Atomistic spin model simulations of complex magnets

Richard F L Evans

Acknowledgements

Sam Westmoreland, Ramon Cuadrado,
Roy Chantrell, Matt Probert

T. Shoji, M. Yano, M. Ito, A. Manabe

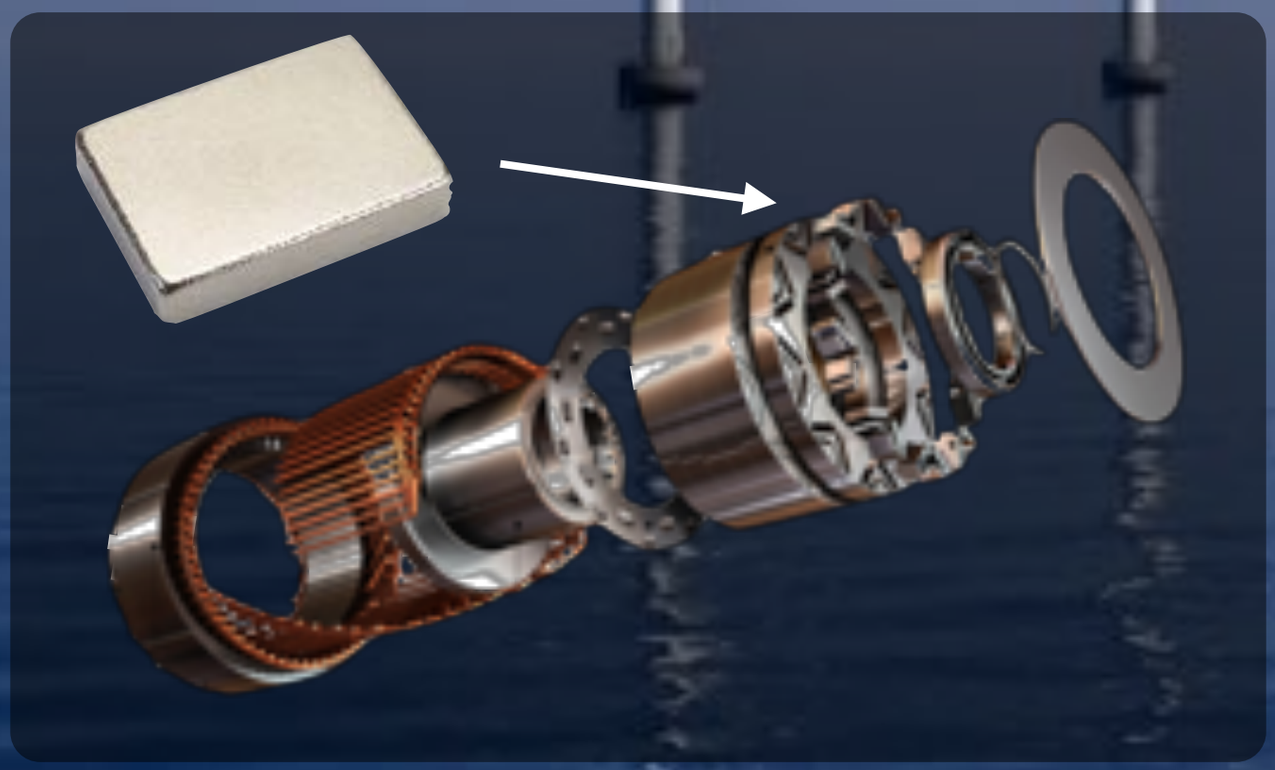
Dominique Givord

Gino Hrkac

Thomas Schrefl

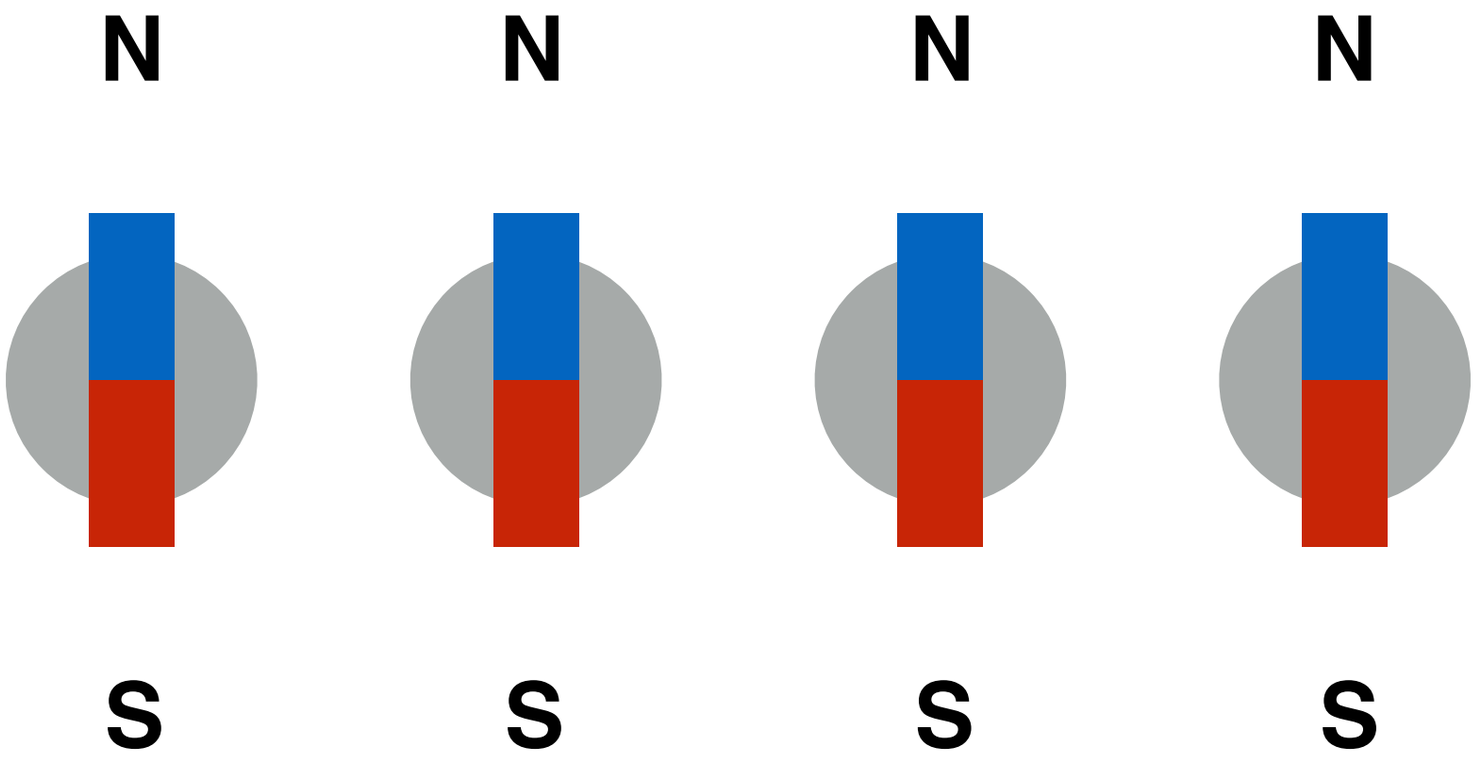
Permanent magnetic materials

Source: siemens.com



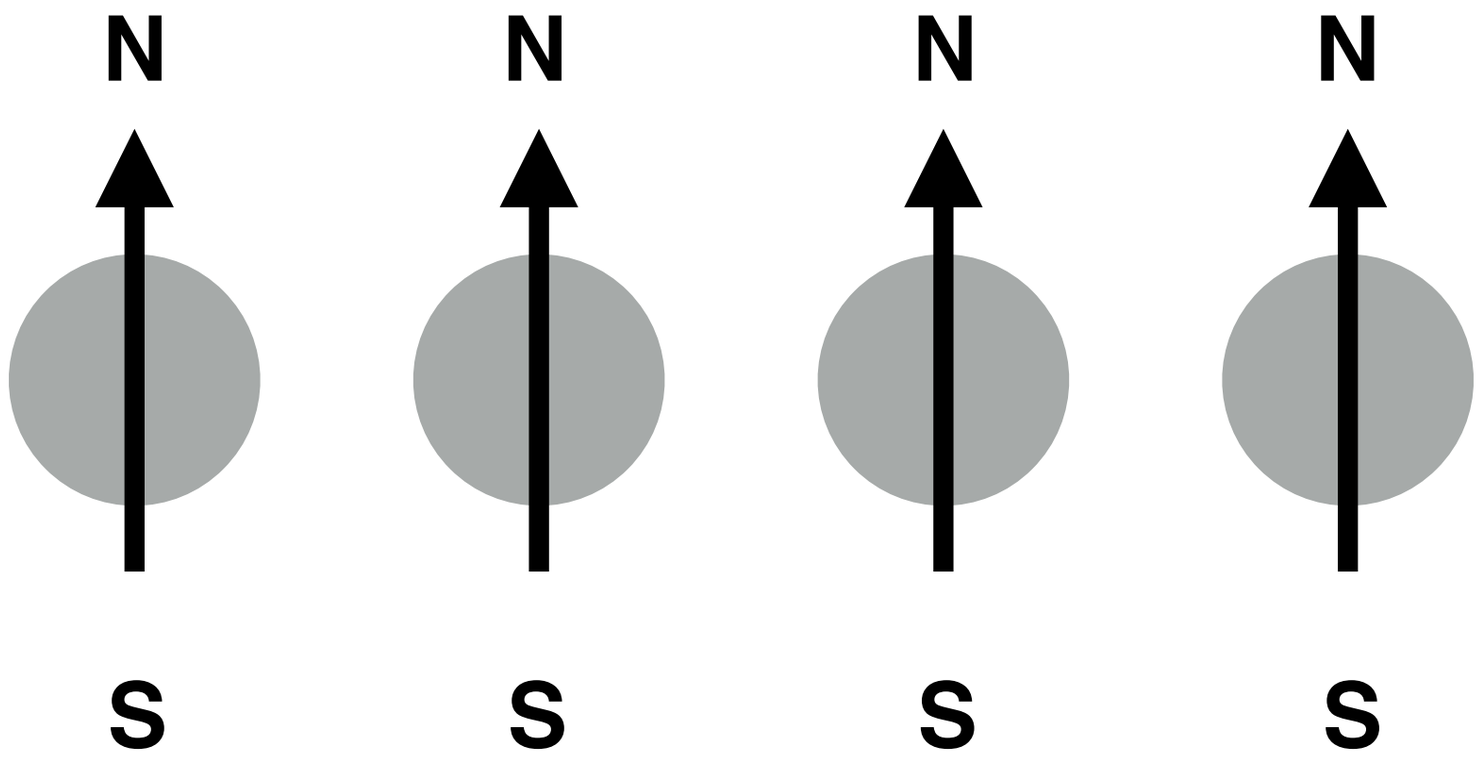
Where does ‘magnetism’ come from?

Magnetism comes from quantum mechanical ‘spin’ of the electron



Can think of these as atomic bar magnets

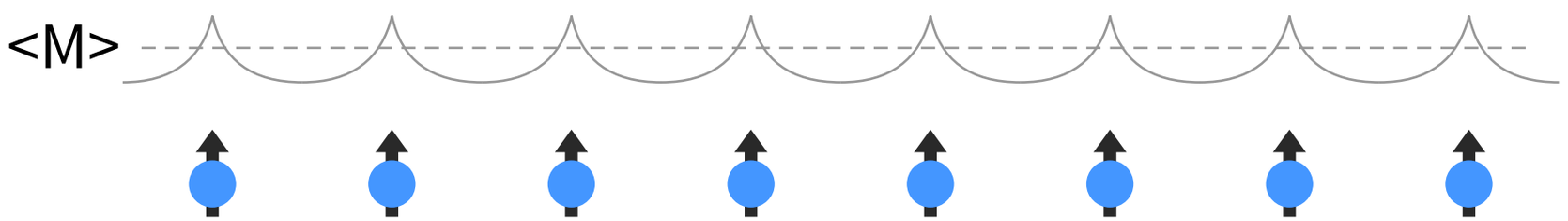
Magnetism comes from quantum mechanical ‘spin’ of the electron



Can think of these as atomic bar magnets

Modelling magnets: numerical micromagnetics

Treat magnetisation as a **continuum approximation**



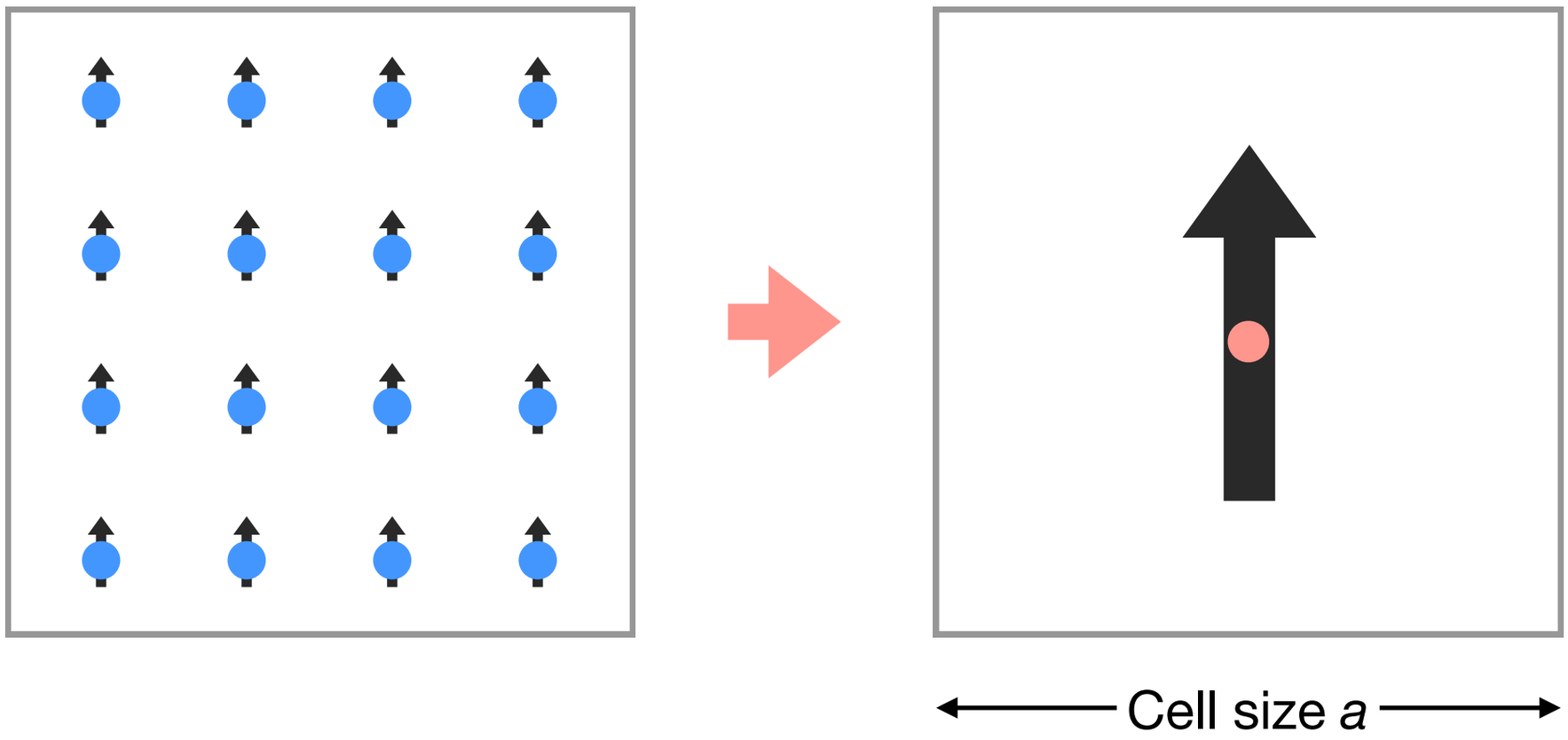
Average over the local atomic moments to give an *average* moment density (magnetization) that is assumed to be continuous

Then consider a small volume of space (1 nm)^3 - (10 nm)^3 where the magnetization (and all atomic moments) are assumed to point along the same direction

