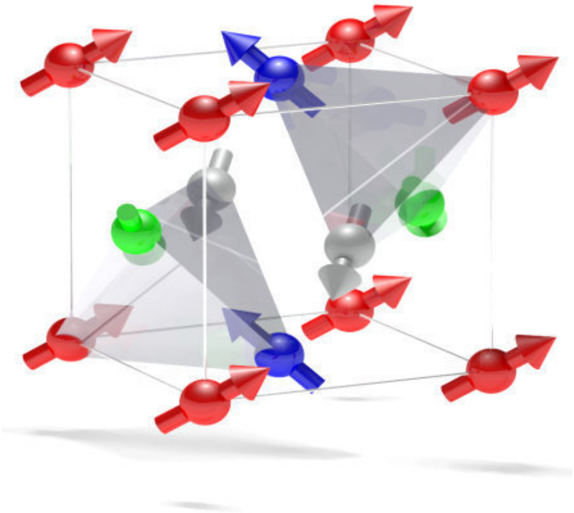
Advanced micromagnetics and atomistic simulations of magnets

Richard F L Evans

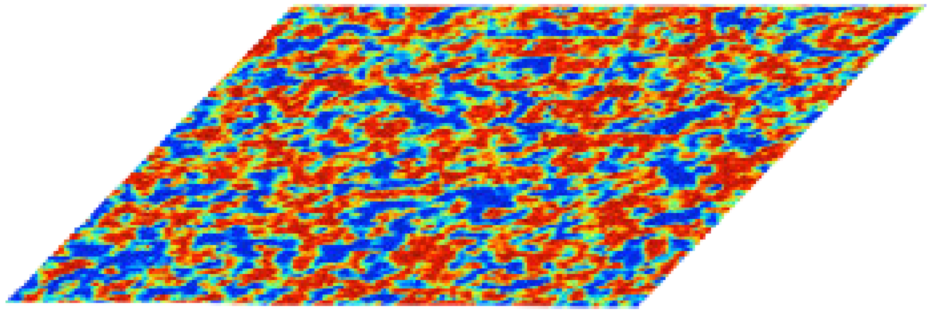
ESM 2018

Overview

- Landau-Lifshitz-Bloch micromagnetics
- Applications of atomistic spin dynamics



- Simulations of ultrafast magnetisation processes



Landau Lifshitz Bloch micromagnetics

Next generation micromagnetics: Landau Lifshitz Bloch equation

- Conventional micromagnetics ubiquitous but does a poor job of thermodynamics of magnetic materials

- Atomistic models in principle resolve this but horrendously computationally expensive

- **Landau Lifshitz-Bloch micromagnetics** is an advanced micromagnetic approach which attempts to correctly simulate the intrinsic thermodynamic properties of magnets

- Still only a partial solution - crystal structure, interfaces, surfaces, local defects, finite size effects all still not really accessible to a micromagnetic model

Landau Lifshitz Bloch (LLB) equation

- An additional dynamic term compared to the LLG equation

$$\dot{\mathbf{m}} = \gamma[\mathbf{m} \times \mathbf{H}_{\text{eff}}] + \frac{|\gamma|\alpha_{||}}{m^2}(\mathbf{m} \cdot \mathbf{H}_{\text{eff}})\mathbf{m} - \frac{|\gamma|\alpha_{\perp}}{m^2}[\mathbf{m} \times [\mathbf{m} \times (\mathbf{H}_{\text{eff}} + \boldsymbol{\eta}_{\perp})]] + \boldsymbol{\eta}_{||}$$

- Derived from the thermodynamic behaviour of a collection of classical spins by D. Garanin [1]

- Longitudinal fluctuations (and damping) of the magnetization are now included in the dynamics, enabling simulations up to and above the Curie temperature

- Also quantum flavours of the LLB

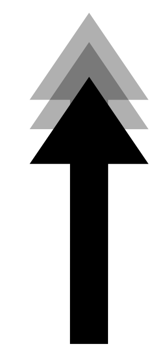
[1] D. A. Garanin, Phys. Rev. B 55, 3050 (1997)

Longitudinal term in the Landau Lifshitz Bloch (LLB) equation

- Longitudinal fluctuations of the magnetization have their own dynamics

$$\frac{|\gamma|\alpha_{||}}{m^2}(\mathbf{m}\cdot\mathbf{H}_{\text{eff}})\mathbf{m}$$

- Different effects below and above the Curie temperature, T_{c}



- The effective magnetic field that constrains the magnetization length is given by

$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \mathbf{H}_A + \begin{cases} \frac{1}{2\tilde{\chi}_{\|}}\left(1-\frac{m^2}{m_{\text{e}}^2}\right)\mathbf{m}, & T \lesssim T_{\text{c}} \\ -\frac{1}{\tilde{\chi}_{\|}}\left(1+\frac{3}{5}\frac{T_{\text{c}}}{T-T_{\text{c}}}m^2\right)\mathbf{m}, & T \gtrsim T_{\text{c}} \end{cases}$$

Energy terms in the Landau Lifshitz Bloch (LLB) equation

- Conventional energy terms used in micromagnetics cause numerical issues for the LLB, as any “applied” magnetic field will cause the moment length to grow

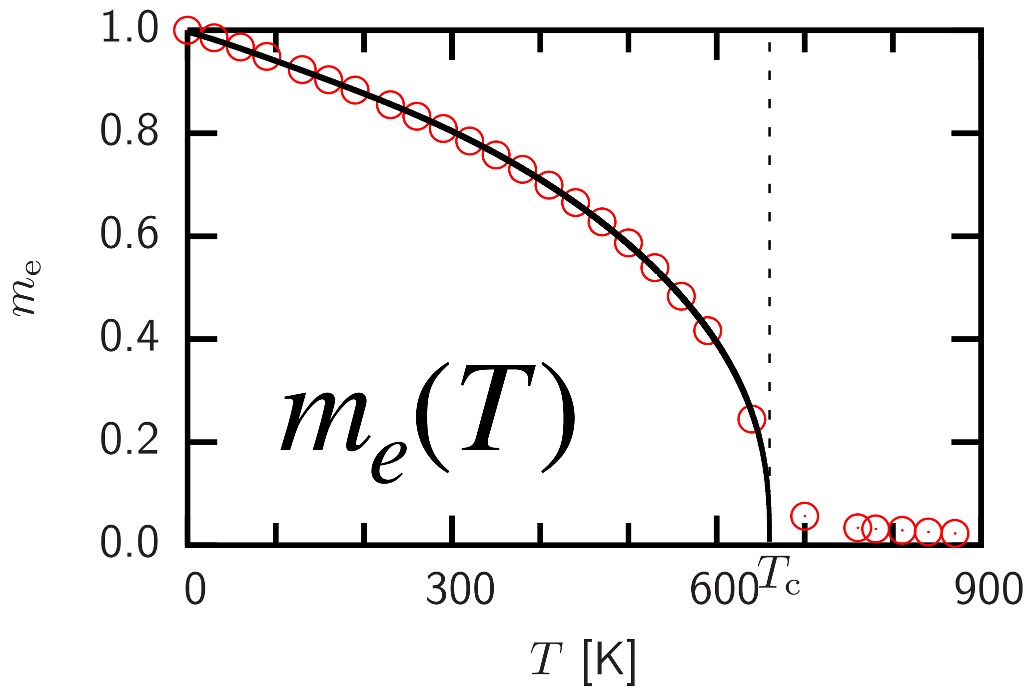
$$\frac{|\gamma|\alpha_{||}}{m^2}(\mathbf{m}\cdot\mathbf{H}_{\mathrm{eff}})\mathbf{m}$$

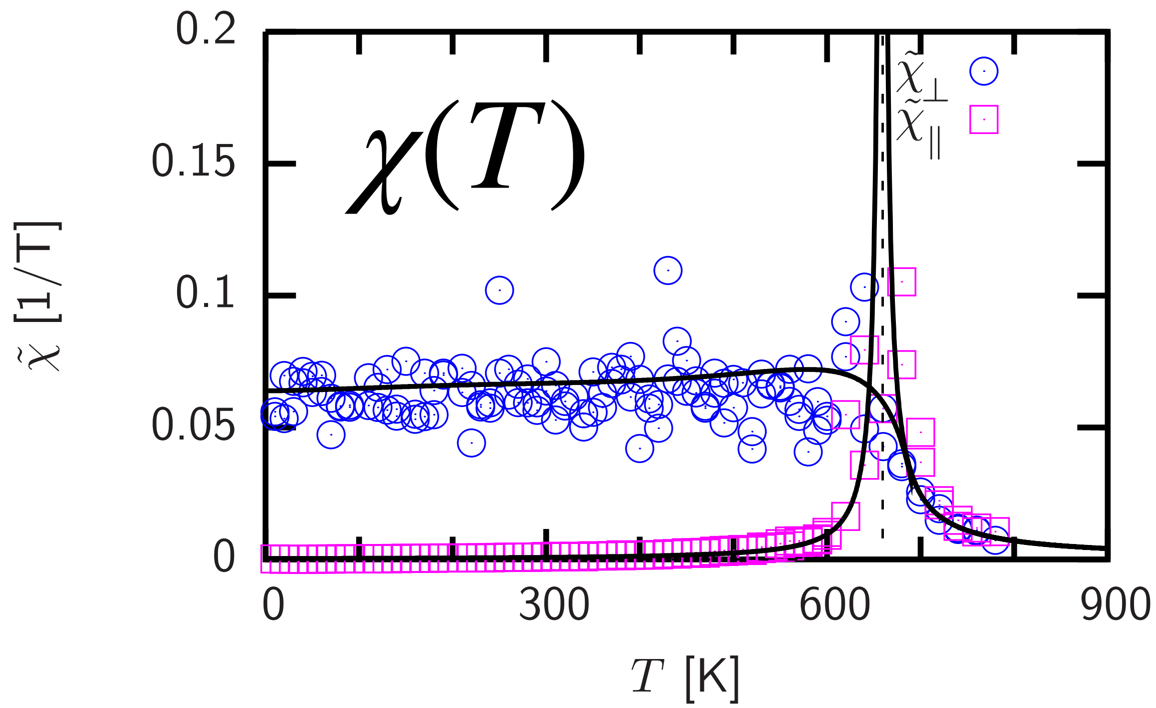
- Therefore need to treat internal fields in a special way so that in **thermal equilibrium**, the net magnetic field is **zero**

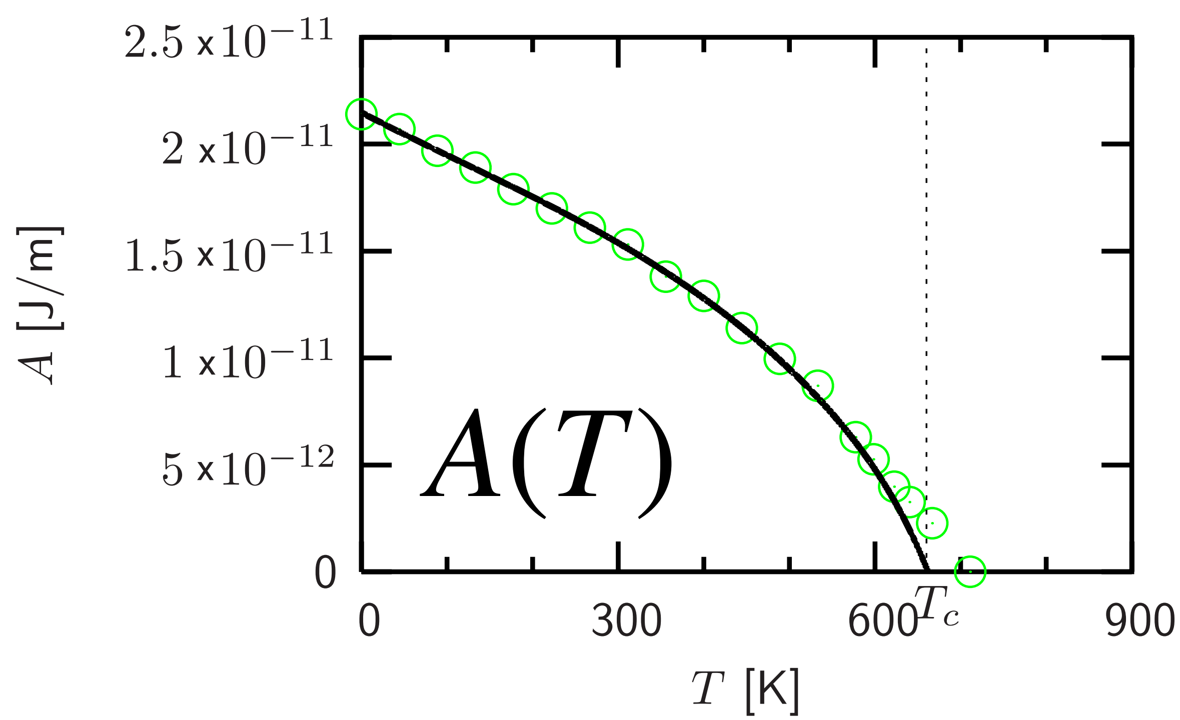
$$\frac{F}{M_s^0 V} = \begin{cases} \frac{m_x^2+m_y^2}{2\tilde{\chi}_\perp} + \frac{\left(m^2-m_e^2\right)^2}{8\tilde{\chi}_\| m_e^2}, & T \leqslant T_c \\ \frac{m_x^2+m_y^2}{2\tilde{\chi}_\perp} + \frac{3}{20\tilde{\chi}_\|}\frac{T_c}{T-T_c}\left(m^2+\frac{5}{3}\frac{T-T_c}{T_c}\right)^2, & T > T_c \end{cases}$$

Evans *et al*, Phys. Rev. B **85**, 014433 (2012)

Parameters for the LLB equation can be derived from mean field or atomistic/multiscale simulations

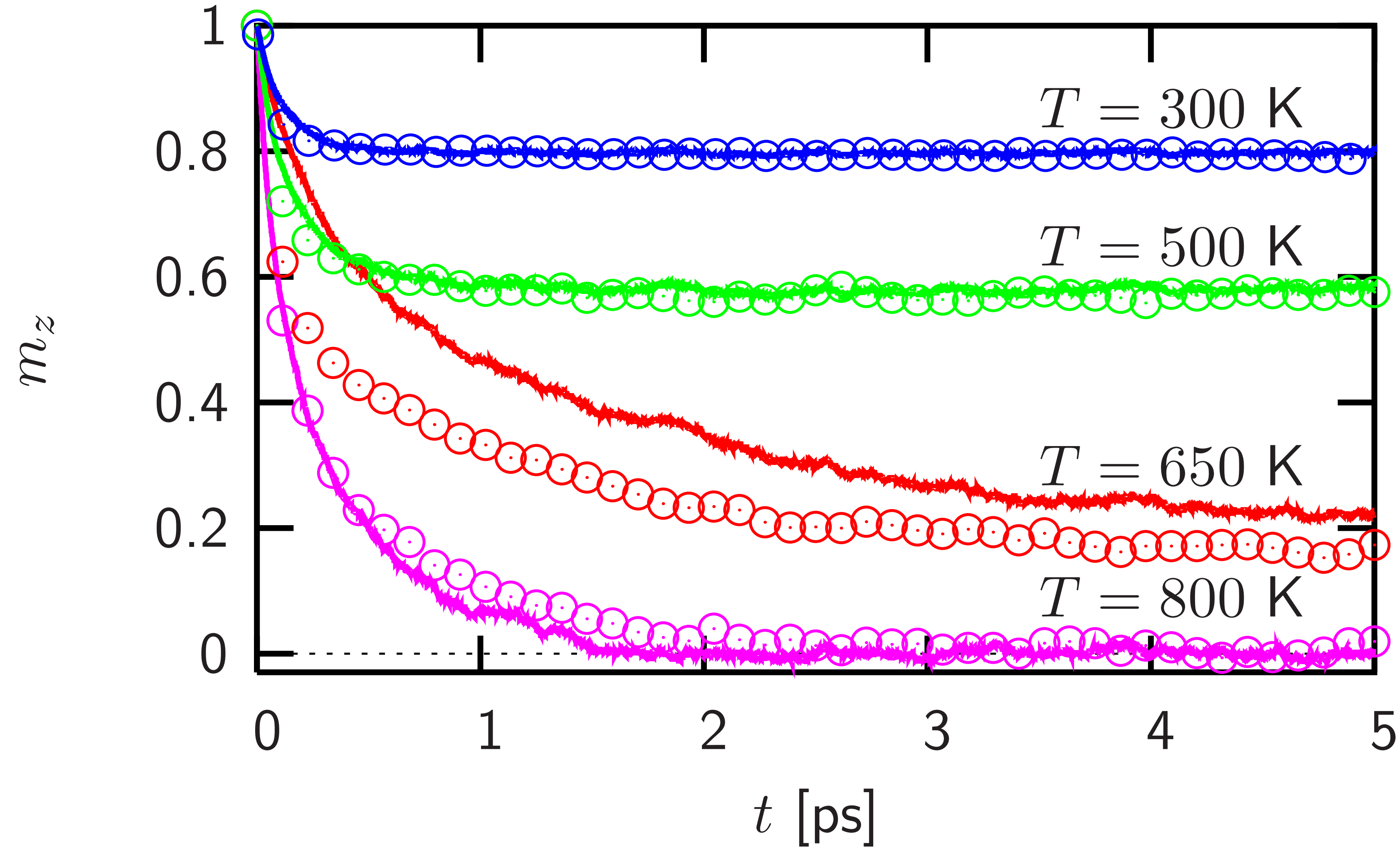






Kazantseva *et al*, Phys. Rev. B **77**, 184428 (2008)

Comparative dynamics for LLB and atomistic simulations



Kazantseva *et al*, Phys. Rev. B **77**, 184428 (2008)

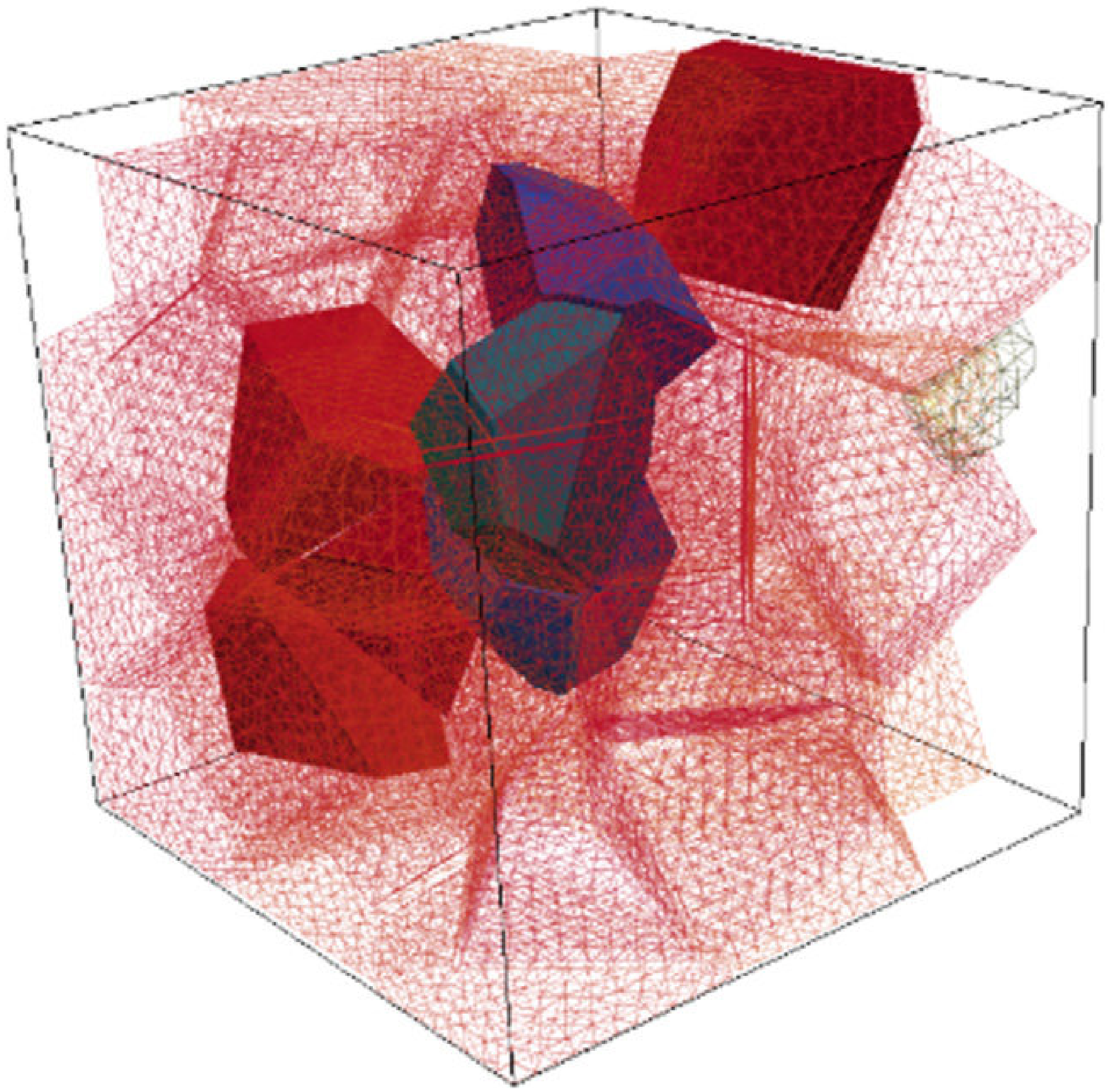
Applications of atomistic spin dynamics

Atomistic spin dynamics and temperature dependent properties of $Nd_2Fe_{14}B$

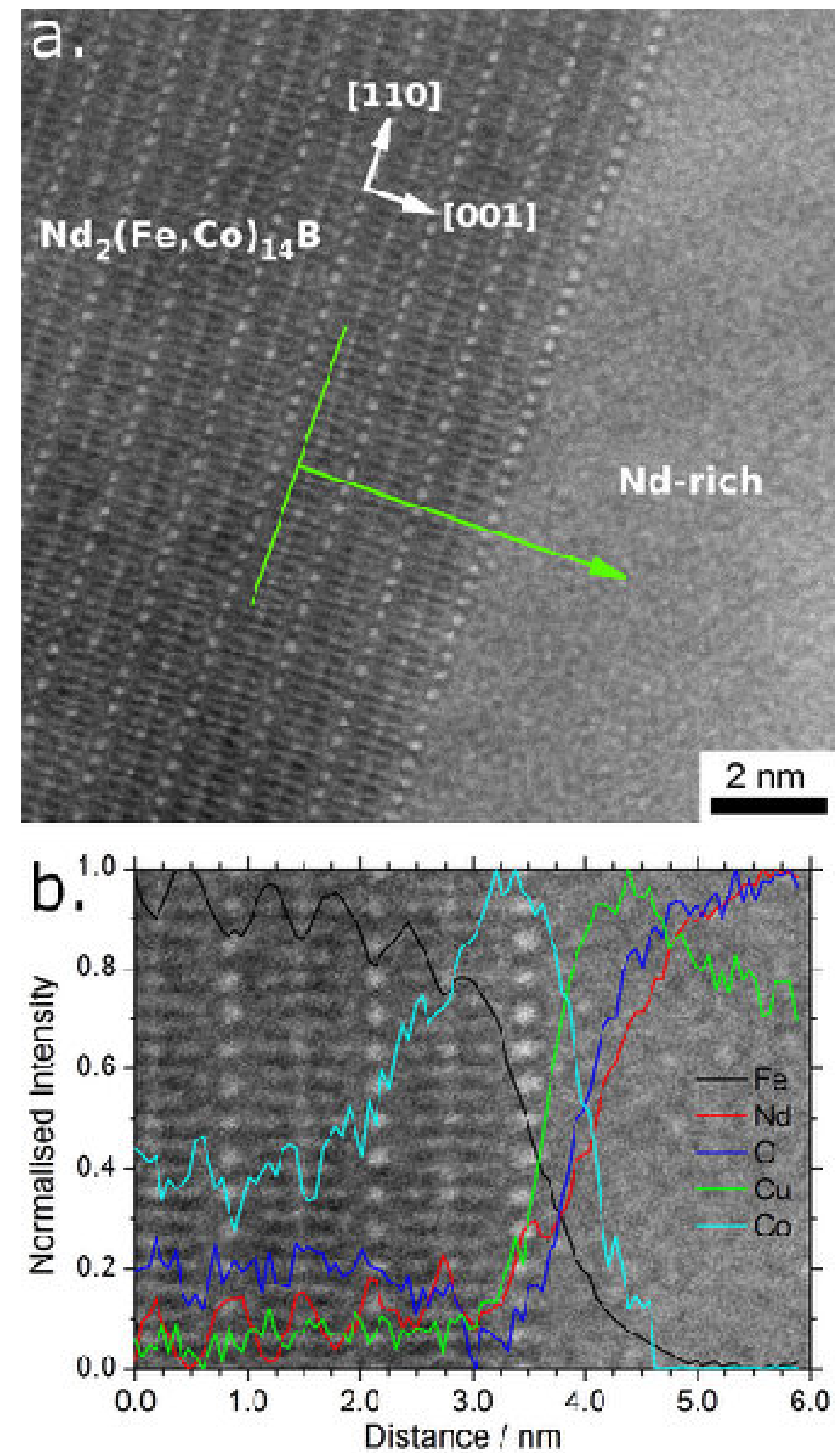
UNIVERSITY of York

Permanent magnetic materials

Structure at atomic and granular length scales determines overall material performance



Acta Materialia **77**, 111-124 (2014)

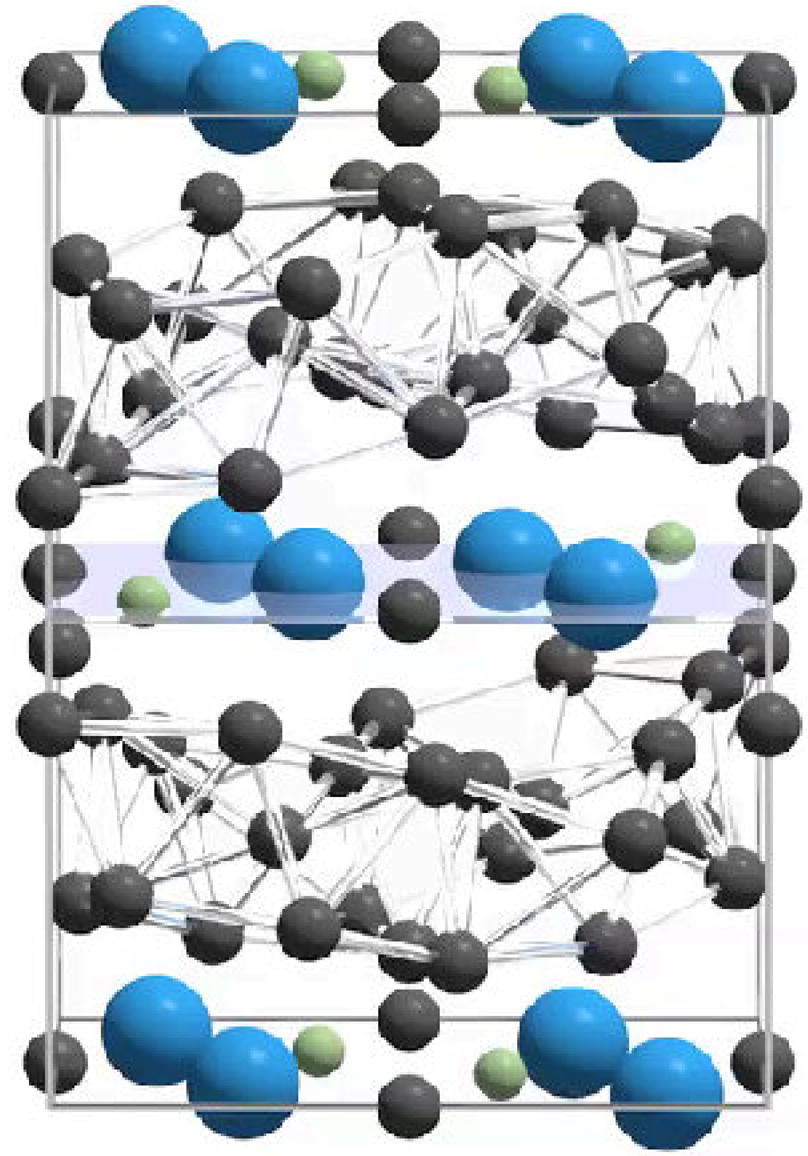


Atomistic spin Hamiltonian for $Nd_2Fe_{14}B$

$$\mathscr{H} = \mathscr{H}_{\mathrm{Nd}} + \mathscr{H}_{\mathrm{Fe}}$$

$$\mathscr{H}_{\mathrm{Nd}} = -\sum_{i,\delta} J_{\mathrm{NdFe}} \mathbf{S}_i \cdot \mathbf{S}_\delta - \sum_i E_i^{k,\mathrm{Nd}} - \mu_{\mathrm{Nd}} \sum_i \mathbf{H}_{\mathrm{app}} \cdot \mathbf{S}_i$$

