Magnetic Small-Angle Neutron Scattering: A Probe for Mesoscale Magnetism Analysis

Andreas Michels

Department of Physics and Materials Science, University of Luxembourg

UNIVERSITÉ DU LUXEMBOURG

CEMAG Club Español de Magnetismo

The EUROPEAN MAGNETISM ASSOCIATION

IEEE MAGNETICS spain.eu

andreas.michels@uni.lu

Acknowledgements

- Mathias Bersweiler, Ivan Titov, Venus Rai, Elizabeth Jefremovas, Evelyn Pratami Sinaga, Michael Adams, Stefan Liscak (University of Luxembourg)
- Joachim Kohlbrecher (PSI), Dirk Honecker & Diego Alba Venero (ISIS), Sebastian Mühlbauer (TUM), Nina-Juliane Steinke (ILL)
- María del Puerto Morales (ICMM-CSIC, Madrid)
- Luis F. Barquín (U Cantabria)
- Hamid Kachkachi (U Perpignan)
- Konstantin Metlov (Donetsk)
- Sergey Erokhin, Dmitry Berkov (General Numerics Research Lab, Jena)

UNIVERSITÉ DU LUXEMBOURG

Fonds National de la Recherche Luxembourg

DFG

Outline

- ➢ **The very basics of magnetic neutron scattering**
  - ✓ Properties of the neutron
  - ✓ Basic interactions, Born approximation, magnetic scattering cross section...

- ➢ **Magnetic Small-Angle Neutron Scattering (SANS)**
  - ✓ Origin of magnetic SANS
  - ✓ Analytical SANS theory
  - ✓ Analysis of magnetic microstructure
  - ✓ Real-space analysis

- ➢ **Selected Examples**
  - ✓ Impact of DMI: Symmetry breaking at defect sites
  - ✓ Scaling in magnetic SANS
  - ✓ Signatures of hopfions

- ➢ **Conclusion**

Basic properties of the neutron

- Neutron is an elementary particle, which has been discovered by James Chadwick in 1932 (Nobel Prize 1935)
- mass $m = 1.675 \times 10^{-27}$ kg (-> de Broglie wavelength in Å regime; allows to study static and dynamic structure of matter)
- spin angular momentum of $S = \pm\frac{1}{2}\,\hbar$ and associated magnetic dipole moment of $\mu = -1.913\ \mu_N$ (-> allows to probe magnetism)
- zero net electrical charge (-> weak interaction; interpretation of scattering data in terms of Born approximation)
- average lifetime of a free neutron is ~ 886 seconds (long enough)

→ neutrons are extremely attractive for research purposes, in particular, for investigating the structure and dynamics of matter on a wide range of length and time scales

Classification of research neutrons

	Energy [meV]	Temperature [K]	Wavelength [Å]	Velocity [m/s]
hot neutrons	100–500	1200–6000	1–0.4	4000–10000
thermal neutrons	10–100	120–1200	3–1	1000–4000
cold neutrons	0.1–10	1–120	30–3	130–1300

H. Schober, J. Neutron Research 17, 109 (2014).

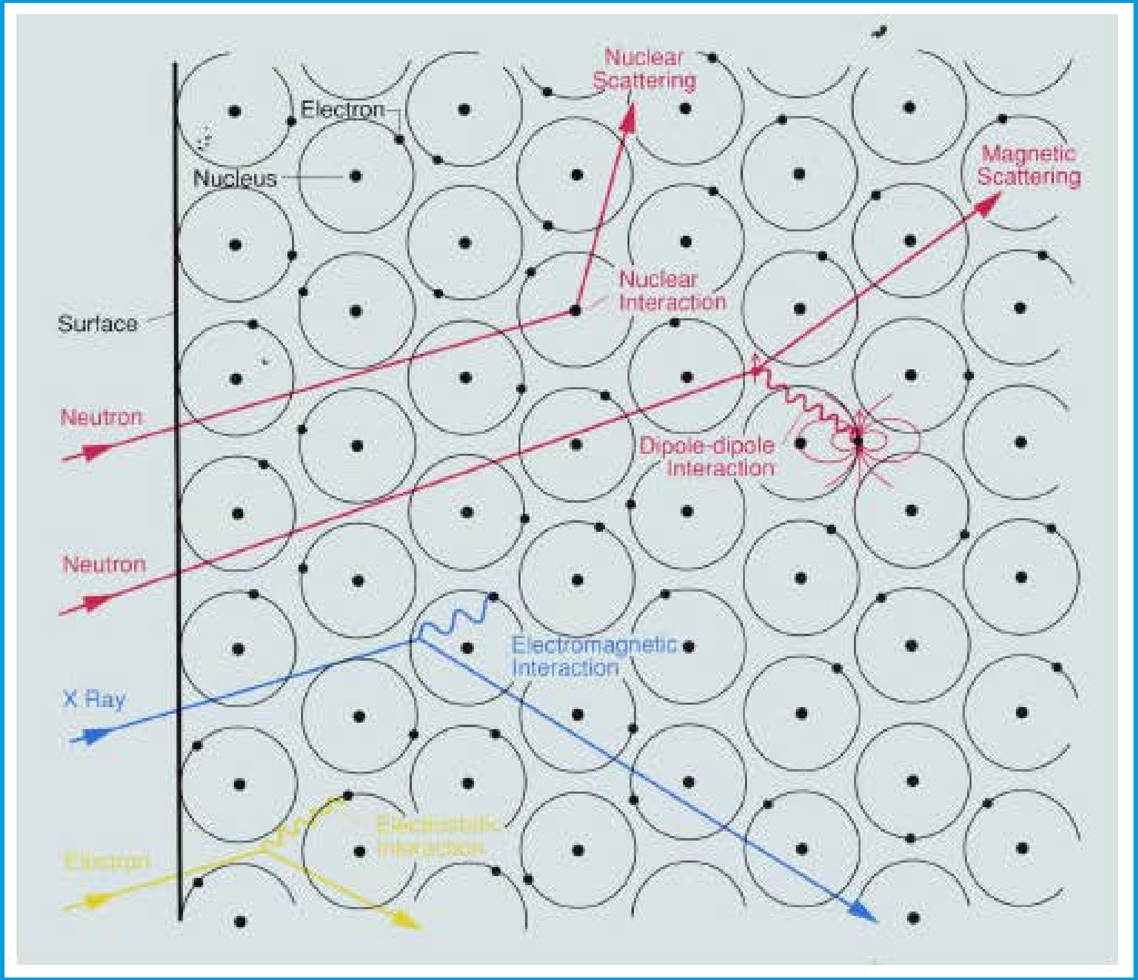
$$E = kT = \tfrac{1}{2}\, m\, v^2$$

$$\lambda = h/(mv)$$

$$k = 2\pi/\lambda$$

$$\mathbf{p} = \hbar\mathbf{k}$$

Neutron-Matter Interaction Mechanisms



R. Pynn, in *Neutron Scattering: A Primer*, Los Alamos Science (1990).

- ❑ **Neutrons interact with atomic nuclei via very short-range (~ fm) forces**
- ❑ **Neutrons also interact with unpaired electrons via a magnetic dipole interaction**

The cross section: Born approximation

- In general we consider the scattering process of neutrons by a sample during which the sample state changes from s_0 to s_1 (e.g., via the excitation or annihilation of a phonon or magnon) while the state of neutron changes from $\mathbf{k}_0$, $\boldsymbol{\sigma}_0$ to $\mathbf{k}_1$, $\boldsymbol{\sigma}_1$
- For <u>elastic scattering</u> ($s_0 = s_1$) and ignoring the spin degree of freedom of the neutron ($\boldsymbol{\sigma}$), the cross section is given by (only direction of neutron beam changes)

$$\frac{d\Sigma}{d\Omega} = \frac{1}{V}\frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\mathbf{k}_1 \text{ in } d\Omega} \overbrace{W_{\mathbf{k}_0\rightarrow\mathbf{k}_1}}^{\text{transition rate}}$$

$$\sum_{\mathbf{k}_1 \text{ in } d\Omega} W_{\mathbf{k}_0\rightarrow\mathbf{k}_1} = \frac{2\pi}{\hbar}\rho_{\mathbf{k}_1}\left|\langle\mathbf{k}_1|V_{\text{int}}|\mathbf{k}_0\rangle\right|^2$$

Fermis Golden Rule

- where V_{int} denotes the neutron-matter interaction potential (to be specified)
- Born approximation: incoming and outgoing neutron waves are in a plane-wave state
- In Born approximation, the matrix element reduces to the Fourier transform of V_{int}

Basic interactions of research neutrons with matter

Modeled by <u>Fermi Pseudo potential</u>; very short range; gives correct result in first Born approximation; Neutron wavelength (a few Å) >> size of the nucleus -> <u>isotropic</u> s-wave scattering

Nuclear Scattering

$$\sum_{\mathbf{k}_1 \text{ in } d\Omega} W_{\mathbf{k}_0 \to \mathbf{k}_1} = \frac{2\pi}{\hbar} \rho_{\mathbf{k}_1} \left| \langle \mathbf{k}_1 | V_{\text{int}} | \mathbf{k}_0 \rangle \right|^2$$

$$\boxed{V_{\text{int}}^{\text{nuc}}(\mathbf{r}) = \frac{2\pi\hbar^2}{m_{\text{n}}} b\delta(\mathbf{r})}$$

$$b = b' - ib''$$

nuclear scattering length (bound); b ~ a few fm = 10^{-15} m
b″ describes absorption (^{3}He, B, Cd, Gd); for most materials b″ << b′

$$\frac{d\sigma_{\text{nuc}}}{d\Omega}(\mathbf{q}) = \left| \sum_{m=1}^{N} b_m e^{-i\mathbf{q}\mathbf{r}_m} \right|^2 = \sum_{m,n} b_m b_n^* e^{-i\mathbf{q}(\mathbf{r}_m - \mathbf{r}_n)}$$

Basic interactions of research neutrons with matter

- The magnetic moment of the neutron μ_n interacts with the magnetic field B, which is produced by the spin (B_S) and orbital motion (B_L) of the electrons

Magnetic Scattering

$$\sum_{\mathbf{k}_1 \text{ in } d\Omega} W_{\mathbf{k}_0 \to \mathbf{k}_1} = \frac{2\pi}{\hbar} \rho_{\mathbf{k}_1} \left| \langle \mathbf{k}_1 | V_{\text{int}} | \mathbf{k}_0 \rangle \right|^2$$

$$\boxed{V_{\text{int}}^{\text{mag}}(\mathbf{r}) = -\boldsymbol{\mu}_{\text{n}} \cdot \mathbf{B}(\mathbf{r})}$$

$$\mathbf{B} = \mathbf{B}_{\text{S}} + \mathbf{B}_{\text{L}} = \frac{\mu_0}{4\pi} \left(\nabla \times \frac{\boldsymbol{\mu}_{\text{e}} \times \mathbf{r}}{r^3} - \frac{2\mu_{\text{B}}}{\hbar} \frac{\mathbf{p} \times \mathbf{r}}{r^3} \right)$$