The micromagnetic cell

This gives the fundamental unit of micromagnetics: the micromagnetic cell

The magnetisation is resolved to a single point **magnetic moment**



Generally a good approximation for simple magnets (local moment variations are weak) at low temperatures ($T < T_c/2$)

Micromagnetic problems

A typical problem is then divided (discretised) into multiple micromagnetic cells

Can now generally treat any micromagnetic problem by solving system of equations describing magnetic interactions

Often we need to consider problems where continuum micromagnetics is a poor approximation

Multi-sublattice ferro, ferri and antiferromagnets

Realistic particles with surface effects

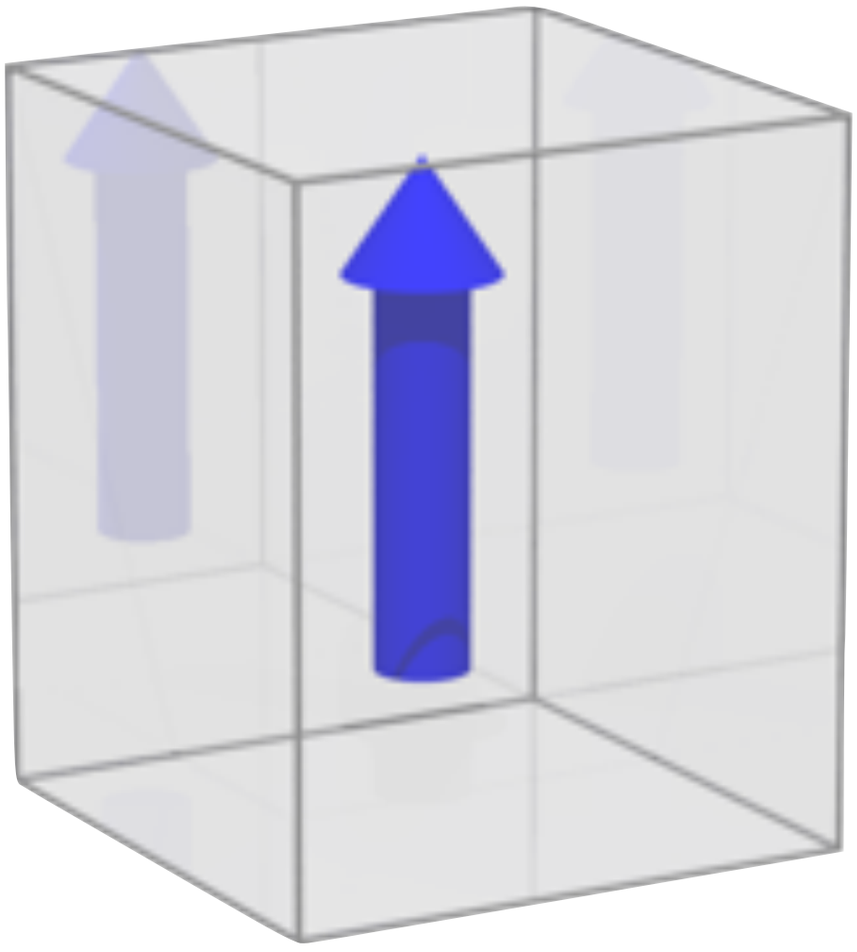
Elevated temperatures near T_c

Magnetic interfaces

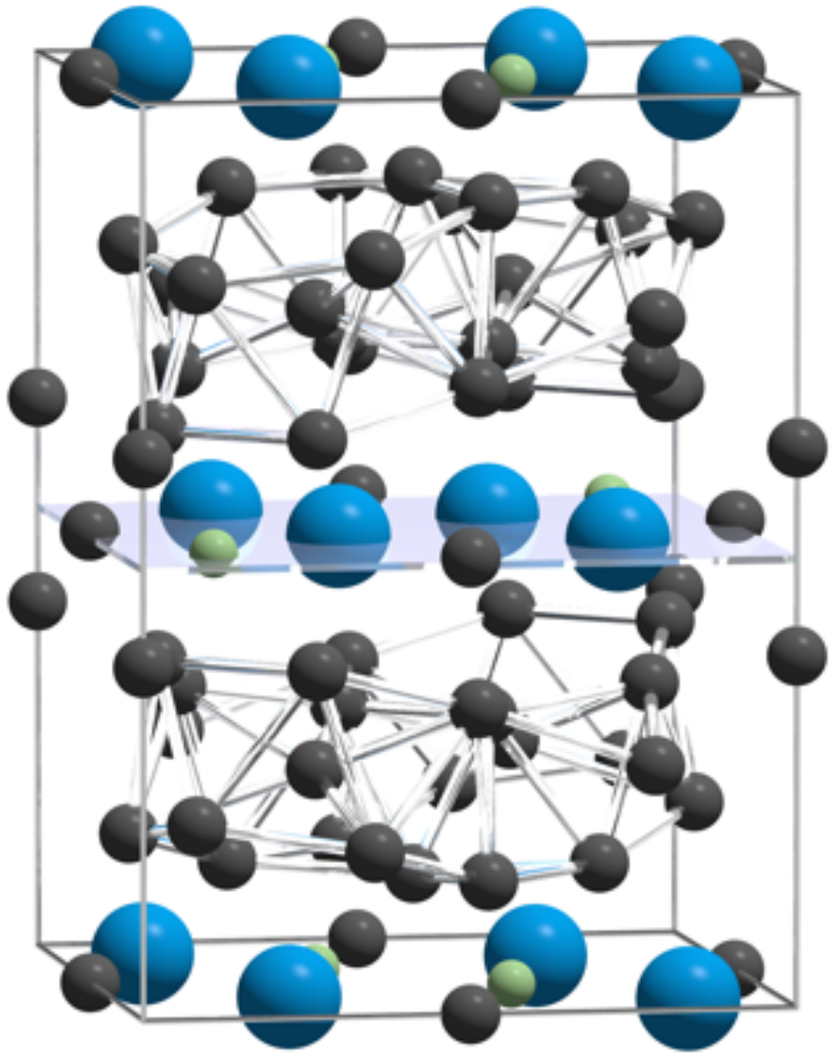
Crystal defects and disorder

Example 1: $Nd_2Fe_{14}B$ permanent magnets

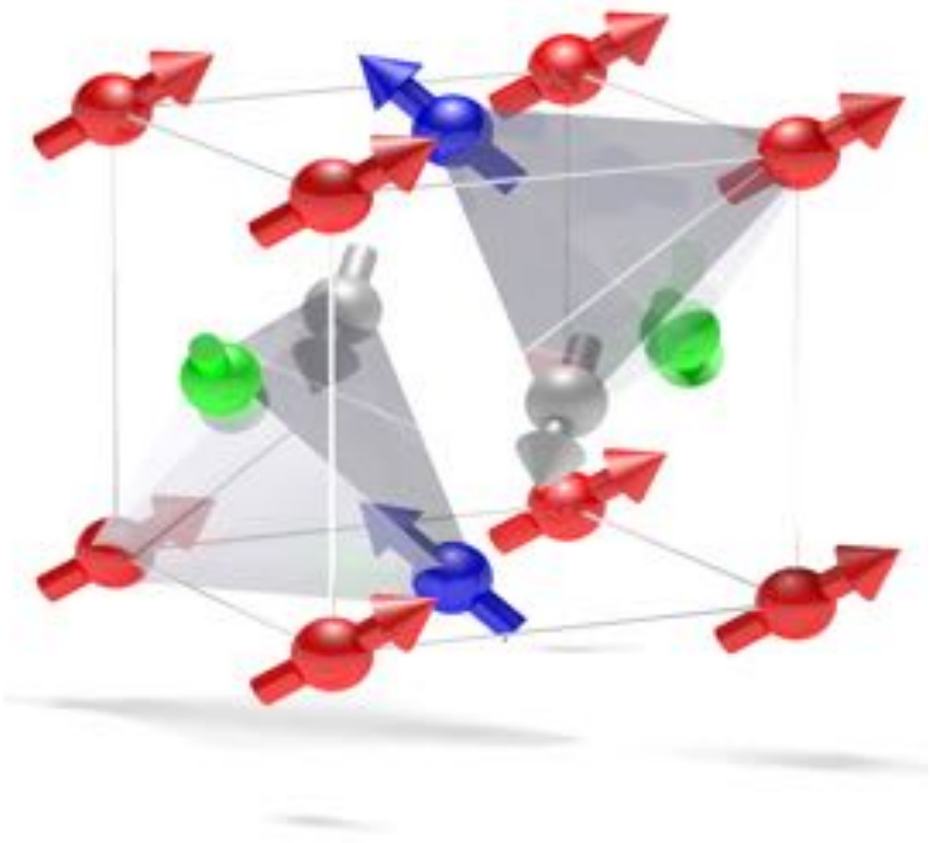
Micromagnetics



Atomistic



Example 2: Antiferromagnets (next talk!)

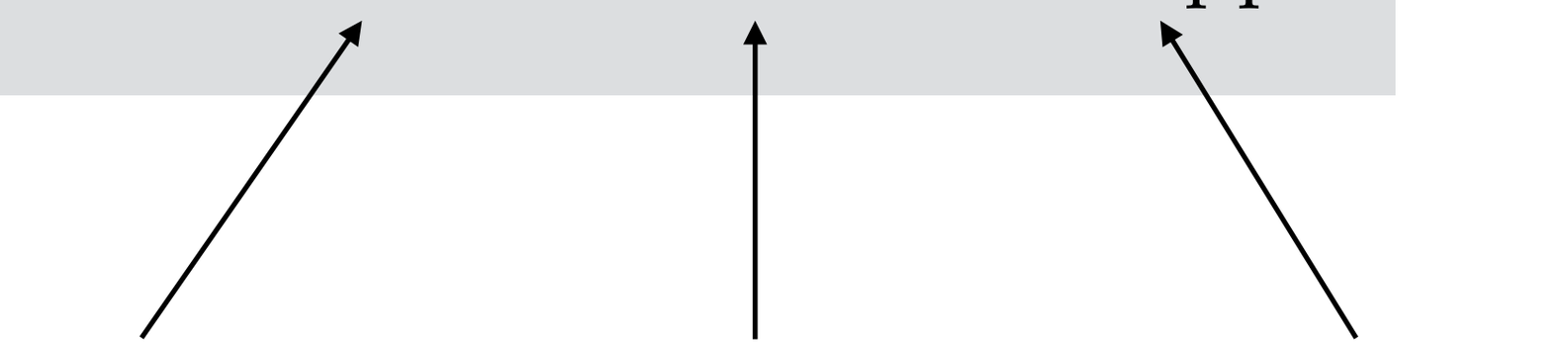


$IrMn_3$

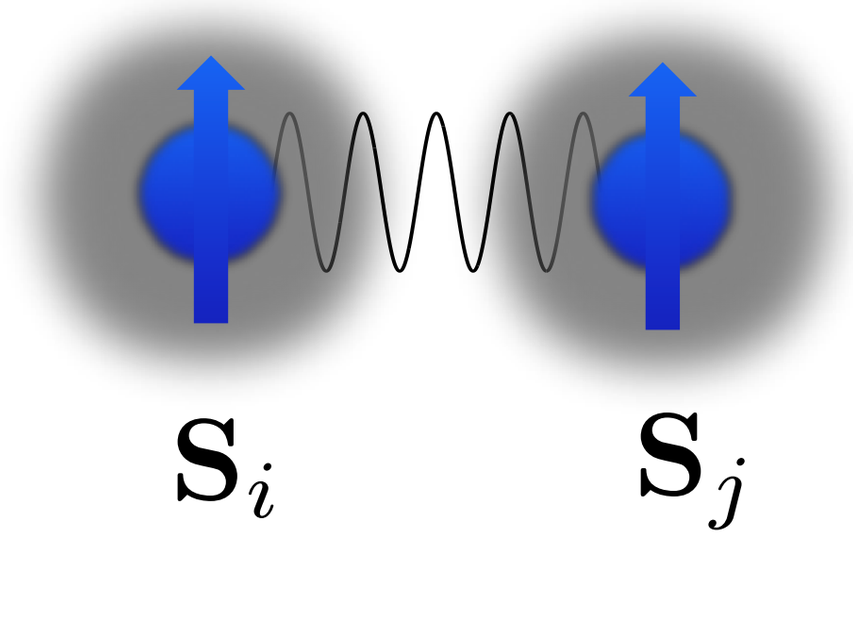
Atomistic spin models

The ‘spin’ Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\mathrm{exc}} + \mathcal{H}_{\mathrm{ani}} + \mathcal{H}_{\mathrm{app}}$$



Foundation of the atomistic model is Heisenberg exchange

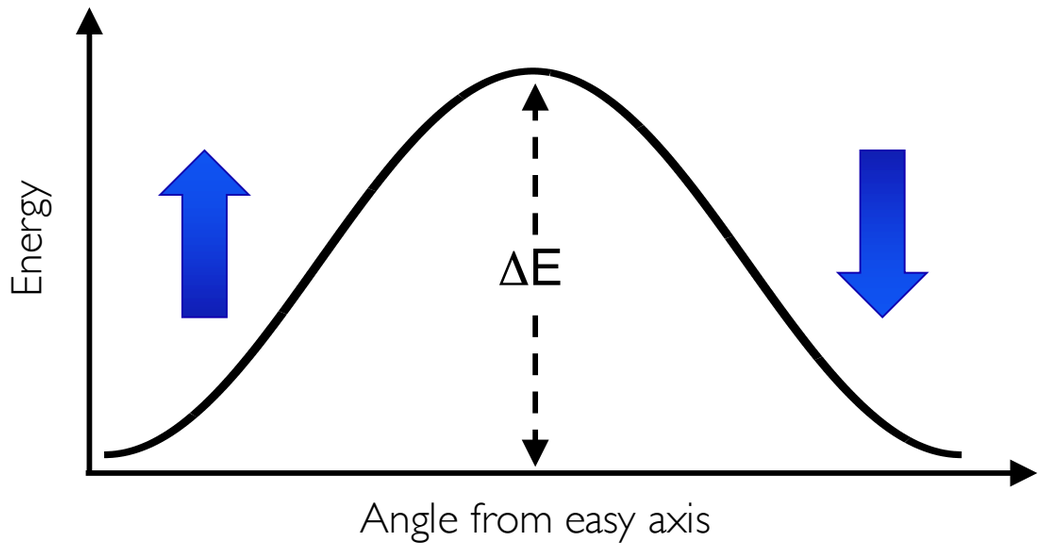


$$\mathcal{H}_{\text{exc}} = -\frac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$