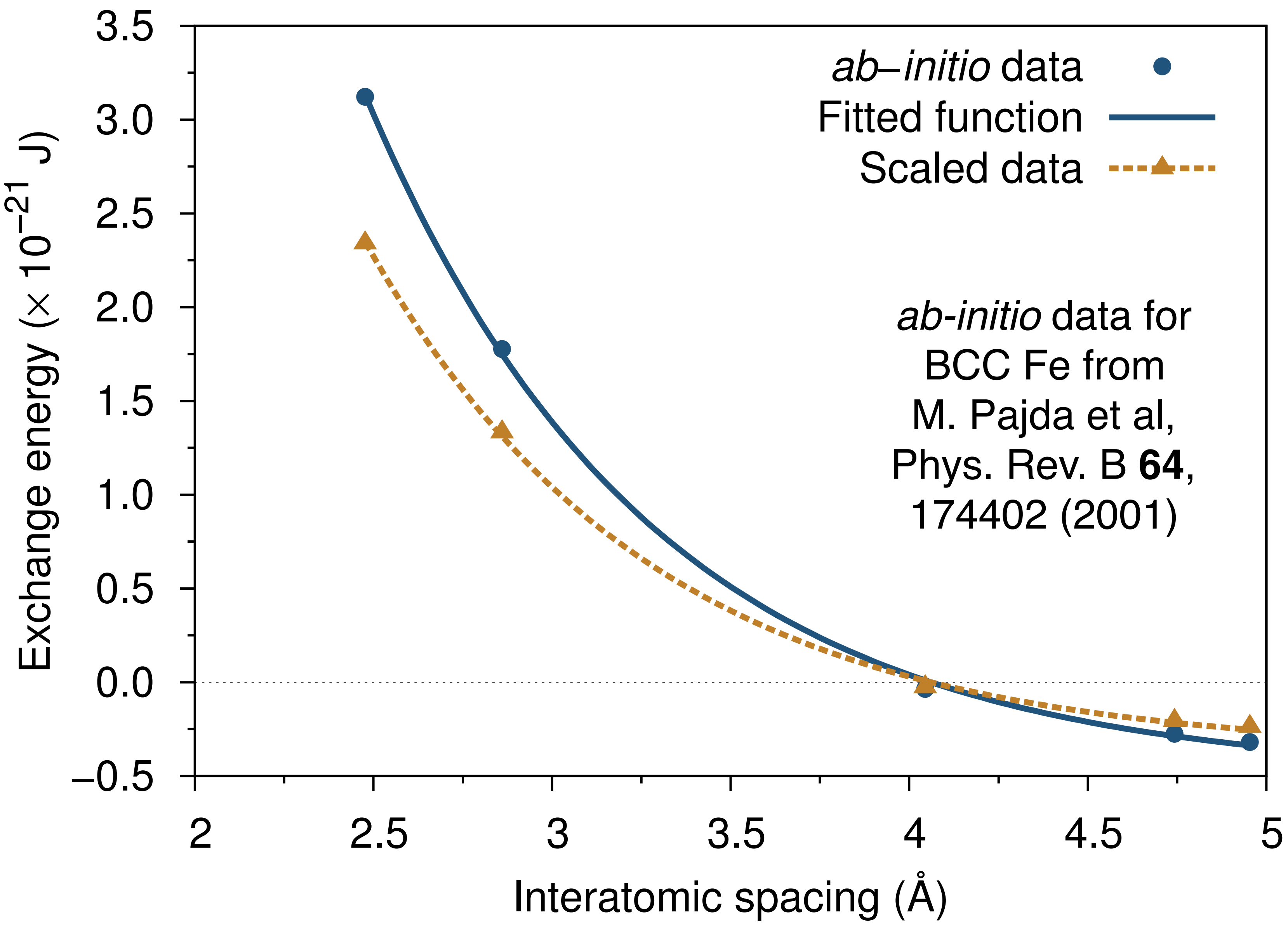
$$\mathscr{H}_{\mathrm{Fe}} = -\sum_{\nu,\delta} J_{\mathrm{Fe}}(r) \mathbf{S}_\nu \cdot \mathbf{S}_\delta - \sum_{\nu,j} J_{\mathrm{NdFe}} \mathbf{S}_\nu \cdot \mathbf{S}_j - \sum_\nu E_\nu^{k,\mathrm{Fe}} - \mu_{\mathrm{Fe}} \sum_\nu \mathbf{H}_{\mathrm{app}} \cdot \mathbf{S}_\nu$$



UNIVERSITY of York

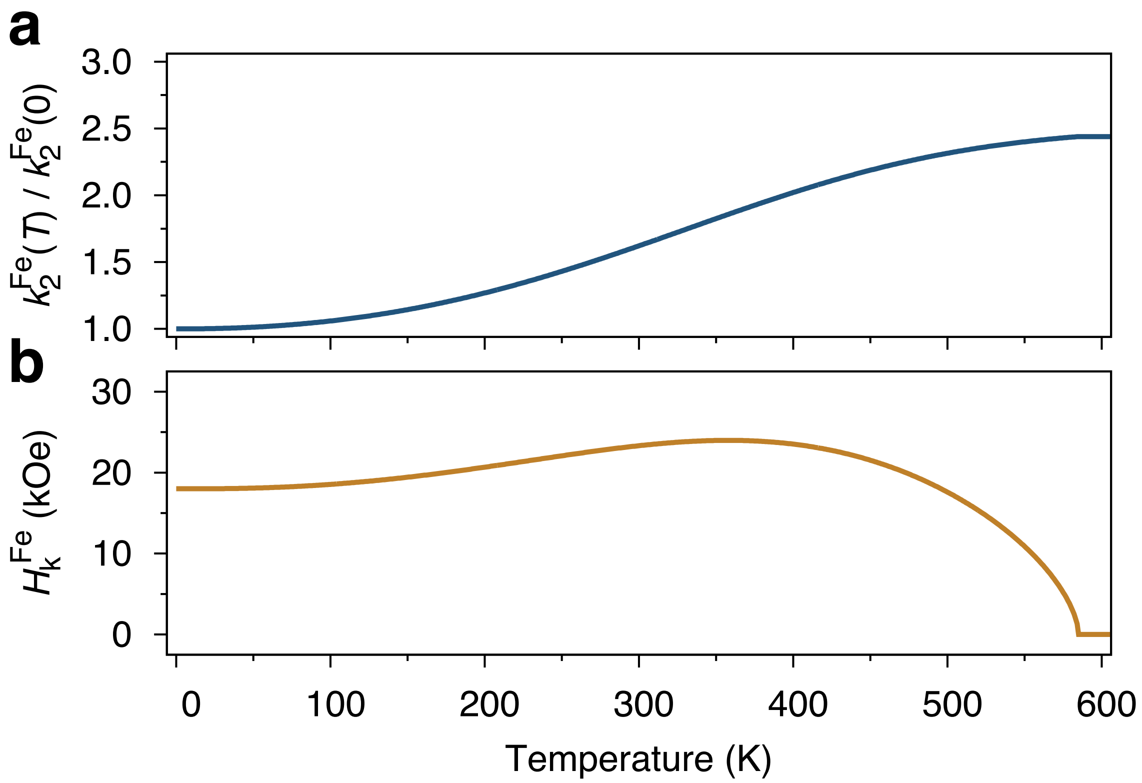
Fe-Fe Exchange interactions

$$J_{\mathrm{Fe}}(r) = J_0 + J_{\mathrm{r}} \exp(-r/r_0)$$



Magnetic anisotropy energy

Fe



$$k_2^{\mathrm{Fe}}(\widetilde{T}) = f(\sigma(\widetilde{T}))$$

$$f(\widetilde{\sigma}) = 1 + \frac{\kappa_{\mathrm{ca}}}{r} \tanh(r\widetilde{\sigma})$$

Nd

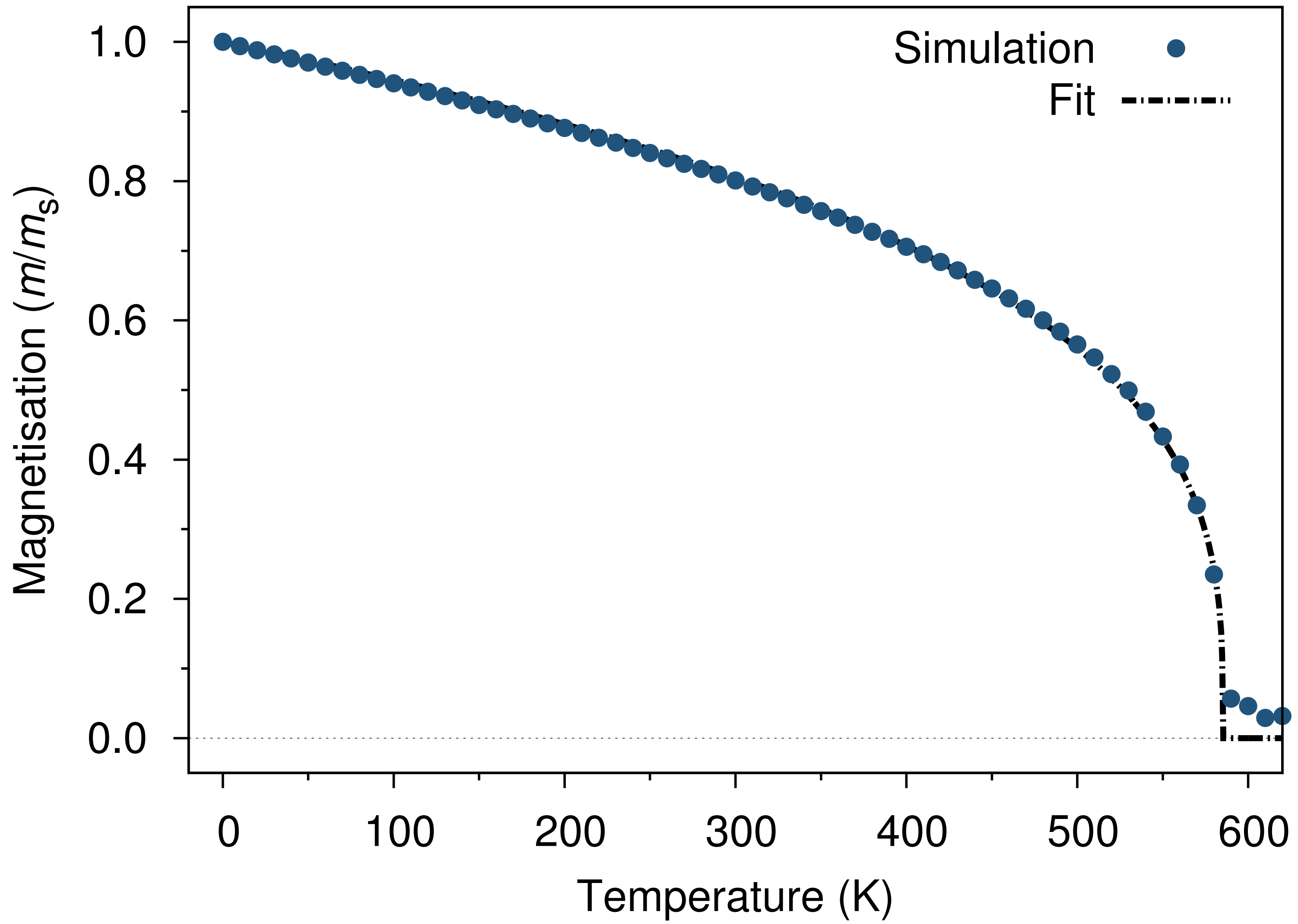
$$E_i^{k,\mathrm{Nd}} = -\kappa_2^{\mathrm{Nd}} \widetilde{P}_2 - \kappa_4^{\mathrm{Nd}} \widetilde{P}_4$$

$$\widetilde{P}_2 = -\tfrac{1}{3}(3S_z^2 - 1)$$

$$\widetilde{P}_4 = -\tfrac{1}{12}(35S_z^4 - 30S_z^2 + 3)$$

J. F. Herbst, Rev. Mod. Phys. 63, 819 (1991)

Simulated temperature dependent magnetization



$$m(T) = (1 - T/T_c)^{\beta}$$

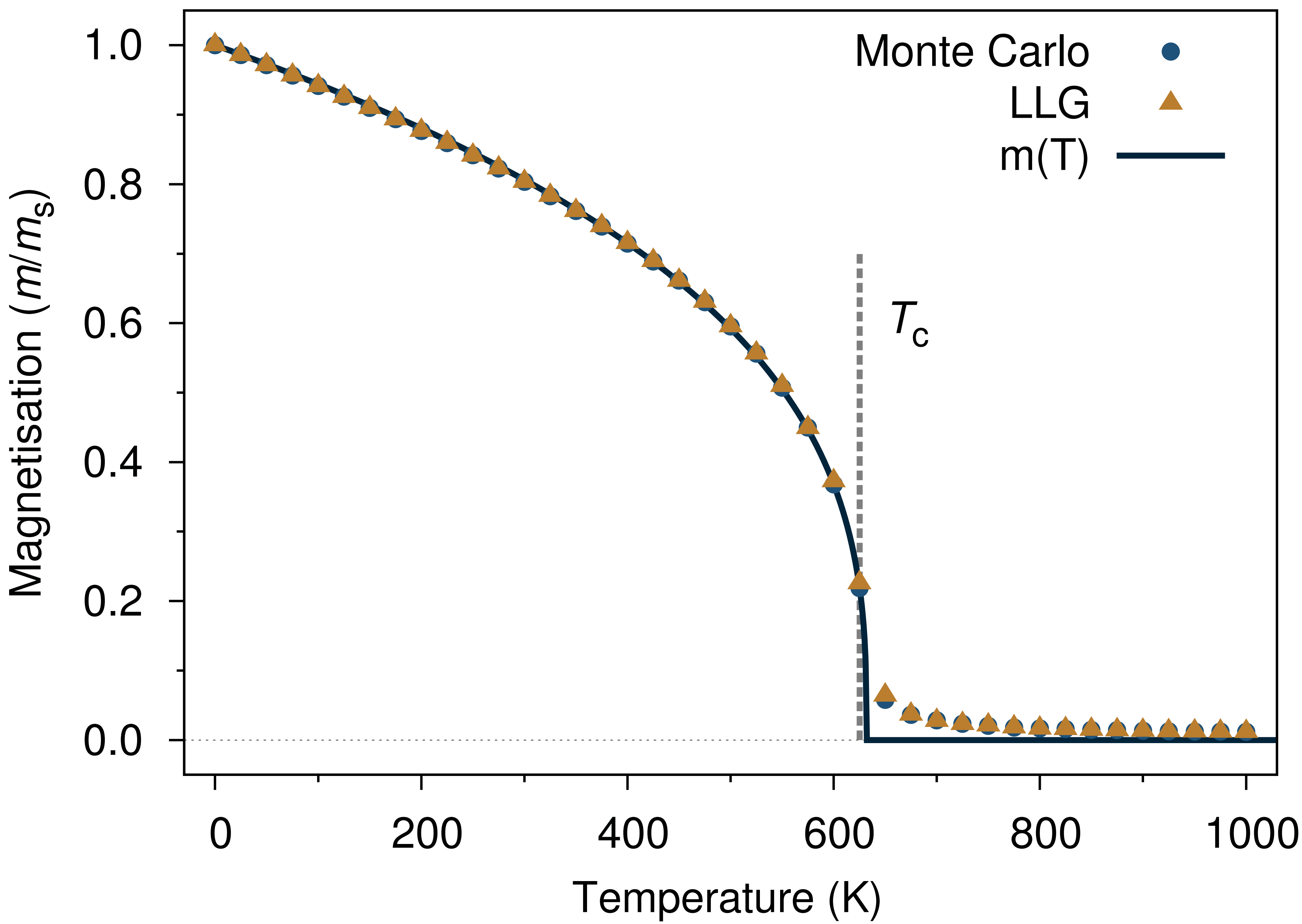
Quantitative modelling of temperature dependent properties in ferromagnets

Richard F L Evans, Unai Atxitia and Roy W Chantrell

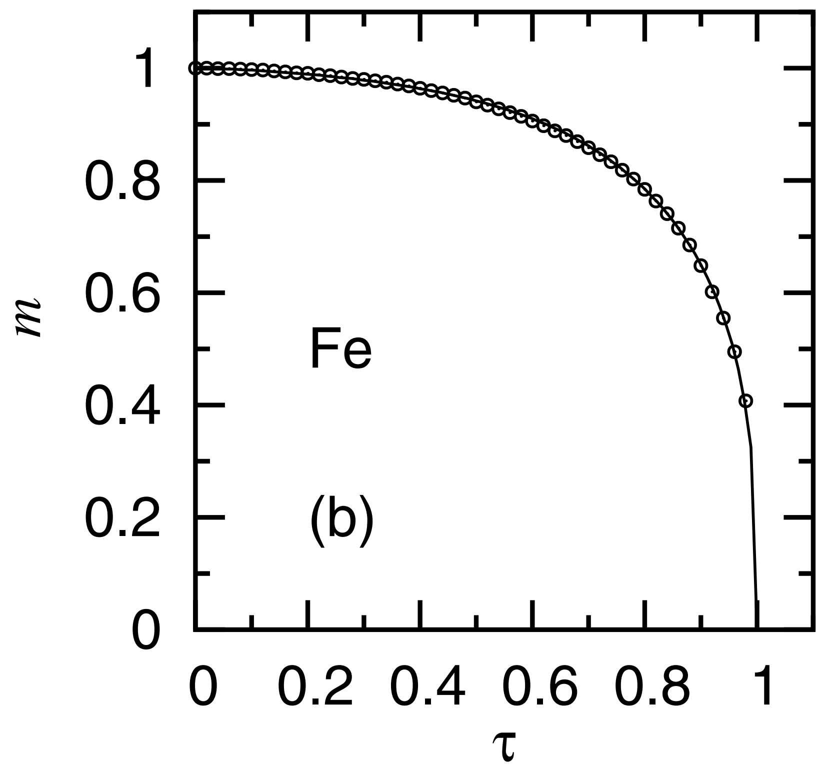
UNIVERSITY *of York*

Evans *et al*, Phys. Rev. B **91**, 144425 (2015)

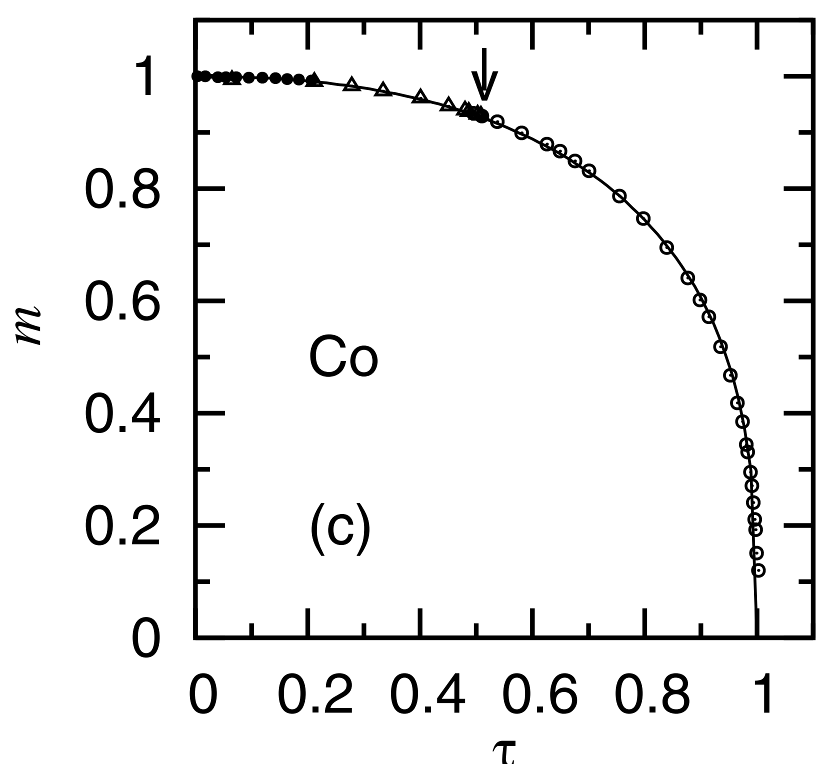
Classical spin model *m(T)* simulation



Real ferromagnets: Kuz'min equation



$$m(\tau) = [1 - s\tau^{3/2} - (1-s)\tau^{p}]^{1/3}$$



Real ferromagnets very different from classical model → problem!

M. D. Kuz'min, Phys. Rev. Lett. **94**, 107204 (2005)

Phenomenological temperature rescaling

Classical model

$$m(T) = (1 - T/T_c)^{\beta}$$

Assume m(T) well fitted by Curie-Bloch equation

$$m(\tau) = (1 - \tau^{\alpha})^{\beta}$$

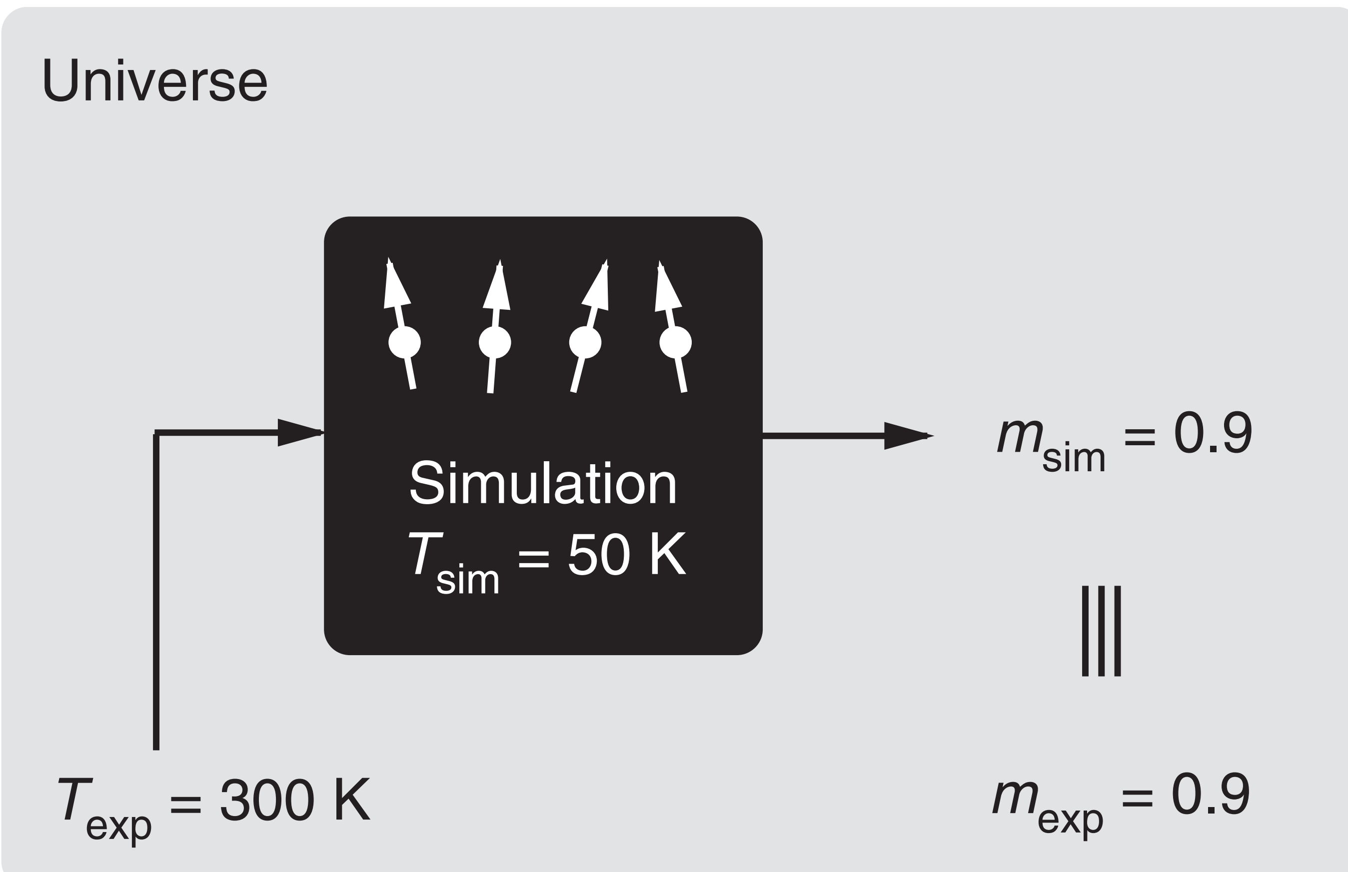
Classical model: $\alpha = 1$

Real ferromagnets: $\alpha \neq 1$

Simplest rescaling:

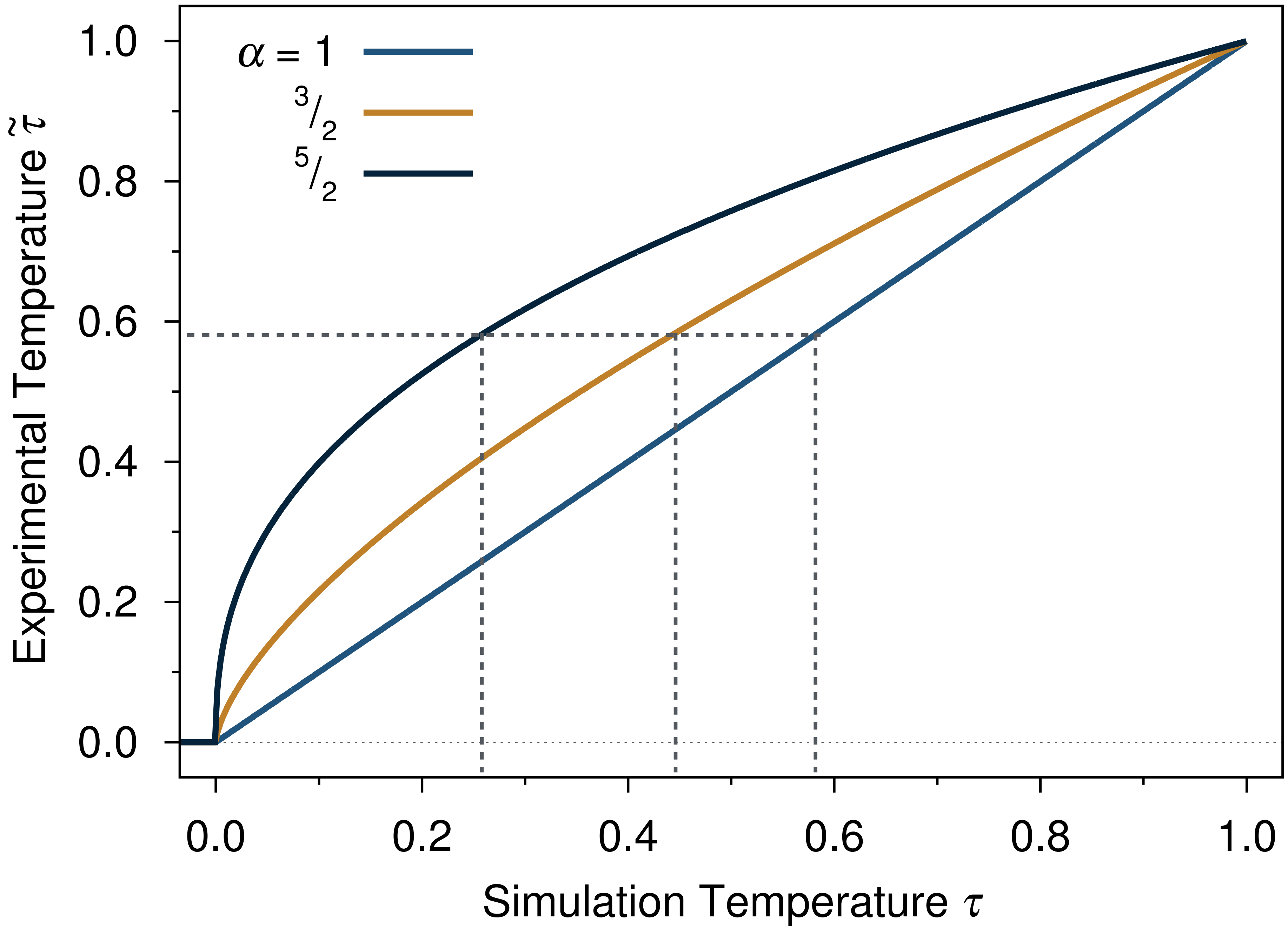
$$\widetilde{\tau} = \tau^{\frac{1}{\alpha}}$$

