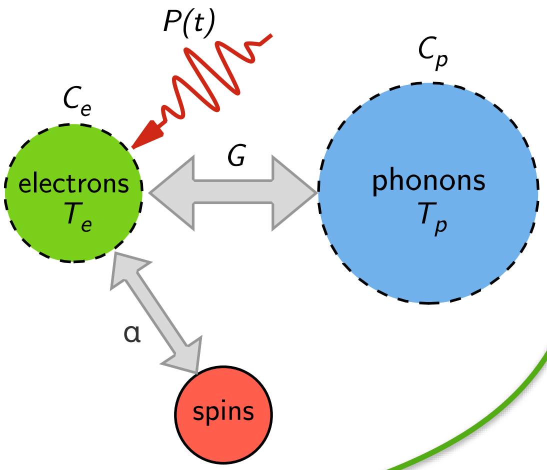
Laser heating

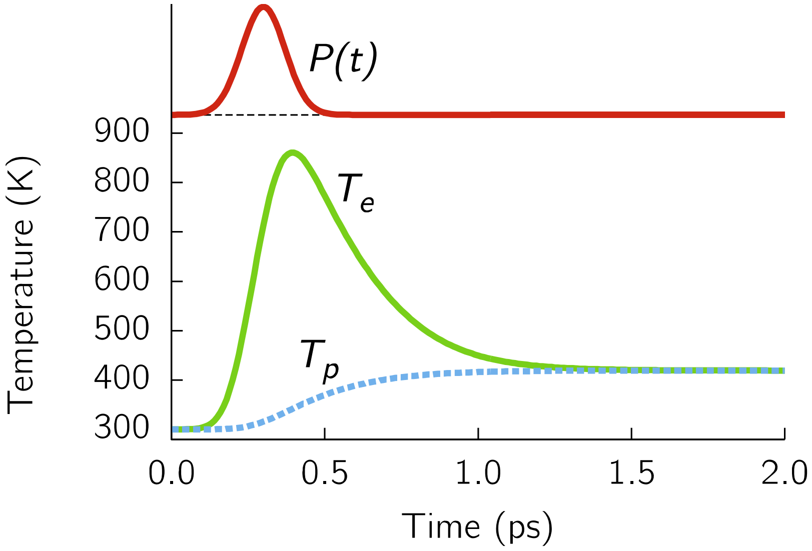


$$\boldsymbol{H}_i = -\frac{\partial \mathcal{H}}{\partial \boldsymbol{S}_i} + \boldsymbol{\xi}_i$$

$$\langle \zeta_i^a(t)\zeta_j^b(t)\rangle = \frac{2\lambda_i k_{\mathrm{B}} T(t) \mu_{i,s}}{\gamma_i}\delta_{ij}\delta_{ab}\delta(t-t')$$

$$\langle \zeta_i^a(t)\rangle = 0$$





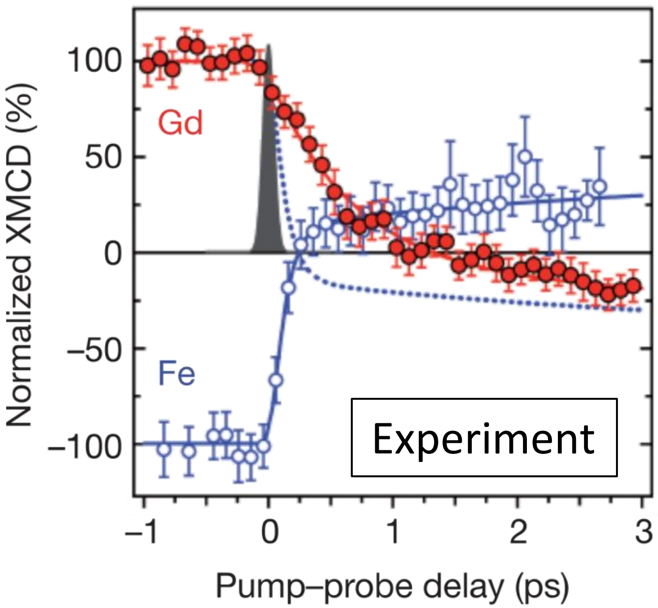
$$C_e \frac{dT_e}{dt} = -G_{e-p}(T_e - T_p) + P(t)$$