Natural discrete limit of magnetization

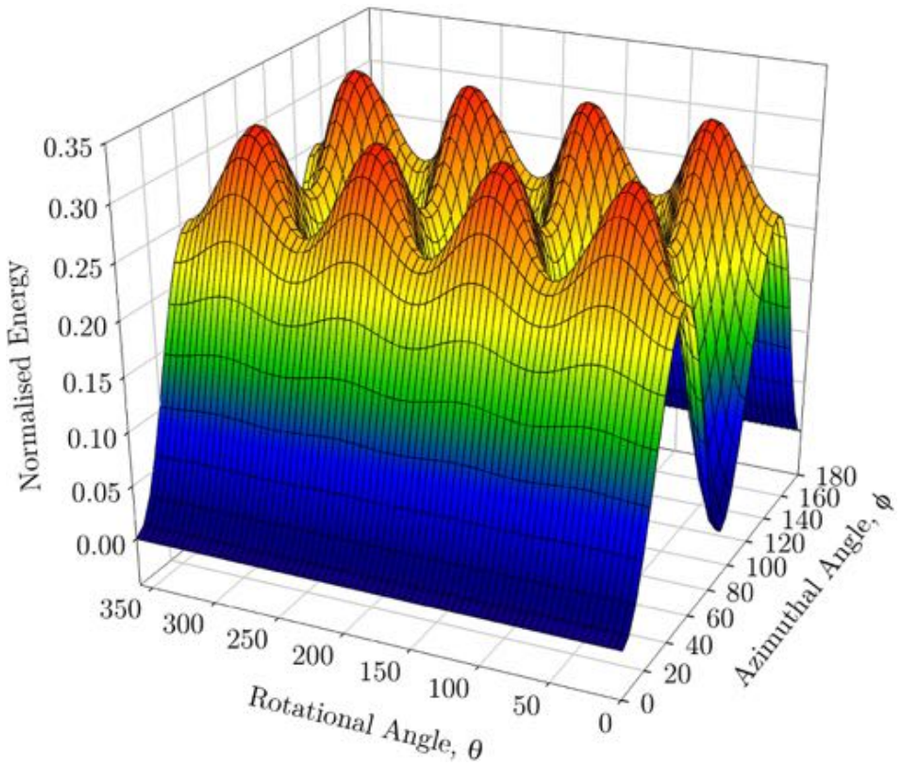
Magnetic anisotropy energy

Uniaxial



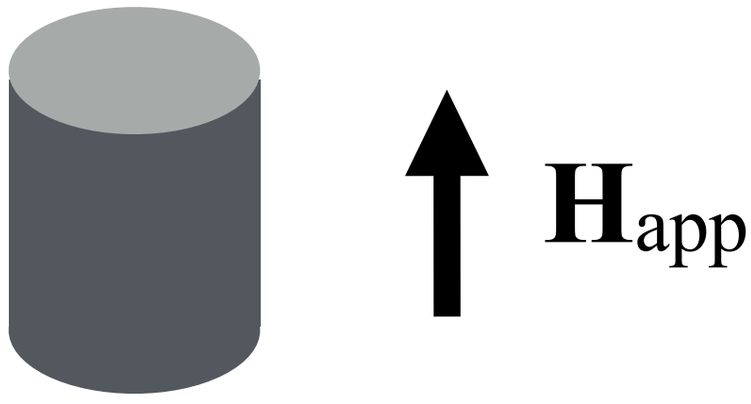
$$\mathcal{H}_{\text{ani}}^{\text{uni}} = -k_{\text{u}} \sum_i \left(\mathbf{S}_i \cdot \boldsymbol{e}\right)^2$$

Cubic



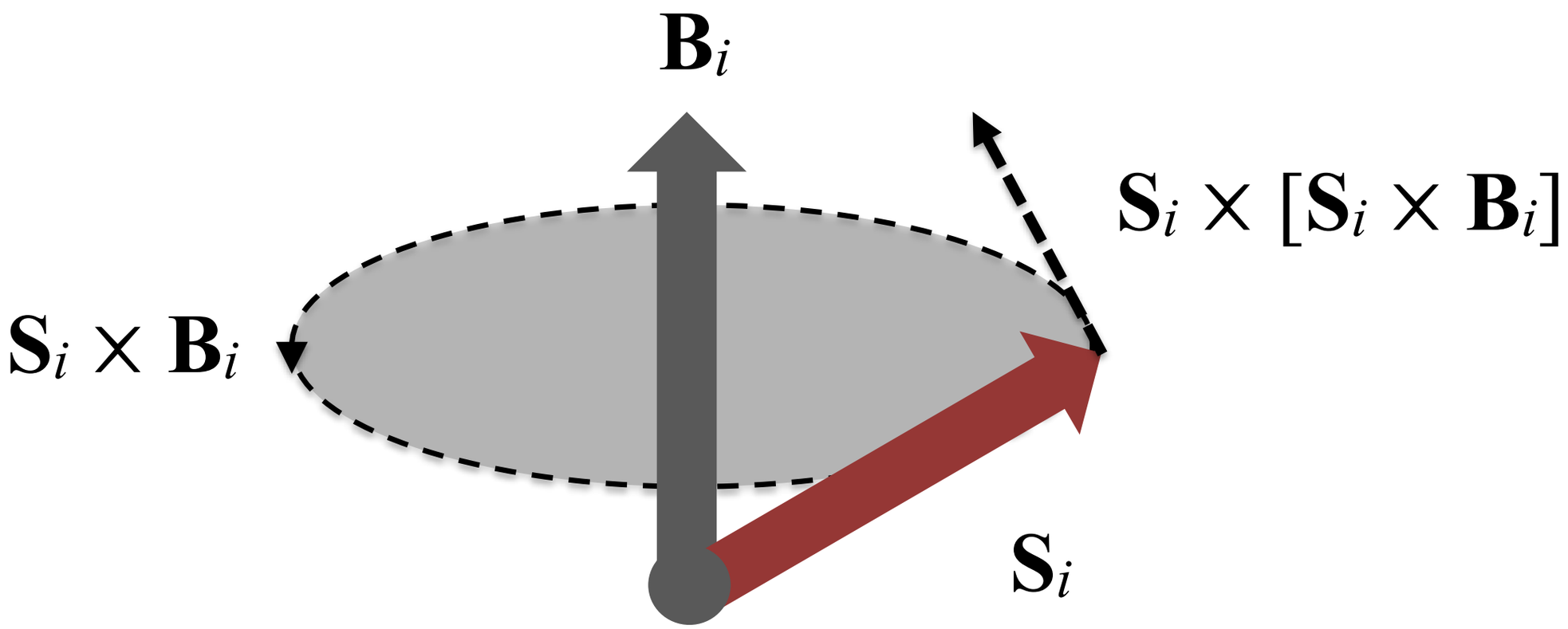
$$\mathcal{H}_{\text{ani}}^{\text{cub}} = \frac{k_{\text{c}}}{2} \sum_i \left(S_x^4 + S_y^4 + S_z^4\right)$$

Externally applied fields



$$\mathcal{H}_{\mathrm{app}} = -\sum_i \mu_{\mathrm{s}} \mathbf{S}_i \cdot \mathbf{H}_{\mathrm{app}}$$

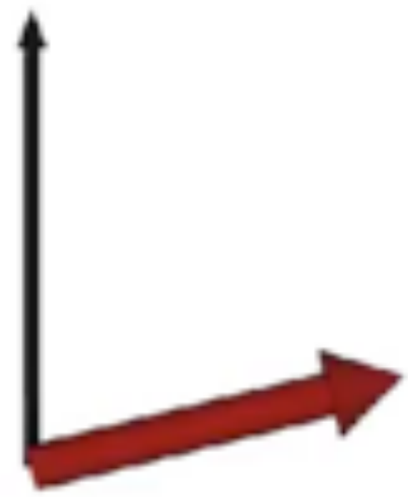
Atomistic *Spin Dynamics*



$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma_i}{(1+\lambda_i^2)}\left[\mathbf{S}_i \times \mathbf{B}_i + \lambda_i \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{B}_i)\right]$$

Stochastic Landau-Lifshitz-Gilbert equation

$$\mathbf{B}_i = \zeta_i(t) - \frac{1}{\mu_i}\frac{\partial \mathscr{H}}{\partial \mathbf{S}_i}$$



$$\zeta_i = \langle \zeta_i^a(t)\zeta_j^b(t)\rangle = 2\delta_{ij}\delta_{ab}(t-t')\frac{\lambda_i k_B T}{\mu_i \gamma_i}$$

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

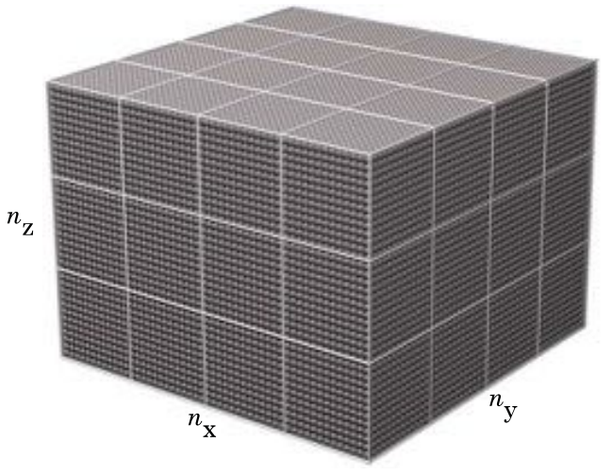
Spin dynamics is the magnetic analogue of molecular dynamics

But typically more complicated dynamics

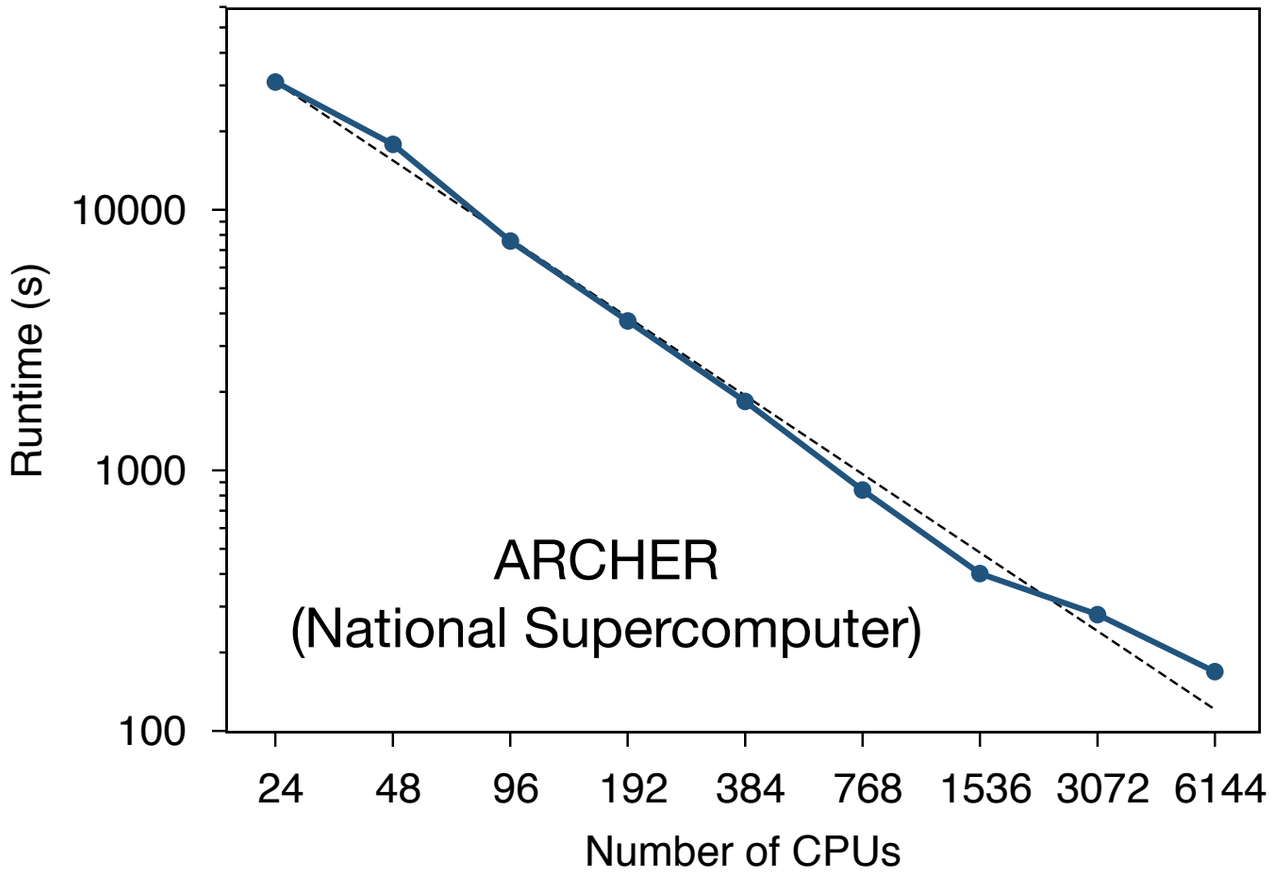
VAMPIRE

vampire.york.ac.uk

Parallel performance of VAMPIRE



Parallelisation for supercomputers and clusters

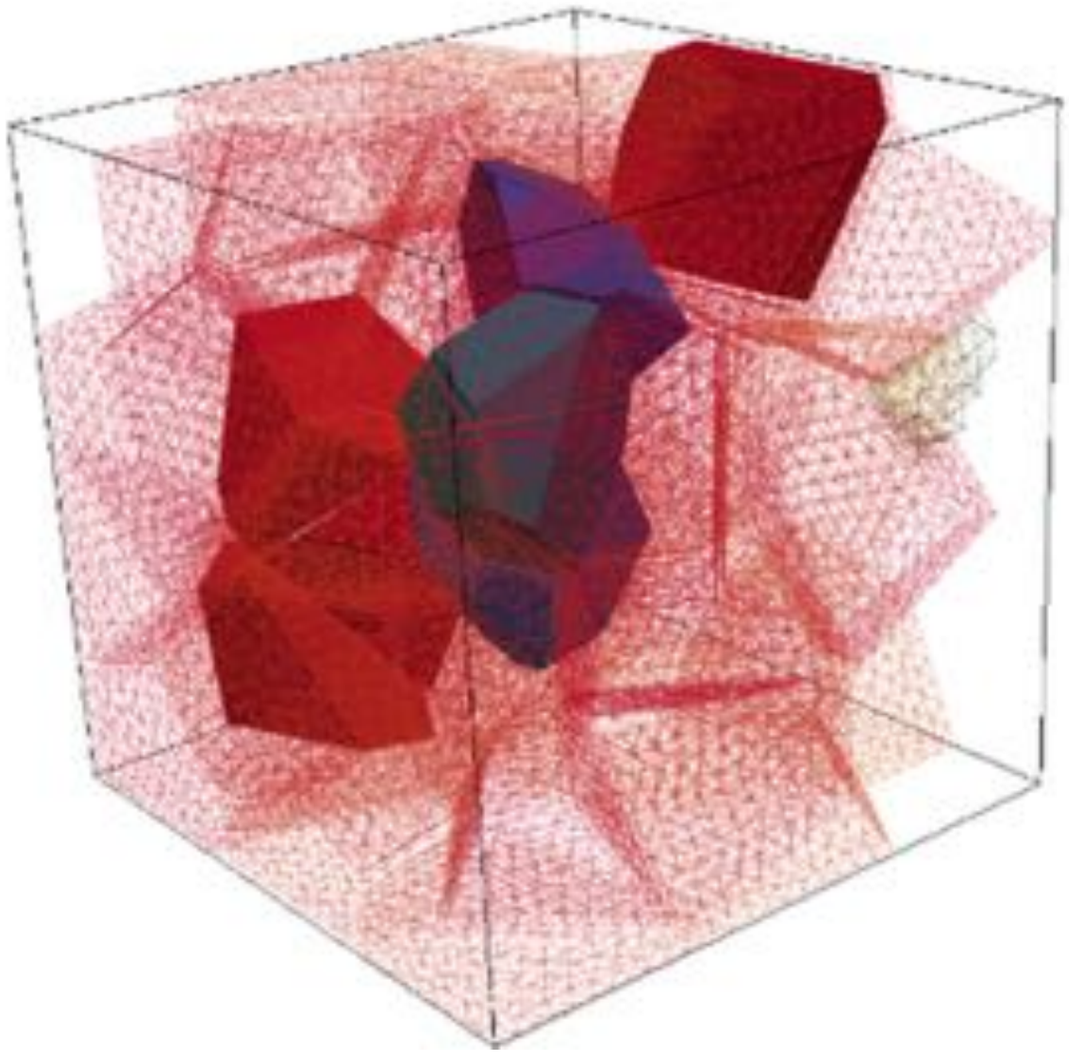


GPU acceleration with CUDA (20-50 x faster than serial)