Spin temperature rescaling (STR) method



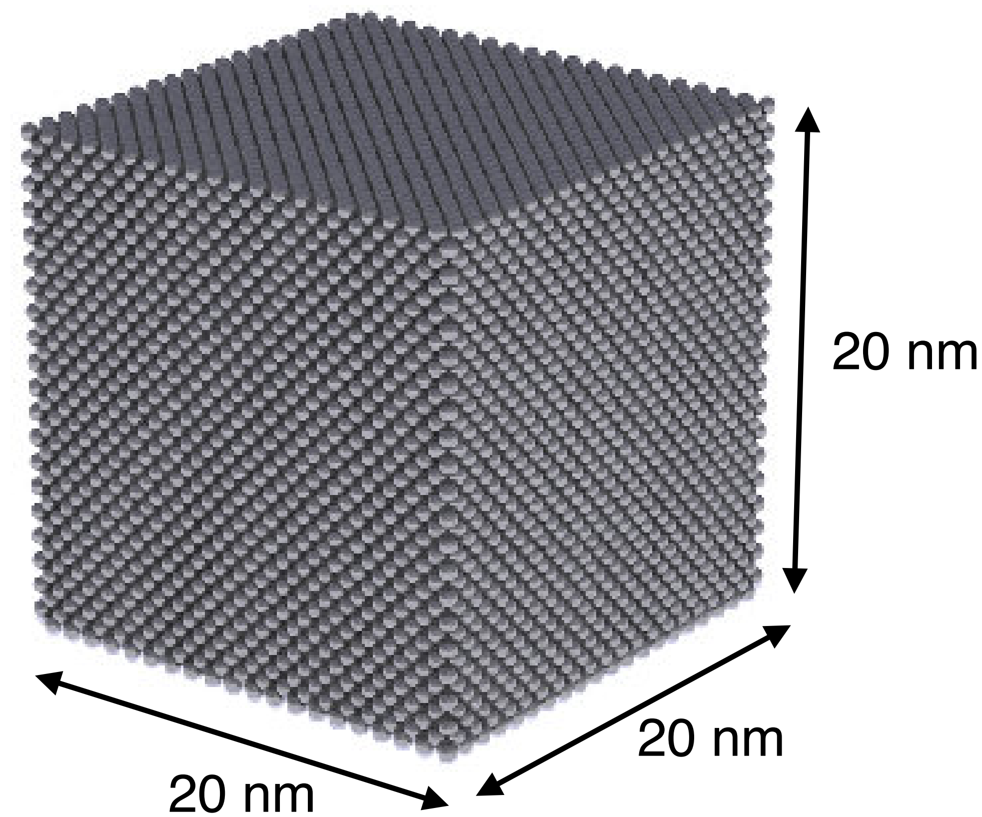
$$\frac{T_{\mathrm{sim}}}{T_{\mathrm{c}}} = \left(\frac{T_{\mathrm{exp}}}{T_{\mathrm{c}}}\right)^{\alpha}$$

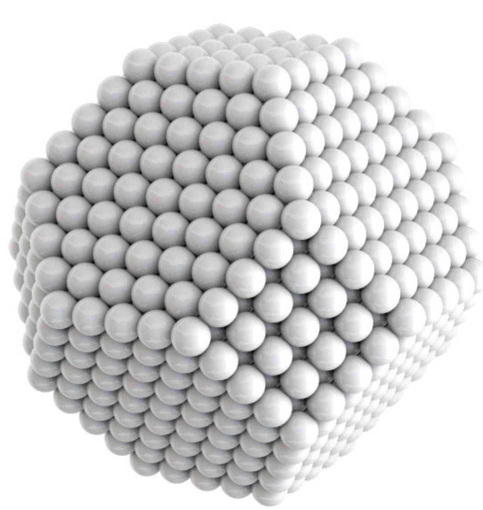
Spin temperature rescaling (STR) method



Classical spin model with Heisenberg exchange

$$\mathcal{H}_{\mathrm{exc}} = -\sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

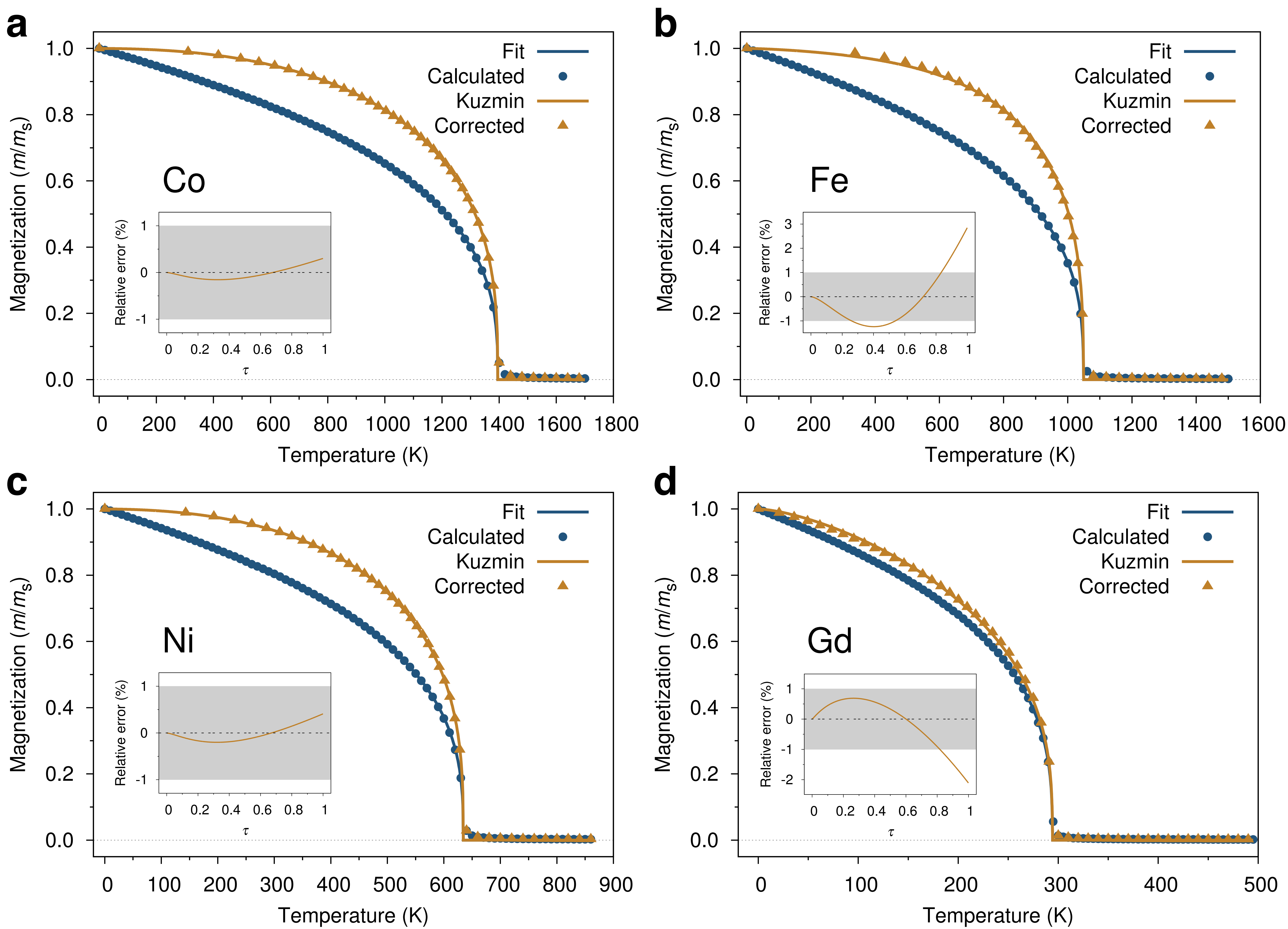




VAMPIRE

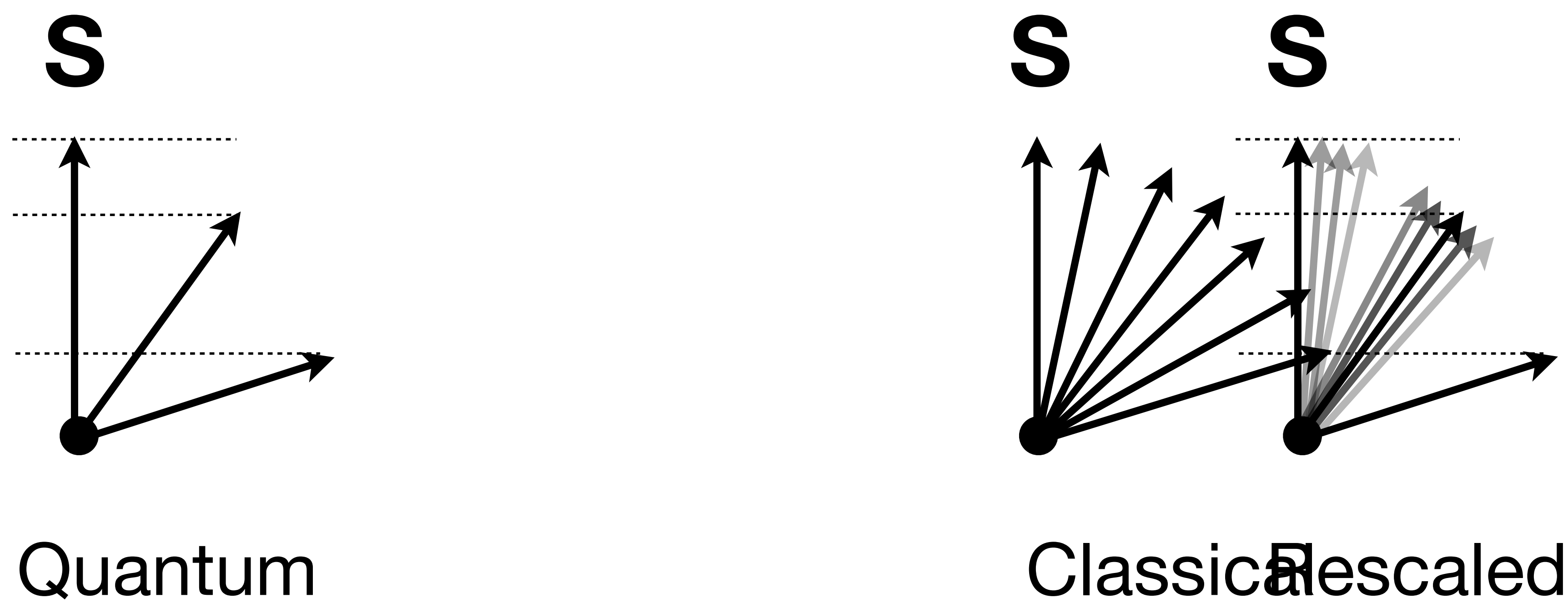
vampire.york.ac.uk

R F L Evans *et al*, J. Phys.: Condens. Matter **26** 103202 (2014)



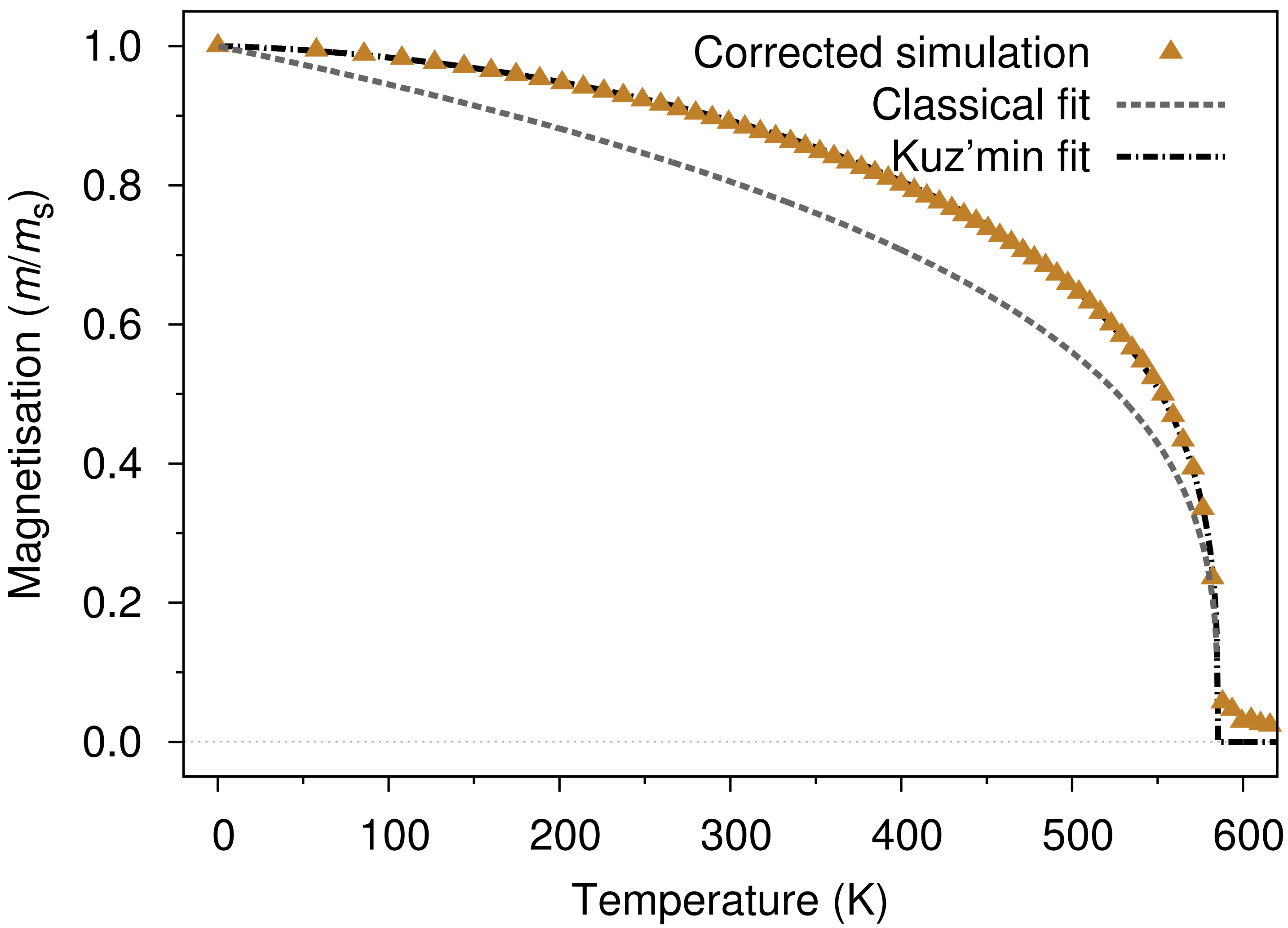
a
b
c
d
Co
Fe
Ni
Gd
Fit
Calculated
Kuzmin
Corrected
Magnetization (m/m_s)
Temperature (K)
Relative error (%)
τ

Physical picture of temperature rescaling



Back to NdFeB

Apply temperature rescaling to achieve exact agreement with experimental M_s(T)



Temperature rescaling

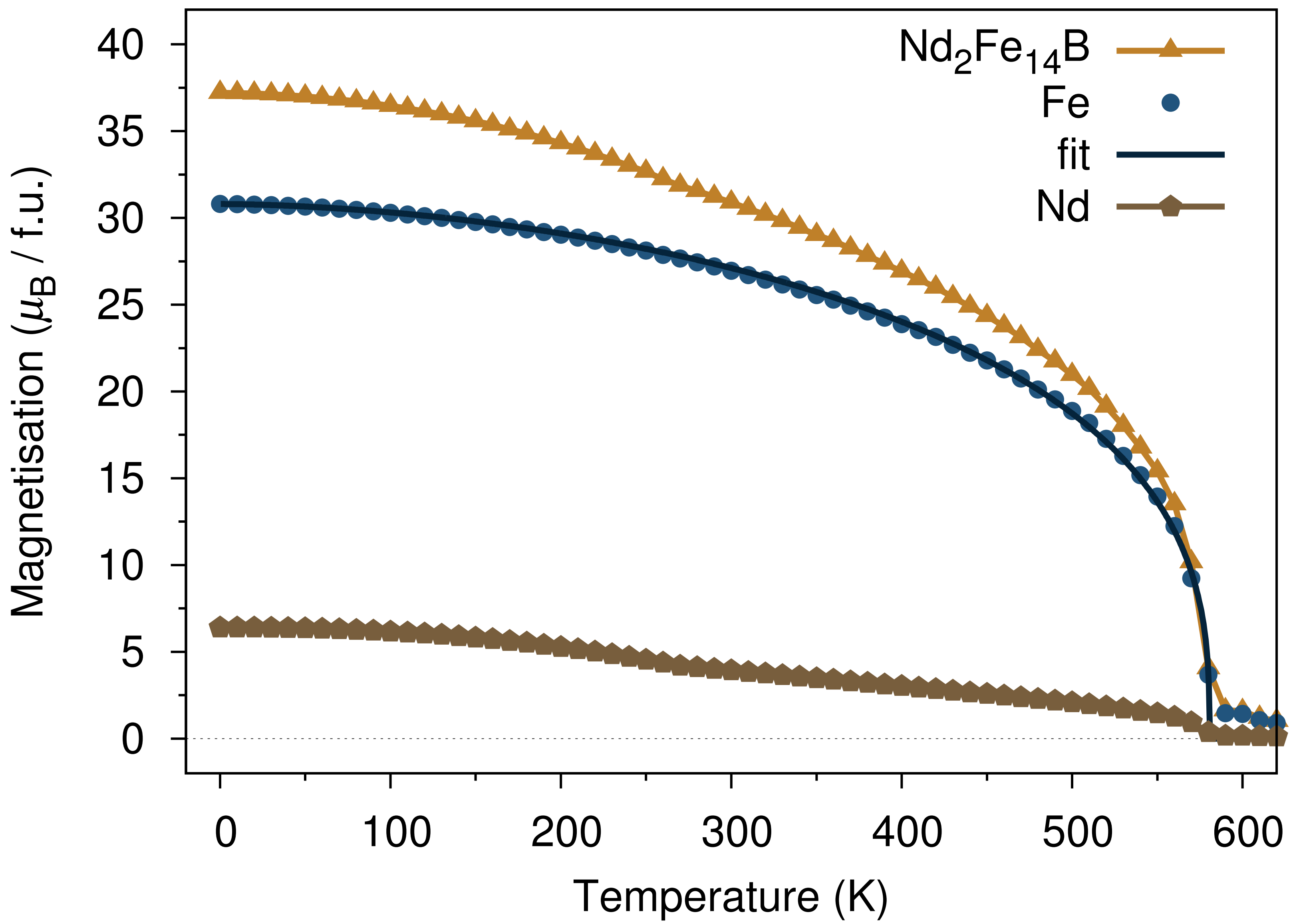
$$m(\tau) = (1 - \tau^{\alpha})^{\beta}$$

$$\frac{T_{\rm sim}}{T_{\rm c}} = \left(\frac{T_{\rm exp}}{T_{\rm c}}\right)^{\alpha}$$

R. F. L. Evans *et al*,

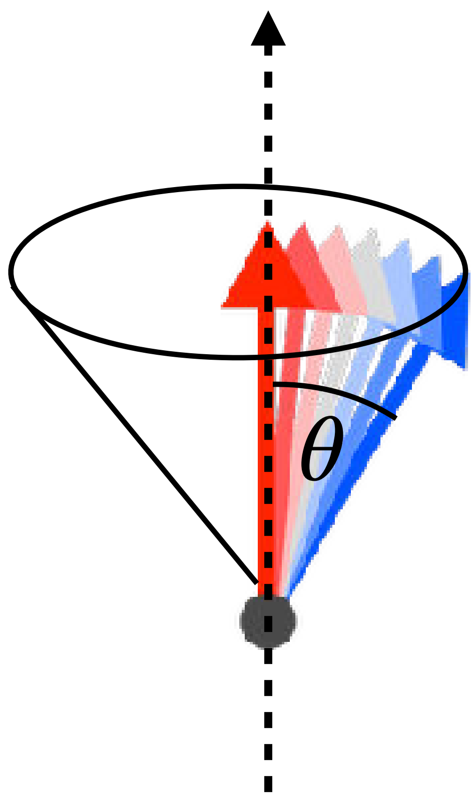
Phys. Rev. B **91**, 144425 (2015)

Temperature dependent magnetization with temperature rescaling

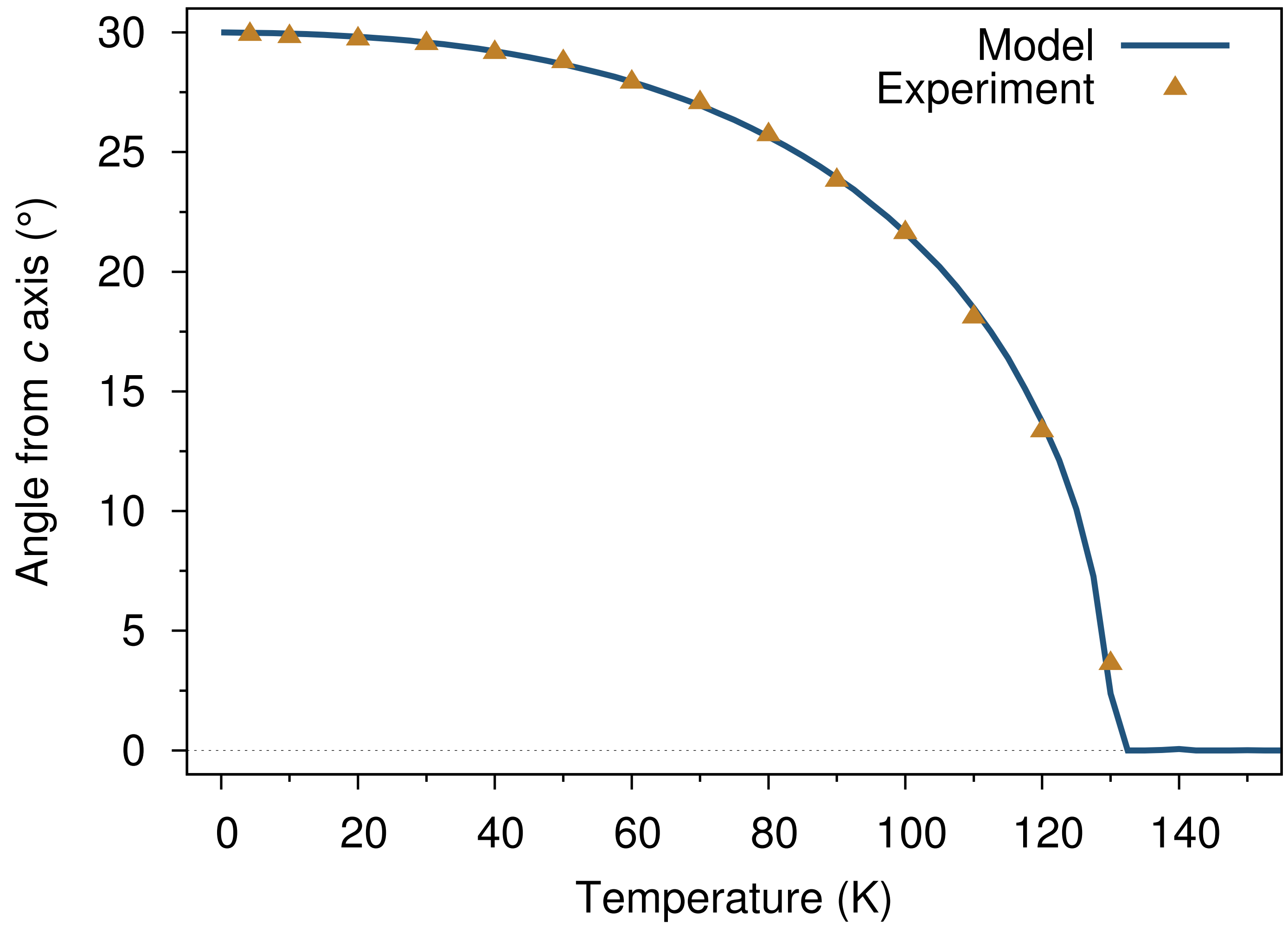


UNIVERSITY of York

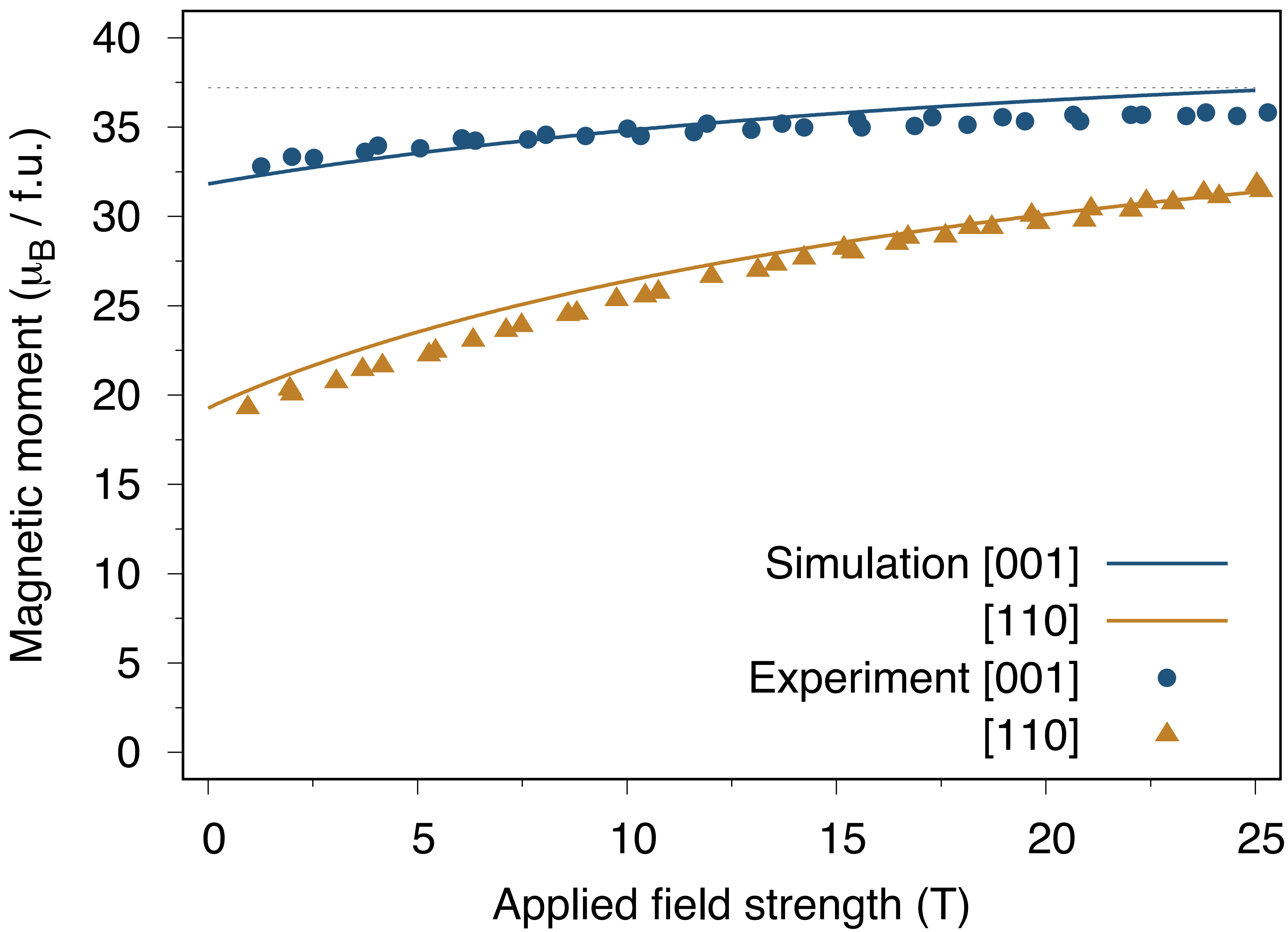
Spin-reorientation transition



$$E_i^{k,\mathrm{Nd}} = -\kappa_2^{\mathrm{Nd}} \widetilde{P}_2 - \kappa_4^{\mathrm{Nd}} \widetilde{P}_4$$