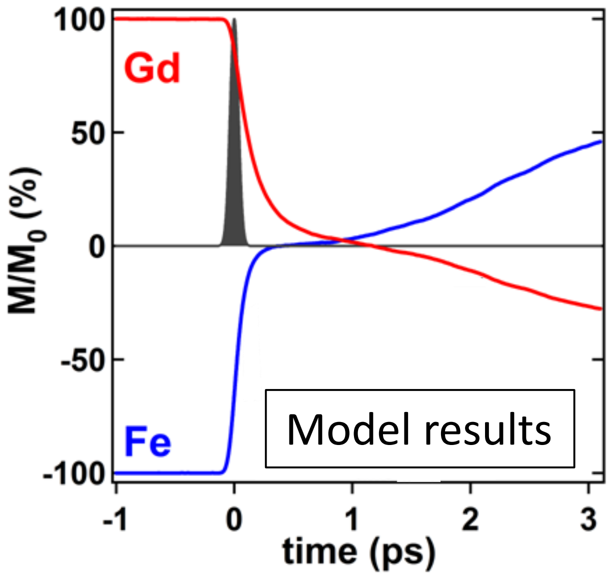
$$C_l \frac{dT_p}{dt} = G_{e-p}(T_e - T_p)$$

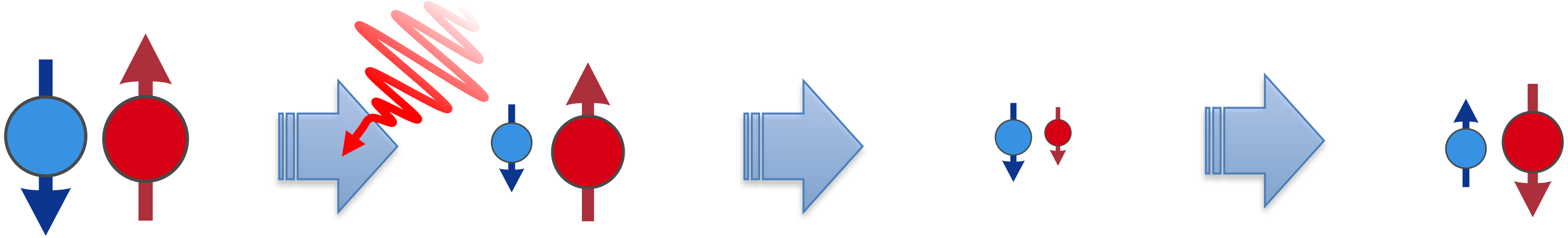
Chen *et al. Int. Journ. Heat and Mass Transfer.* **49**, 307-316 (2006)

‘Magic’ reversal?

Element-resolved dynamics.