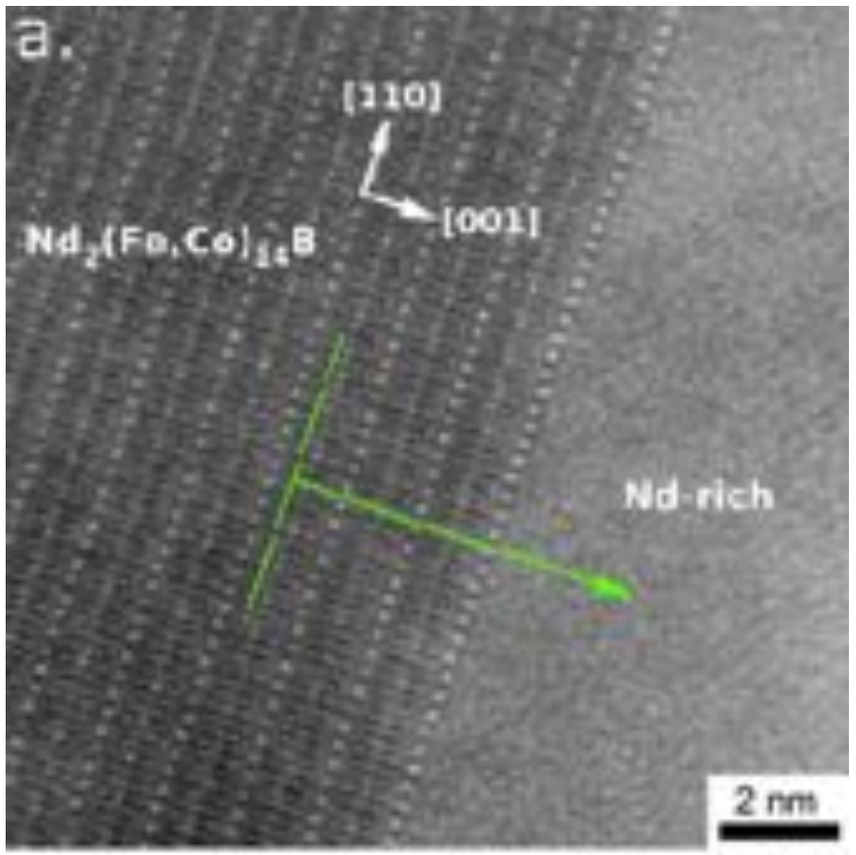
Atomistic spin dynamics and temperature dependent properties of $Nd_2Fe_{14}B$

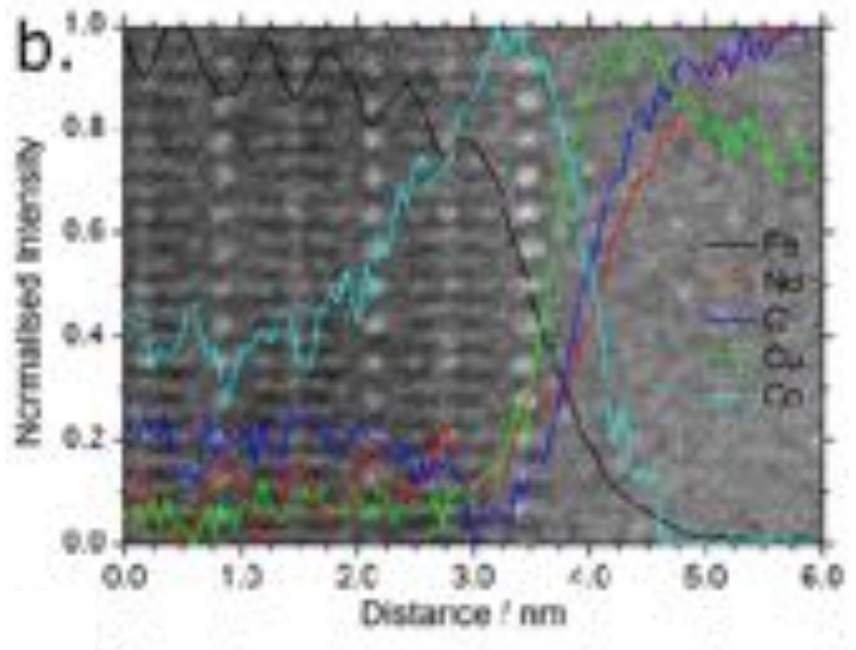
UNIVERSITY of York

Structure at atomic and granular length scales determines overall material performance



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



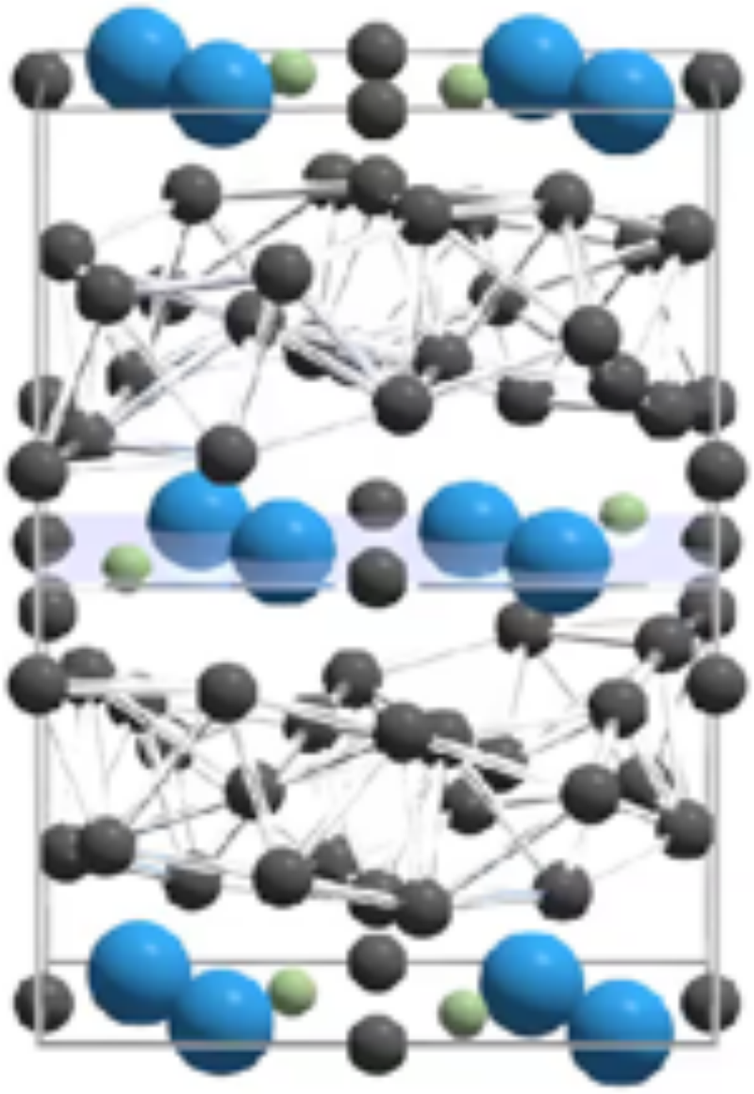


Atomistic spin Hamiltonian for $Nd_2Fe_{14}B$

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

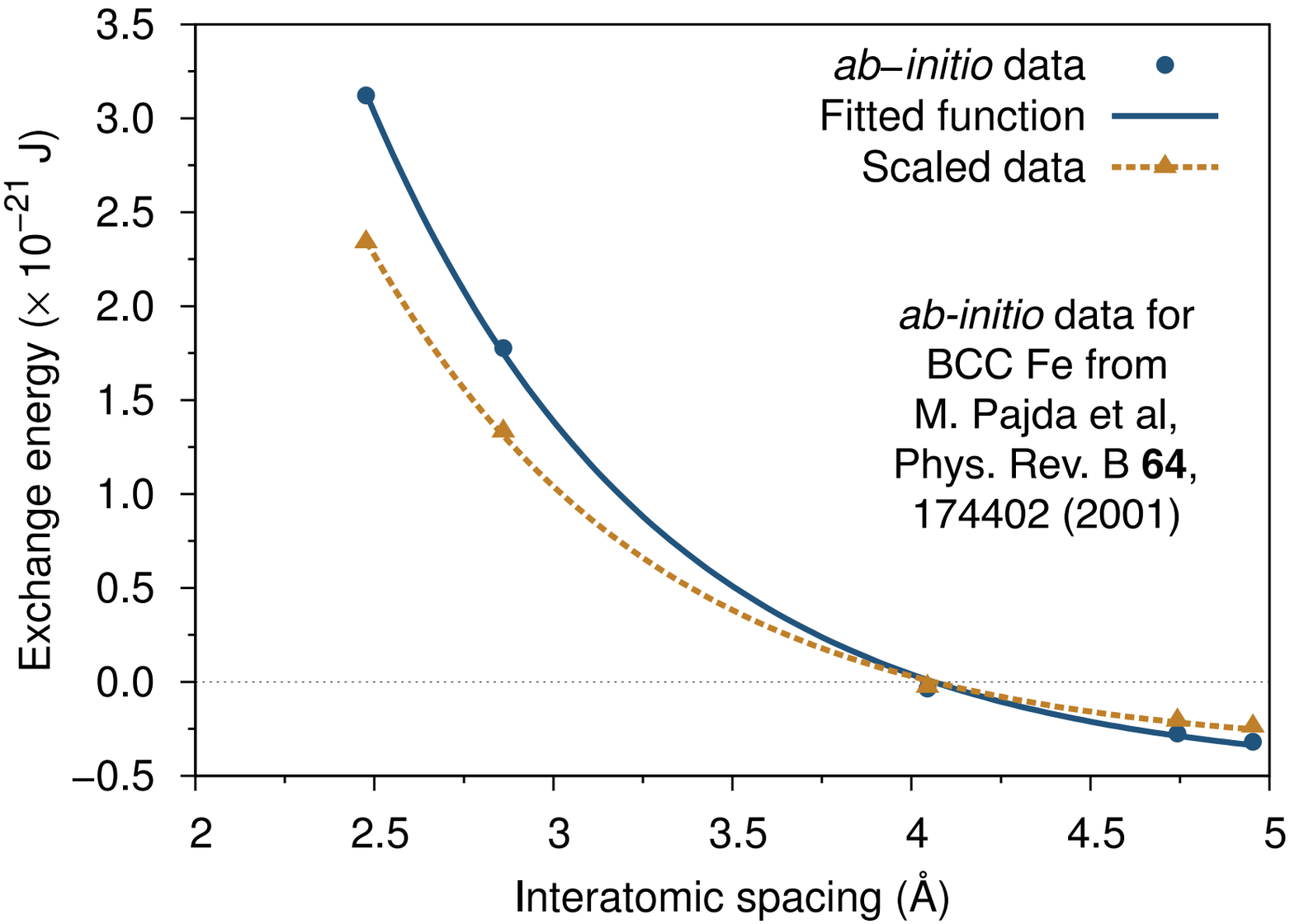
$$\mathscr{H}_{\mathrm{Nd}} = -\sum_{i,\delta} J_{\mathrm{NdFe}} \mathbf{S}_i \cdot \mathbf{S}_\delta - \sum_i E_i^{k,\mathrm{Nd}} - \mu_{\mathrm{Nd}} \sum_i \mathbf{H}_{\mathrm{app}} \cdot \mathbf{S}_i$$

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



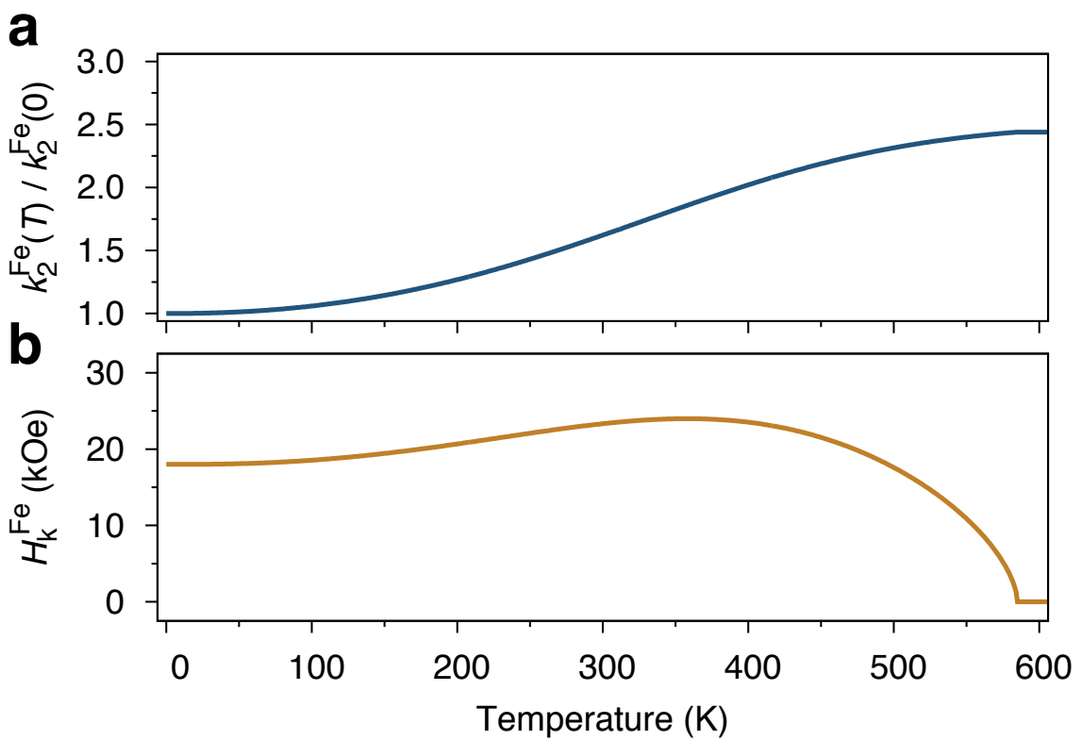
Fe-Fe Exchange interactions

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



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

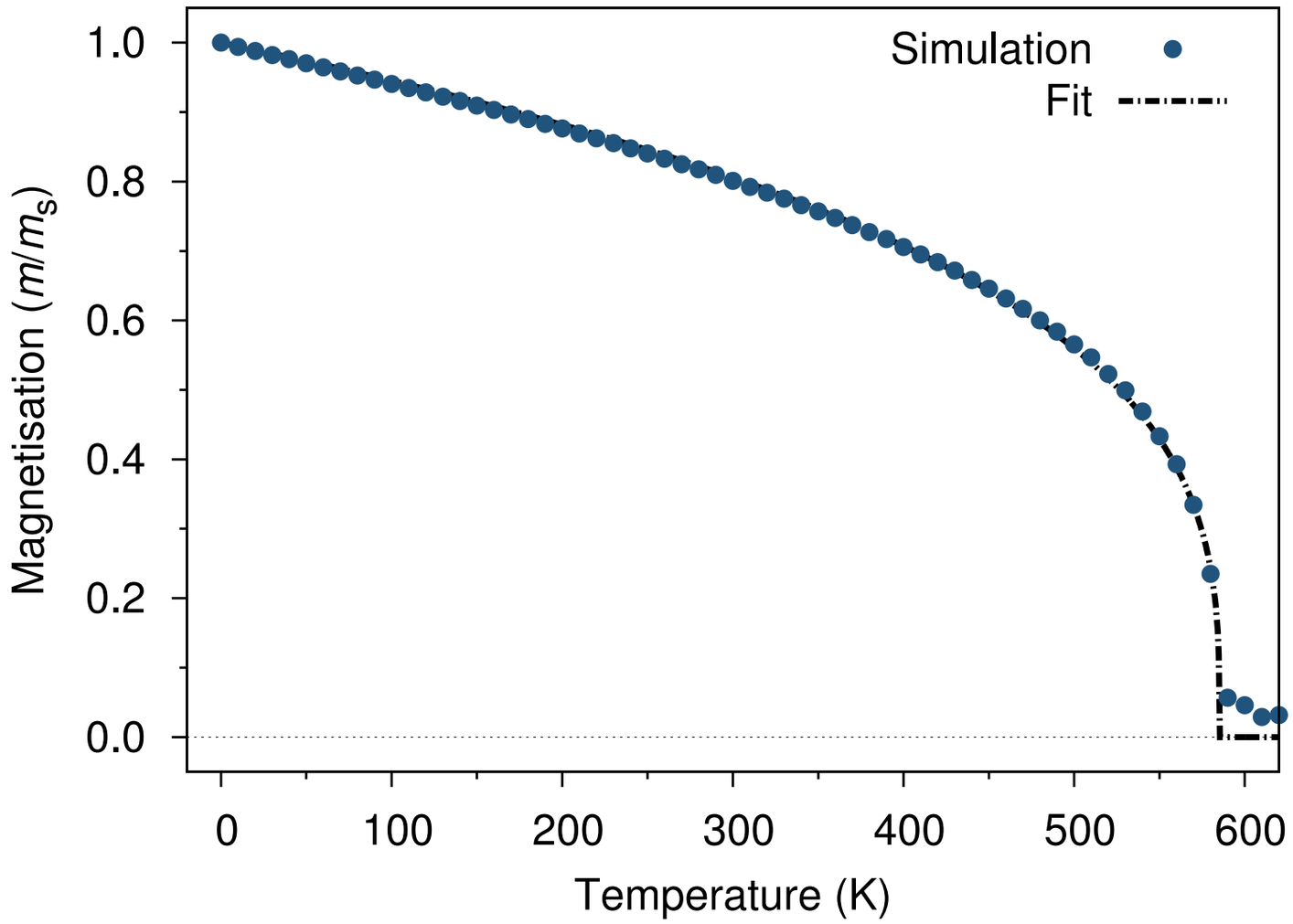
$$E_i^{k,\mathrm{Nd}} = -\kappa_2^{\mathrm{Nd}}\widetilde{P}_2 - \kappa_4^{\mathrm{Nd}}\widetilde{P}_4$$