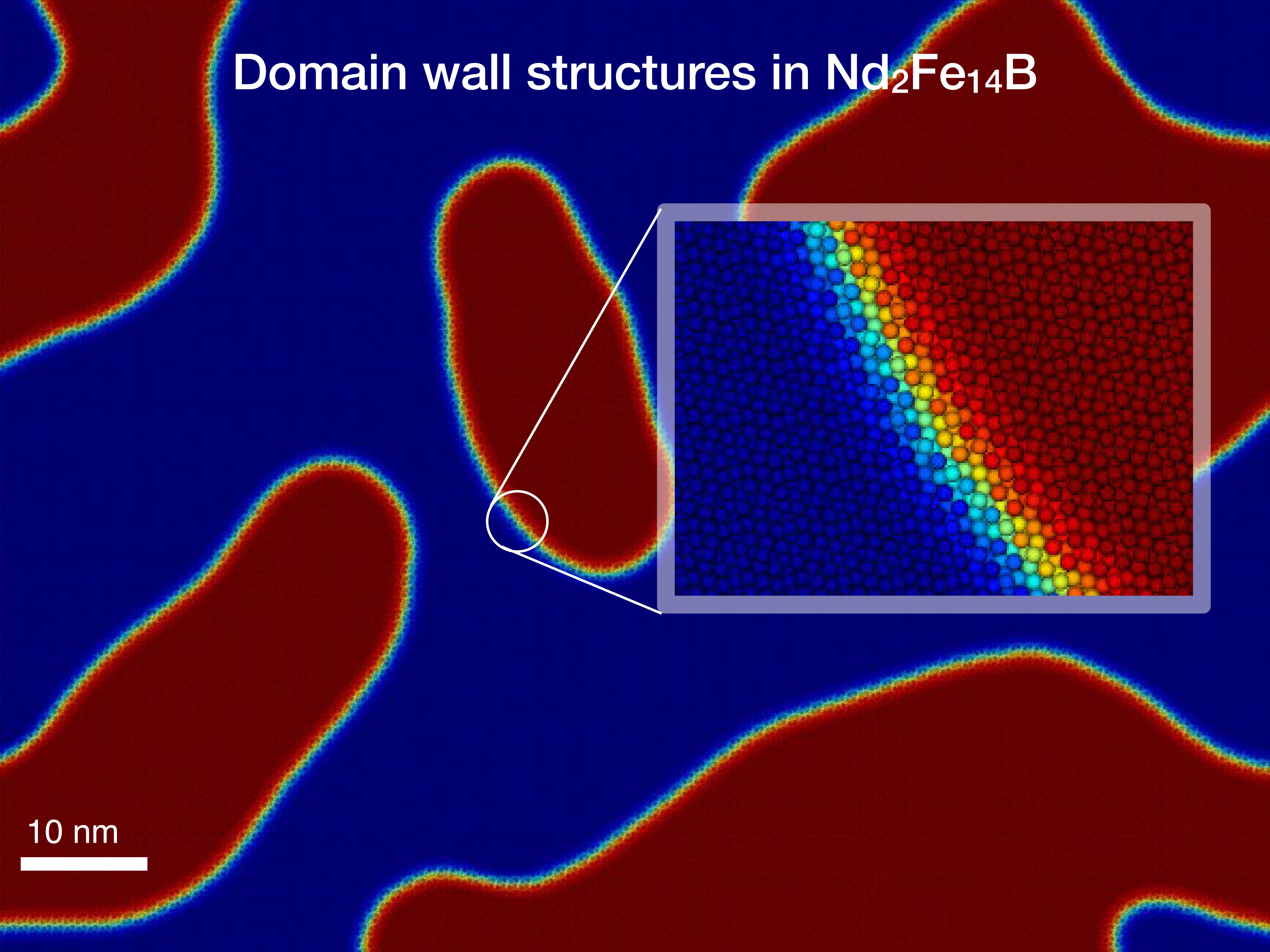


Anisotropy field calculation

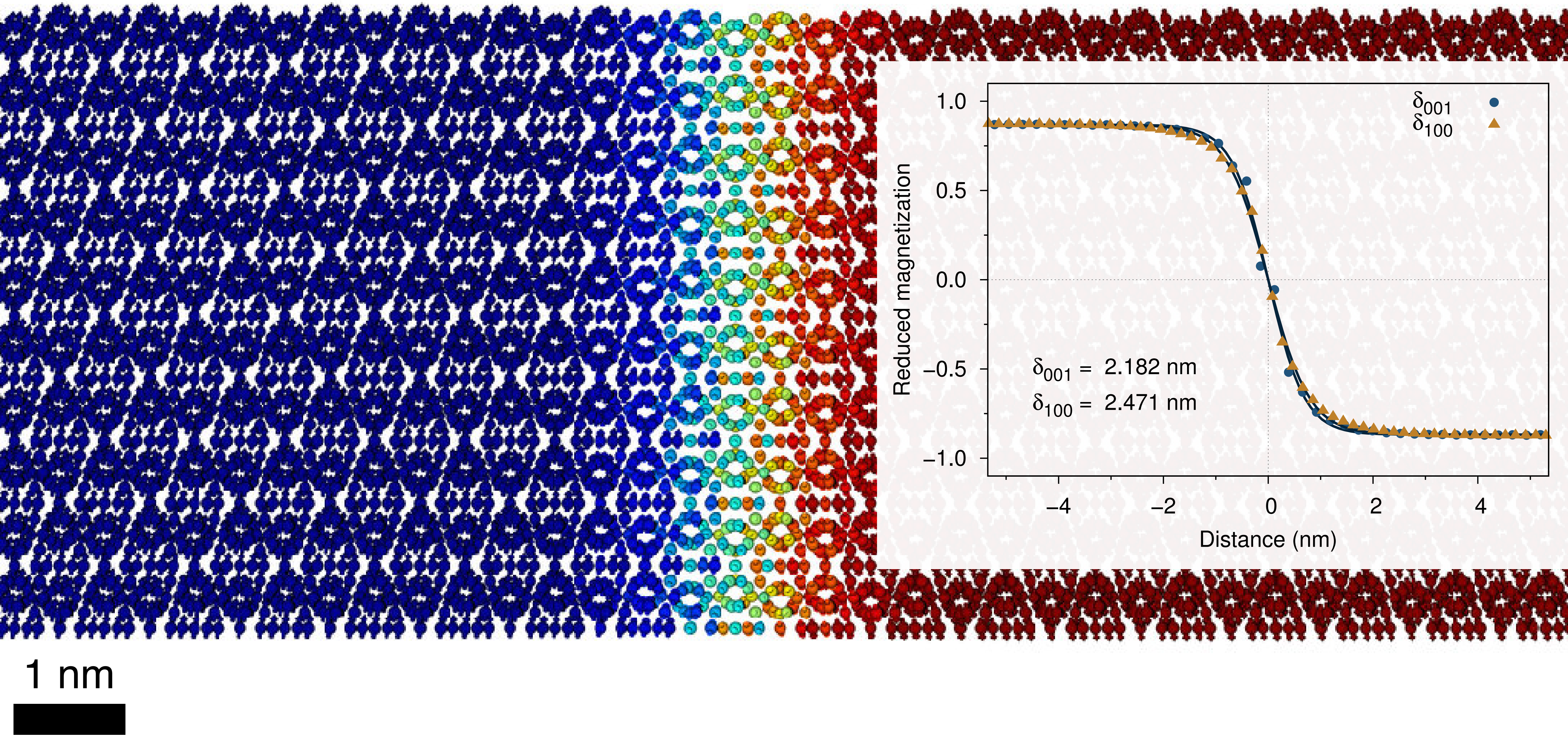


UNIVERSITY of York

Domain wall structures in $Nd_2Fe_{14}B$

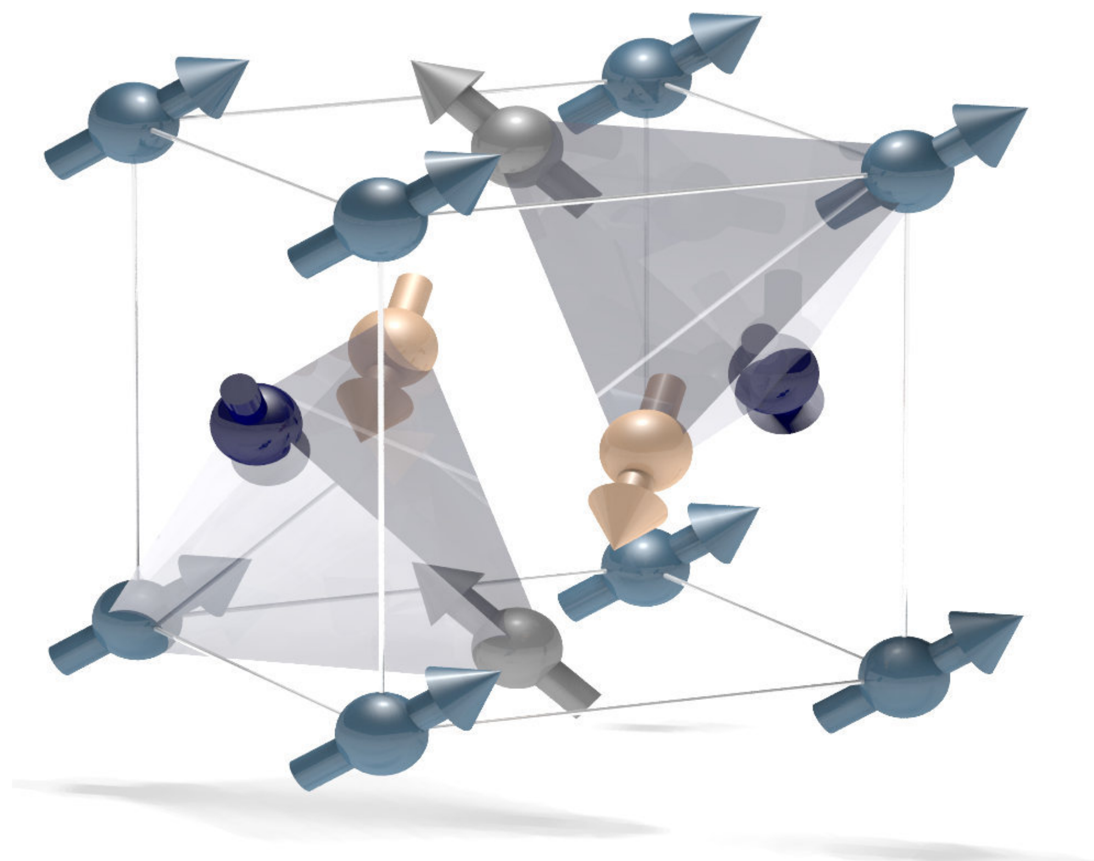


Domain wall profile



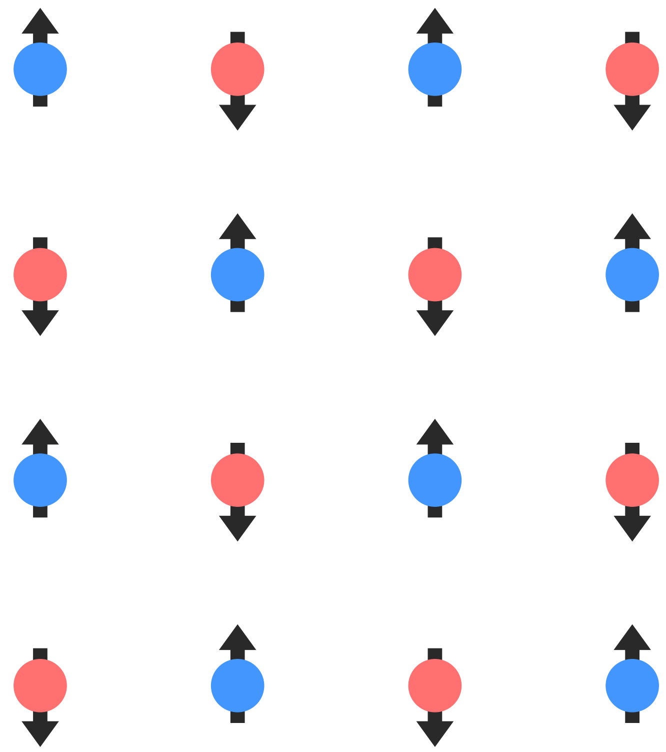
UNIVERSITY of York

Temperature dependent properties and dynamics of $IrMn_3$ antiferromagnets



Sarah Jenkins and Richard F L Evans

Simple antiferromagnets



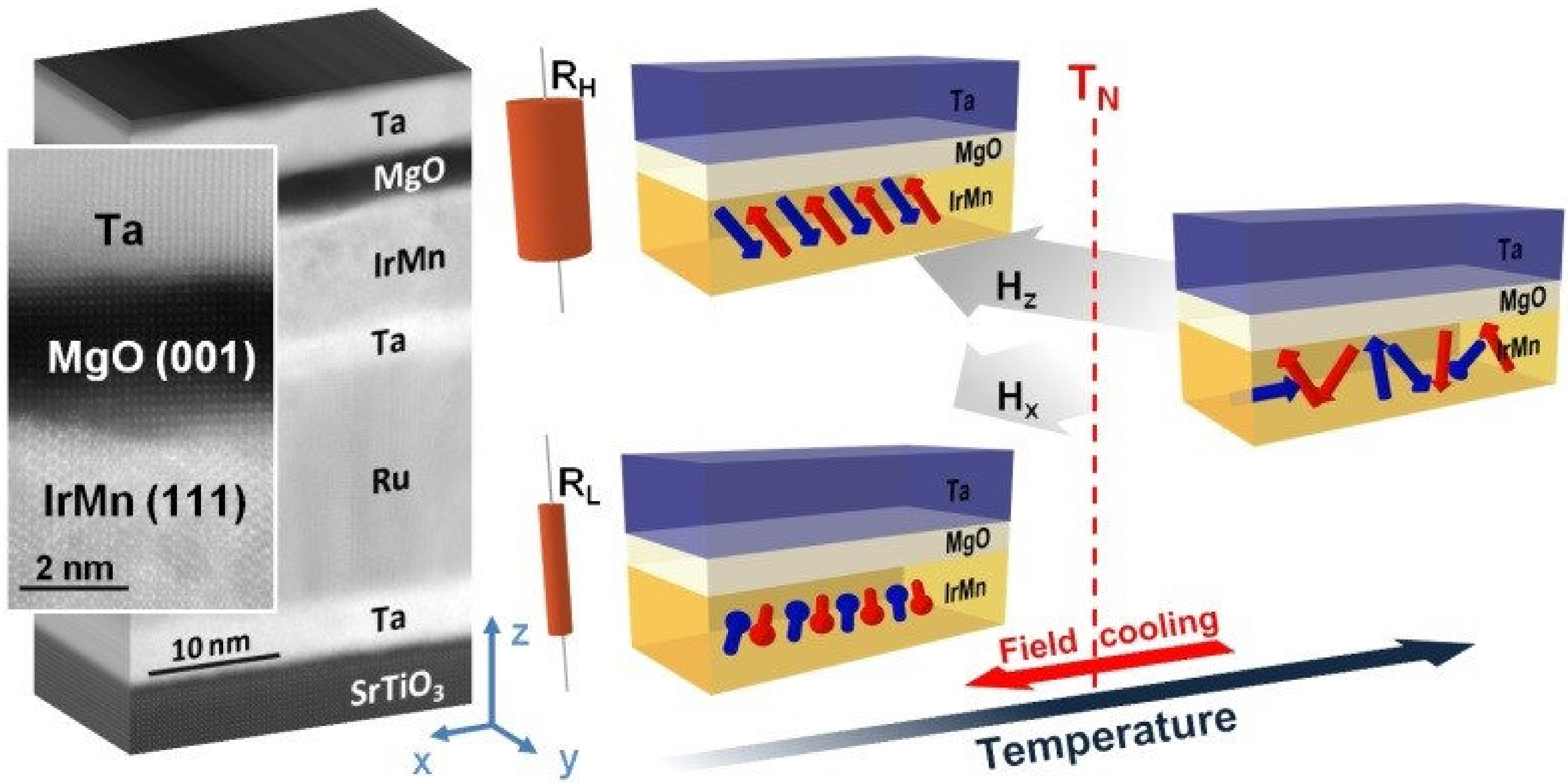
- ‘Simple’ antiferromagnets consist of two magnetic sublattices
- Total magnetic moment is zero (macroscopically)
- Can consider two antiparallel contributions from each ‘colour’ of spin

$$\mathbf{m}_a = \sum_a \mathbf{S}_a \qquad \mathbf{m}_b = \sum_b \mathbf{S}_b$$

- This is called the **sublattice magnetization**
- The Néel vector *n* is the equivalent order parameter for antiferromagnets

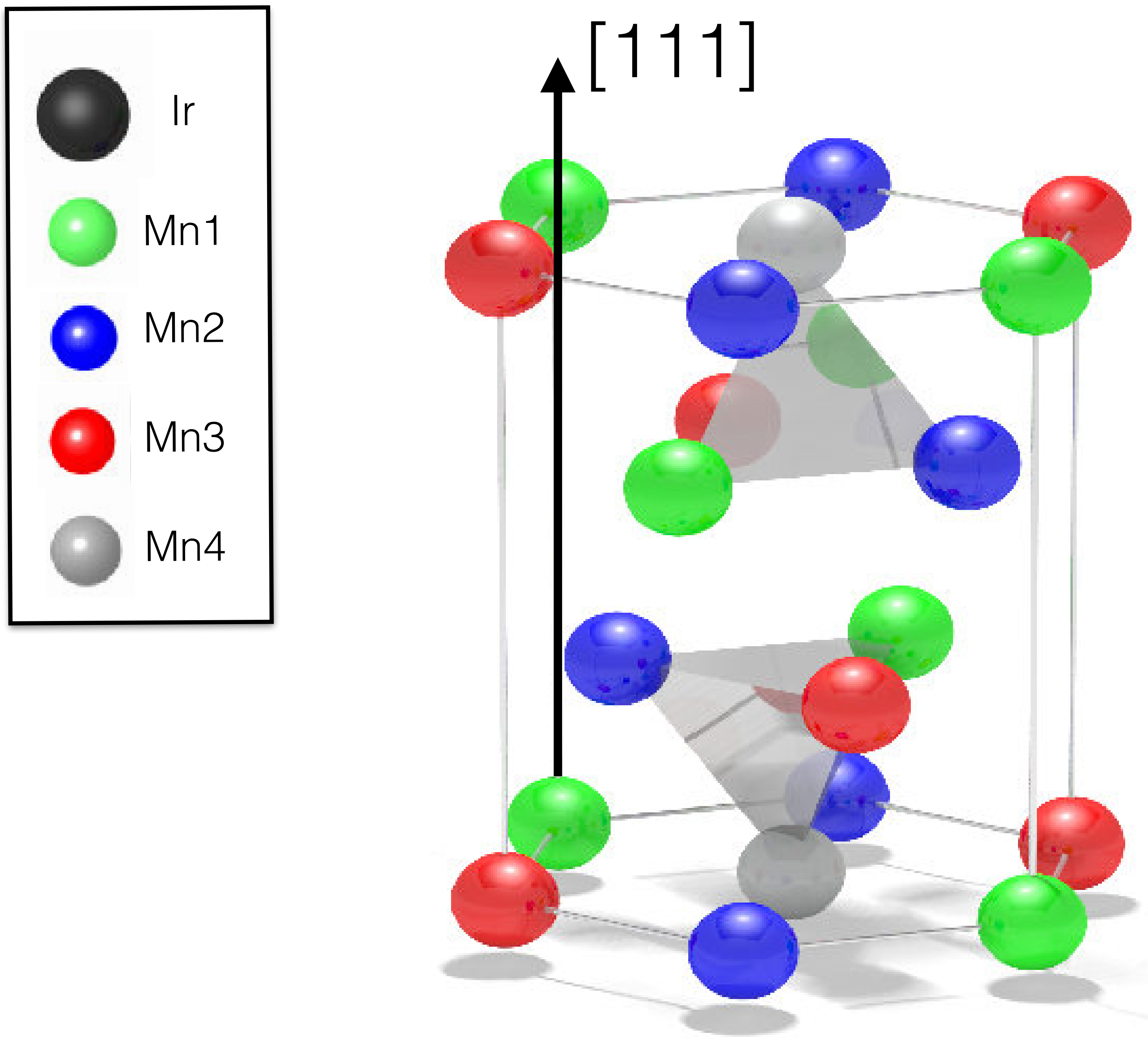
$$\mathbf{n} = \mathbf{m}_a - \mathbf{m}_b$$

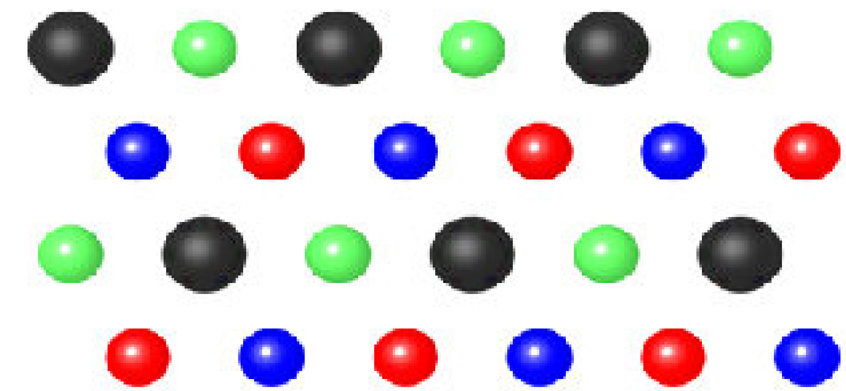
Motivation: exchange bias and antiferromagnetic spintronics



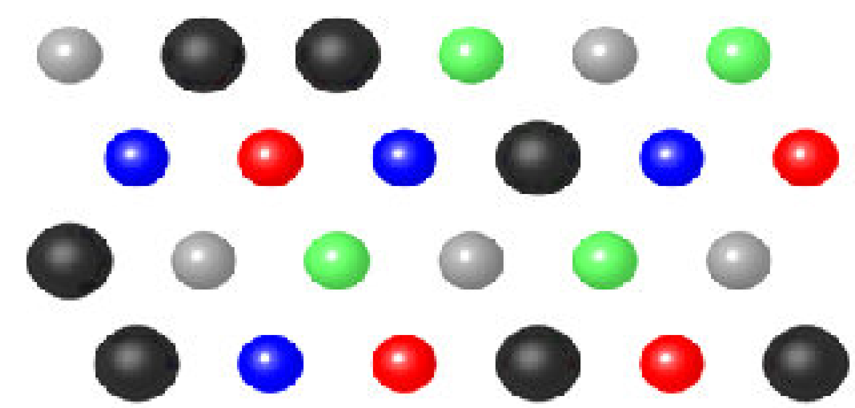
http://nabis.fisi.polimi.it/research-areas/antiferromagnet-spintronics/

Crystallographic structure





Ordered L1$_2$ IrMn$_3$



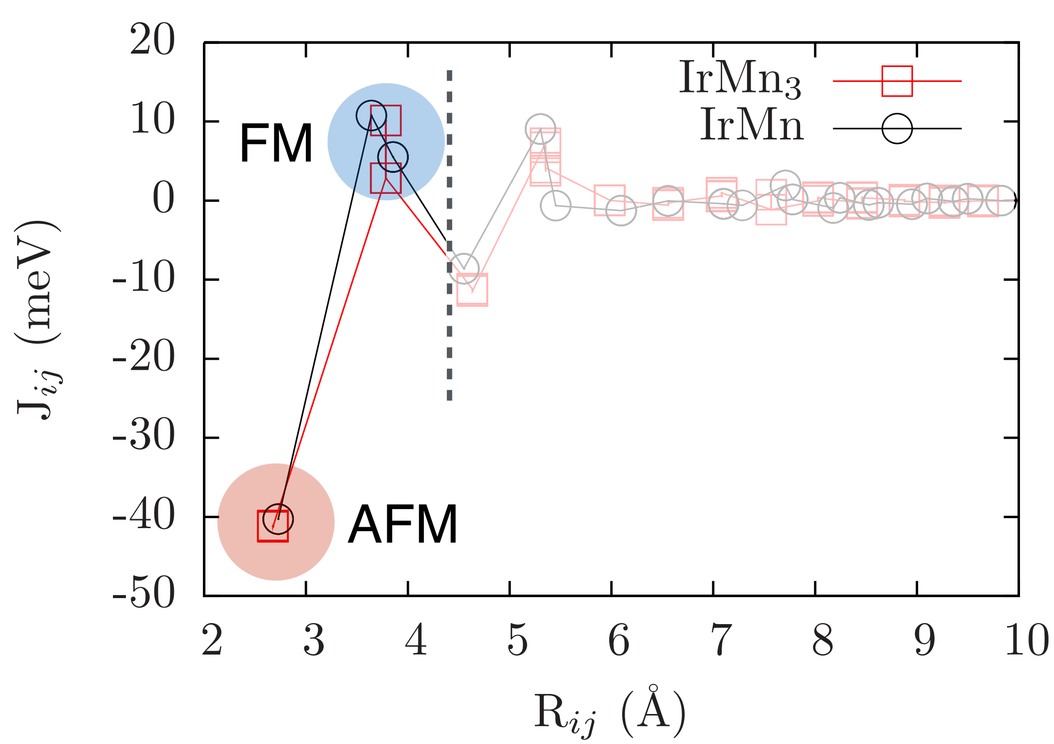
Disordered γIrMn$_3$

UNIVERSITY of York

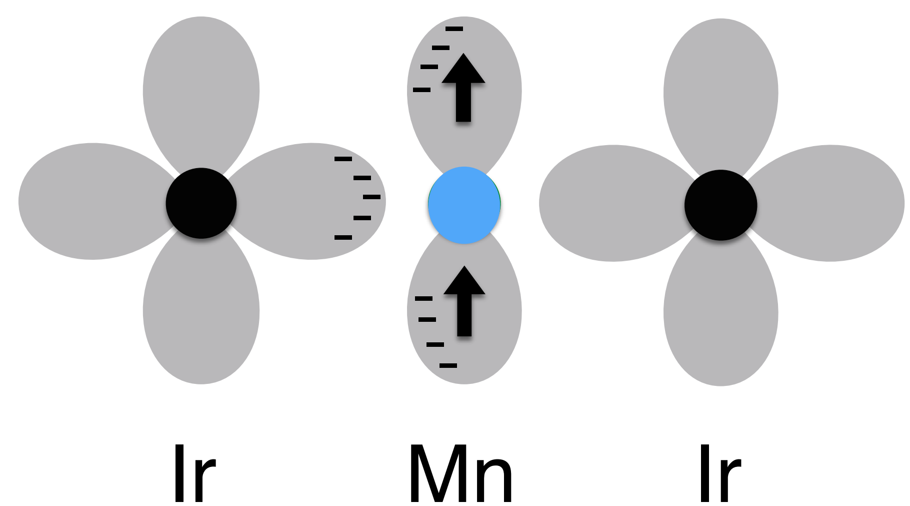
Atomistic spin model

$$\mathscr{H} = -\sum_{i<j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \frac{k_N}{2}\sum_{i \neq j}^{z} (\mathbf{S}_i \cdot \mathbf{e}_{ij})^2$$