Initial State

Different demagnetization times

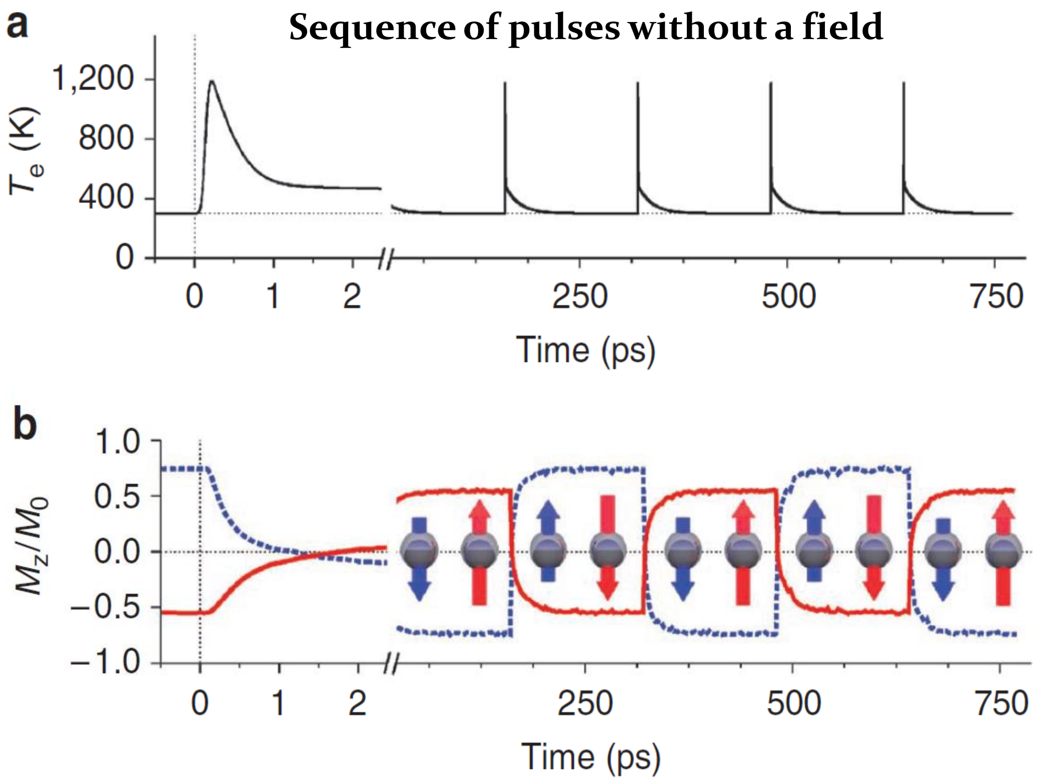
Transient ferromagnetic-like state

Reversal of the sublattices

Radu *et al.* *Nature*, **472**, 205-208 (2011).

Thermally Induced Magnetisation Switching (TIMS)

- What role is the magnetic field playing?
- Model calculations show field playing almost no role!



Do we see the same experimentally?

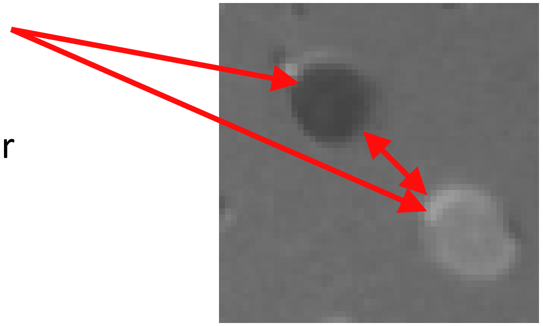
Ostler *et al. Nat. Commun.* **3**, 666 (2012).

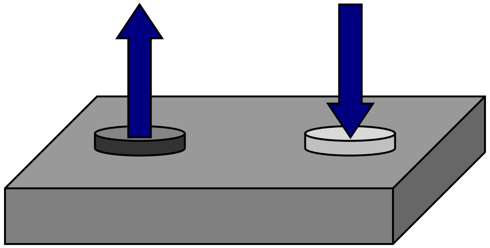
Experimental Verification: GdFeCo Microstructures

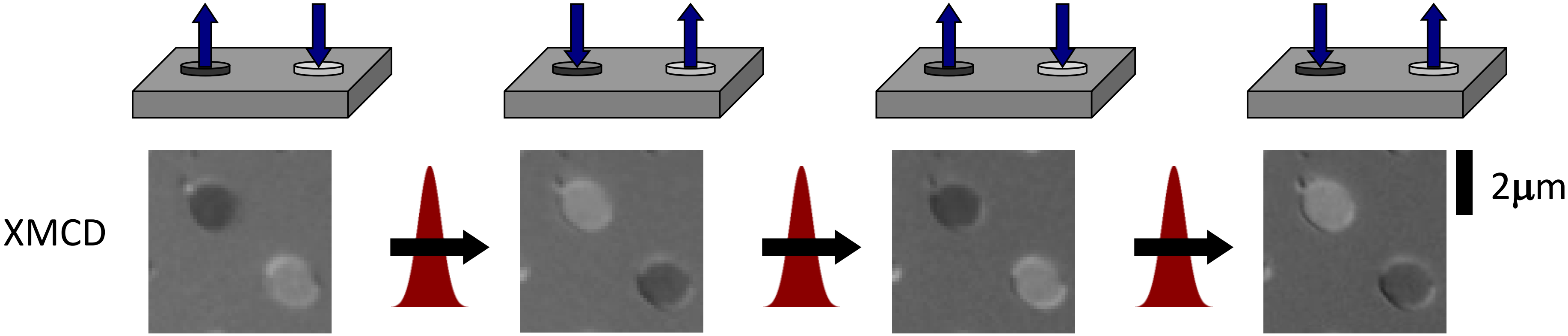
Initial state

- two microstructures with opposite magnetisation

- Separated by distance larger than radius (no coupling)