- Dipole-dipole interaction (long-range and anisotropic)

Elastic Magnetic (Small-Angle) Neutron Scattering

$$\sum_{\mathbf{k}_1 \text{ in } d\Omega} W_{\mathbf{k}_0 \to \mathbf{k}_1} = \frac{2\pi}{\hbar} \rho_{\mathbf{k}_1} \left| \langle \mathbf{k}_1 | V_{\text{int}} | \mathbf{k}_0 \rangle \right|^2$$

$$V_{\text{int}}^{\text{mag}}(\mathbf{r}) = -\boldsymbol{\mu}_{\text{n}} \cdot \mathbf{B}(\mathbf{r})$$

$$\mathbf{M}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int_V \widetilde{\mathbf{M}}(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}} d^3 q$$

$$\widetilde{\mathbf{M}}(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}} \int_V \mathbf{M}(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} d^3 r$$

… final result

$$\begin{aligned}
\frac{d\Sigma_{\text{M}}}{d\Omega}(\mathbf{q}) &= \frac{1}{V} b_{\text{H}}^2 \left| \int_V \mathbf{Q}(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} d^3 r \right|^2 = \frac{8\pi^3}{V} b_{\text{H}}^2 |\widetilde{\mathbf{Q}}|^2 \\
&= \frac{8\pi^3}{V} b_{\text{H}}^2 \left| \hat{\mathbf{q}} \times \left(\widetilde{\mathbf{M}}(\mathbf{q}) \times \hat{\mathbf{q}} \right) \right|^2 \\
&= \frac{8\pi^3}{V} b_{\text{H}}^2 \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta \right) \widetilde{M}_\alpha \widetilde{M}_\beta
\end{aligned}$$

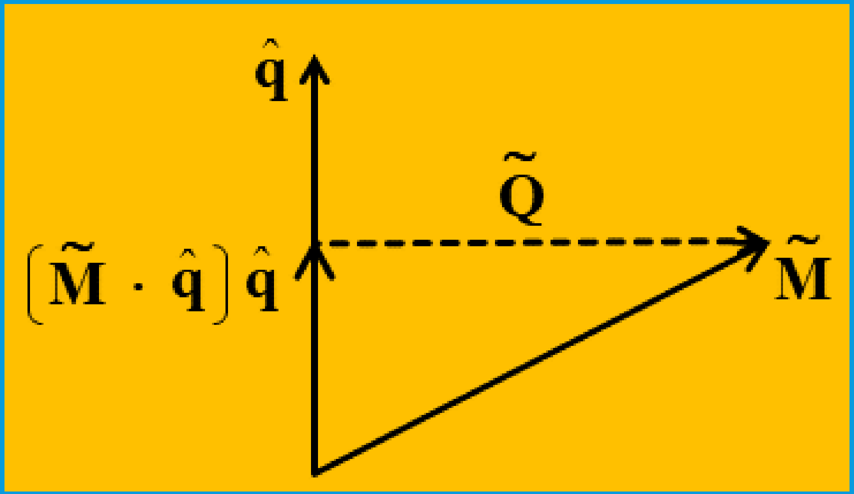
$$b_{\text{m}} = \frac{\gamma_{\text{n}} r_{\text{e}}}{2} \frac{\mu_{\text{a}}}{\mu_{\text{B}}} f(\mathbf{q}) \cong 2.70 \times 10^{-15}\,\text{m} \frac{\mu_{\text{a}}}{\mu_{\text{B}}} f(\mathbf{q}) \cong b_{\text{H}} \mu_{\text{a}}$$

$$b_{\text{H}} = 2.70 \times 10^{-15}\,\text{m}\,\mu_{\text{B}}^{-1} = 2.91 \times 10^{8}\,\text{A}^{-1}\text{m}^{-1}$$

atomic magnetic scattering length: a few fm = 10^{-15} m

Elastic Magnetic (Small-Angle) Neutron Scattering

$$\widetilde{\mathbf{Q}}_i = \hat{\mathbf{q}} \times (\hat{\mathbf{m}}_i \times \hat{\mathbf{q}}) = \hat{\mathbf{m}}_i - \hat{\mathbf{q}}(\hat{\mathbf{q}} \cdot \hat{\mathbf{m}}_i)$$



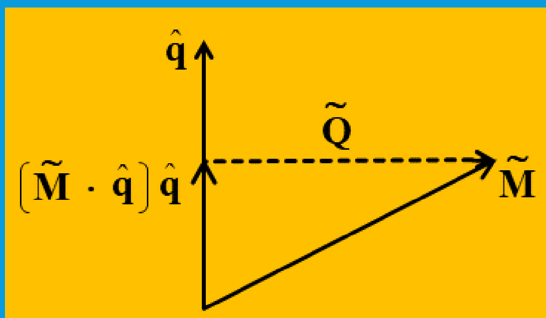
- is called the magnetic interaction or Halpern-Johnson vector
- Embodies anisotropic character of magnetic neutron scattering due to dipole-dipole interaction
- Only the <u>component of M which is perpendicular to the scattering vector q</u> contributes to the magnetic neutron scattering cross section

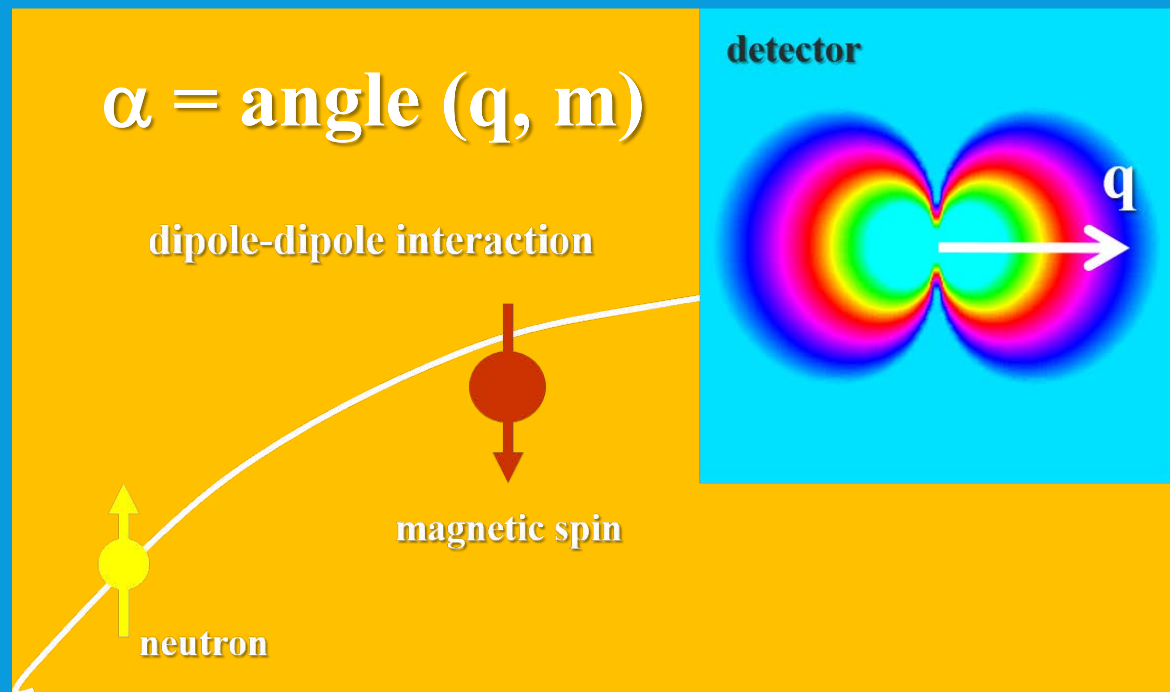
Elastic Magnetic (Small-Angle) Neutron Scattering

For a single magnetic domain

$$\widetilde{\mathbf{Q}}_i = \hat{\mathbf{q}} \times (\hat{\mathbf{m}}_i \times \hat{\mathbf{q}}) = \hat{\mathbf{m}}_i - \hat{\mathbf{q}}(\hat{\mathbf{q}} \cdot \hat{\mathbf{m}}_i)$$

$$|\widetilde{\mathbf{Q}}_i|^2 \propto \sin^2 \alpha_i$$





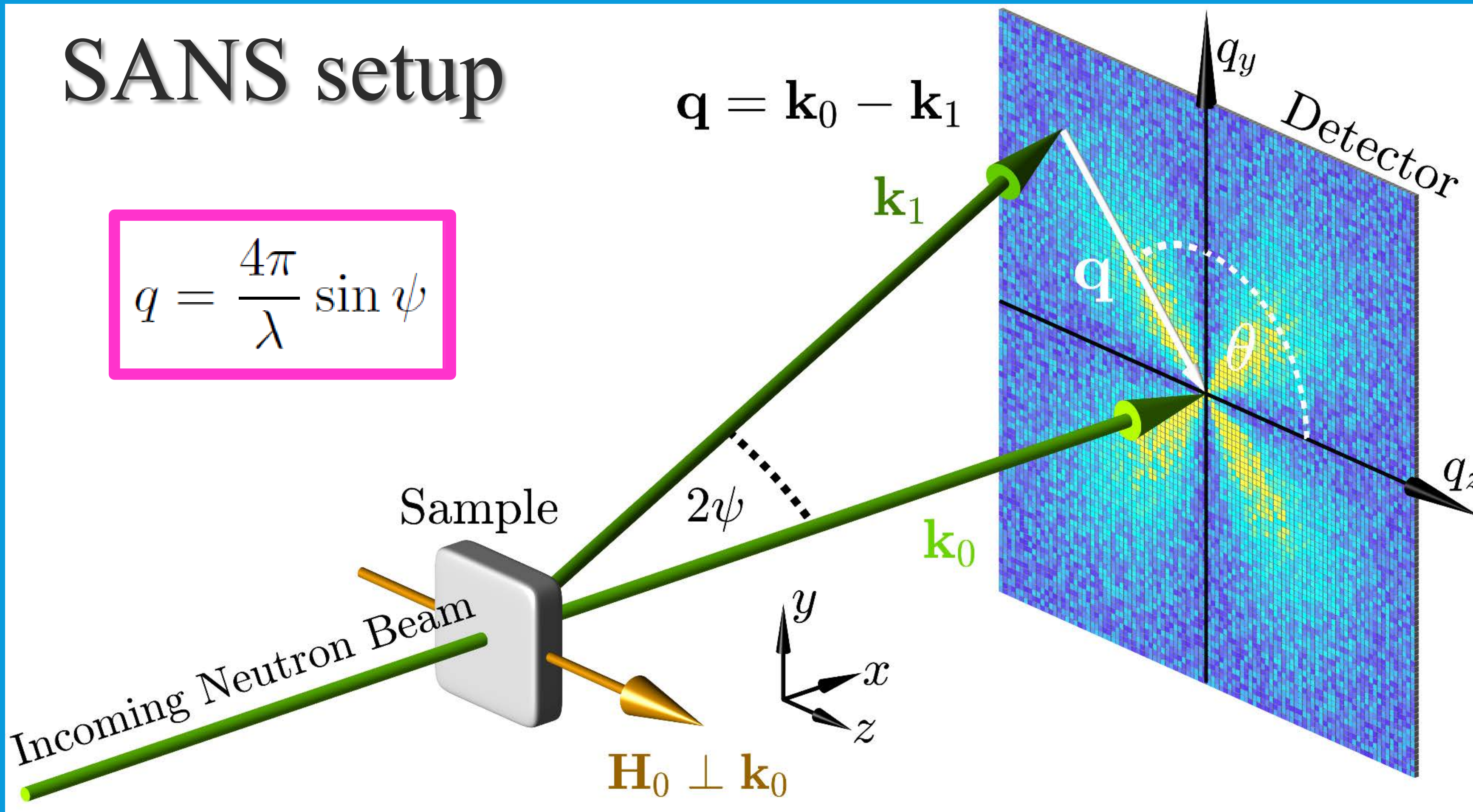
for unpolarized neutrons

$$\frac{d\Sigma_{\text{tot}}}{d\Omega} = \frac{d\Sigma_{\text{nuc}}}{d\Omega} + \frac{d\Sigma_{\text{mag}}}{d\Omega}$$