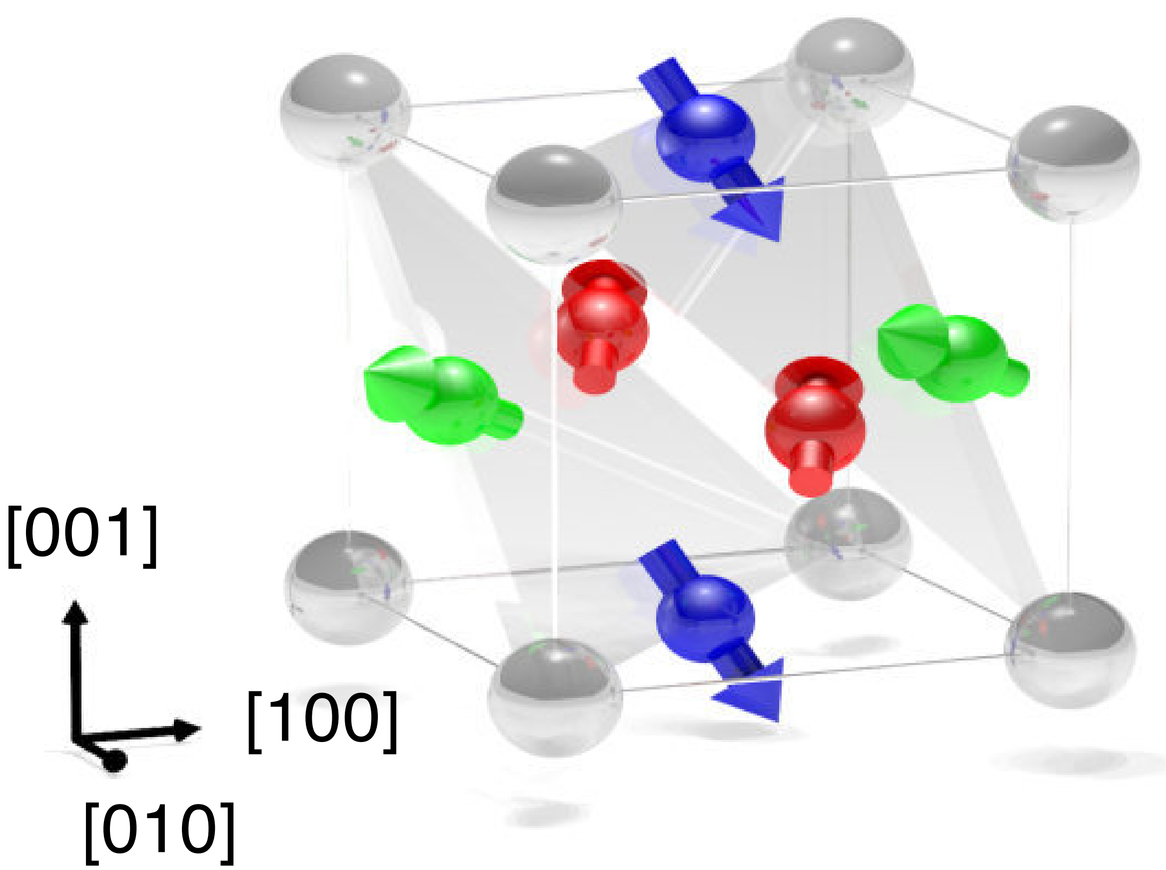
J_{NN}-J_{NNN} model



Néel pair anisotropy

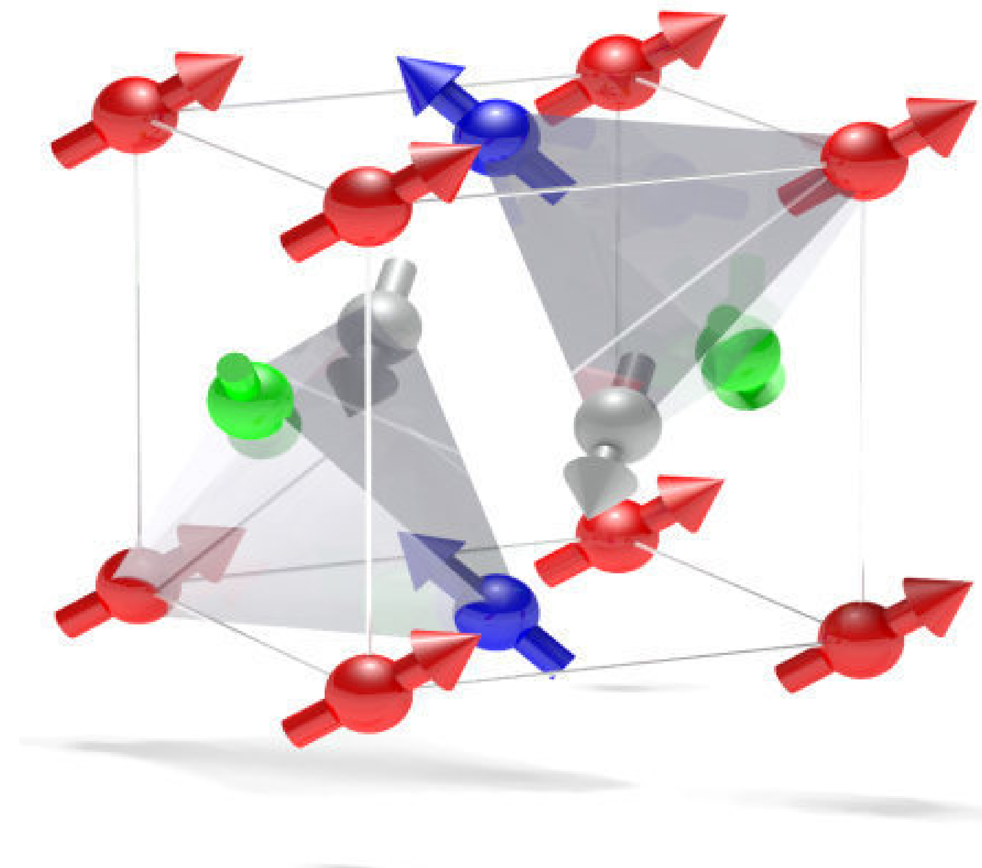


Simulated ground state structures



L1$_2$ - IrMn$_3$

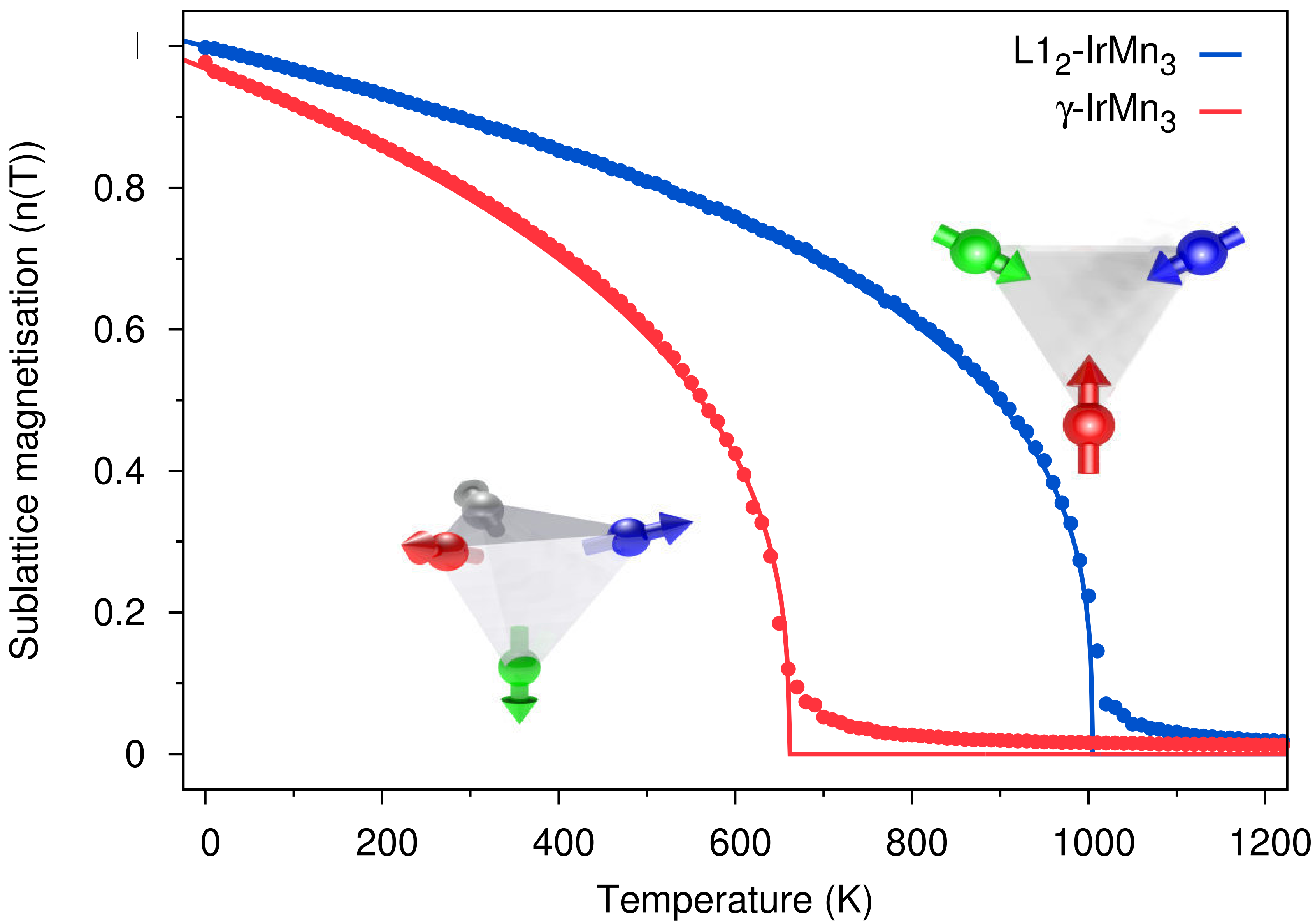
Triangular (T1)



γ - IrMn$_3$

Tetrahedral (3Q)

Simulated Néel temperatures



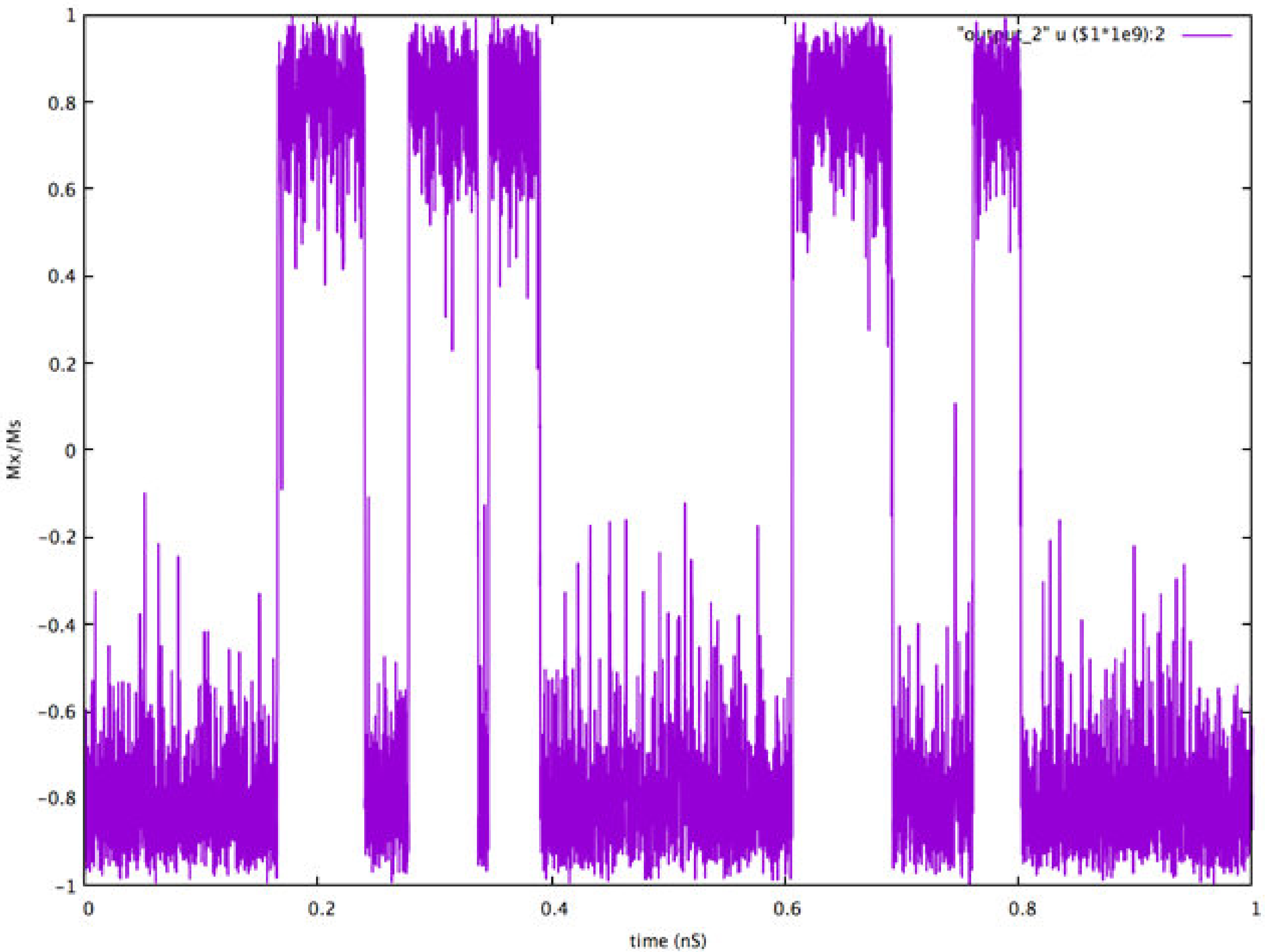
Ordered $L1_2$ $IrMn_3$

T_N = 1000 K

Disordered γ $IrMn_3$

T_N = 680 K

Use spin dynamics to calculate switching rate for small system near blocking temperature



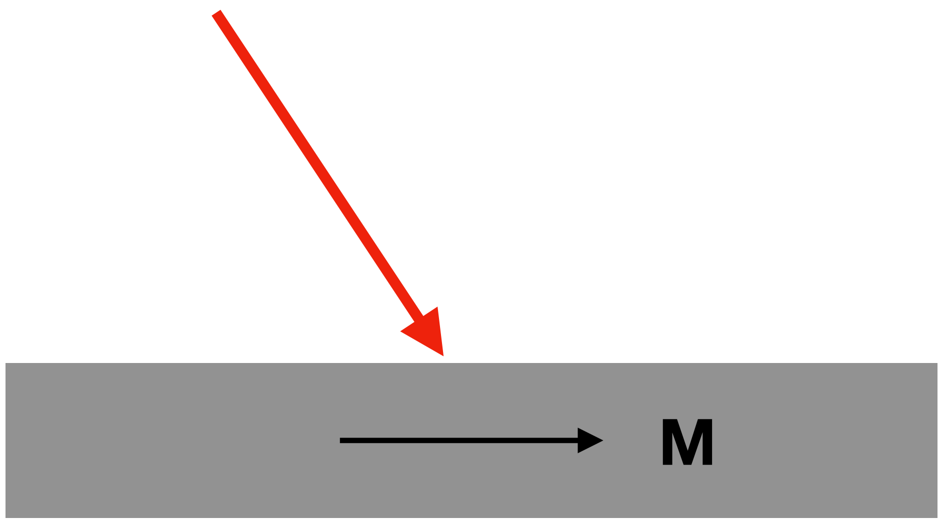
Much higher attempt frequency than equivalent ferromagnets (~10^{10})

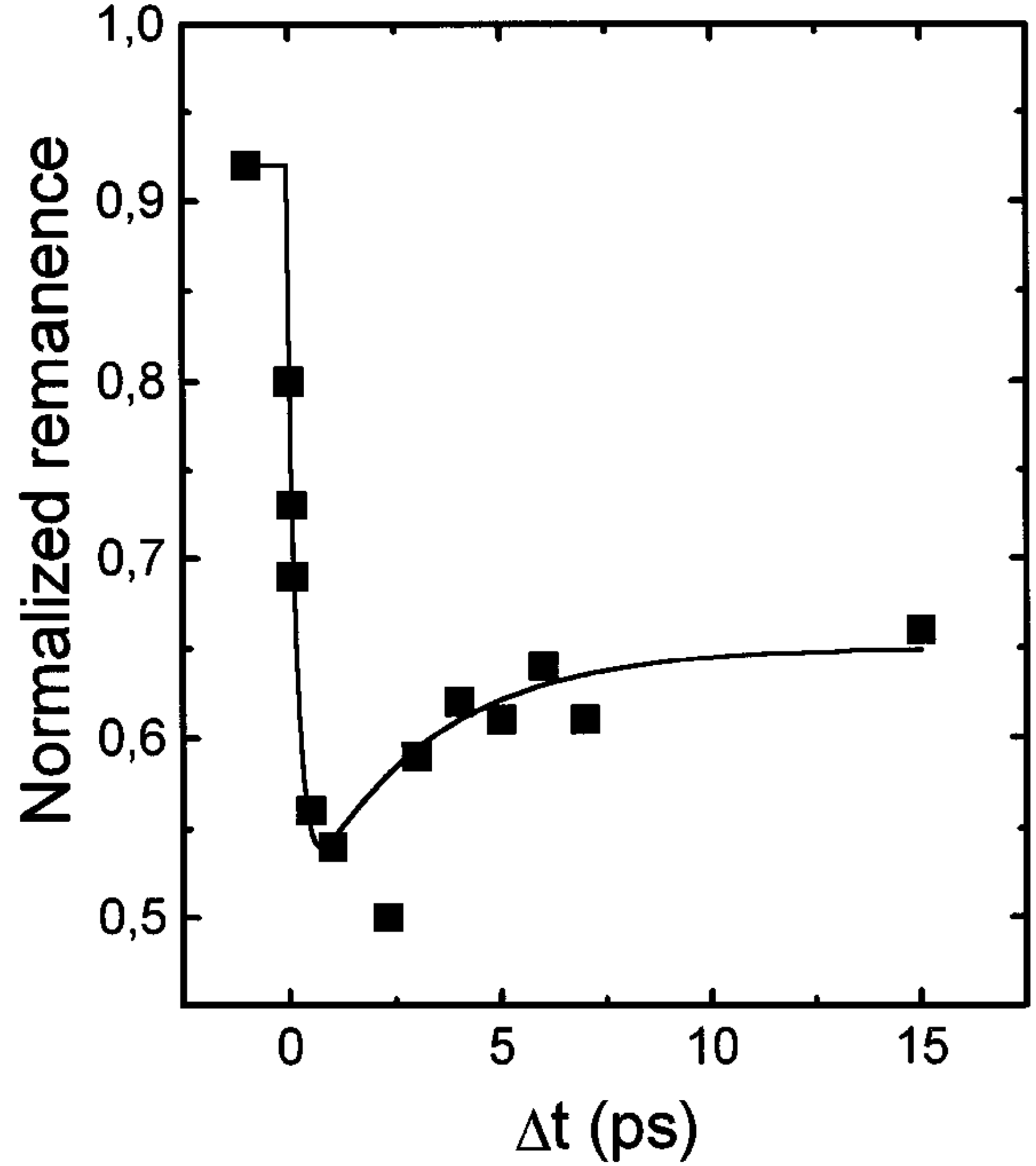
$\tau_0 = 3.84 \times 10^{11}$

Thermodynamics of ultrafast magnetization processes

Ultrafast demagnetization in Ni

Laser excitation

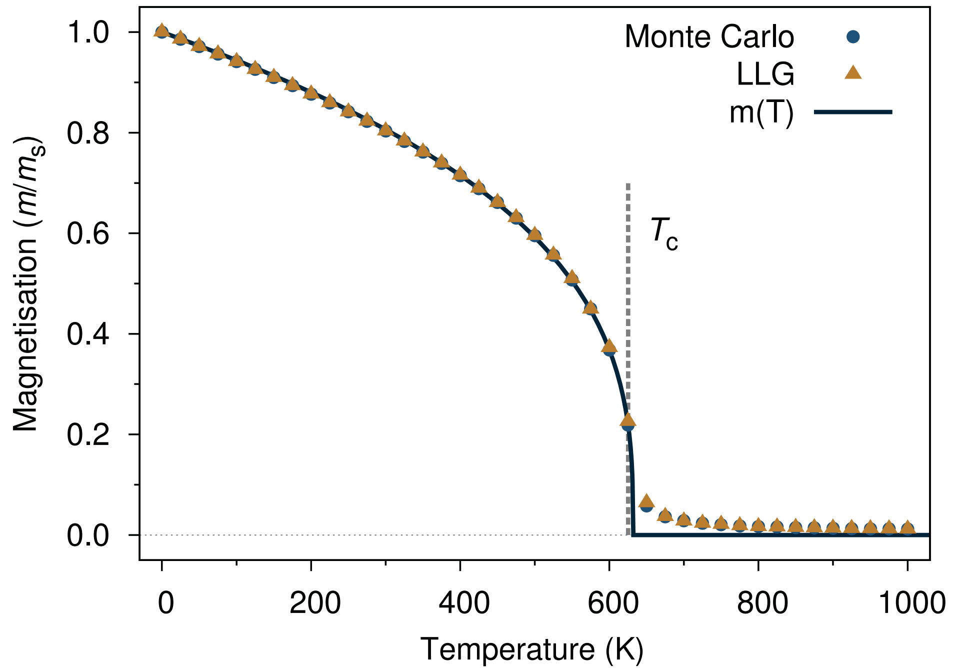


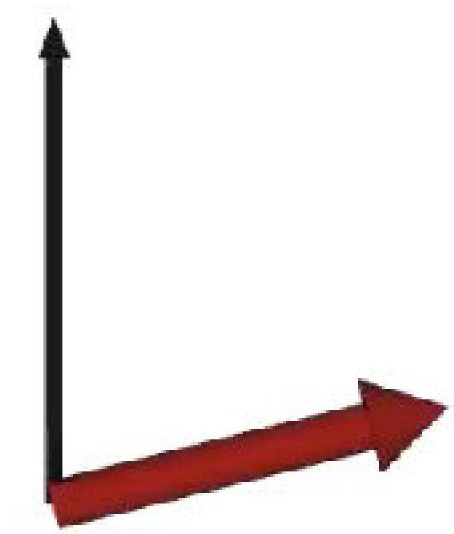


E. Beaurepaire et al, Phys. Rev. Lett. **76** 4250 (1996)

Origin of thermal fluctuations in the atomistic model

- Lets go back to the thermal fluctuations in the atomic model



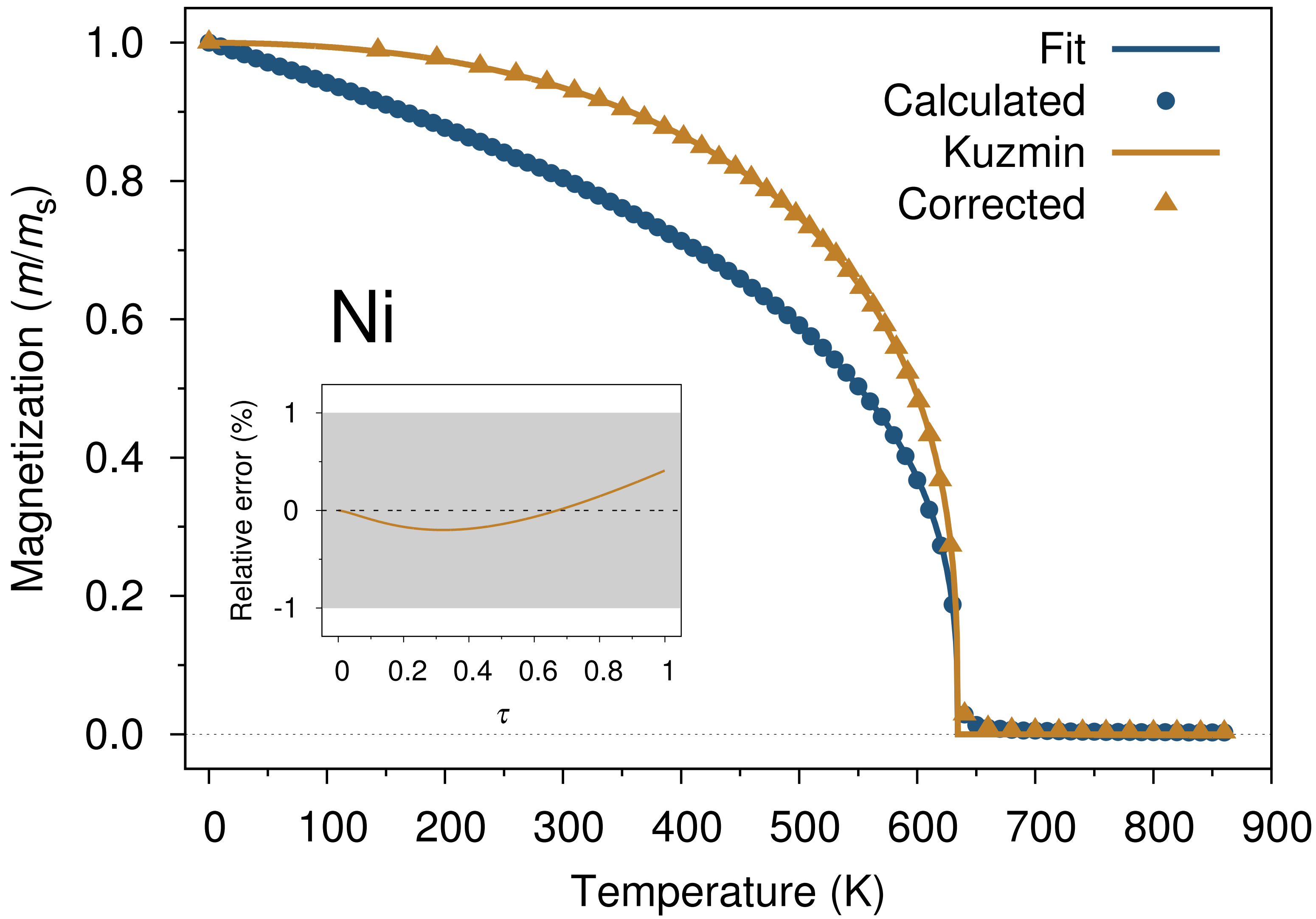


- Physically caused by spin scattering phenomena
  - electron-spin, spin-phonon, spin-photon

- Laser interaction causes heating of the electrons and more scattering events -> fast increase in the effective temperature in the material

Equilibrium properties of Ni

- Use spin temperature rescaling to accurately reproduce temperature dependent magnetization



Evans *et al*, Phys. Rev. B **91**, 144425 (2015)