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

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

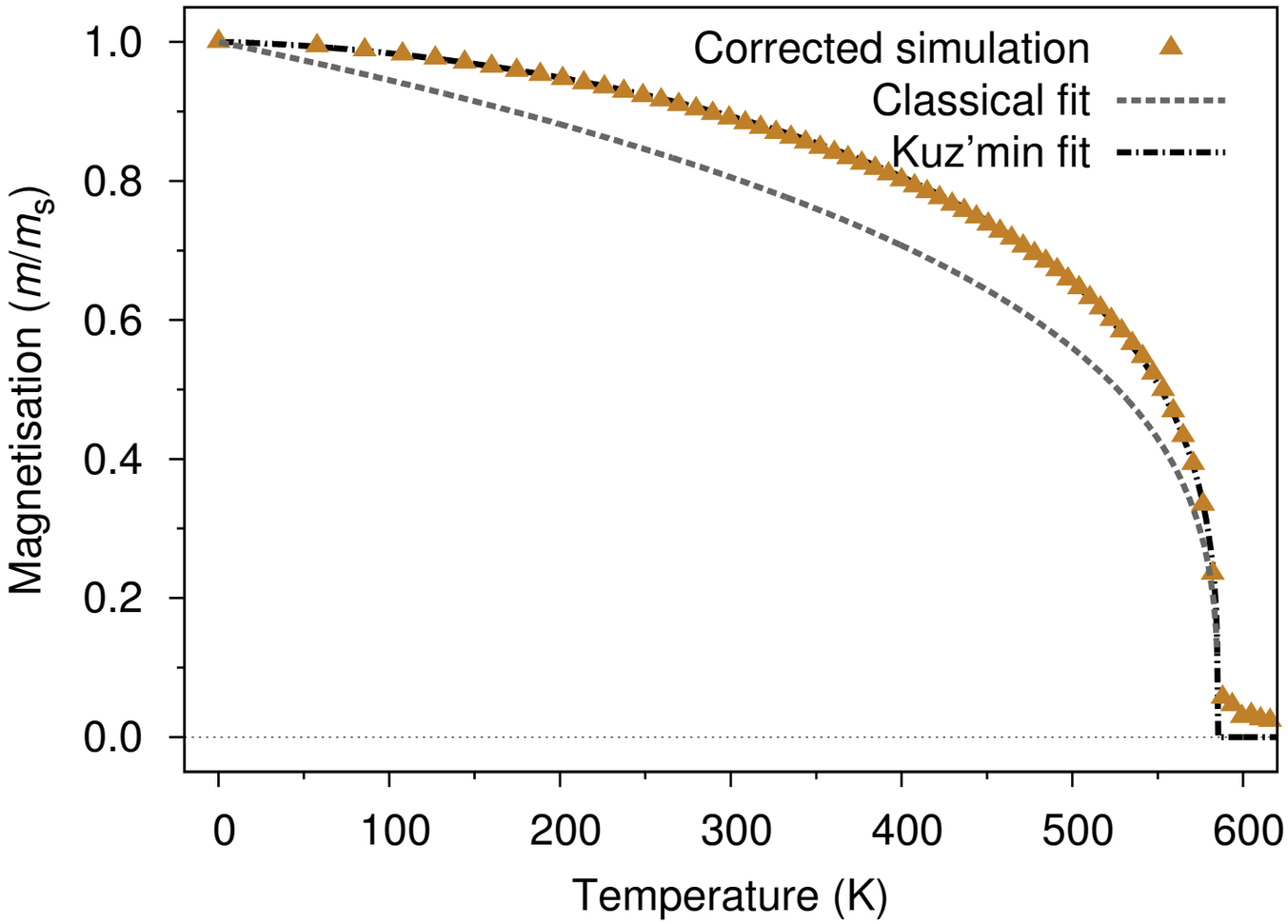
J. F. Herbst, Rev. Mod. Phys. 63, 819 (1991)

Simulated temperature dependent magnetization



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

Problem: poor agreement with experiment due to classical approach



Temperature rescaling

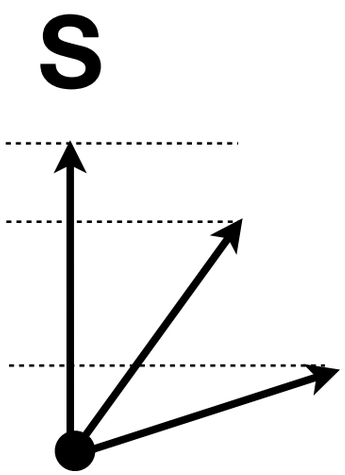
$$m(\tau) = (1 - \tau^{\alpha})^{\beta}$$

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

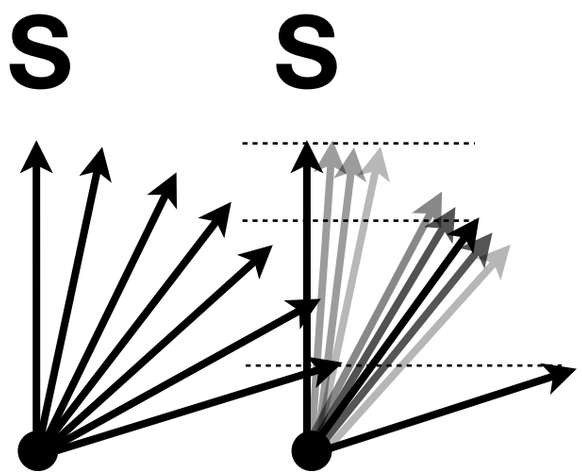
R. F. L. Evans *et al*,

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

Physical picture of temperature rescaling

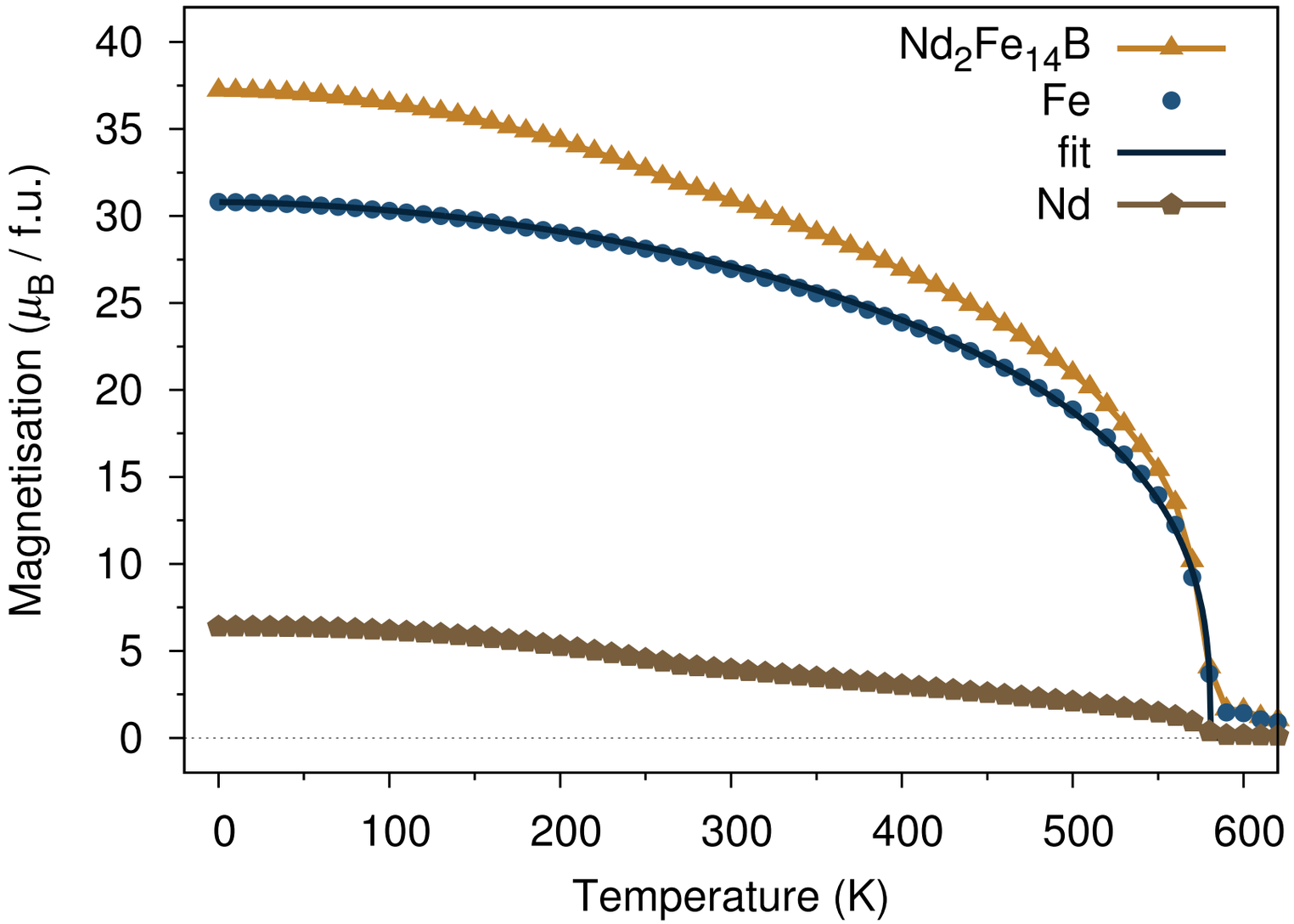


Quantum

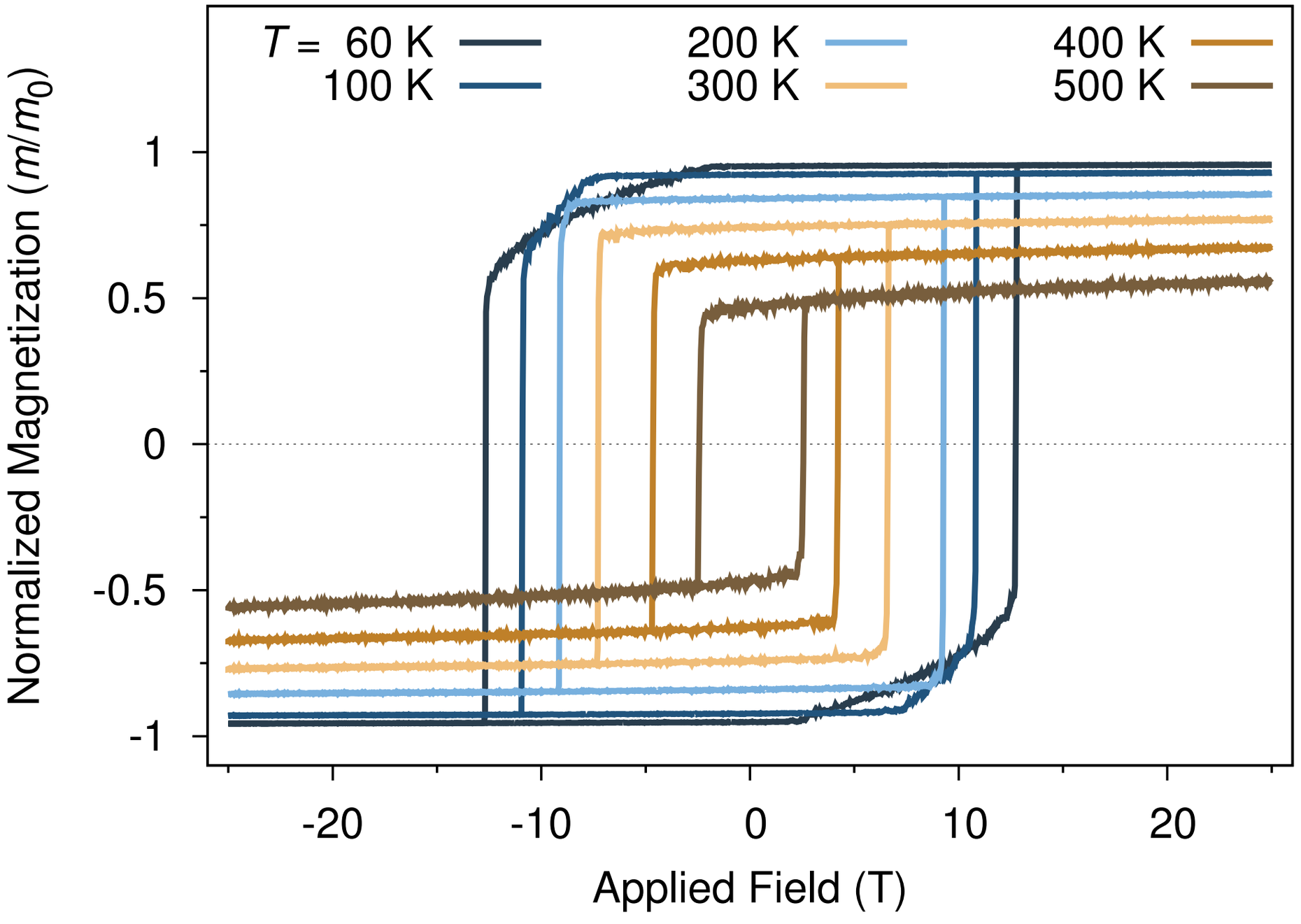


Classical Rescaled

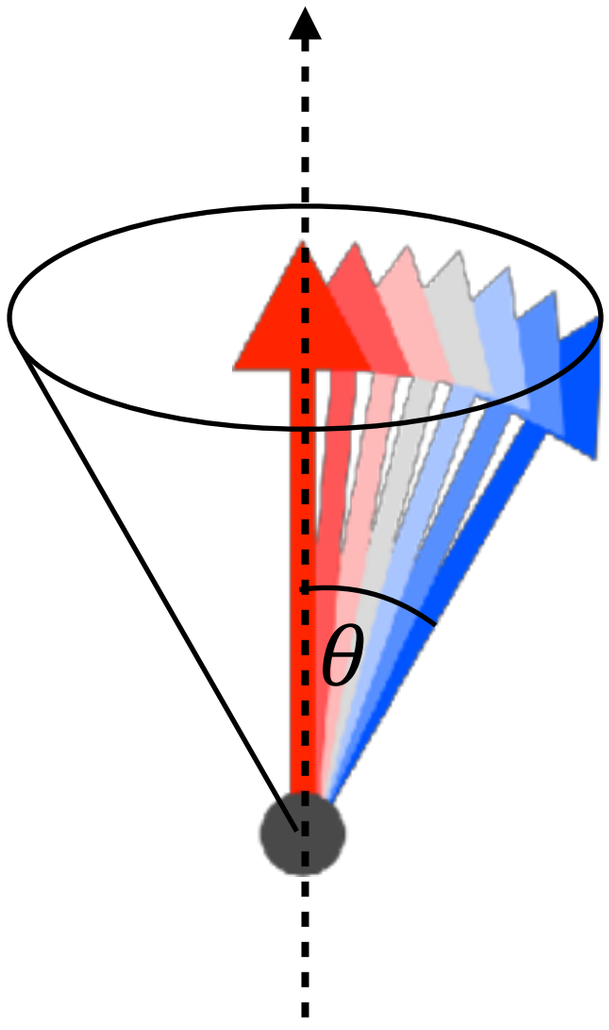
Temperature dependent magnetization with temperature rescaling