$$= \frac{d\Sigma_{\text{nuc}}}{d\Omega} + \widetilde{M}_s^2(q)\sin^2\alpha$$

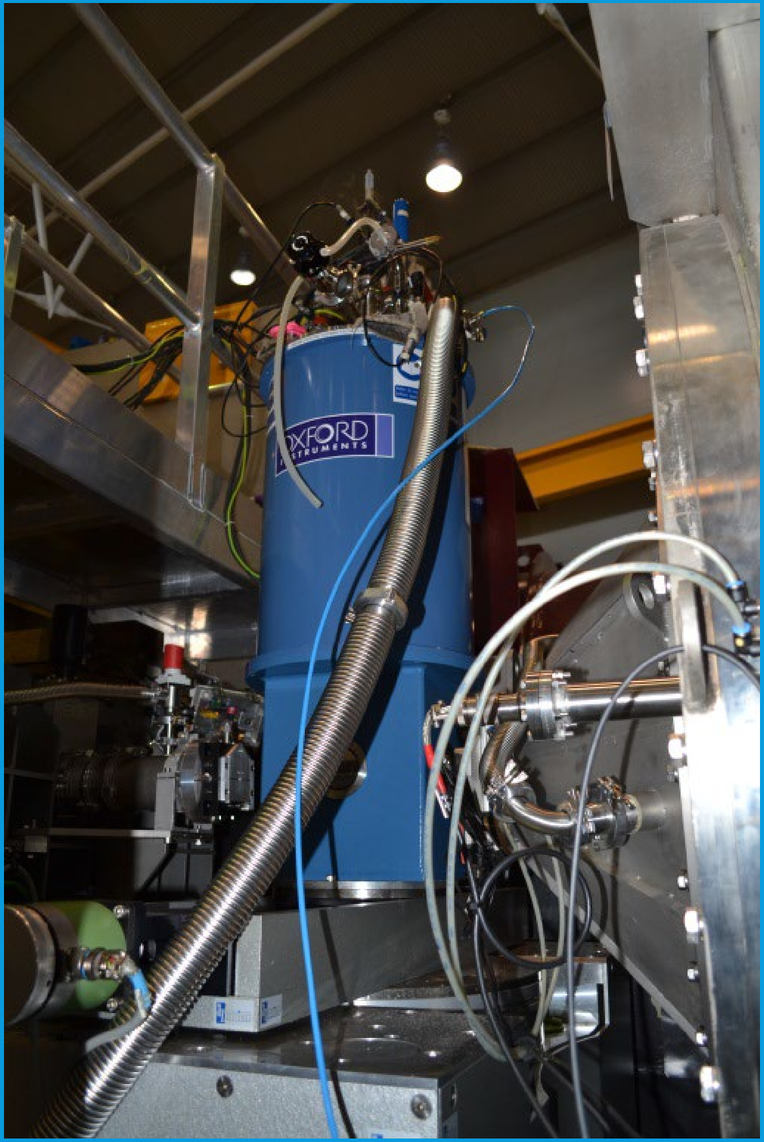
$$\frac{d\Sigma_{\text{tot}}}{d\Omega} = \frac{d\Sigma_{\text{nuc}}}{d\Omega} \qquad (\alpha = 0°)$$

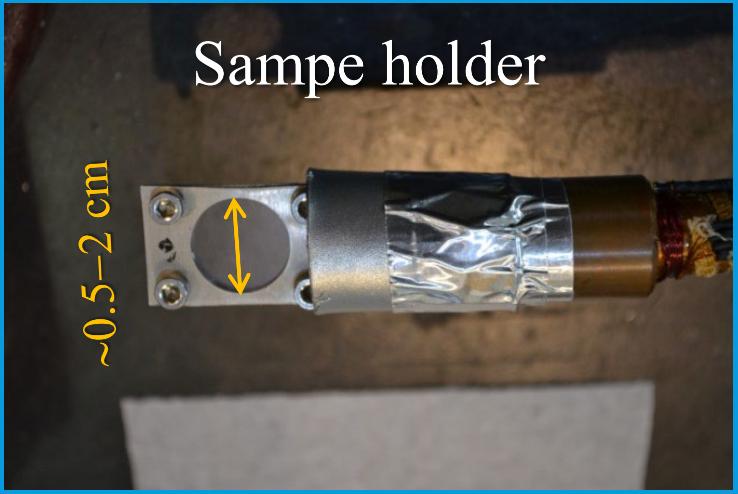
- Measurement of unpolarized cross section in saturated single-domain state allows the separation of nuclear and magnetic scattering



- ➢ SANS probes nuclear (structural) and magnetic inhomogeneities in the bulk and on the mesoscale (~ 1 nm up to 1000 nm)
- ➢ $2\psi < 10°$ small angles; $5Å < \lambda < 20Å \rightarrow 0.001\ \mathrm{nm}^{-1} < q < 1\ \mathrm{nm}^{-1}$

https://kur.web.psi.ch/sans1/sans/sans10.jpg



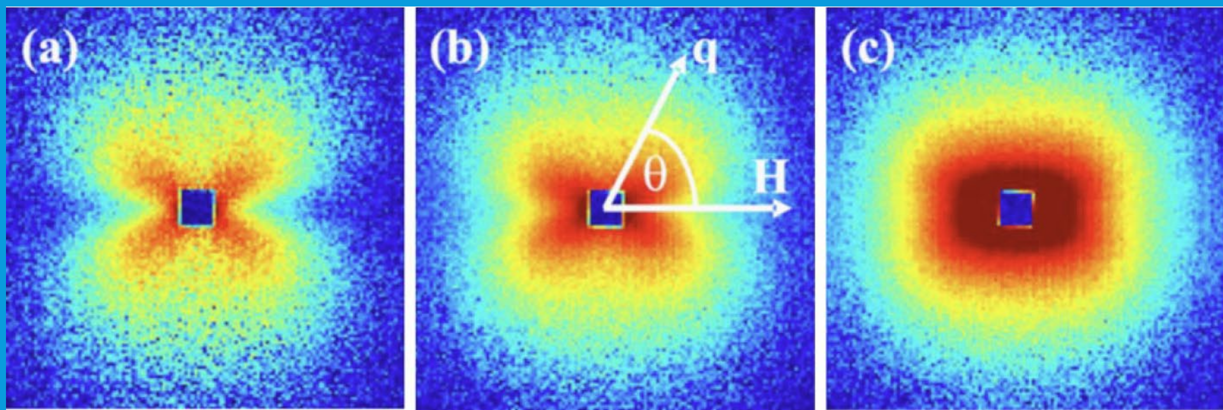


- SANS beamtime is given based on a peer-review process; 1-2 pages proposal; 6-12 month lead time

Richness of magnetic SANS

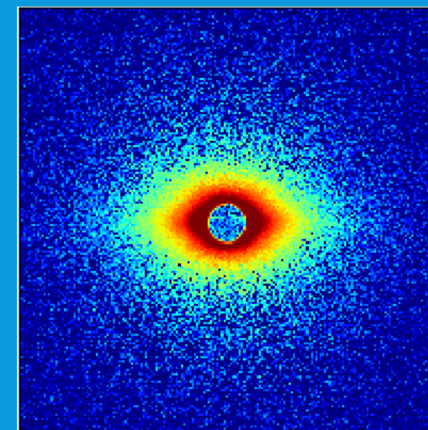
❖ plethora of angular anisotropies and complex interactions

NANOPERM



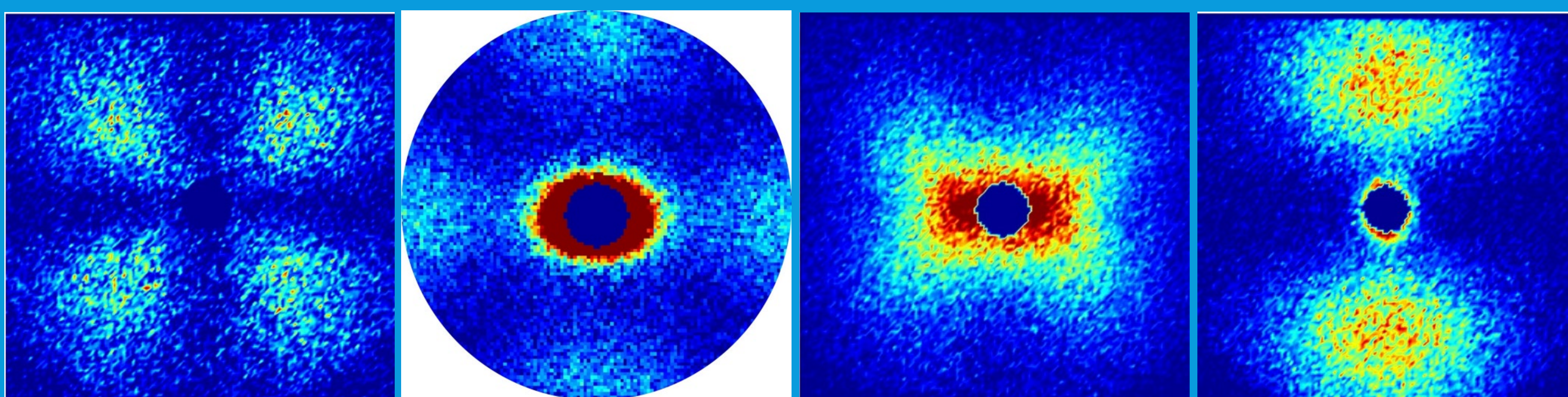
A. Michels *et al.*, PRB 74, 134407 (2006).