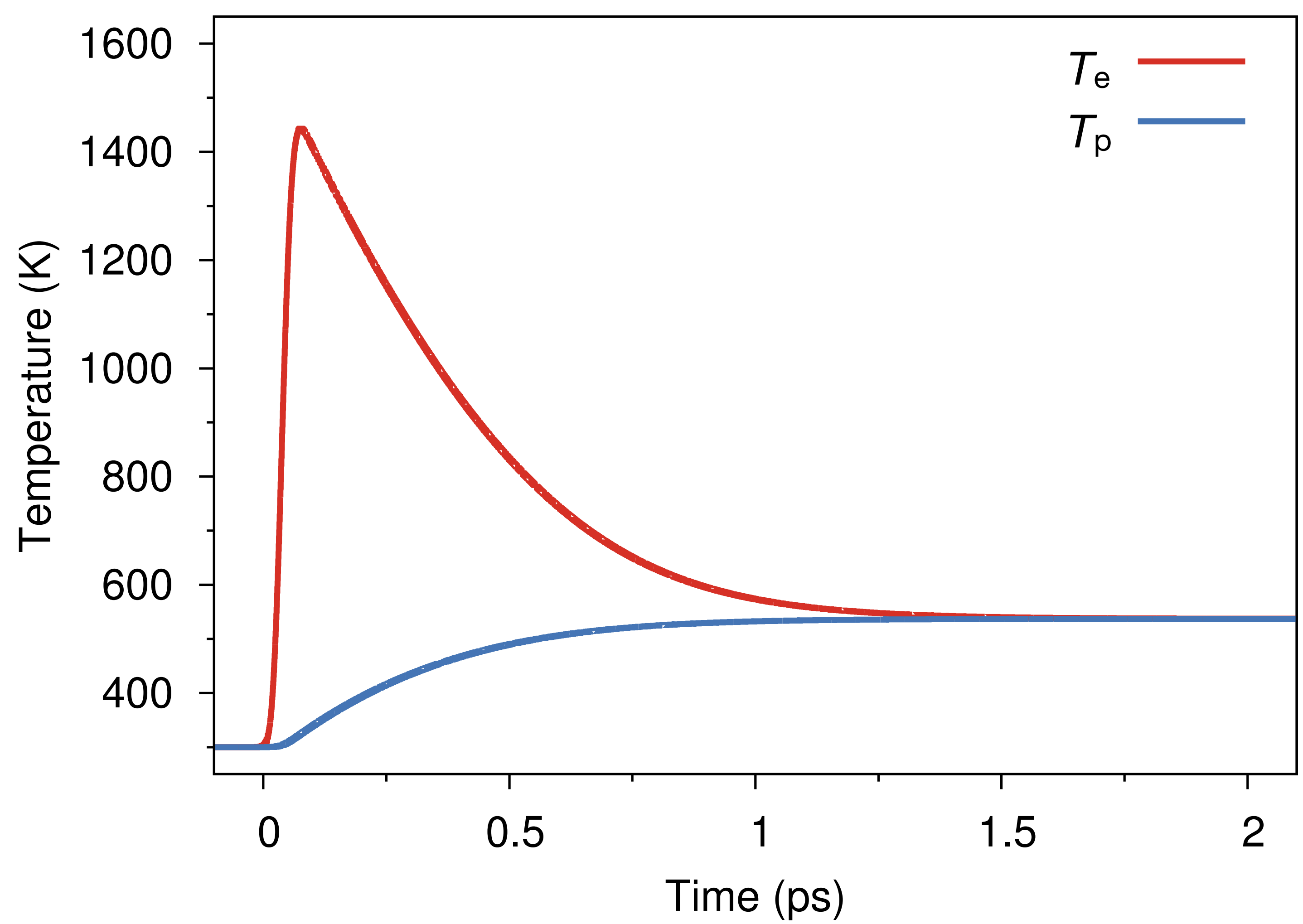
Simulating a laser pulse: two temperature model

$$C_e \frac{\partial T_e}{\partial t} = -G(T_e - T_p) + S(t)$$

$$C_p \frac{\partial T_p}{\partial t} = -G(T_p - T_e)$$

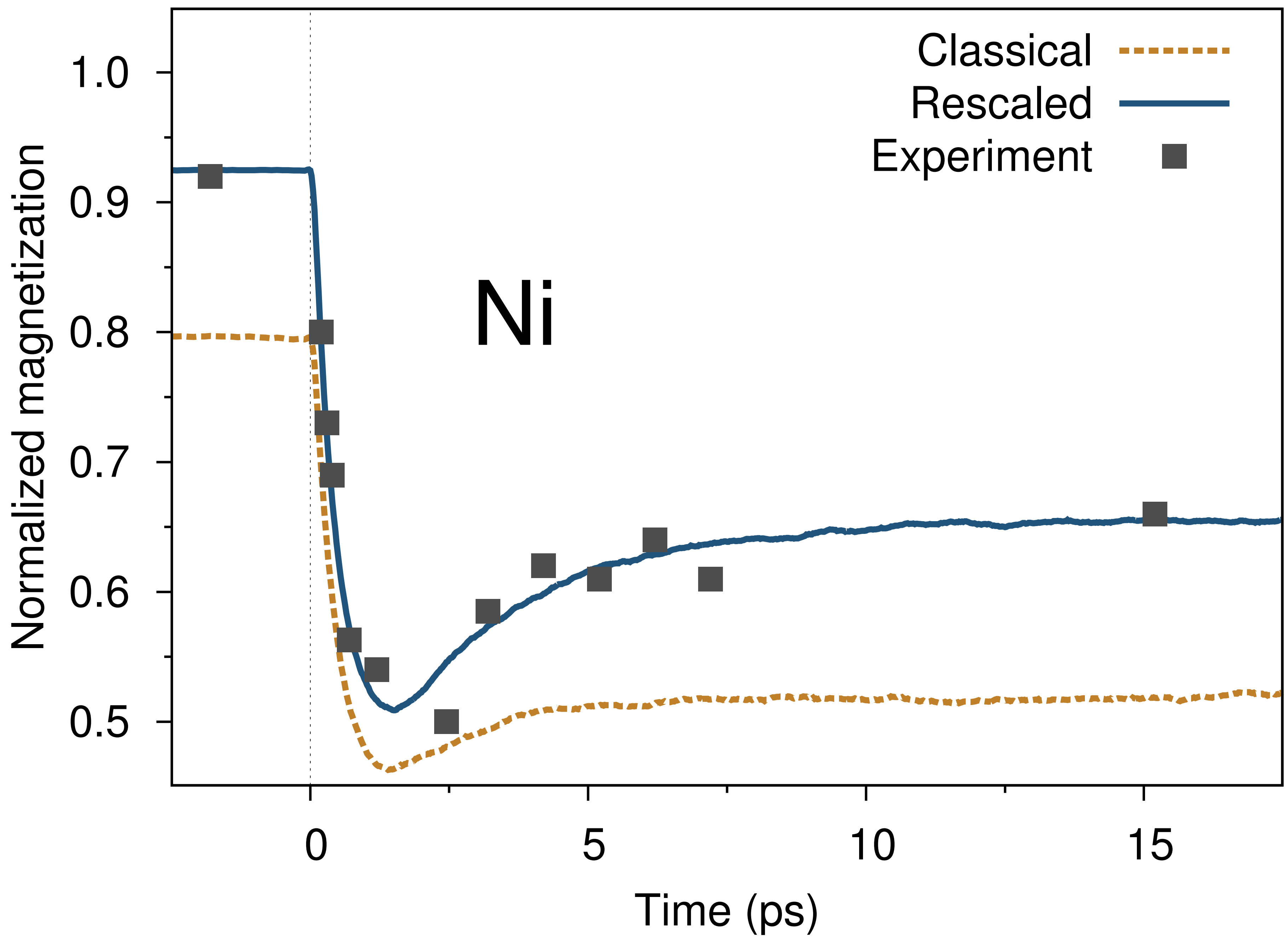
Free electron approximation

$$C_e = C_0 T_e$$



S. Anisimov, B. Kapeliovich, and T. Perelman, Sov. Phys. JETP **39**, 375 (1974).

Ultrafast demagnetization in Ni



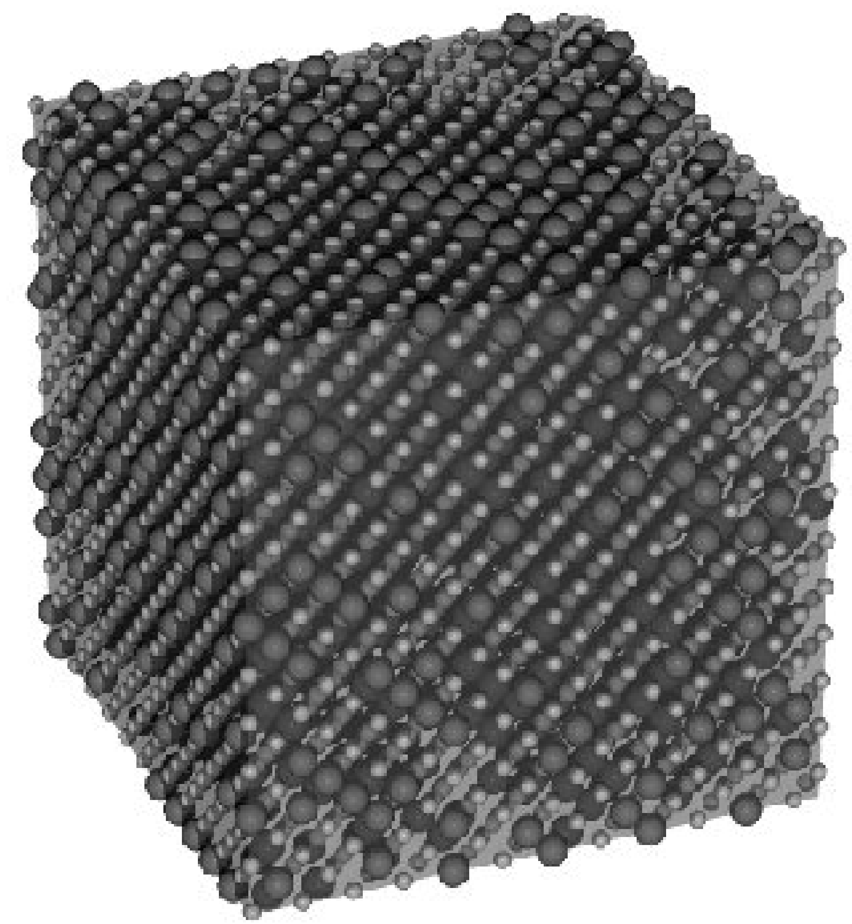
damping-constant = 0.001

E. Beaurepaire *et al*, Phys. Rev. Lett. **76**, 4250 (1996)

R. F. L. Evans *et al*, Phys. Rev. B **91**, 144425 (2015)

What about magnetic alloys?

- Ni shows ultrafast response to a laser excitation?
- What about alloys? How do different magnetic moments inside a material respond to ultrafast laser excitation?
- Consider permalloy - alloy of 80% Ni, 20% Fe
- With XMCD can measure response of each sublattice separately



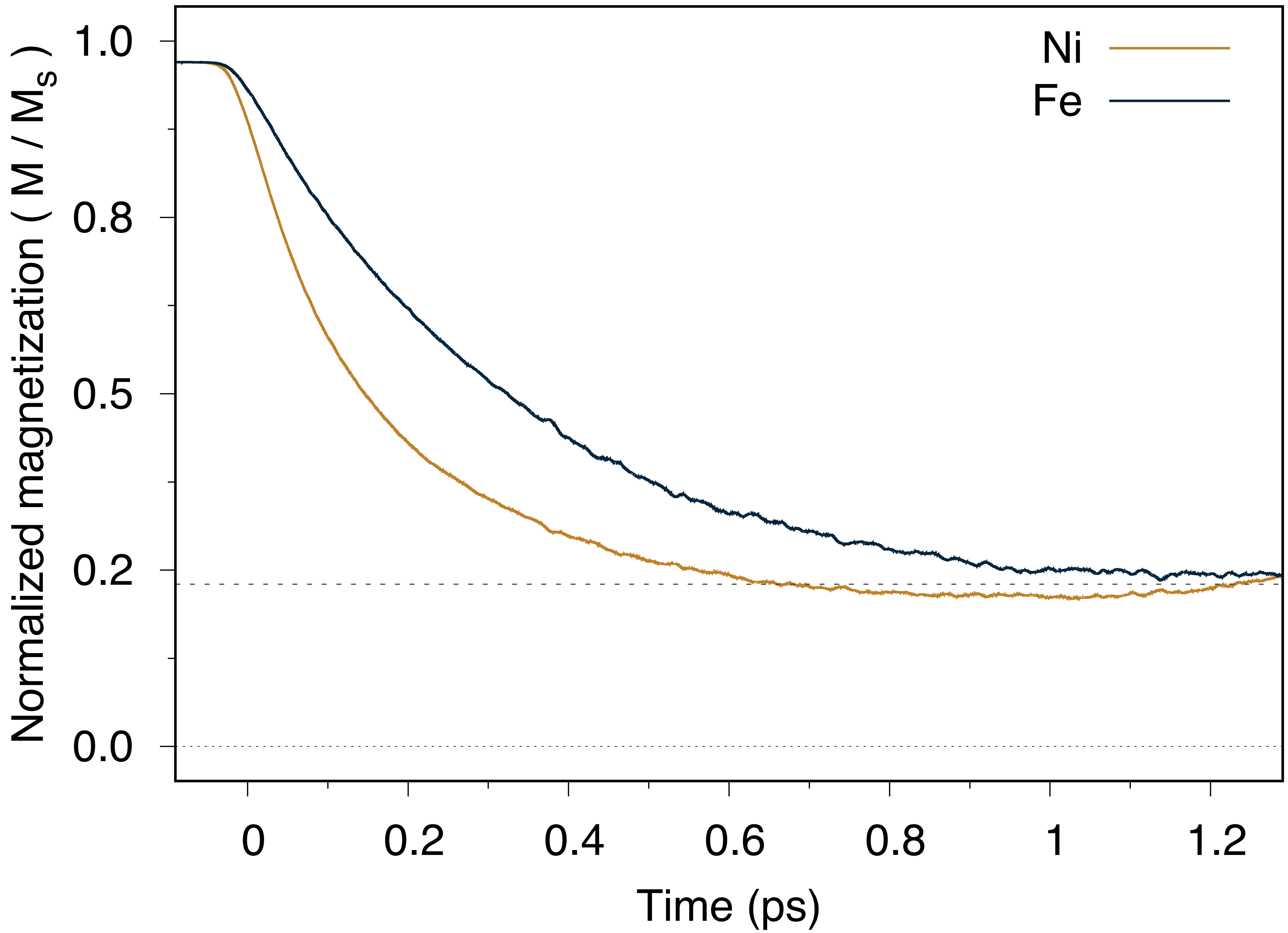
Demagnetization dynamics in bulk $Ni_{80}Fe_{20}$ Permalloy

$\mu_{Fe} = 2.30\ \mu_B$

$\mu_{Ni} = 0.98\ \mu_B$

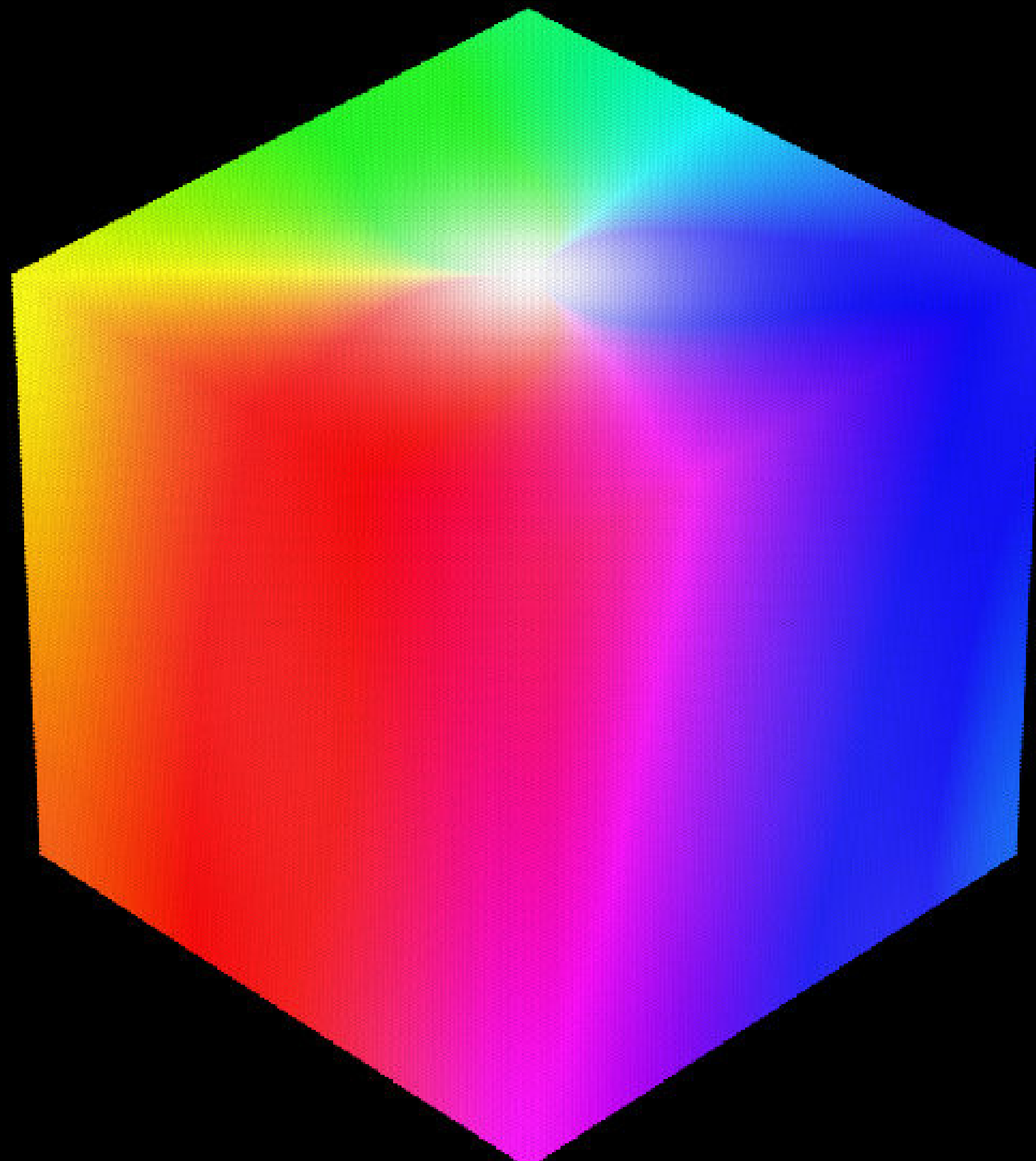
$\alpha = 0.0065$

$$\boldsymbol{\tau} \propto \mu/\alpha$$



I. Radu *et al*, SPIN **5**, 1550004 (2015)

Artificial frustration - a route to **tuneable dynamics**?



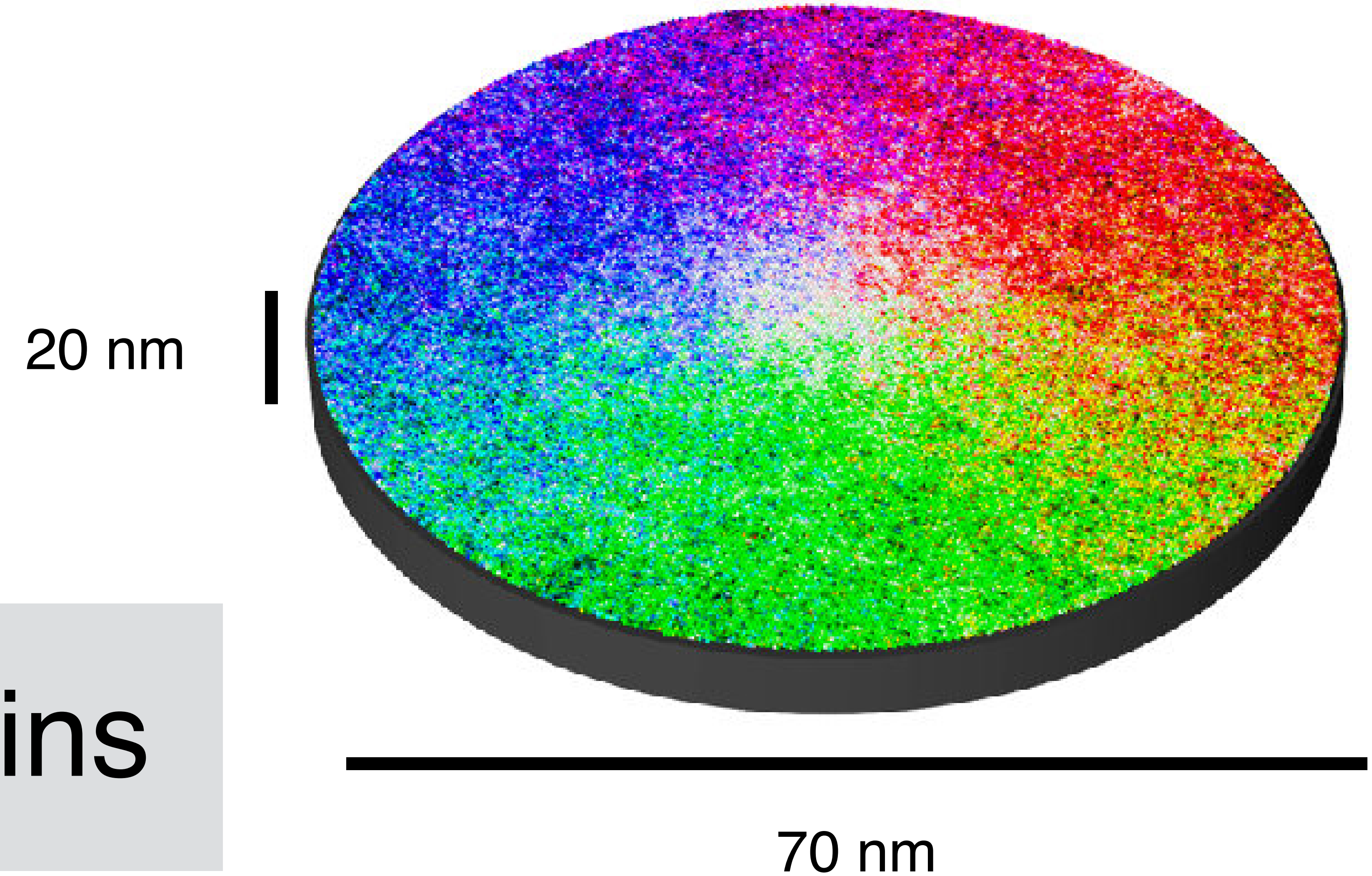
$\mu_{\text{eff}} \sim 0.13\ \mu_{\text{s}}$

$\boldsymbol{\tau} \propto \mu_{\text{eff}}/\alpha$?