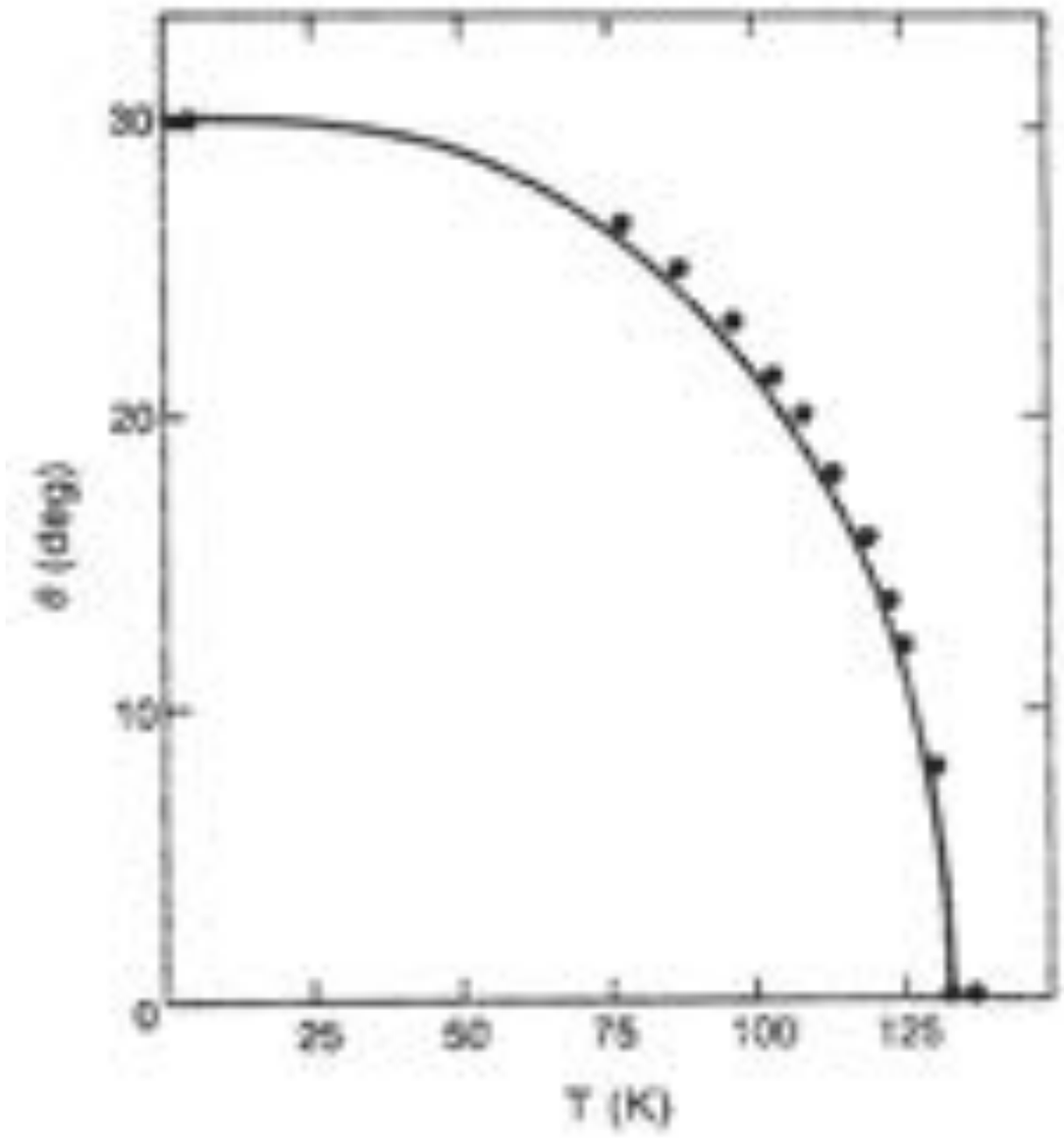


Temperature dependent hysteresis properties



Spin-reorientation transition



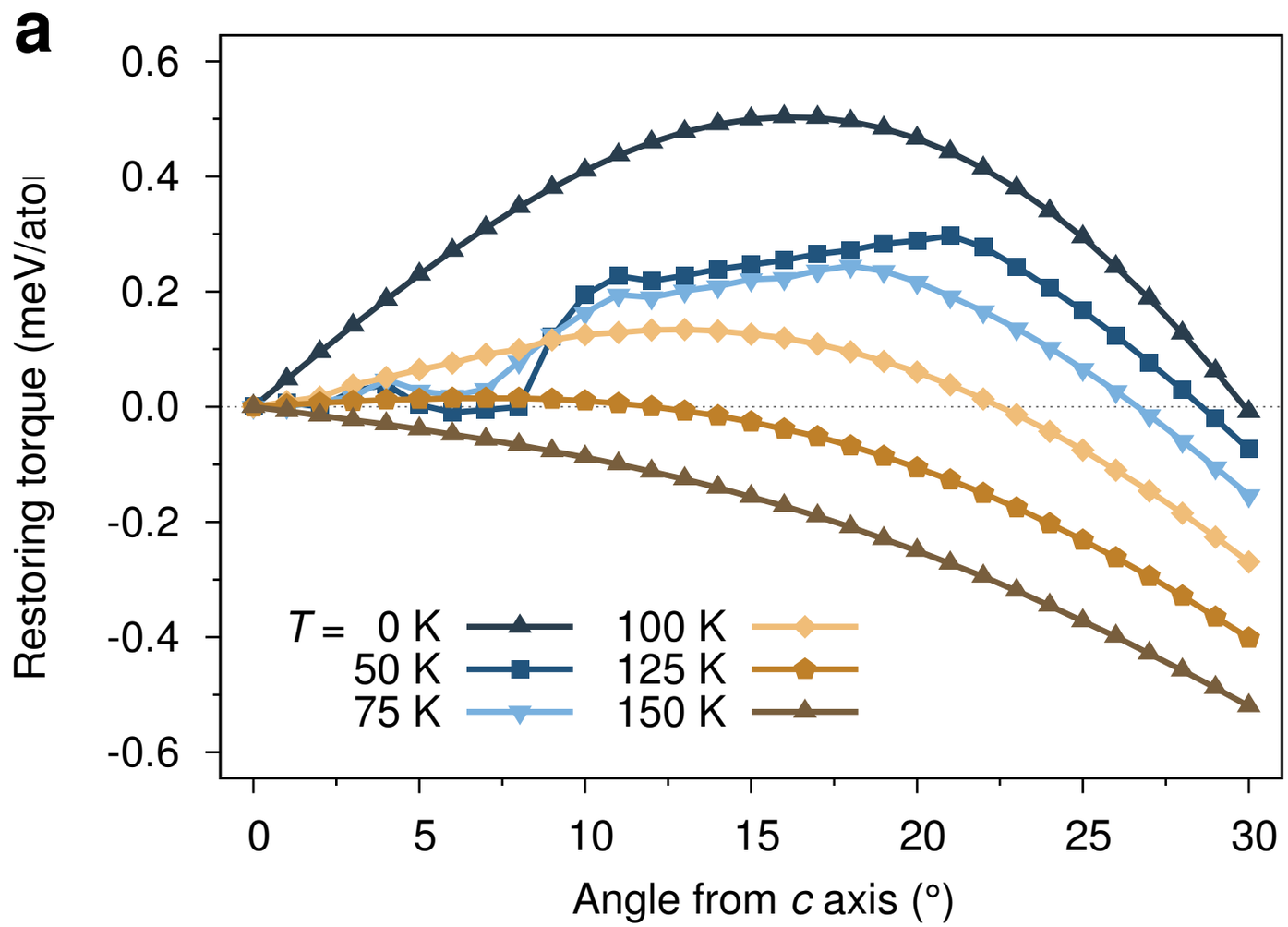


F. T. Parker, J. Appl. Phys. **61**, 2606 (1987)

Spin-reorientation transition: torque method

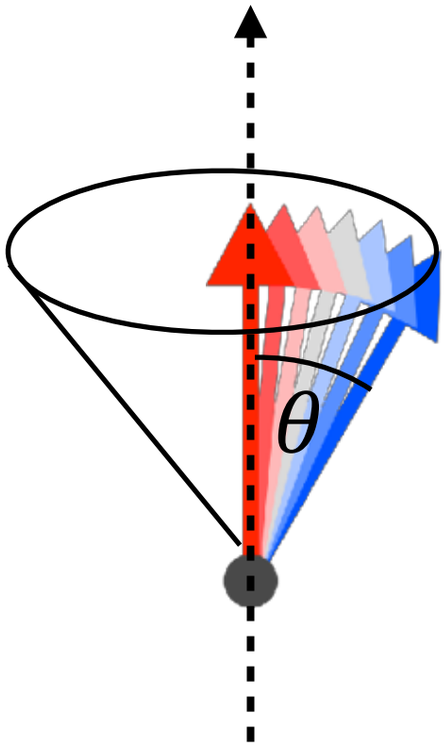
Constrained Monte Carlo method holds *net* magnetization along fixed axis

$$\langle \mathscr{T} \rangle = \langle \sum_i \mathbf{S}_i \times \mathbf{H}_i \rangle$$