Nd-Fe-B



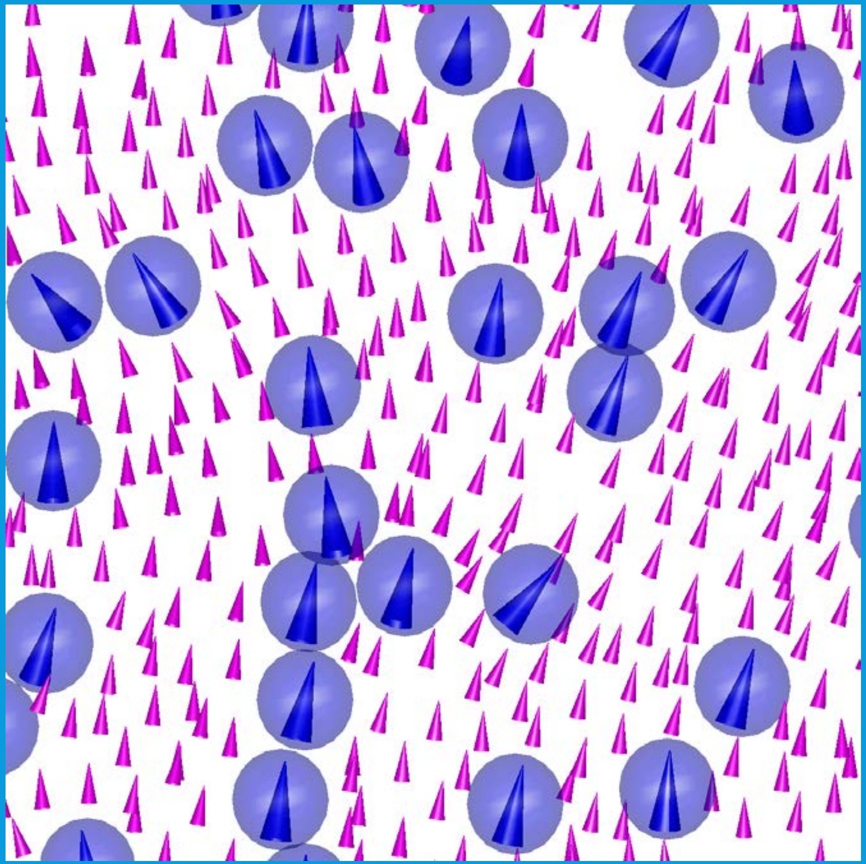
É.A. Périgo *et al.*,
NJP <u>16</u>, 123031 (2014).

Fe-based alloys



D. Honecker *et al.*, EPJ B <u>76</u>, 209 (2010).

➢ Magnetic SANS can be described within a continuum approach: relevant quantity is the magnetization vector field



S. Erokhin, General Numerics Research Lab

$$\mathbf{M} = \mathbf{M}(\mathbf{r}) = \left\{ \begin{array}{c} M_x(x,y,z) \\ M_y(x,y,z) \\ M_z(x,y,z) \end{array} \right\}$$

- ✓ SANS wavelength above Bragg cutoff for many crystalline materials → no information on discrete atomic structure of matter
- ✓ Discrete atomistic or even purely quantum mechanical calculations limited to very small systems

Elastic Magnetic Neutron Scattering Cross Section

$$\begin{aligned}
\frac{d\Sigma_{\mathrm{M}}}{d\Omega}(\mathbf{q}) &= \frac{1}{V} b_{\mathrm{H}}^2 \left| \int_V \mathbf{Q}(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} d^3 r \right|^2 = \frac{8\pi^3}{V} b_{\mathrm{H}}^2 |\widetilde{\mathbf{Q}}|^2 \\
&= \frac{8\pi^3}{V} b_{\mathrm{H}}^2 \left| \hat{\mathbf{q}} \times \left(\widetilde{\mathbf{M}}(\mathbf{q}) \times \hat{\mathbf{q}} \right) \right|^2 \\
&= \frac{8\pi^3}{V} b_{\mathrm{H}}^2 \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta \right) \widetilde{M}_\alpha \widetilde{M}_\beta
\end{aligned}$$

Halpern-Johnson vector

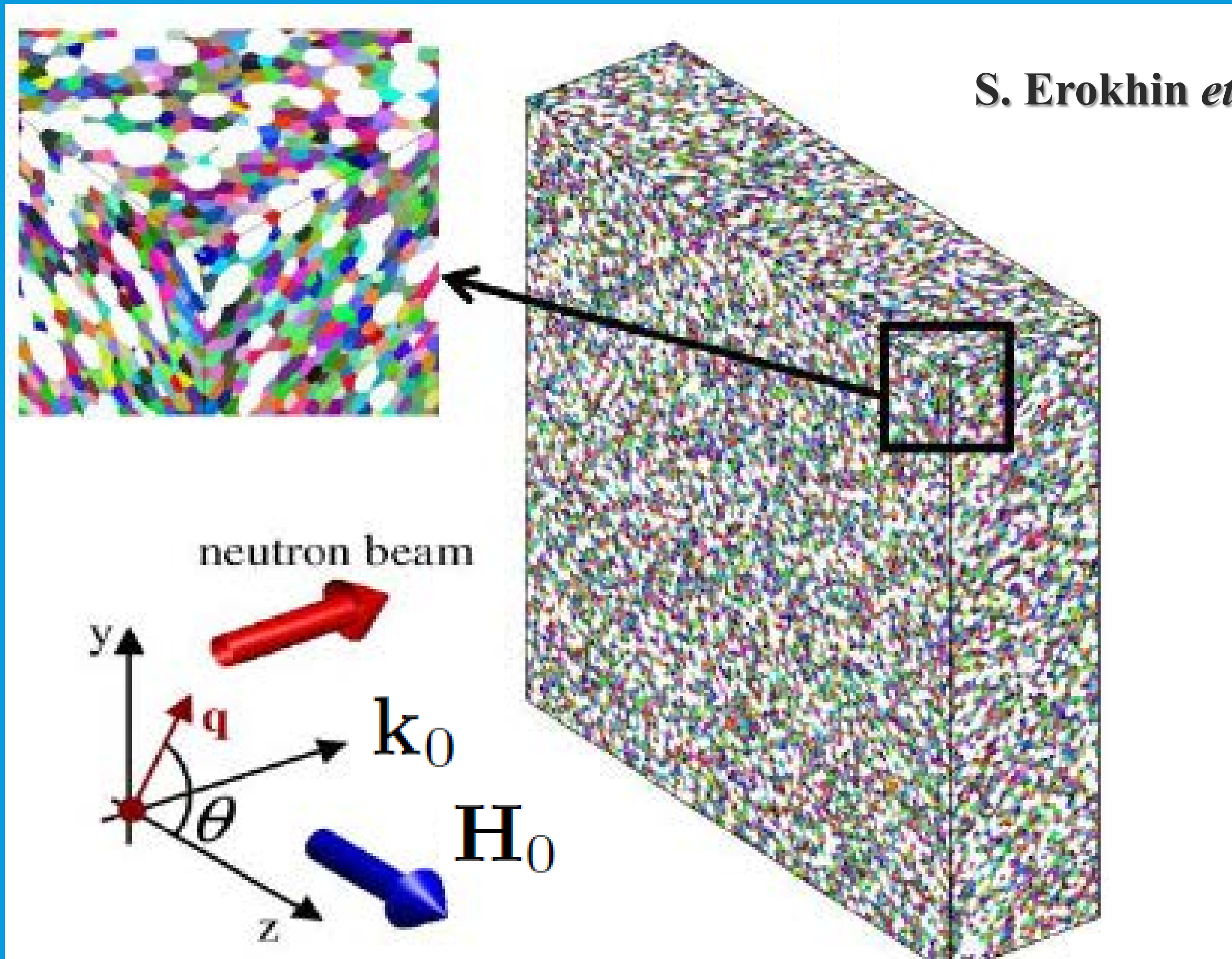
$$\mathbf{M}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int_V \widetilde{\mathbf{M}}(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}} d^3 q$$

$$\widetilde{\mathbf{M}}(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}} \int_V \mathbf{M}(\mathbf{r}) e^{-i\mathbf{q}\mathbf{r}} d^3 r$$

- Central quantity is the Fourier transform of M

$$\boxed{\widetilde{M}_{x,y,z} = \widetilde{M}_{x,y,z}(q, \theta, H, A, D, M_s, K, \lambda, f(R), \ldots)}$$