Permalloy nanodot simulation $Ni_{80}Fe_{20}$

$\mu_{Fe} = 2.30\ \mu_B$

$\mu_{Ni} = 0.98\ \mu_B$

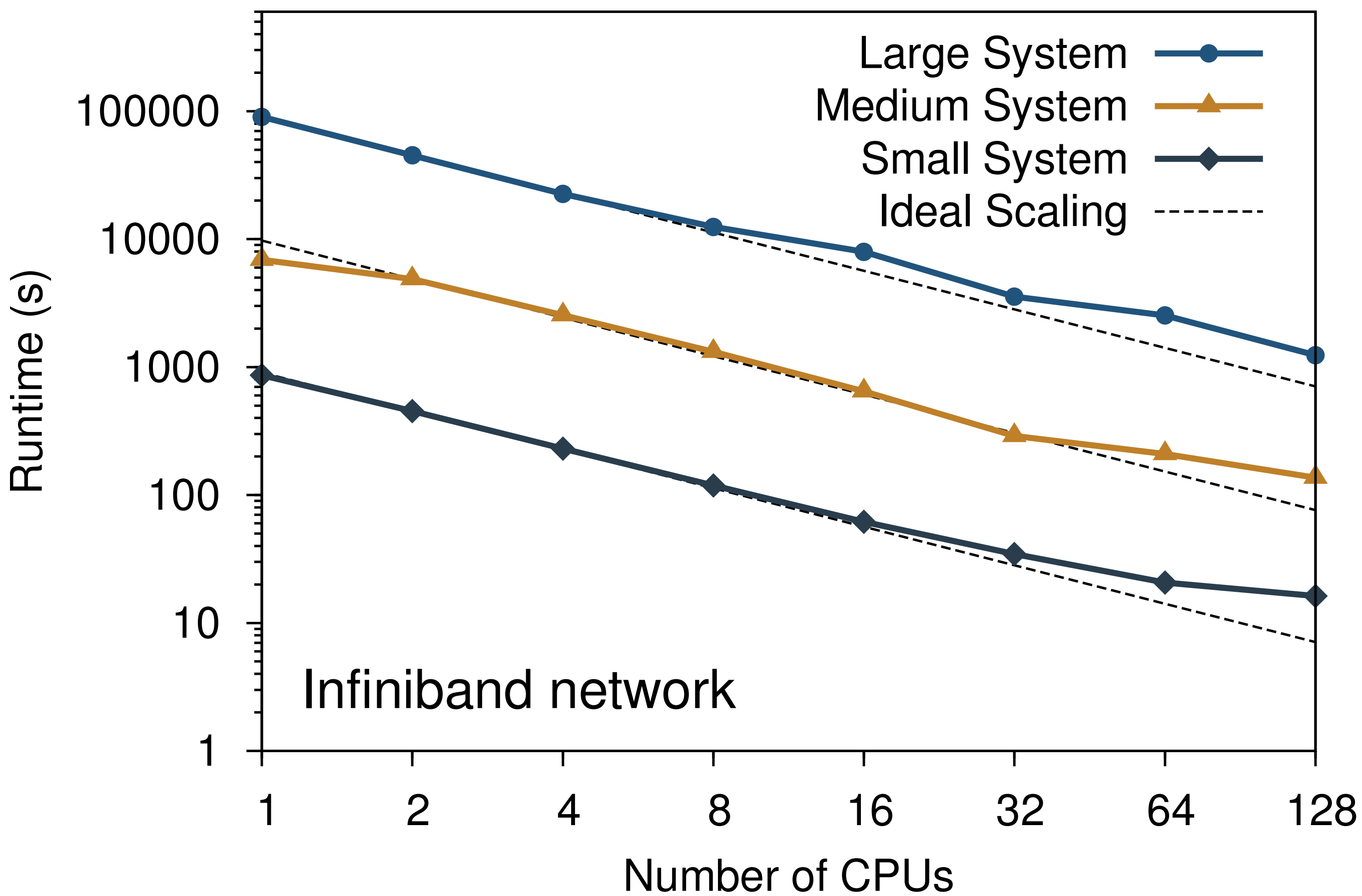


8,815,413 spins

Include spin temperature rescaling to get correct dynamics

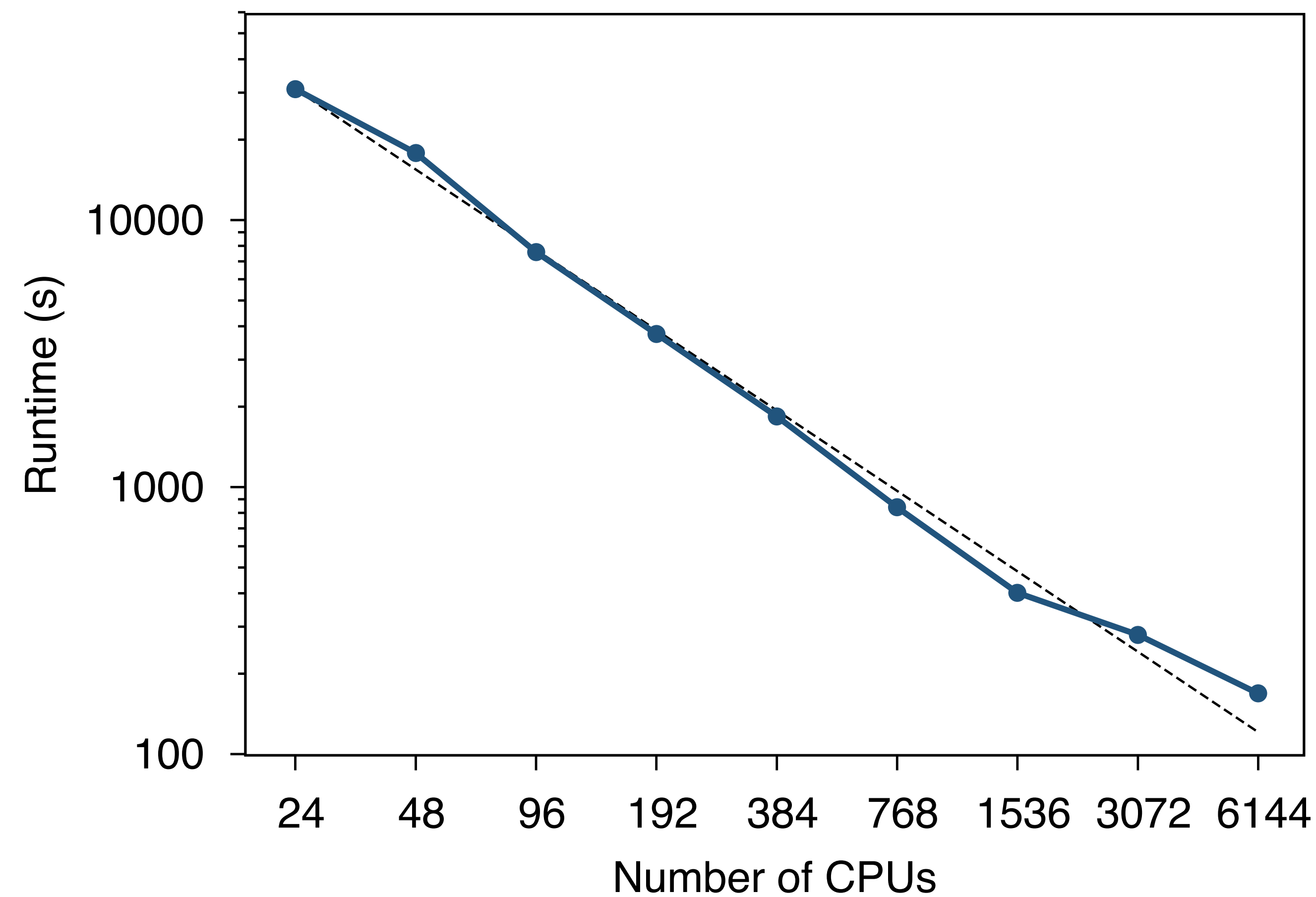
Parallel scaling of VAMPIRE code

Group Cluster



10K, 100K and 1M spins

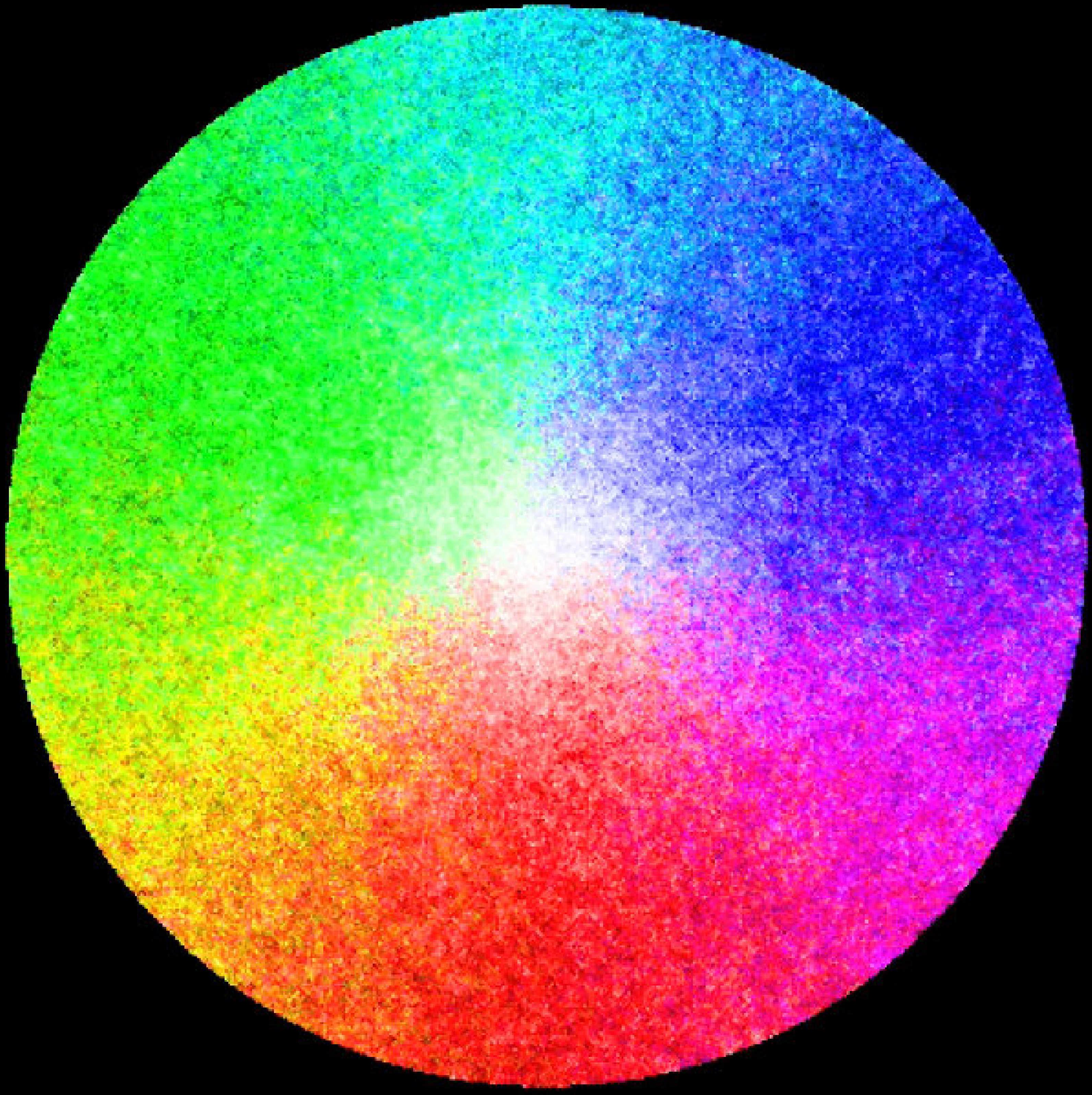
ARCHER



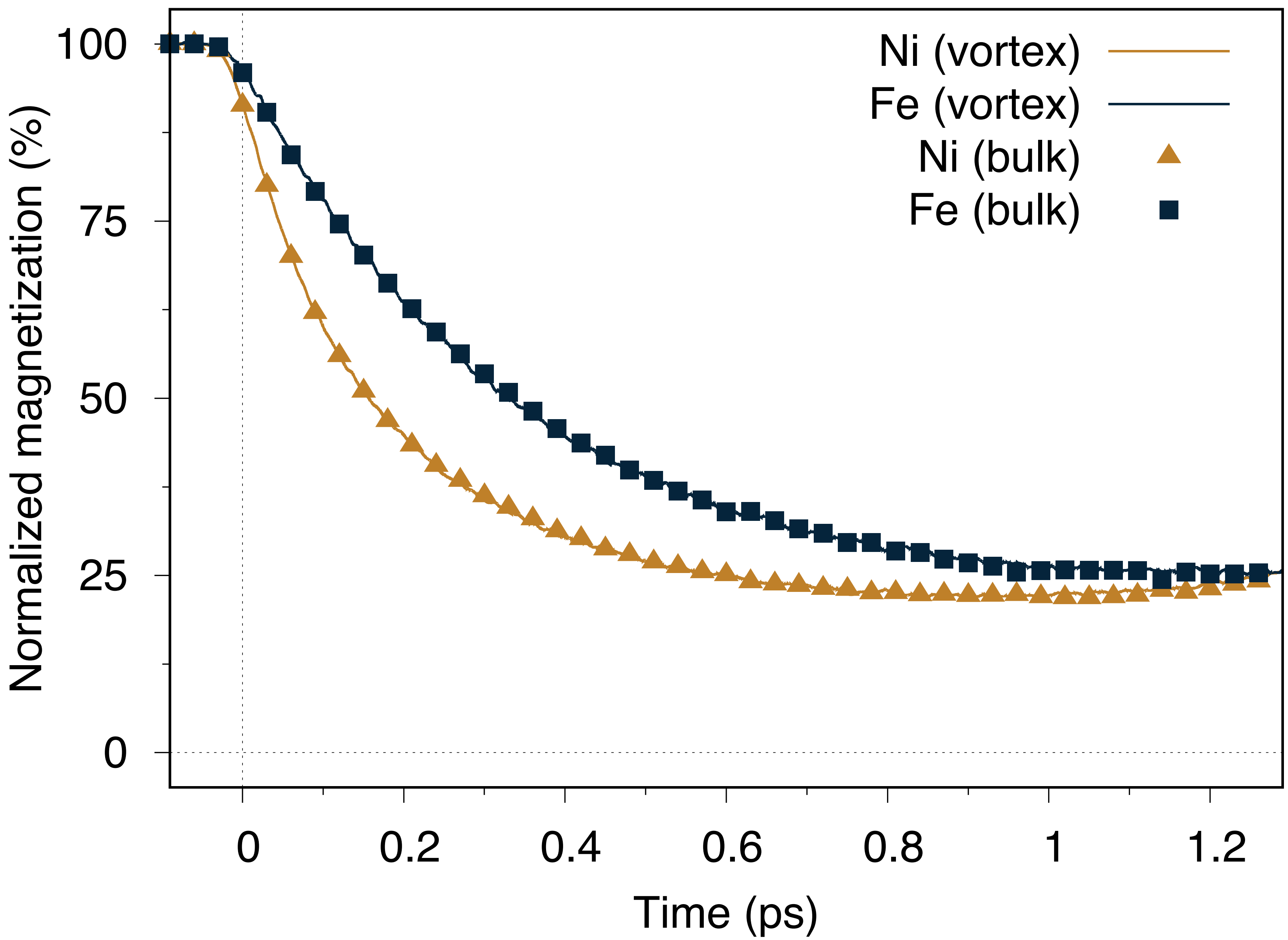
100 nm x 100 nm x 20 nm
(18M spins)

UNIVERSITY of York

Demagnetization process in a $Ni_{80}Fe_{20}$ nanodot

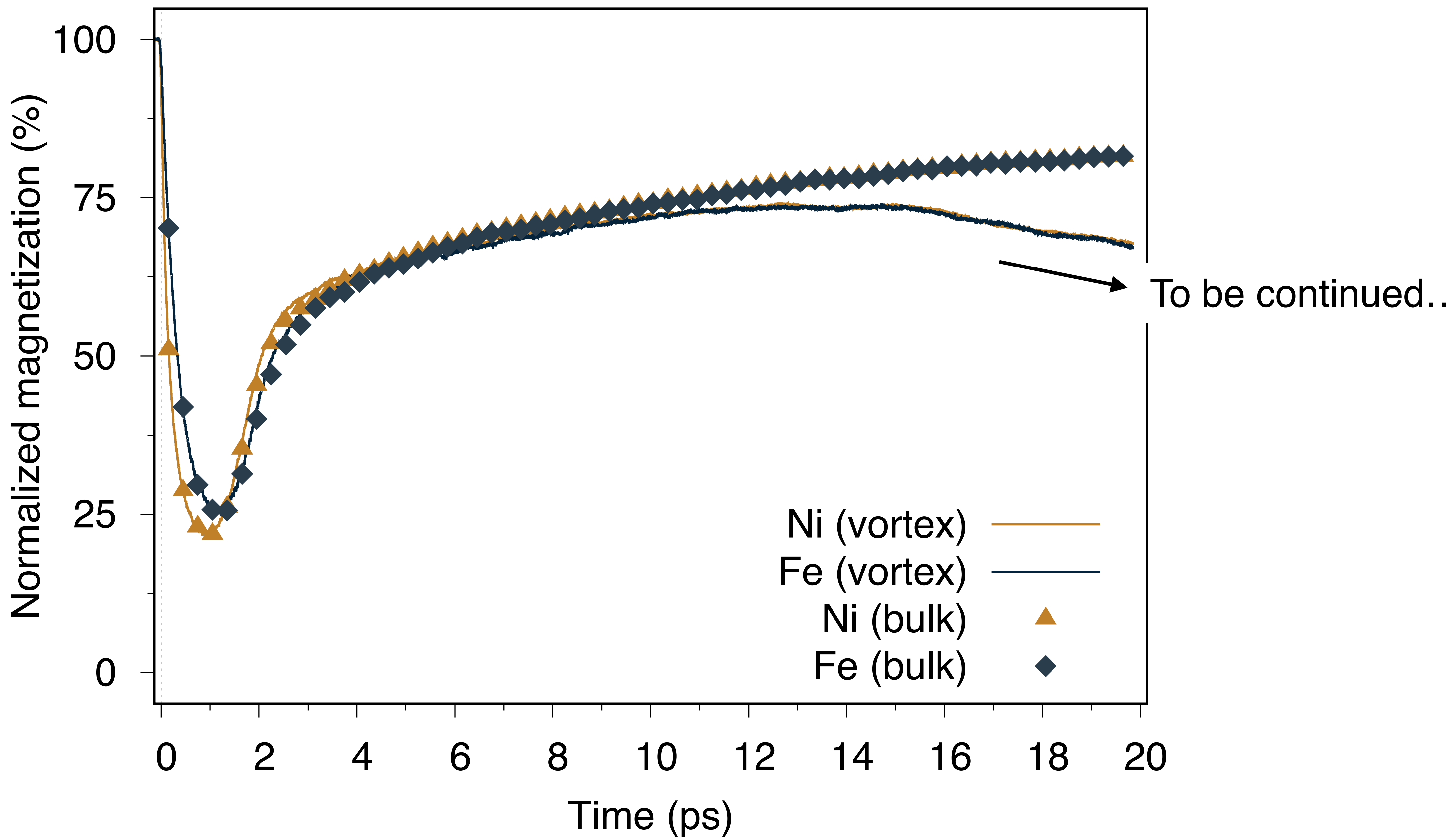


Short time demagnetization dynamics in $Ni_{80}Fe_{20}$ comparing bulk and vortex samples

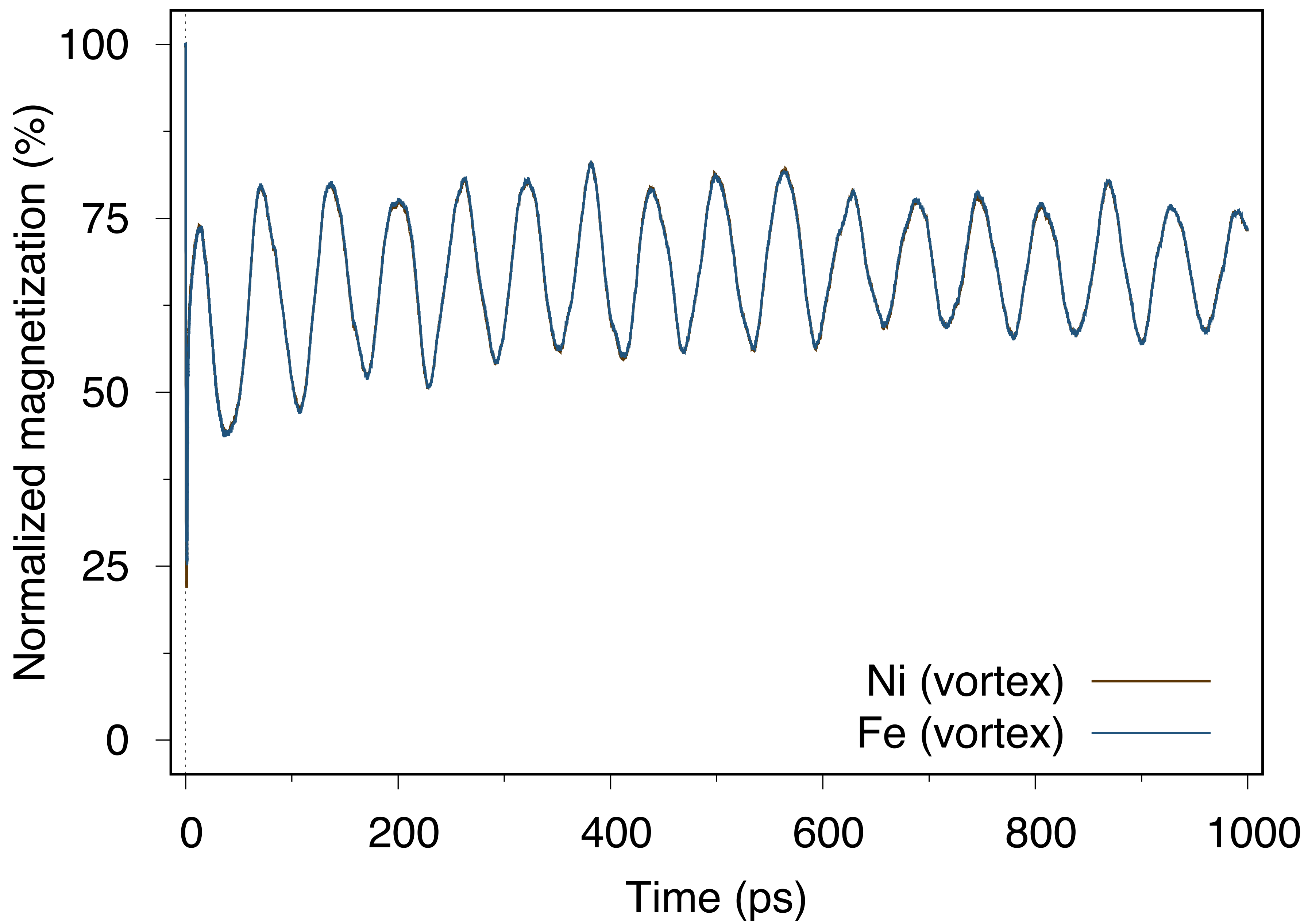


Vortex structure has **no effect** on dynamics!

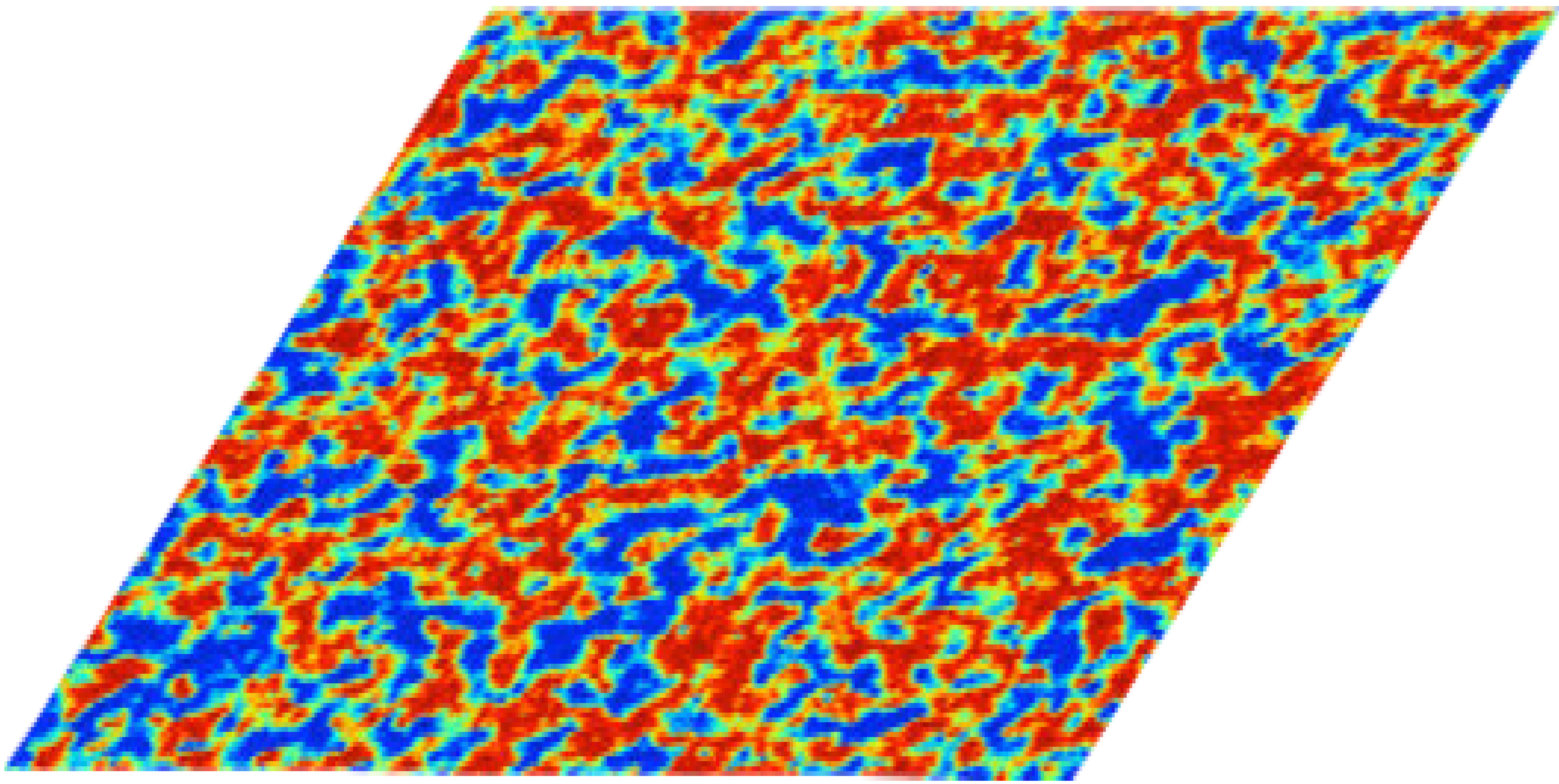
Longer timescale remagnetisation dynamics are different - topology?



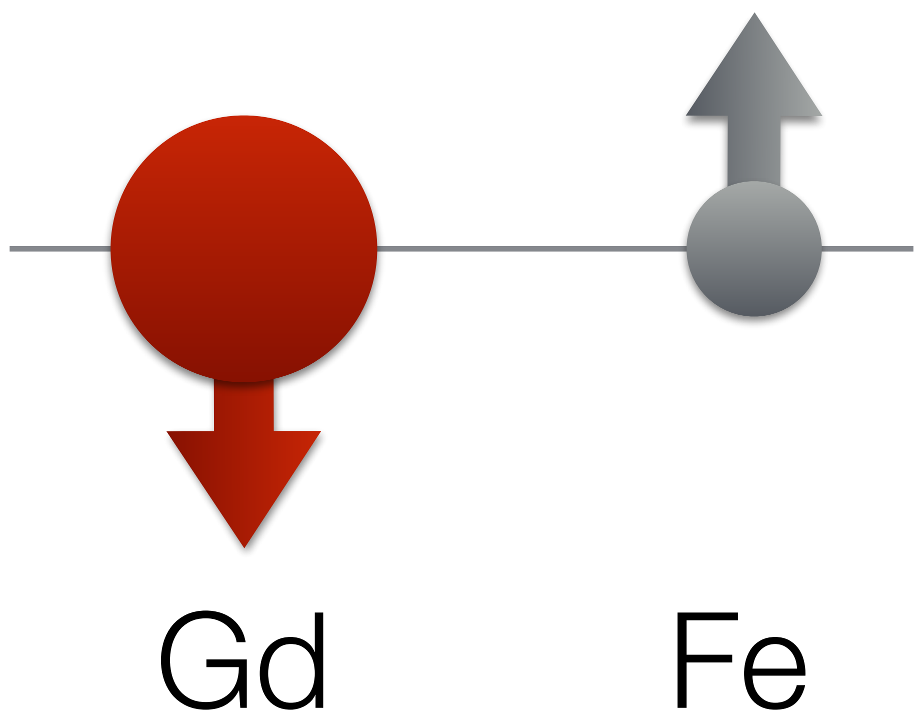
After thermal “kick”, oscillatory dynamics are long lived

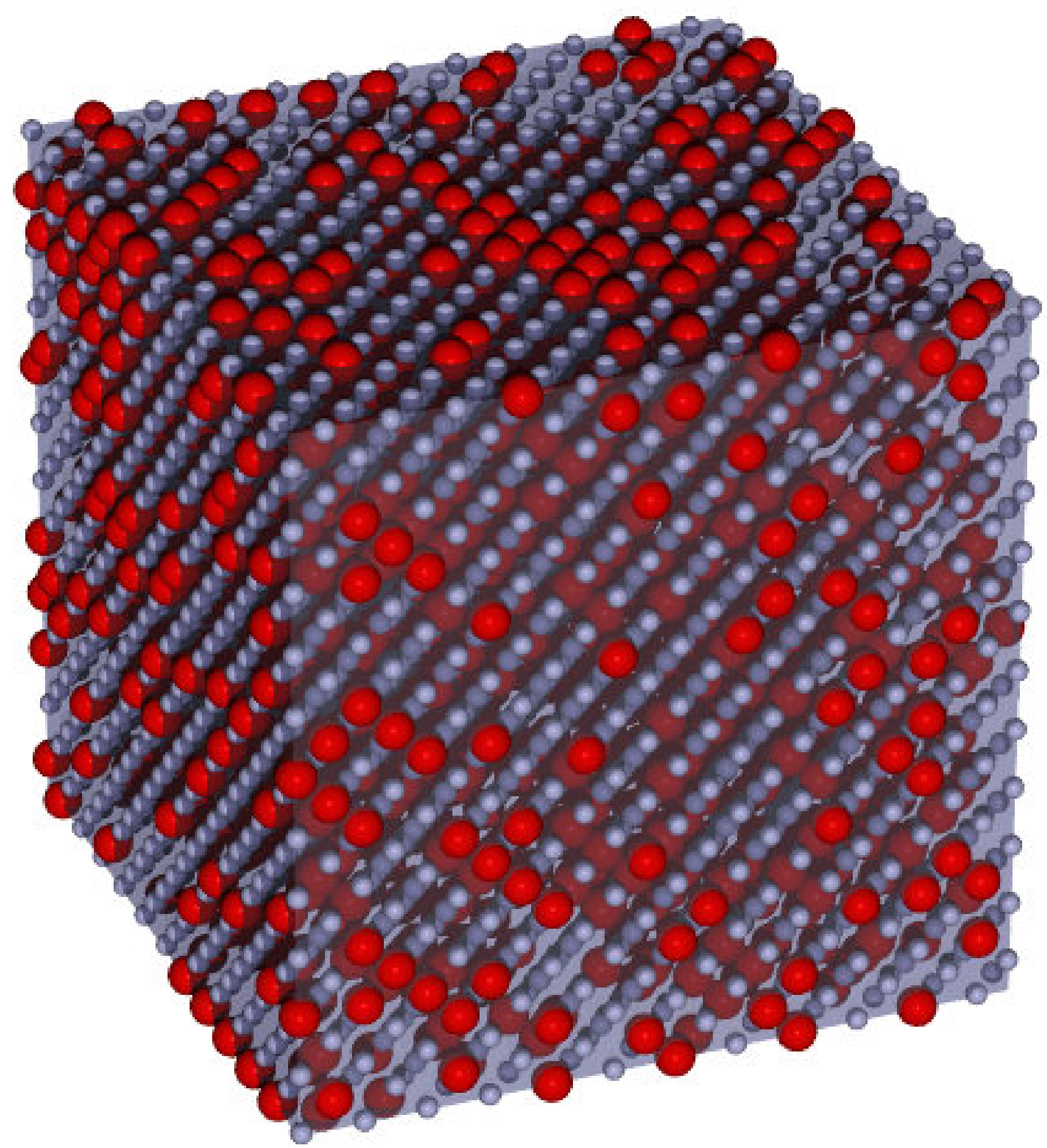


Ultrafast heat-induced switching of GdFeCo



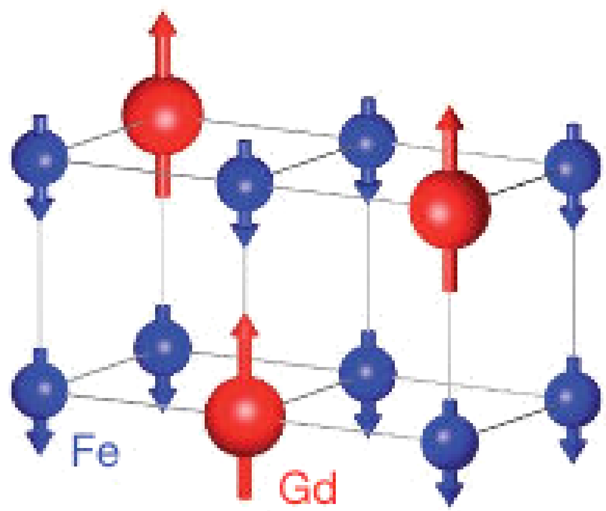
GdFe ferrimagnet

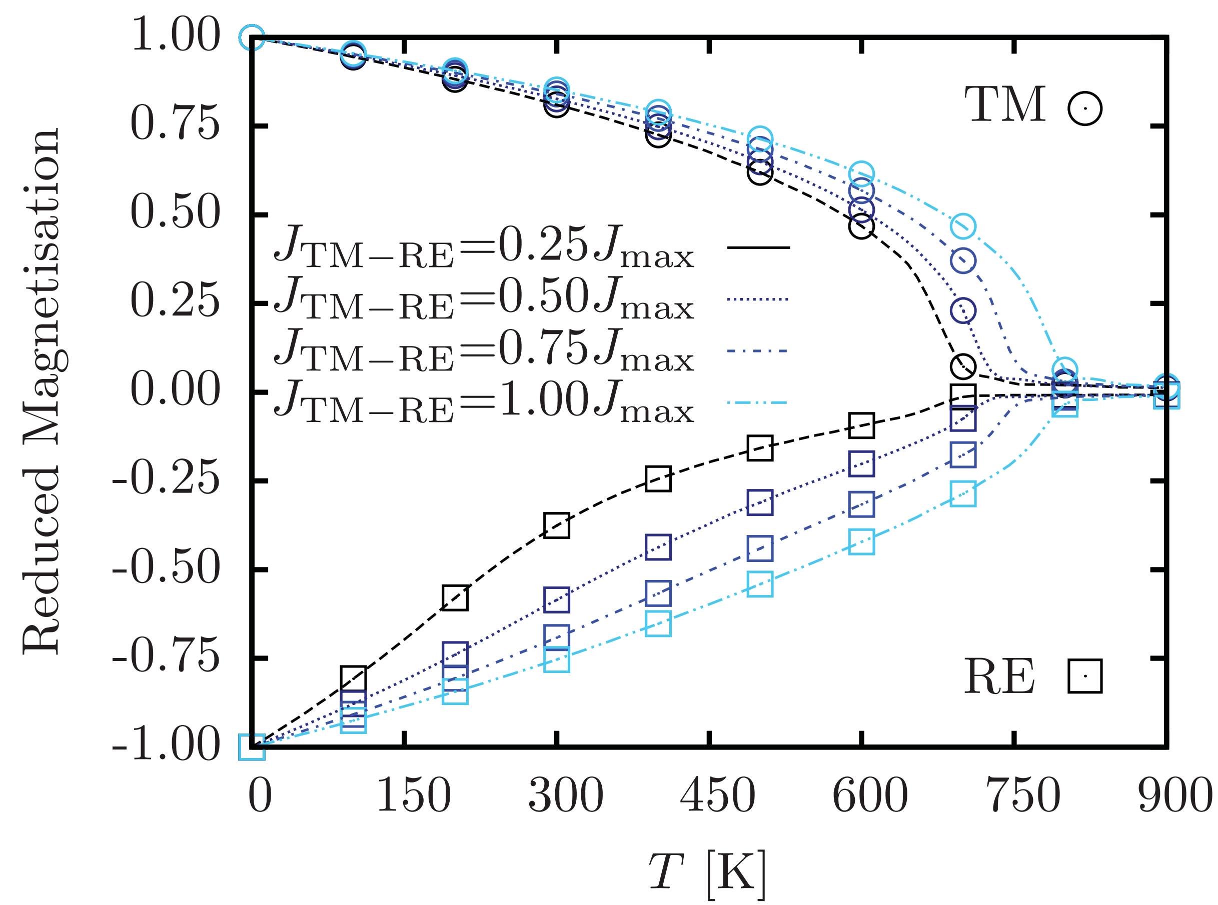




Ferrimagnetic nature of GdFe(Co) and spin models

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i=1}^{\mathcal{N}} D_i(\mathbf{S}_i \cdot \mathbf{n}_i)^2 - \sum_{i=1}^{\mathcal{N}} \mu_i \mathbf{B} \cdot \mathbf{S}_i$$