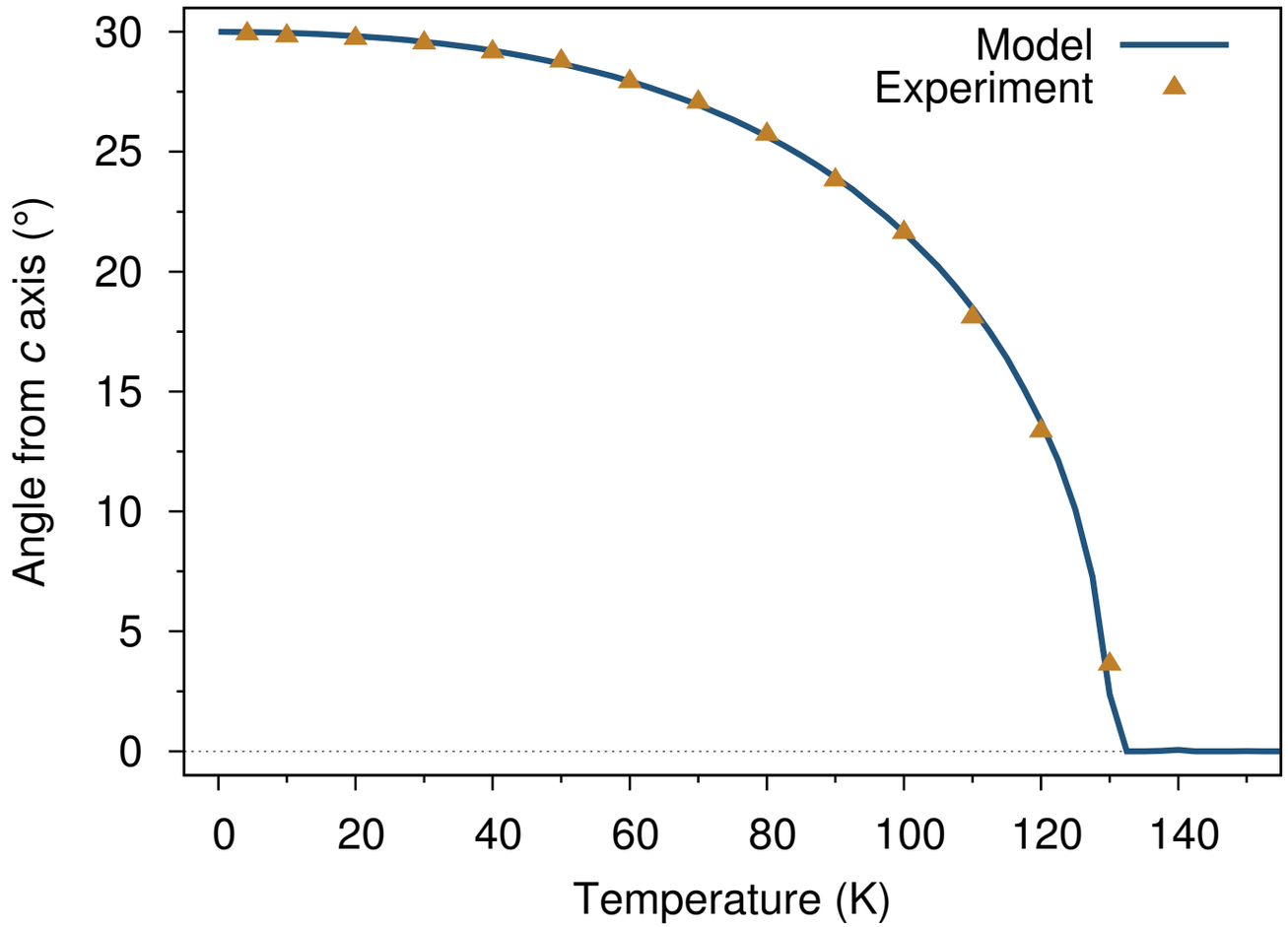


P. Asselin, R. F. L. Evans, *et al* Phys. Rev. B **82**, 054415 (2010)

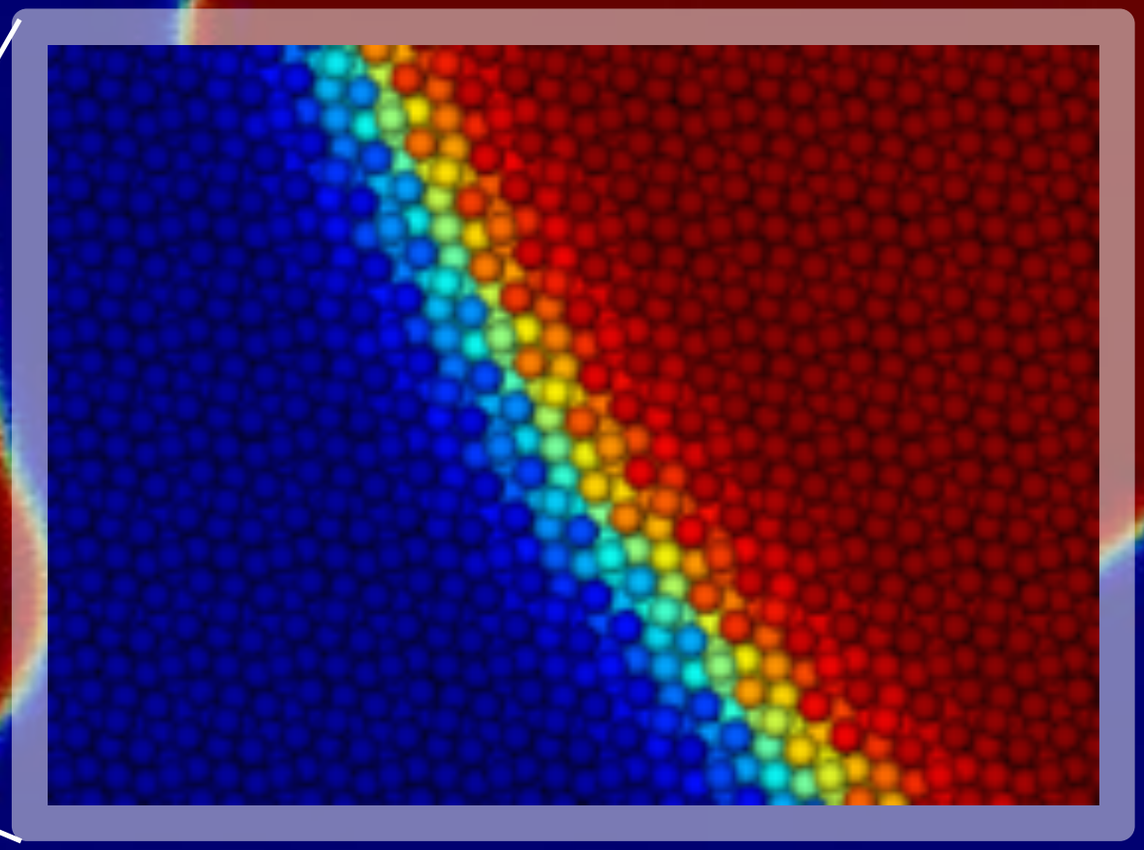
Spin-reorientation transition



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

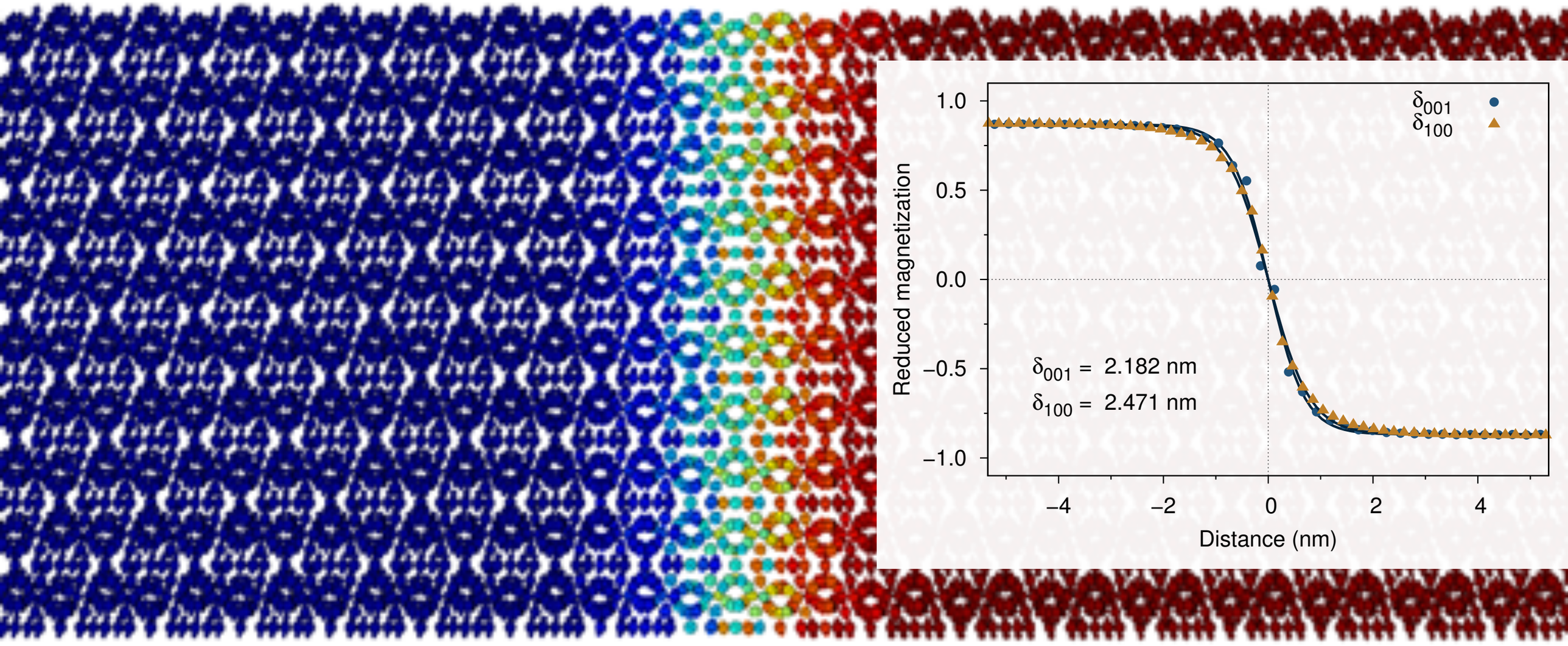


Domain wall structures in $Nd_2Fe_{14}B$



10 nm

Domain wall profile



1 nm

Interfacial atomic structure from molecular dynamics

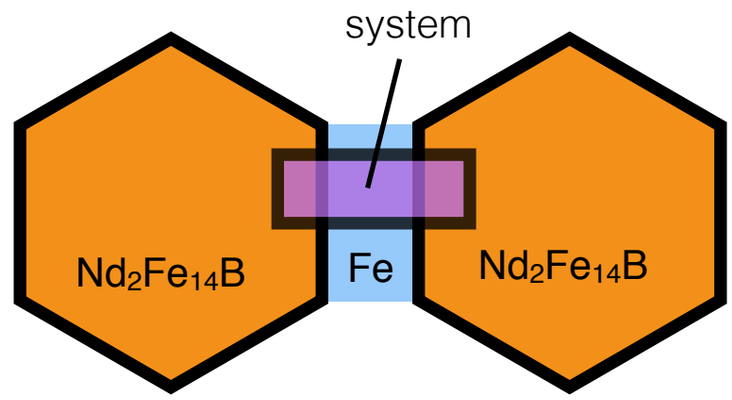
$Nd_2Fe_{14}B$/Fe interface system **relaxed using MD simulation** by G. Hrkac

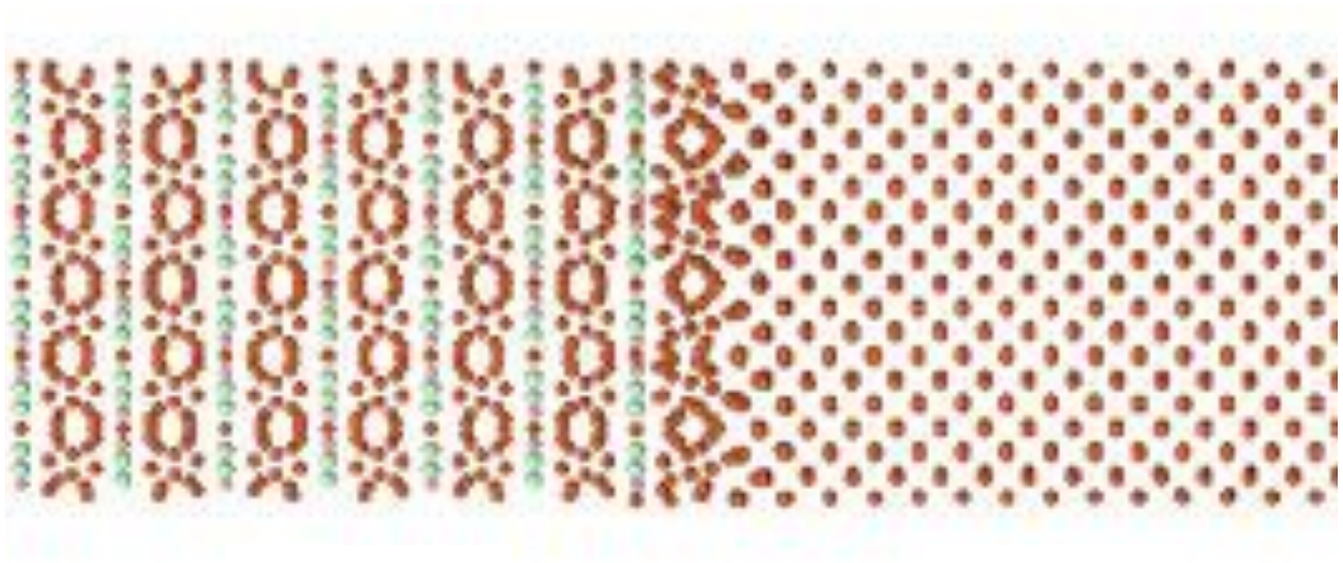
Here we have chosen BCC Fe/ $Nd_2Fe_{14}B$ interface as this is a commonly occurring inter-granular phase

Broken ring structure at interface

Short-range distortion of BCC lattice

System mirrored to create larger area for domain wall propagation simulation





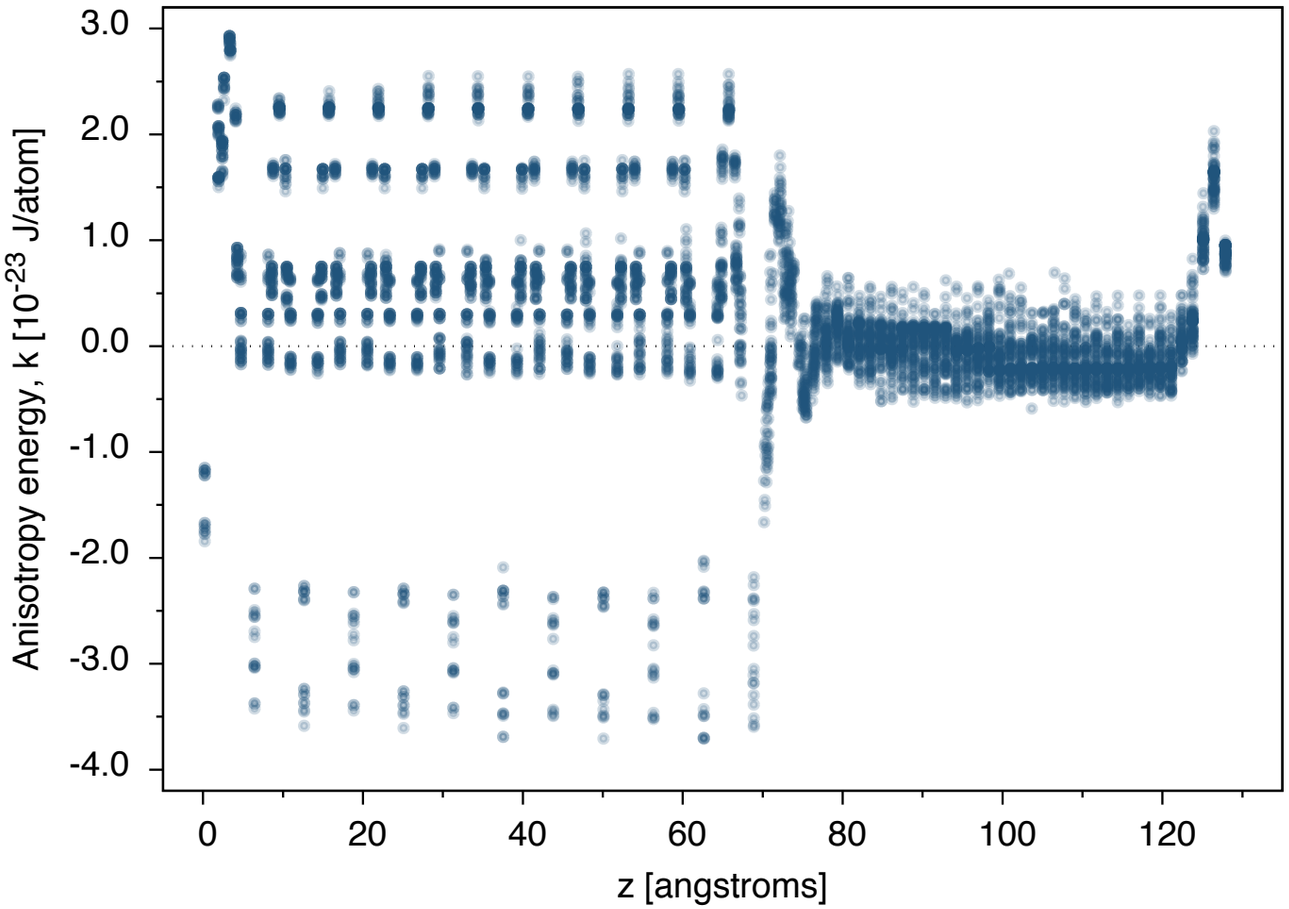
Effective magnetic anisotropy at grain boundary

Fe anisotropy calculated with Neél model, Nd sites using uniaxial constants

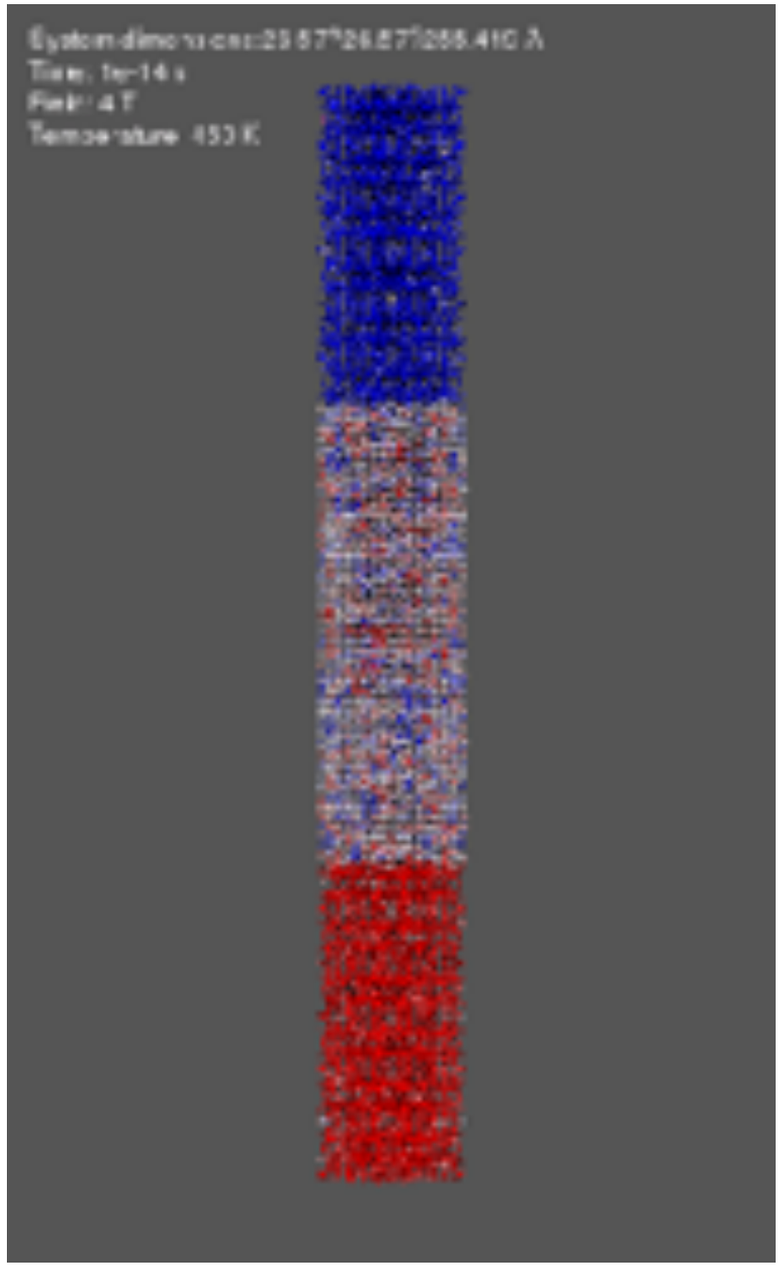
Majority of spins in $Nd_2Fe_{14}B$ phase have out-of-plane anisotropy

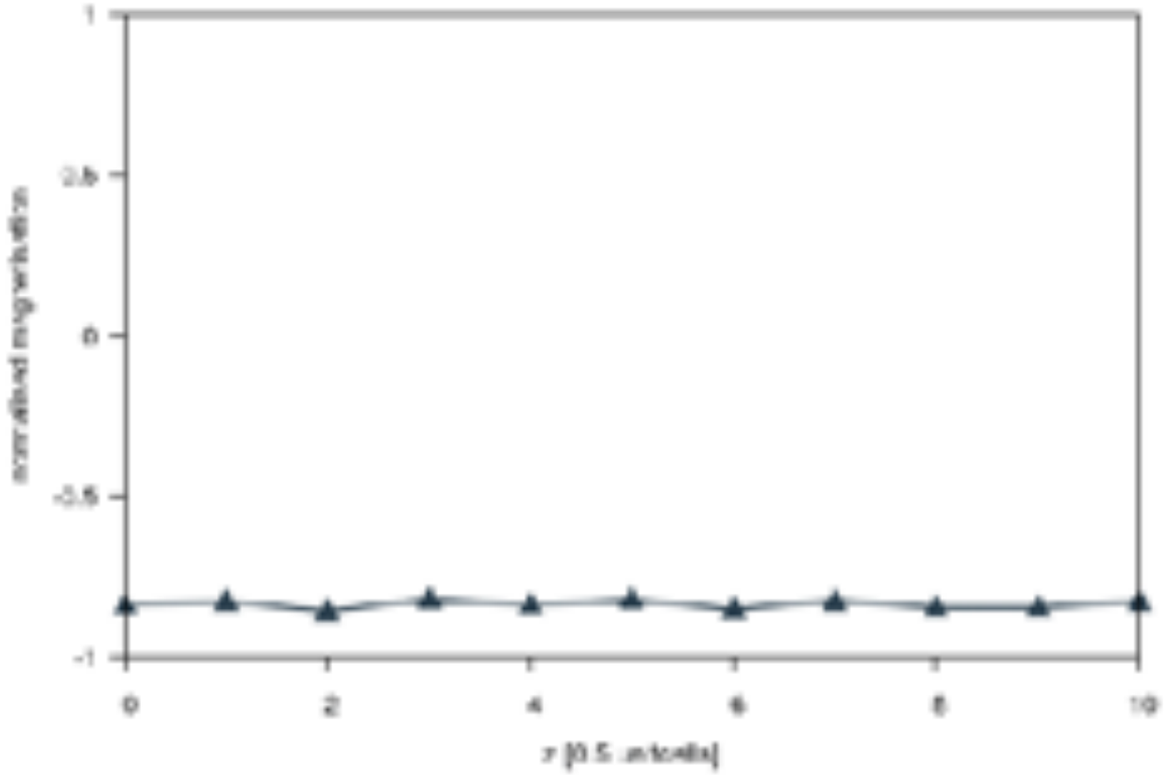
Effect of interface on anisotropy short-ranged