Elastic Magnetic Neutron Scattering Cross Section



S. Erokhin *et al.*, PRB 92, 014427 (2015).

When the applied field is perpendicular to the incoming neutron beam

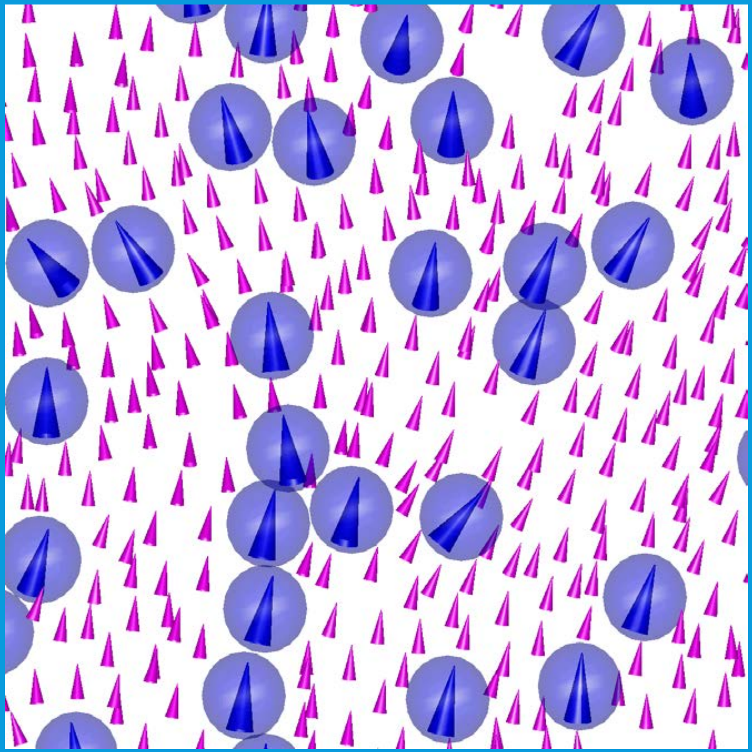
$$\mathbf{k}_0 \perp \mathbf{H}_0$$

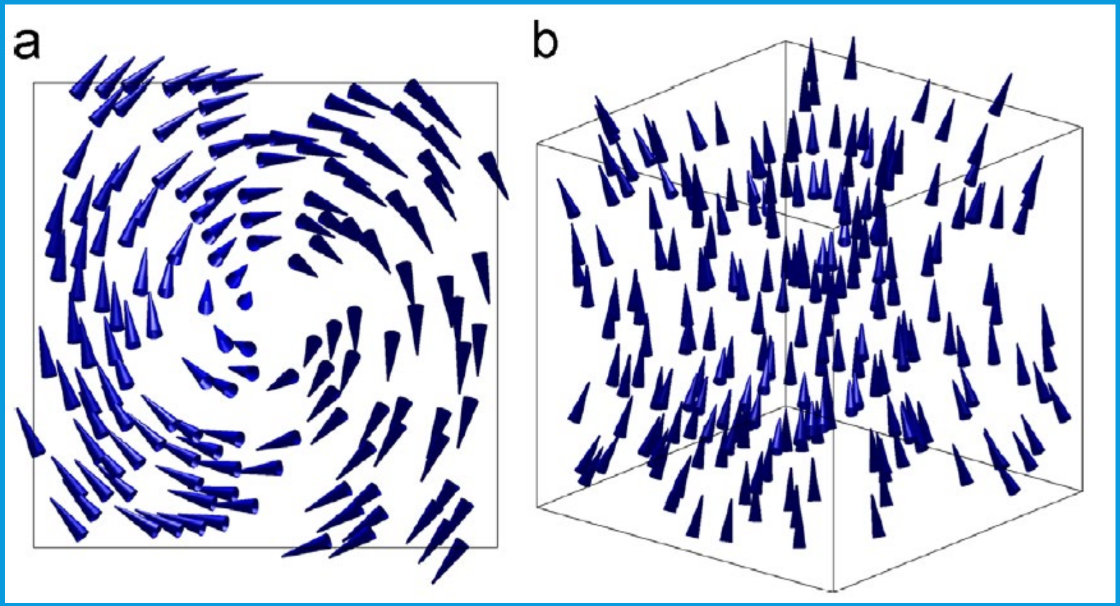
$$\frac{d\Sigma_{\mathrm{M}}}{d\Omega} \sim |\widetilde{M}_x|^2 + |\widetilde{M}_y|^2 \cos^2\theta + |\widetilde{M}_z|^2 \sin^2\theta - (\widetilde{M}_y \widetilde{M}_z^* + \widetilde{M}_y^* \widetilde{M}_z) \sin\theta \cos\theta$$

- Origin of diffuse magnetic SANS?
- Why do we observe a magnetic SANS signal?

Origin of magnetic SANS

➢ **Magnetic SANS is due to nanoscale spatial variations in the <u>magnitude</u> and/or <u>orientation</u> of M(r)**





S. Erokhin *et al.*, PRB 85, 024410 (2012).

What is the origin of magnetic SANS?

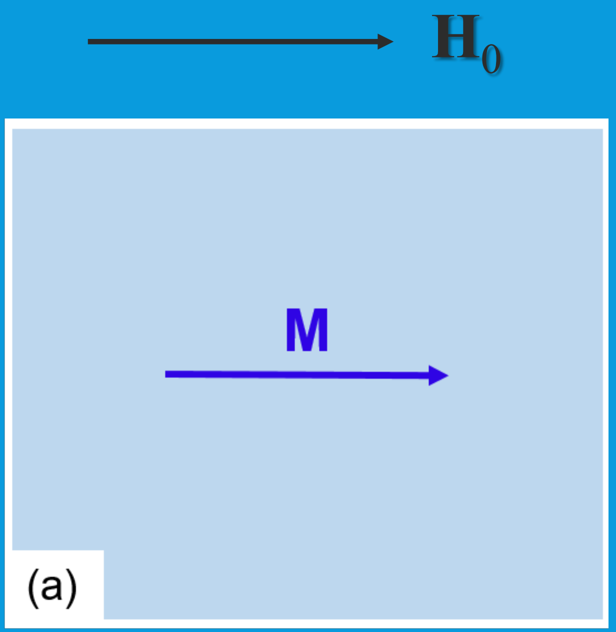
➢ **Magnetic SANS is due to nanoscale spatial variations in the <u>magnitude</u> and/or <u>orientation</u> of the magnetization vector field**

(a) saturated <u>homogeneous</u> ferromagnet

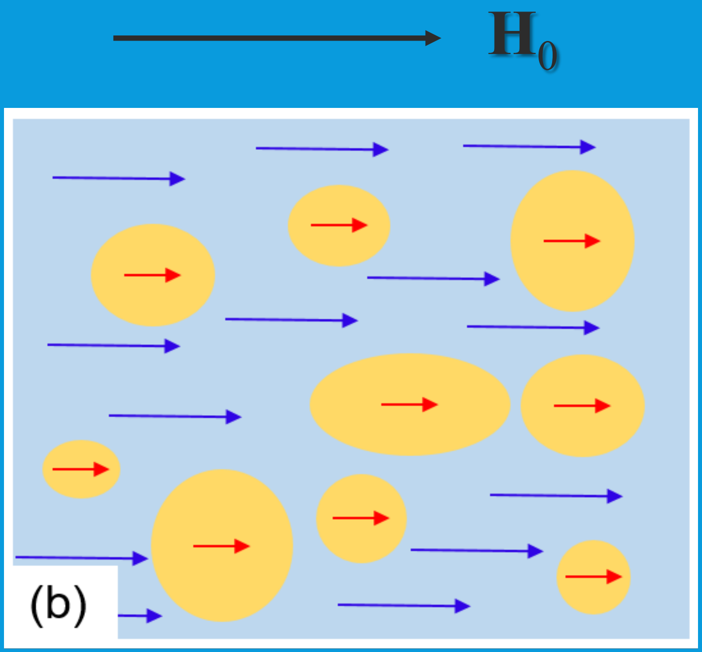
→ M = {0, 0, M_s}, where M_s = constant

$$\frac{d\Sigma_{\mathrm{M}}^{\mathrm{sat}}}{d\Omega} \propto |\delta(\mathbf{q})|^2$$

no magnetic SANS signal



What is the origin of magnetic SANS?



(b) saturated <u>inhomogeneous</u> ferromagnet

$\rightarrow$ $\mathbf{M} = \{0, 0, M_s\}$, where $M_s = M_s(x, y, z)$

$$\frac{d\Sigma_{\mathrm{M}}^{\mathrm{sat}}}{d\Omega} \propto |\widetilde{M}_s(\mathbf{q})|^2$$

magnetic SANS signal

$\widetilde{M}_s(\mathbf{q})$ = Fourier transform of $M_s(\mathrm{r})$

magnetic scattering contrast

$(\Delta M)^2 = (\rightarrow - \longrightarrow)^2 = (M_s^p - M_s^m)^2$

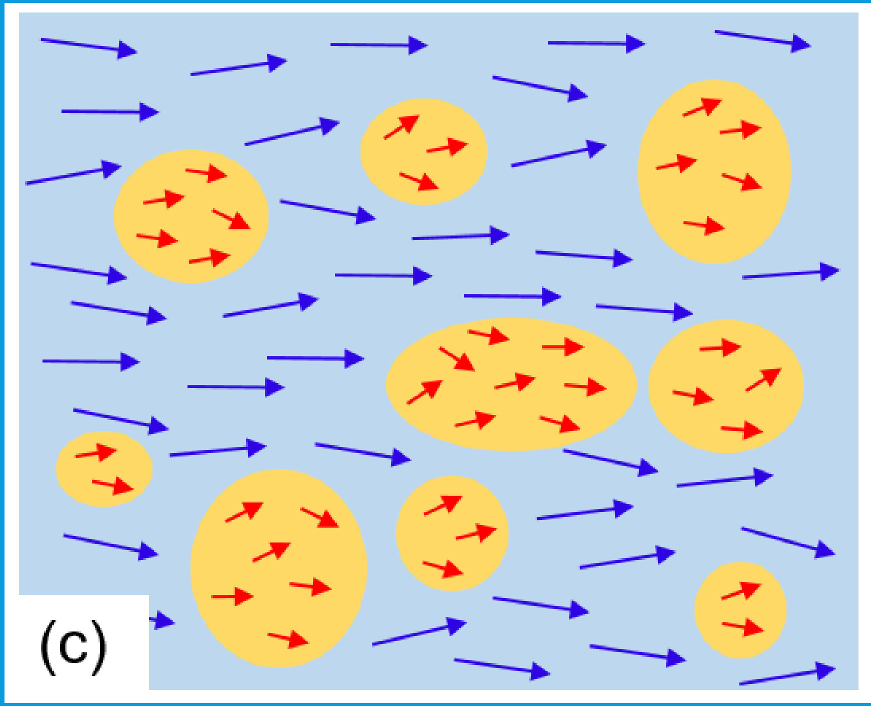
- For case (b), analysis of magnetic SANS cross section provides information on the size (distribution) and shape (form factor), on the contrast $(\Delta M)^2$, and on the interaction potential between „particles“ and „matrix“ (structure factor)
- However, not really magnetic SANS, scalar function $M_s(\mathrm{r})$, can be mapped onto nuclear SANS problem

What is the origin of magnetic SANS?

(c) nonsaturated inhomogeneous ferromagnet

→ M = {M_x(r), M_y(r), M_z(r)}

→ $\mathbf{H}_0$



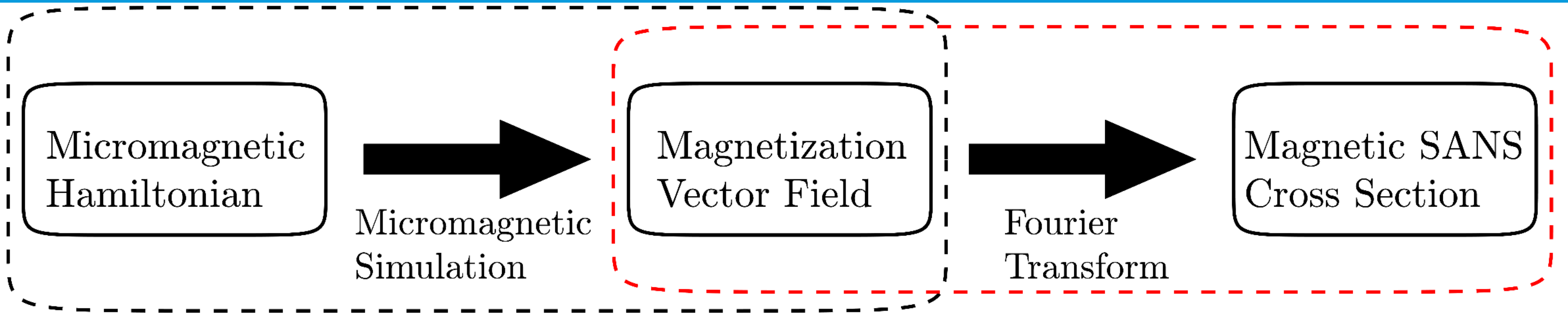
✓ **In the general case (iii), all three magnetization components determine the magnetic SANS cross section**

→ static micromagnetism

$\mathbf{k}_0 \perp \mathbf{H}_0$

$$\frac{d\Sigma_{\mathrm{M}}}{d\Omega} \sim |\widetilde{M}_x|^2 + |\widetilde{M}_y|^2 \cos^2\theta + |\widetilde{M}_z|^2 \sin^2\theta - (\widetilde{M}_y \widetilde{M}_z^* + \widetilde{M}_y^* \widetilde{M}_z) \sin\theta\cos\theta$$

Magnetic SANS Theory



D. Honecker and A. Michels, Phys. Rev. B 87, 224426 (2013); D. Mettus and A. Michels, J. Appl. Cryst. 48, 1437 (2015); K.L. Metlov and A. Michels, Sci. Rep. 6, 25055 (2016); A. Michels *et al.*, PRB 94, 054424 (2016).