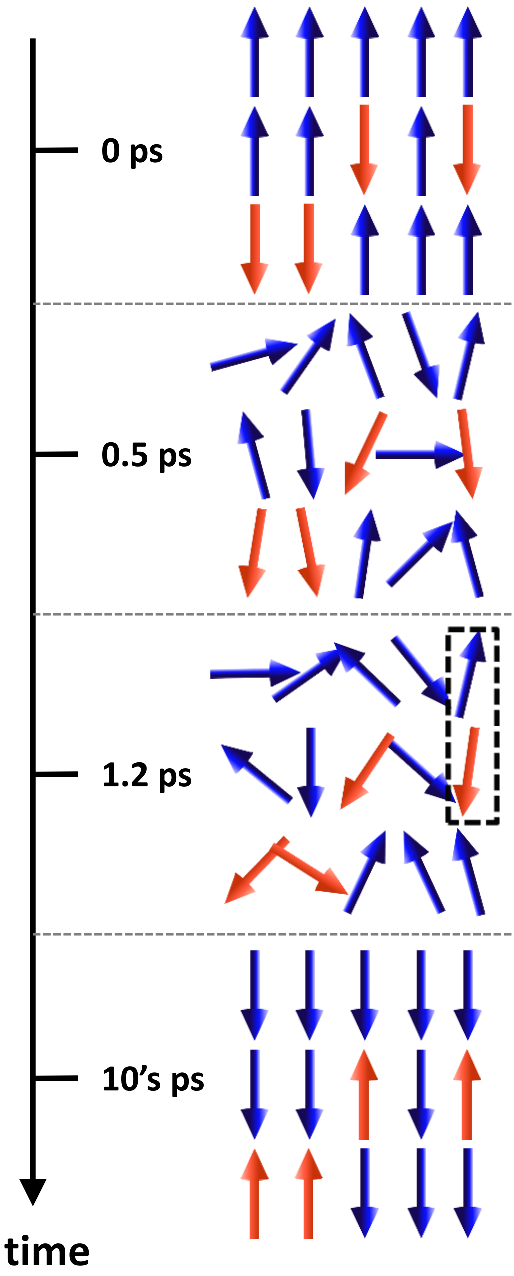




Experimental observation of magnetisation after each pulse.

Ostler *et al. Nat. Commun.* **3**, 666 (2012).

What’s going on?

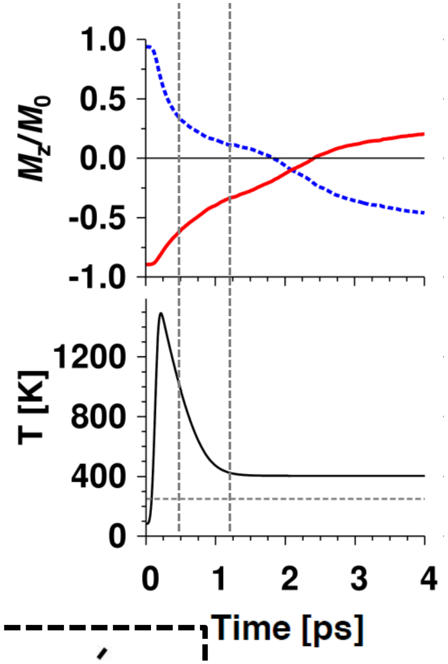


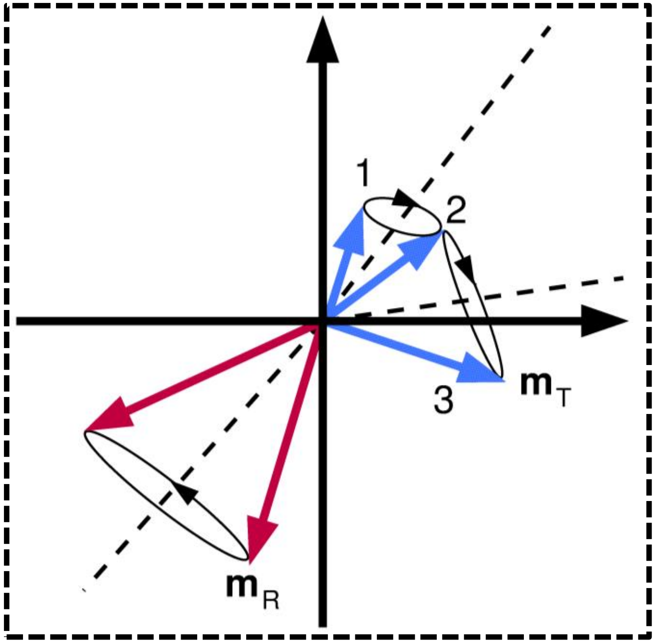
- Ground state

-T>T_C Fe disorders more quickly (μ)