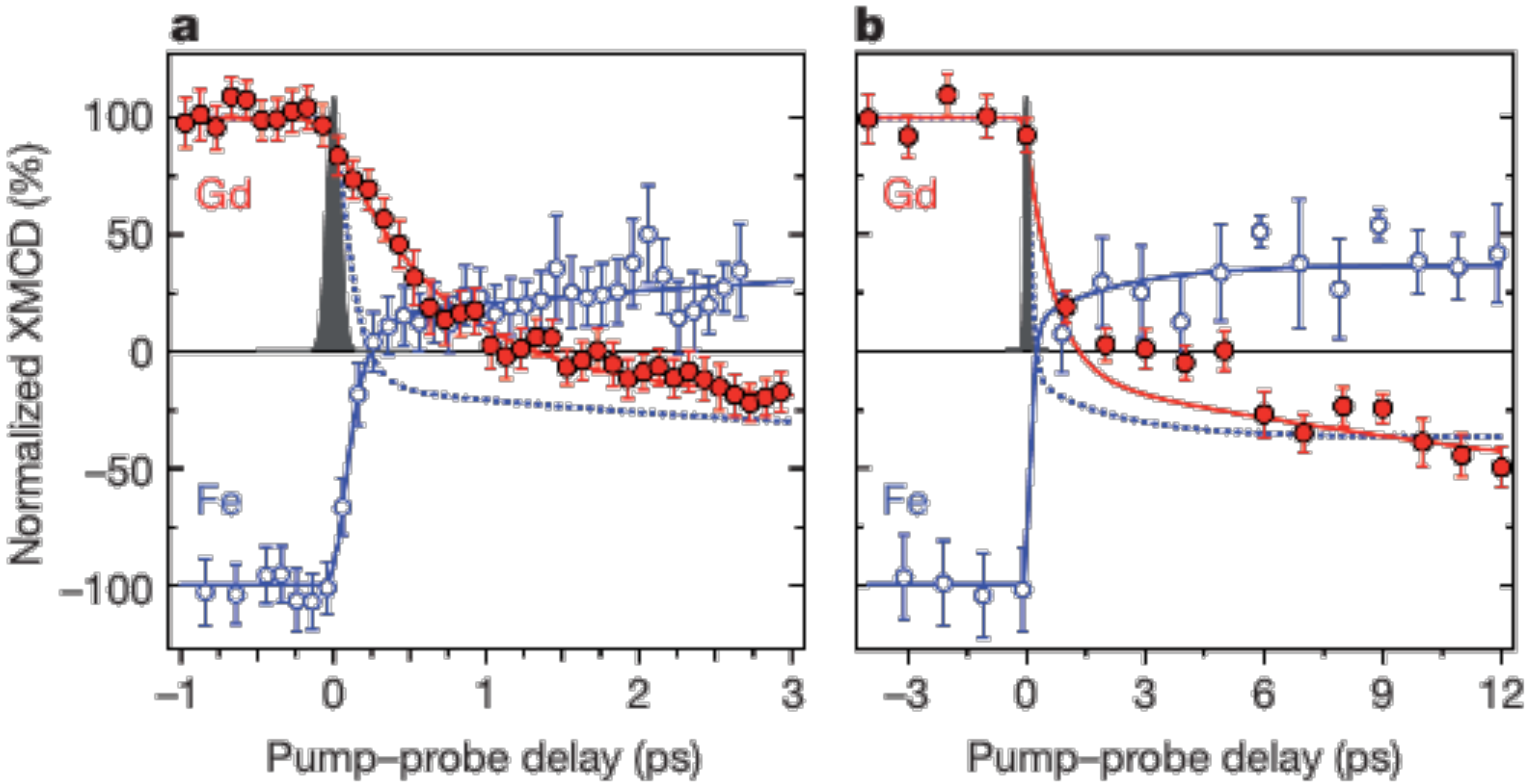




UNIVERSITY of York

T Ostler *et al*, Phys. Rev. B **84**, 024407 (2011)

Ultrafast magnetization dynamics measured with XMCD

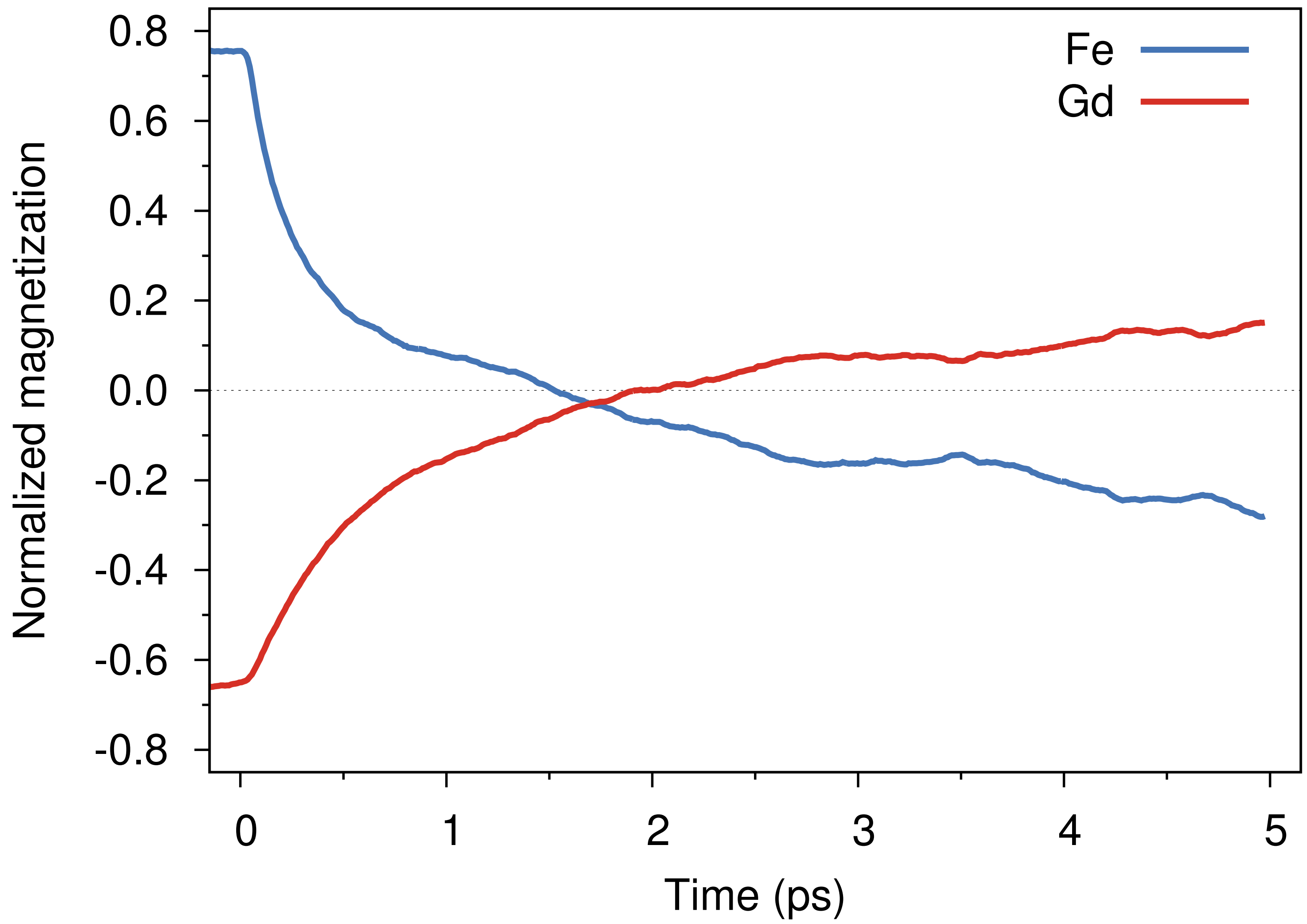


Complex reversal mechanism owing to different sub lattice magnetization dynamics

UNIVERSITY of York

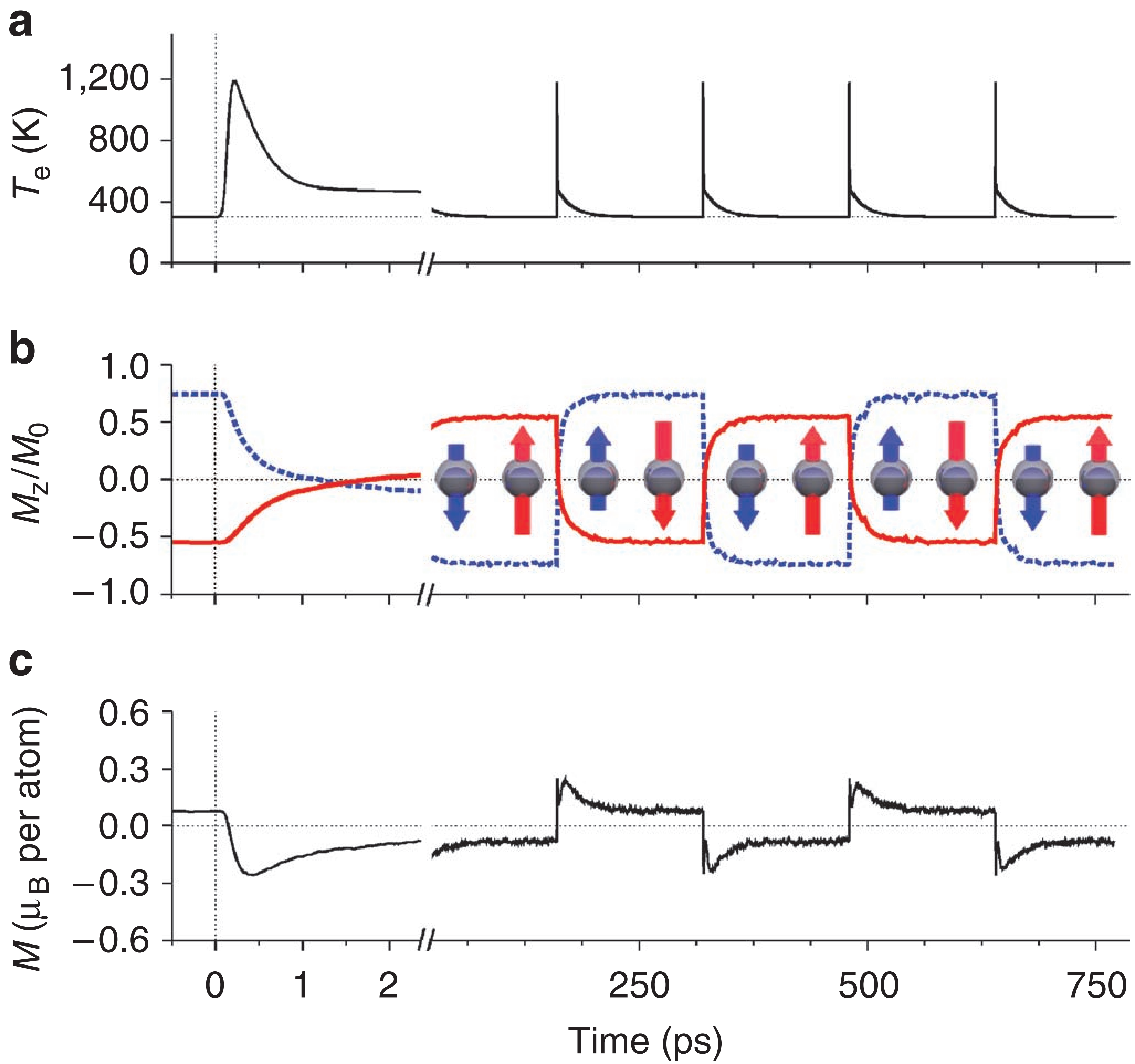
I. Radu *et al*, *Nature* **472**, 205–208 (2011)

Ultrafast magnetization dynamics simulated with atomistic spin model



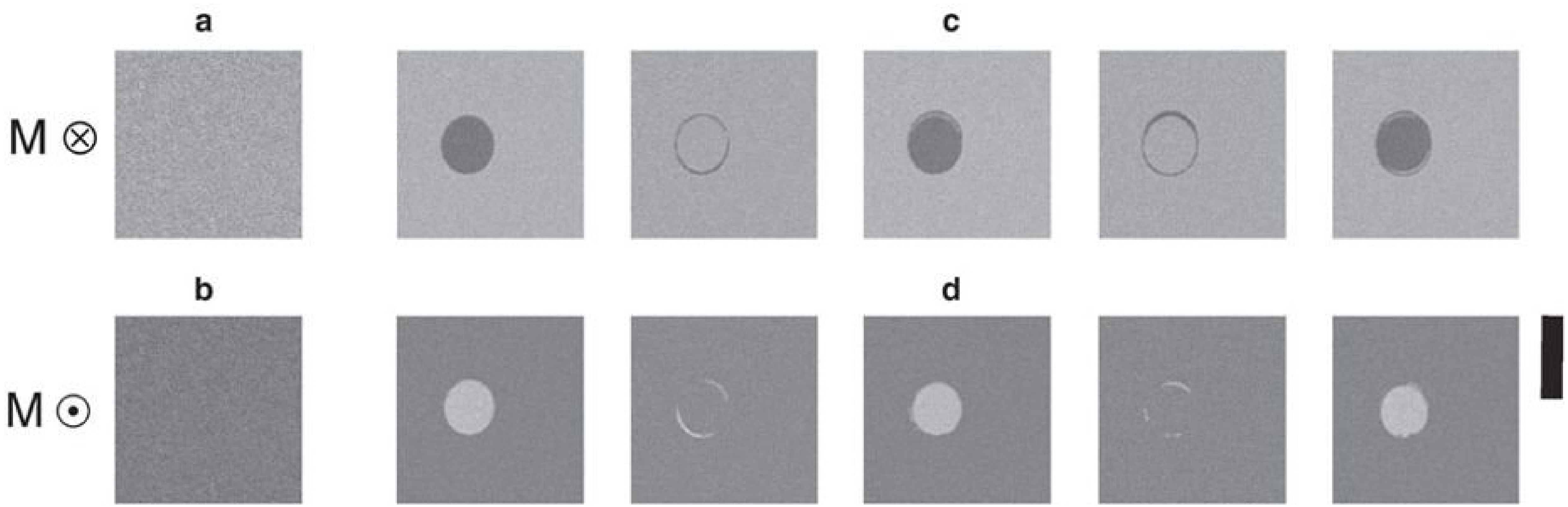
I. Radu *et al*, *Nature* **472**, 205–208 (2011)

Atomistic prediction of heat induced switching



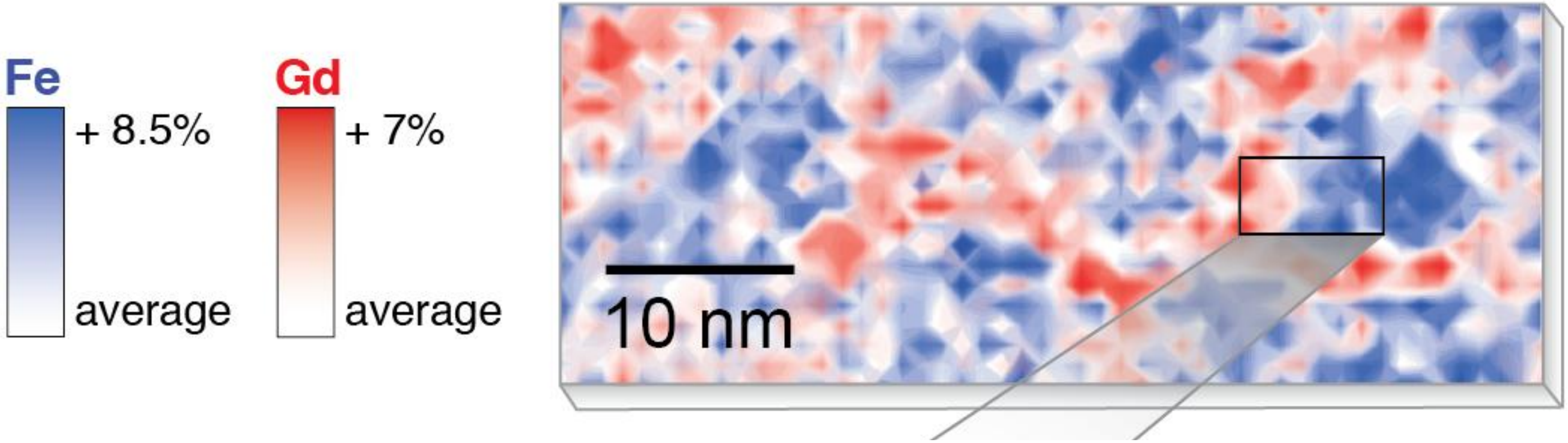
T. Ostler *et al*, *Nat. Commun.* ***3****, 666* (2012)

Experimental confirmation of heat-induced switching



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

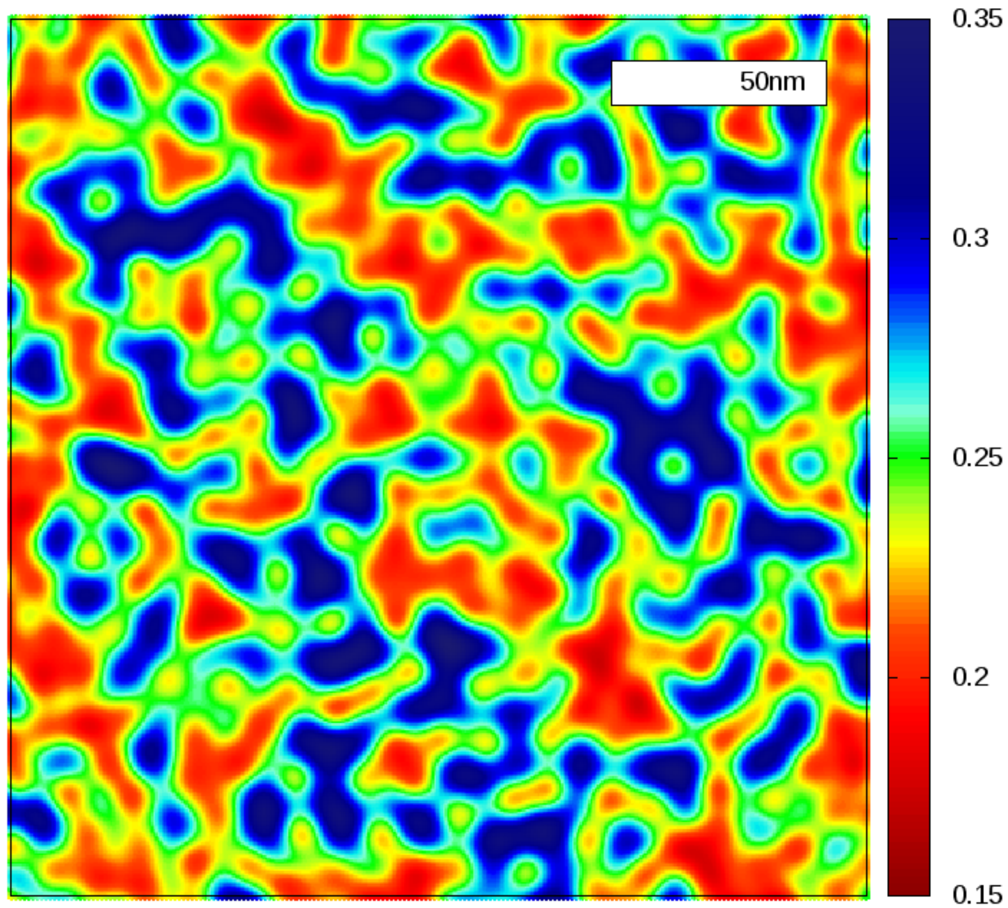
Difference in scale for magnetisation dynamics



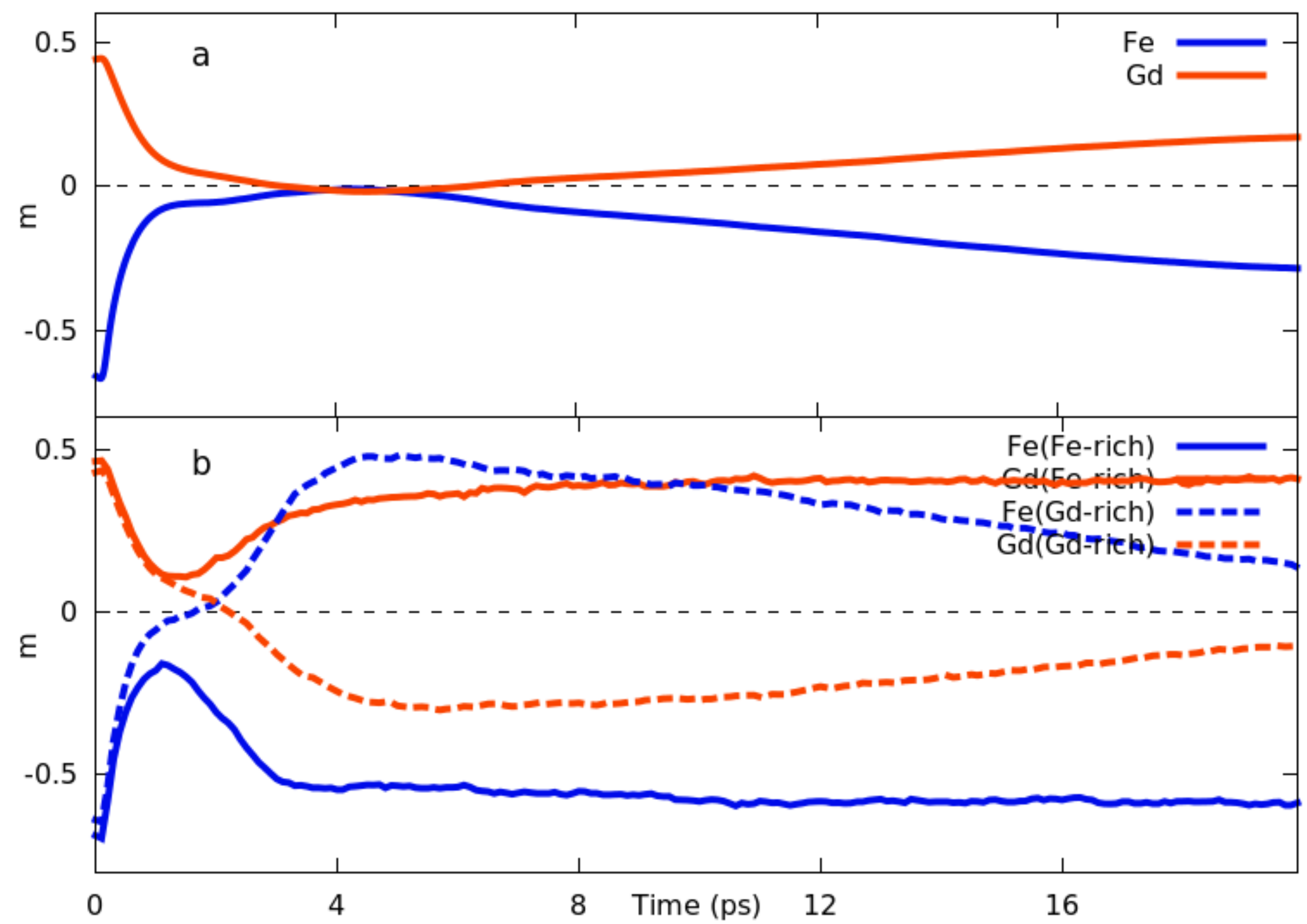
What about the role of inhomogeneity in the sample?

Graves *et al*, *Nature Materials* (2013)

Different dynamics based on Gd and Fe concentrations



Total

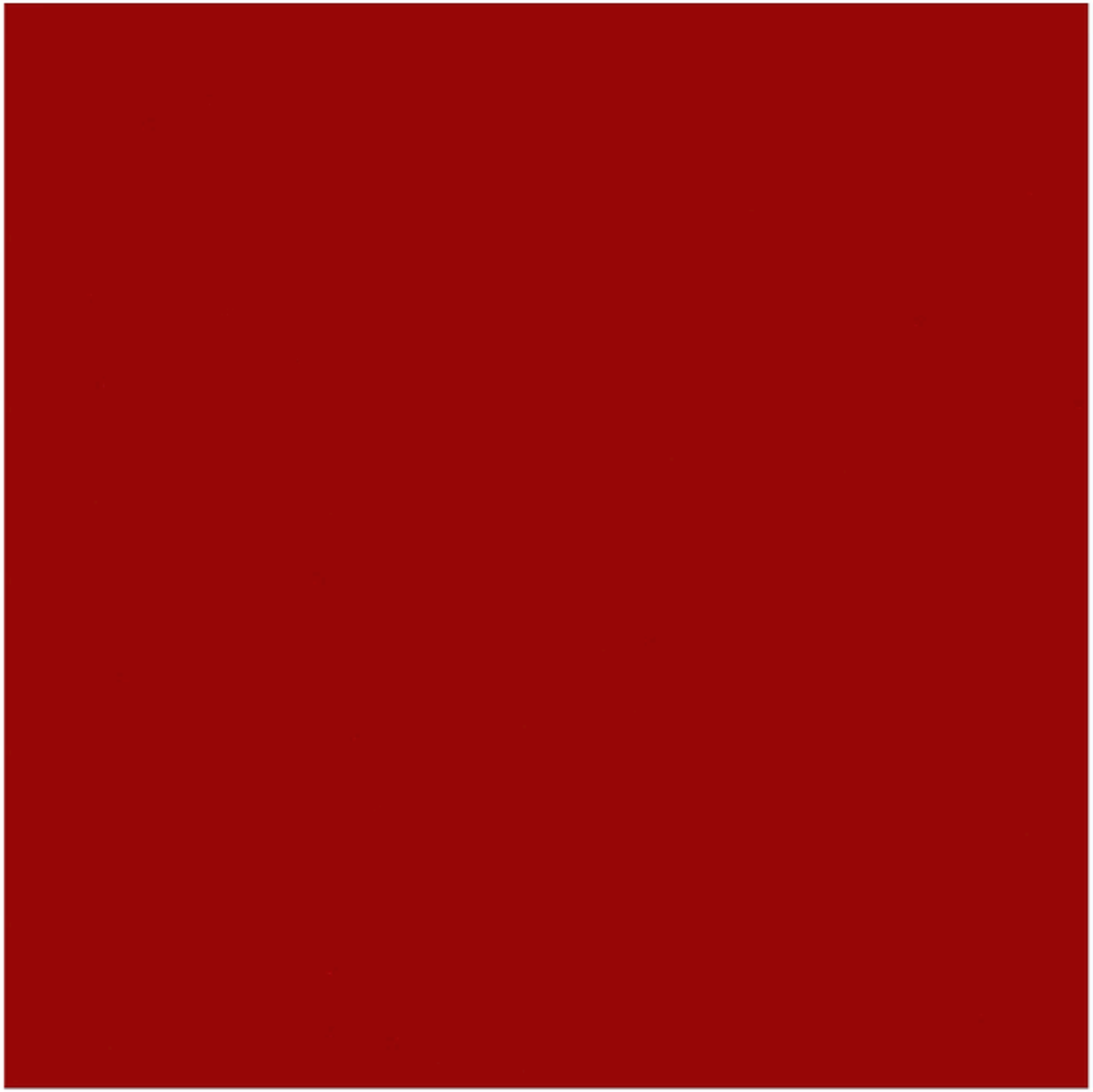


Concentration resolved

UNIVERSITY of York

E. Iococca et al, arXiv:1809.02076

Large scale simulation 1 μm x 1 μm x 10 nm



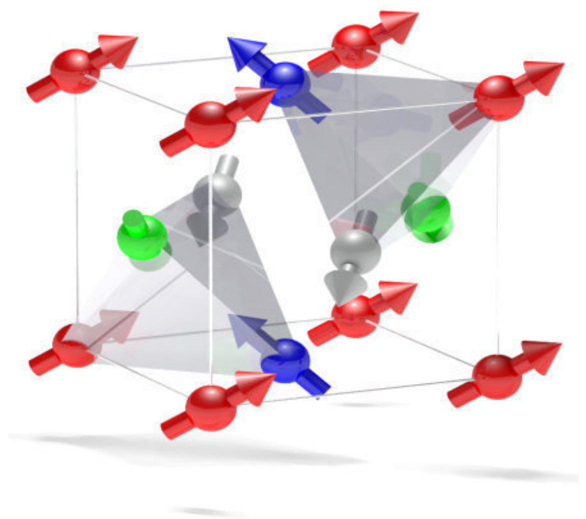
-1.00 ps

E. Iococca et al, arXiv:1809.02076

Summary

- Introduced the basic background of Landau-Lifshitz-Bloch micromagnetics

- Presented simulations of the static and dynamic properties of more complex magnets



- Thermodynamics is a significant and important contribution to ultrafast magnetic processes