Micromagnetic Theory: balance of torques

[L. Landau and E. Lifschitz (1935); W.F. Brown Jr. (1940)]

$$E_{\mathrm{tot}} = \int_V \left(\epsilon_{\mathrm{ex}} + \epsilon_{\mathrm{d}} + \epsilon_{\mathrm{ani}} + \epsilon_{\mathrm{dmi}}\right) d^3 r$$

$\delta E_{tot} = 0$

- Brown's equations of micromagnetics (Euler-Lagrange Eqs.) are a set of nonlinear partial differential equations with complex boundary conditions
- Numerical micromagnetics

$$\left(\underbrace{\mathbf{H}_{\mathrm{ex}}}_{\text{exchange field}} + \underbrace{\mathbf{H}_{\mathrm{d}}}_{\text{magnetostatic field + Zeeman}} + \underbrace{\mathbf{H}_{\mathrm{ani}}}_{\text{anisotropy field}} + \underbrace{\mathbf{H}_{\mathrm{dmi}}}_{\text{DMI field}}\right) \times \mathbf{M} = 0$$

➢ Necessary equilibrium condition

High-field limit: solution for Fourier coefficients

$$\left(\mathbf{H}_{\mathrm{ex}} + \mathbf{H}_{\mathrm{d}} + \mathbf{H}_{\mathrm{ani}} + \mathbf{H}_{\mathrm{dmi}}\right) \times \mathbf{M} = 0$$

based on (cubic symmetry)

$$\mathbf{H}_{\mathrm{dmi}} = -l_D \nabla \times \mathbf{M}$$

$$\widetilde{M}_x = \frac{p\left(\widetilde{H}_{p,x}\left[1 + p\frac{q_y^2}{q^2}\right] - M_s \widetilde{I}_m \frac{q_x q_z}{q^2}\left[1 + p\, l_D^2 q^2\right] - \widetilde{H}_{p,y} p \frac{q_x q_y}{q^2} - i\left[M_s \widetilde{I}_m (1+p) l_D q_y - \widetilde{H}_{p,y} p\, l_D q_z\right]\right)}{1 + p\frac{q_x^2 + q_y^2}{q^2} - p^2 l_D^2 q_z^2}$$

$$\widetilde{M}_y = \frac{p\left(\widetilde{H}_{p,y}\left[1 + p\frac{q_x^2}{q^2}\right] - M_s \widetilde{I}_m \frac{q_y q_z}{q^2}\left[1 + p\, l_D^2 q^2\right] - \widetilde{H}_{p,x} p \frac{q_x q_y}{q^2} + i\left[M_s \widetilde{I}_m (1+p) l_D q_x - \widetilde{H}_{p,x} p\, l_D q_z\right]\right)}{1 + p\frac{q_x^2 + q_y^2}{q^2} - p^2 l_D^2 q_z^2}$$

$$\mathbf{k}_0 \perp \mathbf{H}_0$$

$$\frac{d\Sigma_{\mathrm{mag}}}{d\Omega} \sim |\widetilde{M}_x|^2 + |\widetilde{M}_y|^2 \cos^2\theta + |\widetilde{M}_z|^2 \sin^2\theta - (\widetilde{M}_y \widetilde{M}_z^* + \widetilde{M}_y^* \widetilde{M}_z) \sin\theta\cos\theta$$

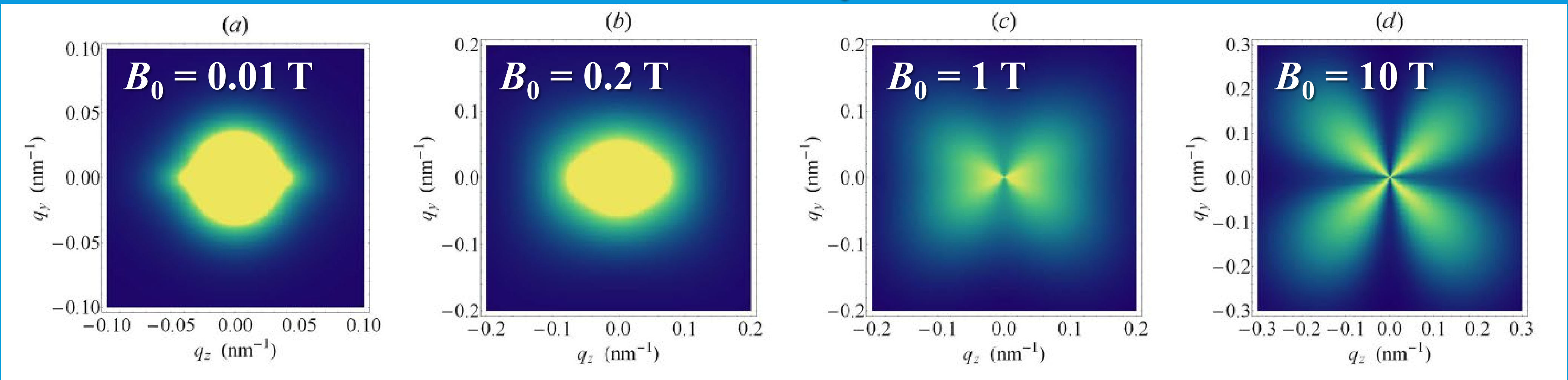
A. Michels *et al.*, PRB 94, 054424 (2016).

$$\widetilde{M}_{x,y,z} = \widetilde{M}_{x,y,z}(q, \theta, H, A, M_s, K, \ldots)$$

Analysis of magnetic SANS data

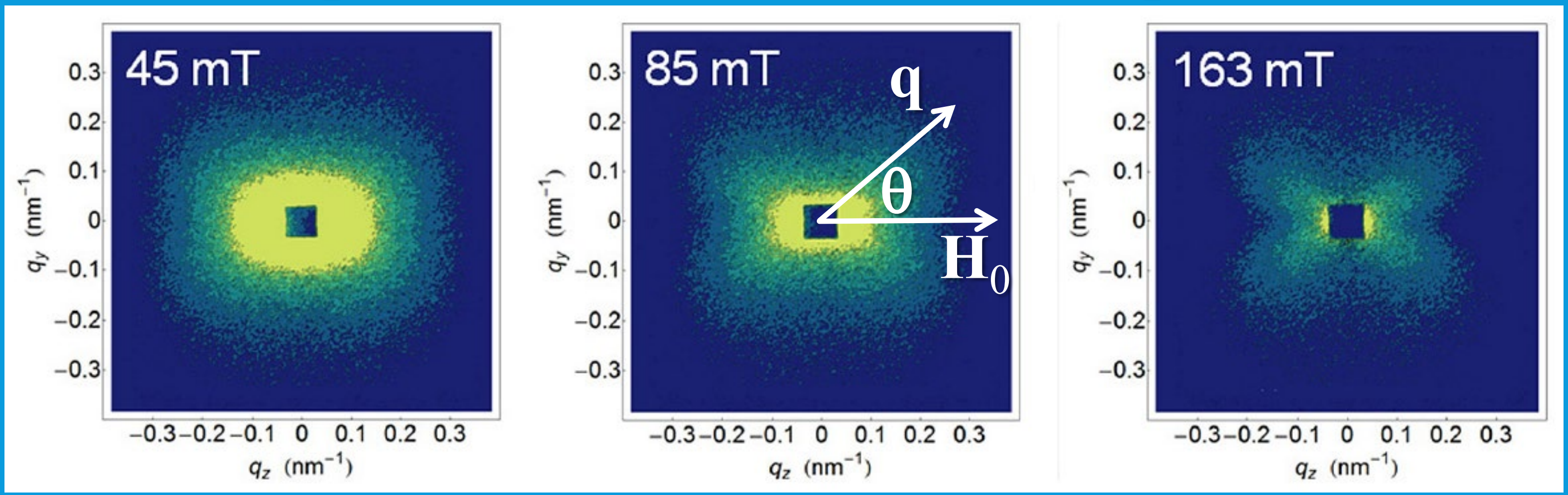
Angular Anisotropy of SANS pattern

Theory



D. Honecker and A .Michels, PRB 87, 224426 (2013).

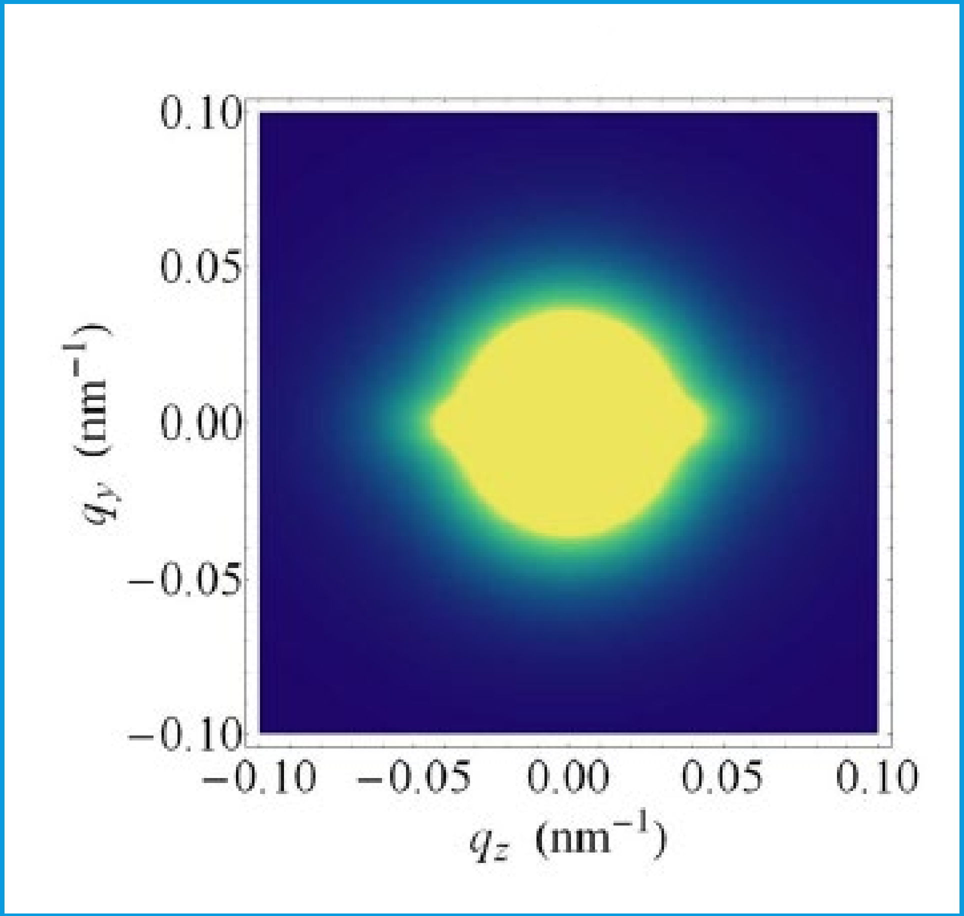
Experiment (Fe based nanocomposite)