-T<T_C precessional switching (on atomic level)
-Exchange mode between TM and RE
- Transient state

-T is lowered when in transient state
-TM is the dominant magnetic species
-RE forced to change direction





Requirements

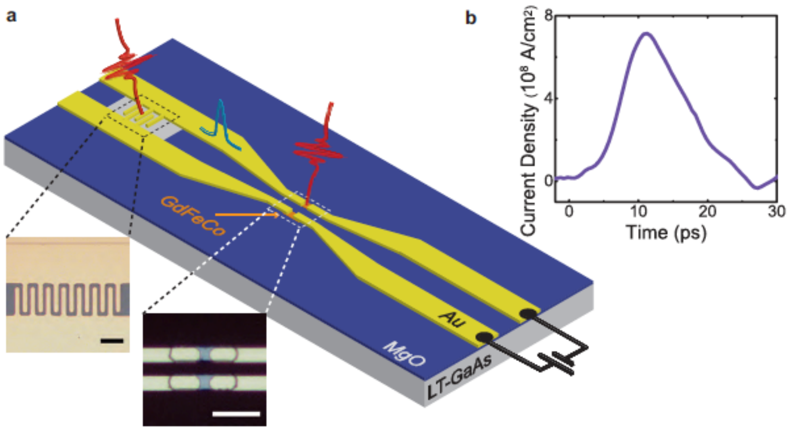
- Switching requirements
  - Distinct sublattices
  - Differential sublattice demagnetisation
  - Antiferromagnetic coupling between sublattices
- NB – effective field arises from exchange. Tens of Tesla needed to prevent reversal. Important for thermal writability
- Ideally - removal of Gd
- Synthetic ferrimagnets?

Advantages

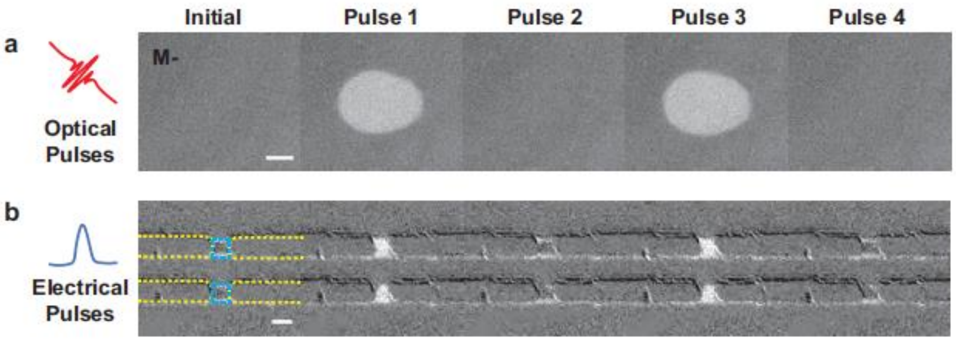
- HAMR head
  - Light delivery + Inductive head
  - Inductive head gives significant design and production issues. >1000 separate production steps
- Optical/electrical recording head
  - Light delivery only
- Advantages
  - Considerable simplification of write heads
  - Significantly reduced energy/write
  - Very large effective fields involved. Important because of ‘quadrilemma’

Recent development: Electrically driven TIMS

Wilson et. al., Phys. Rev. B, **95**, 180409(R) (2017)



Current pulses optically trigged but possibly achievable using CMOS



Single shot optically and electrically driven switching.

- *Evidence that TIMS is indeed a thermodynamic phenomenon*
- *Brings closer the possibility of a practical recording system - ?*

Summary

- Atomistic spin model gives good agreement with ultrafast laser-induced dynamics experiments.
    - Demagnetisation times
    - Differential sublattice dynamics
    - Transient FM-like state
- Model is also powerfully predictive
    - prediction of Thermally Induced Magnetisation Switching (TIMS)
    - Switching times less than 1 picosecond – ultimate speed limit?
- All-optical/electrical recording?
    - X100 data rate
    - Much simplified head design
- Successful model but ……..
    - Classical spin and thermostat
    - Much better connection to quantum models required.