Approximately zero anisotropy in bcc-Fe phase



Effective magnetic anisotropy at grain boundary

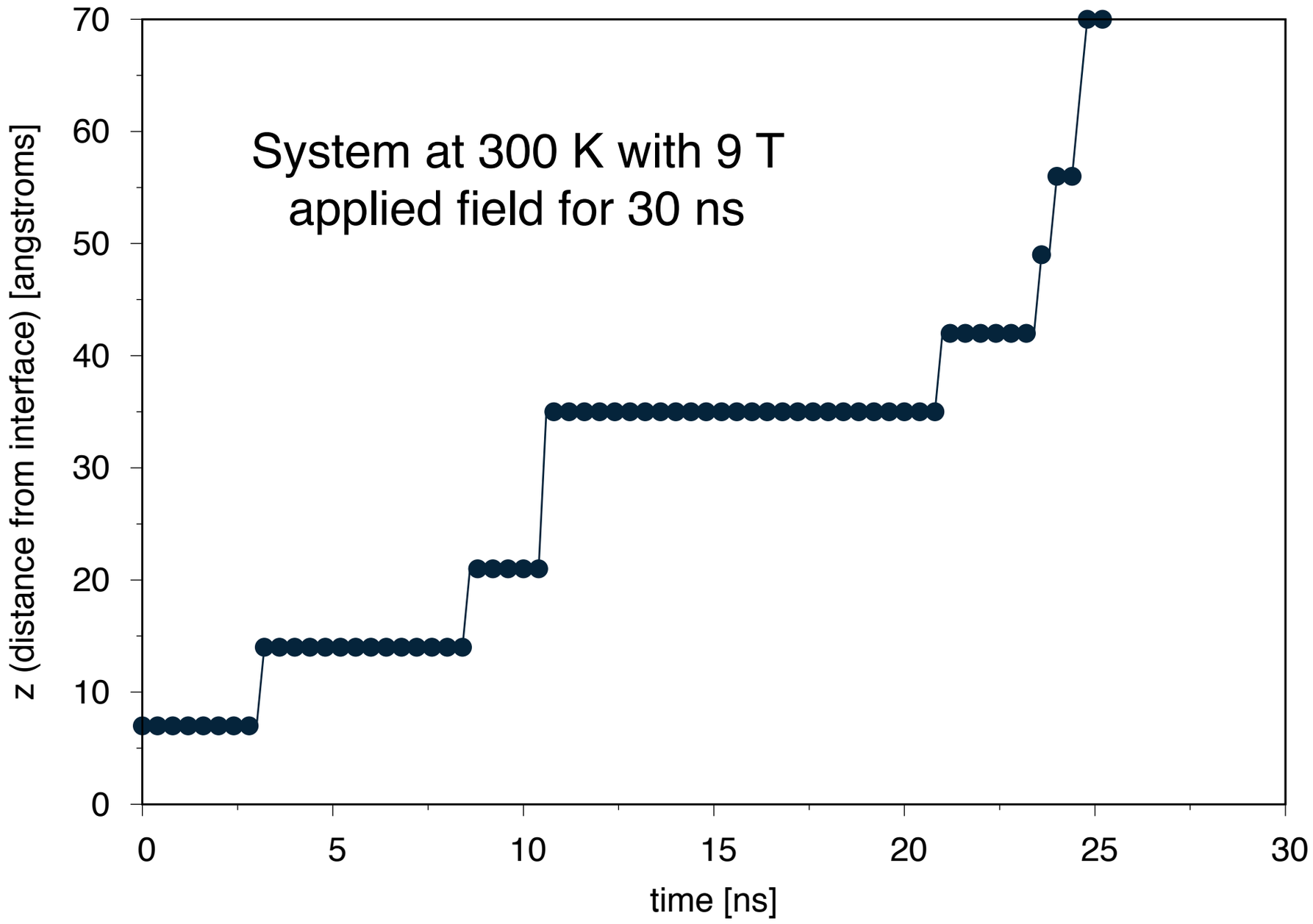




At 450 K, 4 T field required for domain wall to penetrate hard phase on this time scale

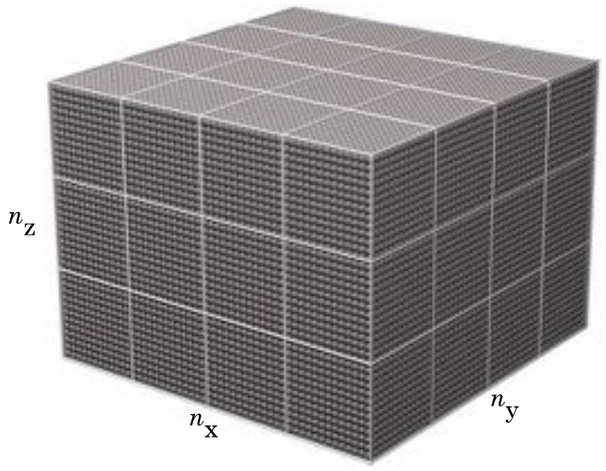
The domain wall propagates faster at higher temperatures due to reduced anisotropy

Barkhausen jumps



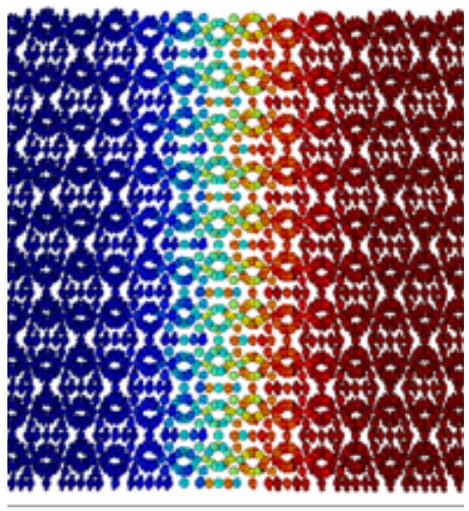
Conclusions

Atomistic spin models provide unprecedented ability to model complex magnetic materials



Parallel computers allow much larger problems to be tackled

New insights into interfacial and thermodynamic properties of Neodymium permanent magnets



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Review article

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

Ising model

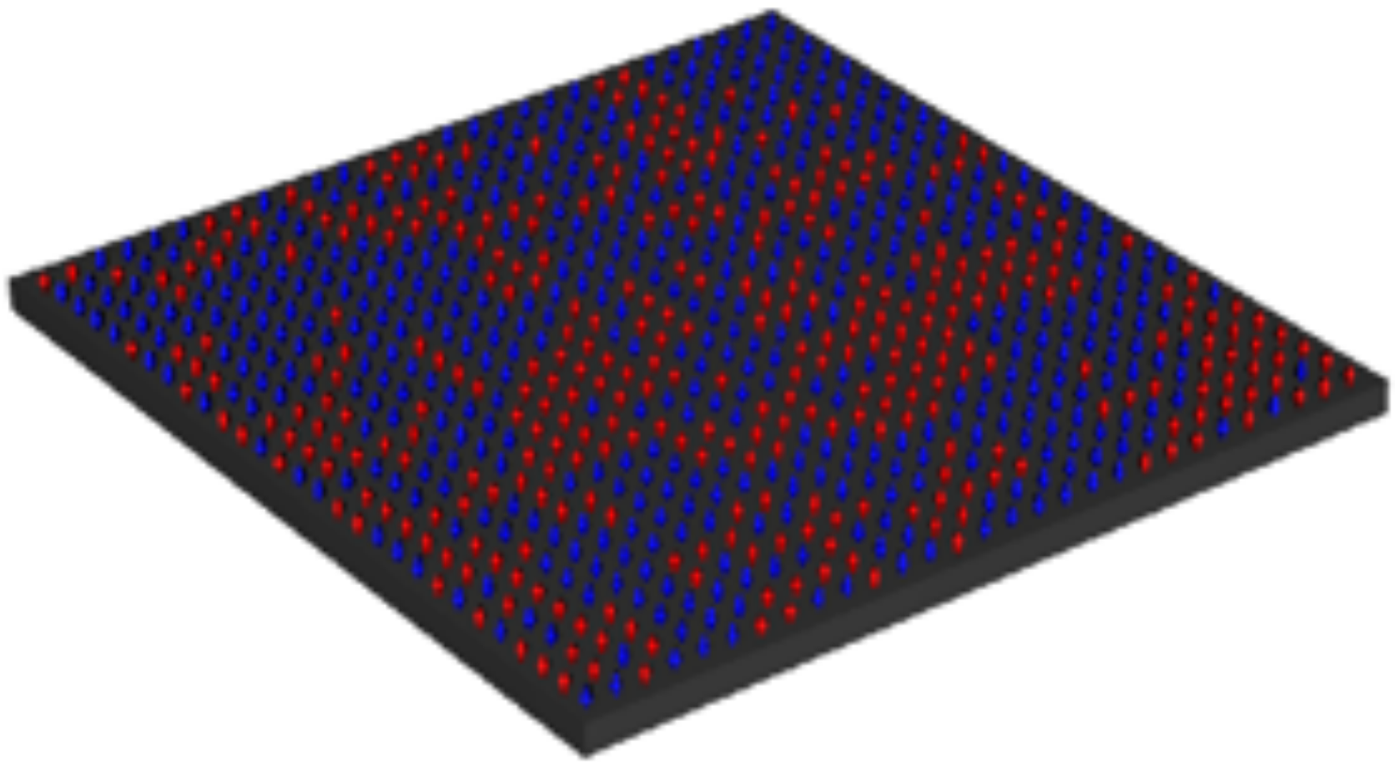
Beitrag zur Theorie des Ferromagnetismus [1].

Von **Ernst Ising** in Hamburg.

(Eingegangen am 9. Dezember 1924.)

Es wird im wesentlichen das thermische Verhalten eines linearen, aus Elementarmagneten bestehenden Körpers untersucht, wobei im Gegensatz zur Weissschen Theorie des Ferromagnetismus kein molekulares Feld, sondern nur eine (nicht magnetische) Wechselwirkung benachbarter Elementarmagnete angenommen wird. Es wird gezeigt, daß ein solches Modell noch keine ferromagnetischen Eigenschaften besitzt und diese Aussage auch auf das dreidimensionale Modell ausgedehnt.

1. Annahmen. Die Erklärung, die P. Weiss [2]) für den Ferromagnetismus gegeben hat, ist zwar formal befriedigend, doch läßt sie besonders die Frage nach einer physikalischen Erklärung der Hypothese des molekularen Feldes offen. Nach dieser Theorie wirkt auf jeden

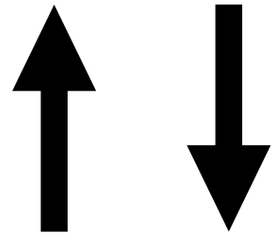


Simplest model of spin-1/2 ferromagnet phase transition

“Toy model”

Ising model

Two allowable states, up, down

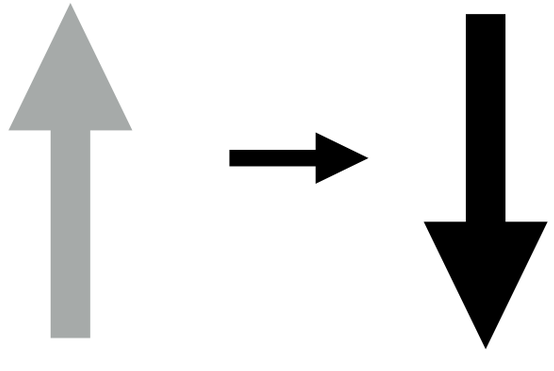


Energy barrier between states defined by exchange energy

$$\mathcal{H}_{\text{exc}} = -\frac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$

Monte Carlo algorithm

1. Pick a new trial state (or move)



2. Evaluate energy before (E_1) and after (E_2) spin flip

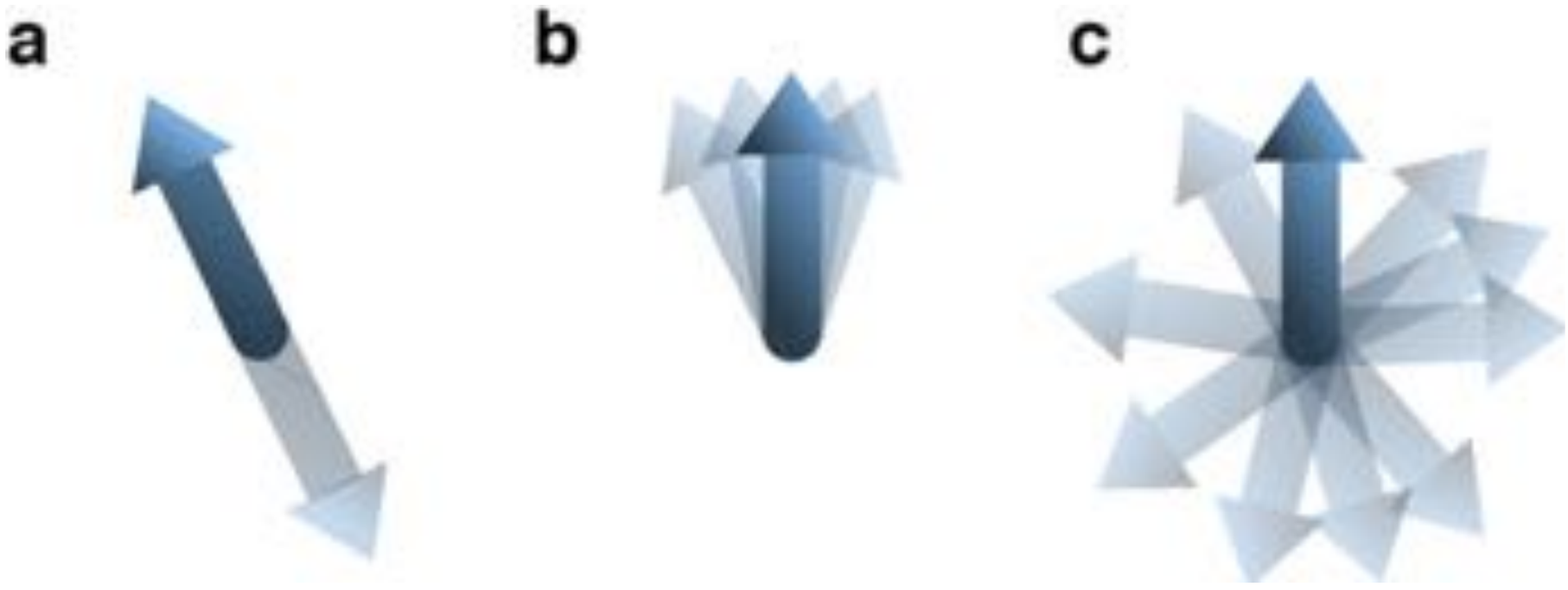
3. Evaluate energy difference between states

$$\Delta E = (E_2 - E_1)$$

4. Accept move with probability

$$\exp(-\Delta E/k_B T)$$

Extension to 3D Heisenberg model straightforward



Use a combination of different trial moves