D. Honecker *et al.*, PRB 88, 094428 (2013).

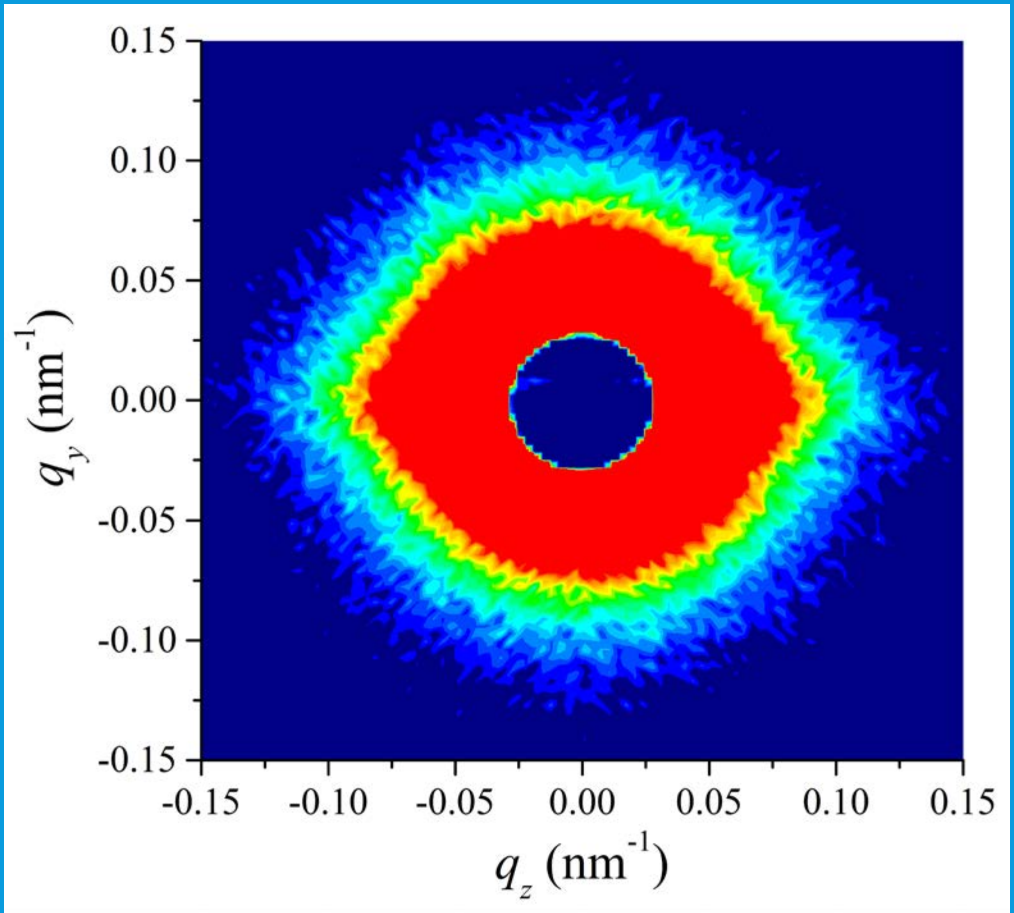
Anisotropy of SANS pattern: flux-closure at nanoscale (due to $\nabla \cdot \mathbf{M} \to 0$)

Theory: spike anisotropy



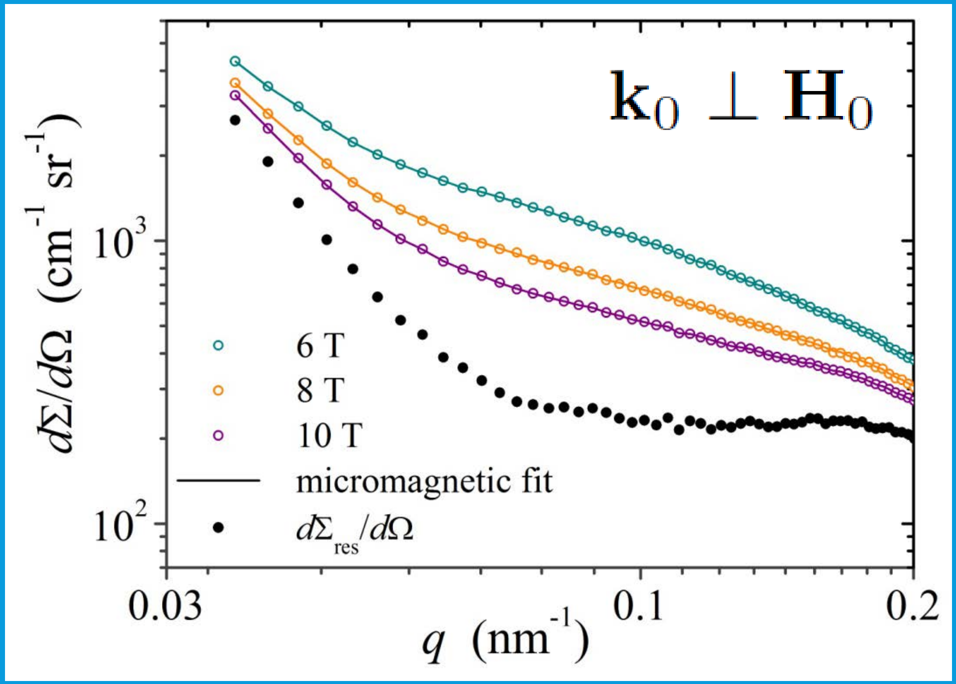
D. Honecker and A .Michels,
PRB 87, 224426 (2013).

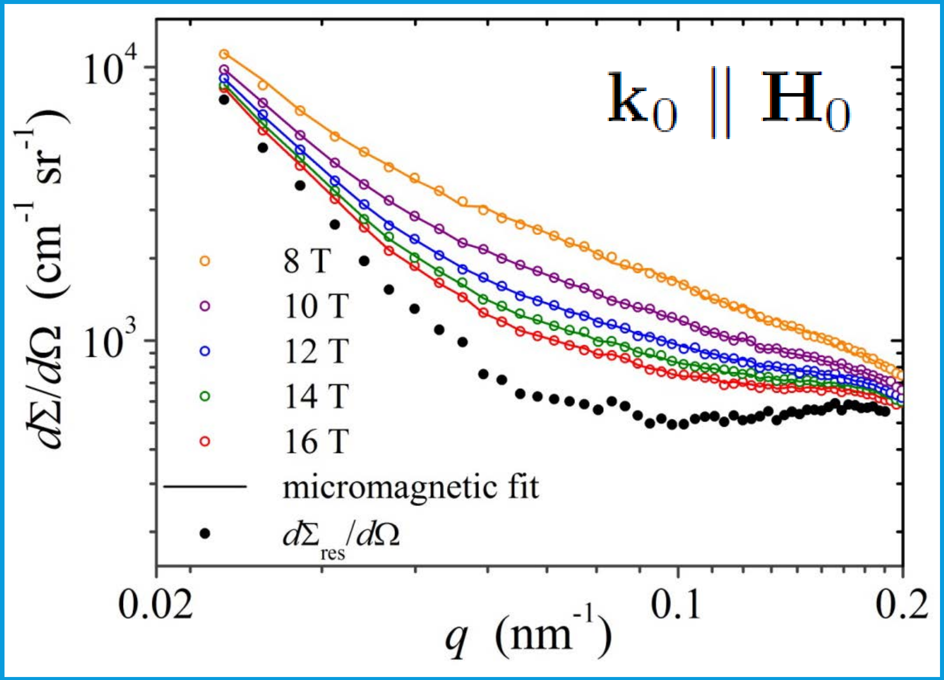
Experiment (Nd-Fe-B)



É.A. Périgo *et al.*, NJP 16, 123031 (2014).
M. Bersweiler *et al.*, PRB 108, 094434 (2023).

Micromagnetic data analysis (Nd-Fe-B nanocomposite)





exchange-stiffness constant

$$A \simeq 12.5 \times 10^{-12}\ \mathrm{J/m}$$

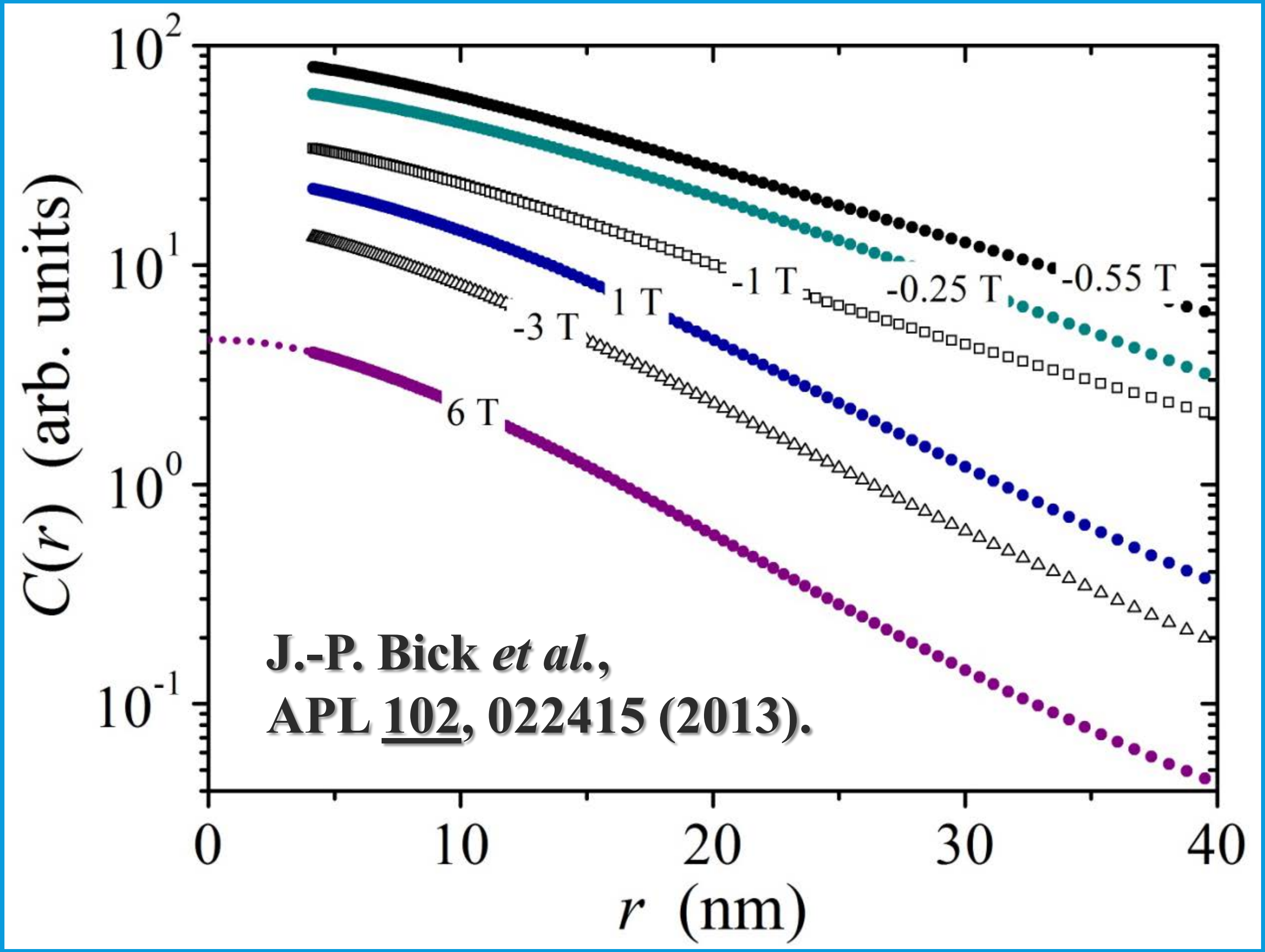
plus information about

- **magnetic anisotropy field**
- **magnetostatics**
- **correlation lengths**
- **...**

J.-P. Bick *et al.*, APL 102, 022415 (2013).
J.-P. Bick *et al.*, APL 103, 122402 (2013).

Real-space analysis: correlation function

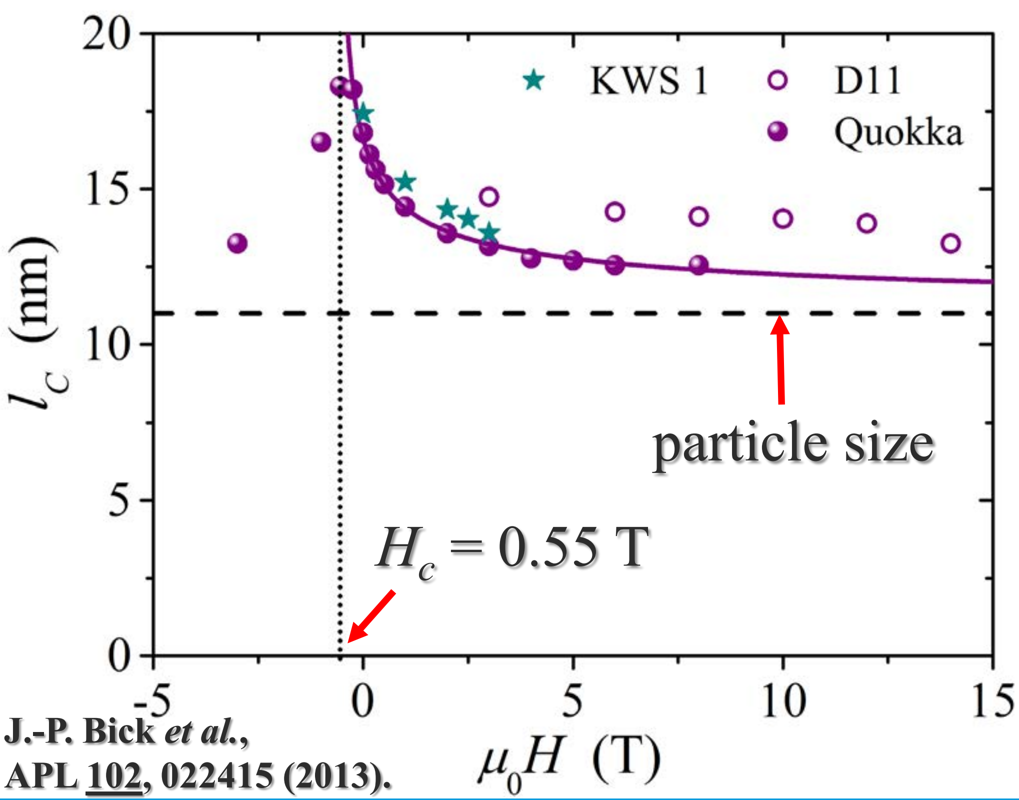
$$C(r) \propto \frac{1}{r}\int_0^\infty \frac{d\Sigma_M}{d\Omega}(q)\sin(qr)q\,dq$$



- Nanomagnets exhibit non-exponential long-range decay of correlations

Magnetization reversal: Correlation length

Nd-Fe-B nanocomposite



J.-P. Bick *et al.*,
APL <u>102</u>, 022415 (2013).

micromagnetic model

$$l_C(H) = R + \sqrt{\frac{2A}{J_s(H + H^*)}}$$

R **= defect size (e.g., *R* ≅ particle radius)**
H* **= effective magnetic field**
<u>Note:</u> for *H* = 0 and *H = $H_K = 2K/J_s$**

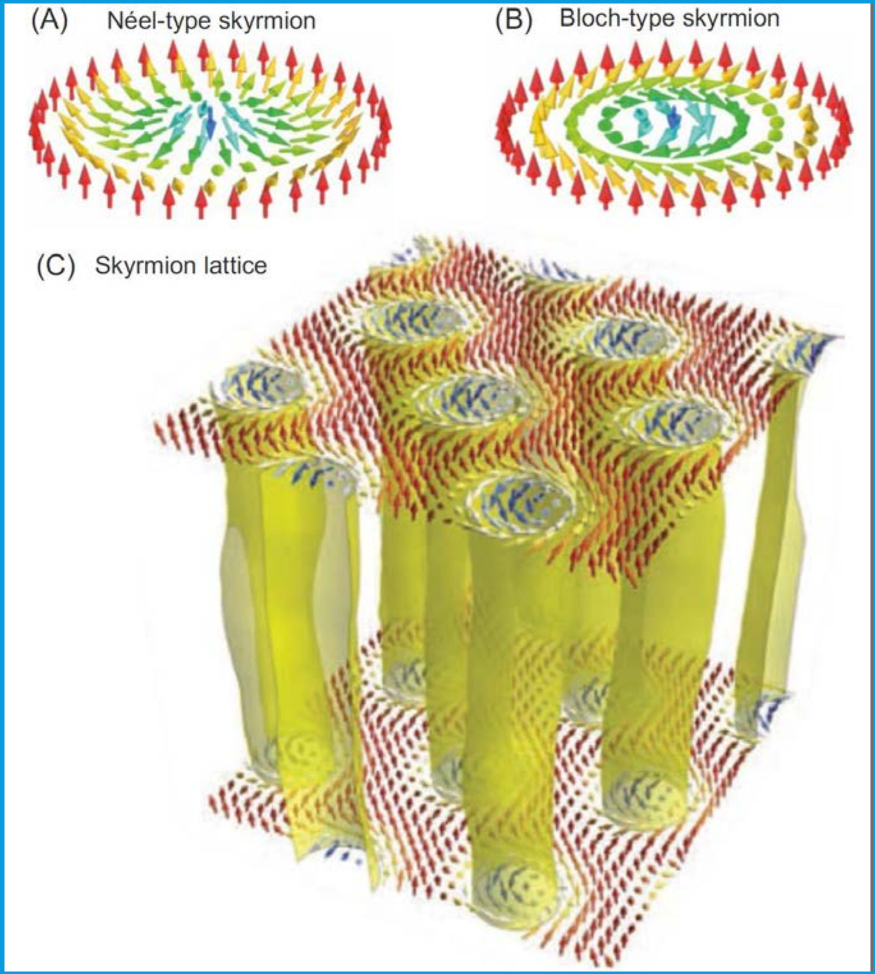
$$l_C(H) = R + \sqrt{\frac{A}{K}}$$

- **fit to data: *R* = 10.9 nm and $\mu_0 H^*$ = 0.60 T**
- **at remanent state: penetration depth of spin disorder into Fe_3B phase $\Delta l_C = l_C(H) - R$ ~ 5-6 nm**

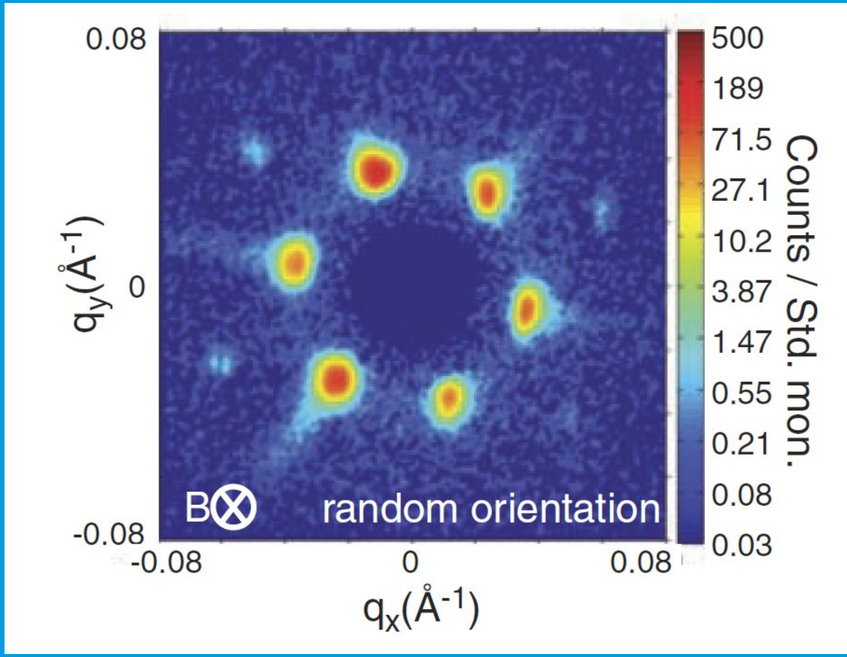
Selected Results

- **Signature of DMI in magnetic SANS cross section?**

DMI relevant in the context of skyrmion physics



$$H_{DMI} = \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$



Mühlbauer, Pfleiderer et al., Science (2009).

- intrinsic DMI due to inversion-asymmetric crystal-field environment (MnSi, FeGe, Cu_2OSeO_3, Heusler-type alloys, …)
- important for the stabilization of skyrmion lattices

Microstructural-defect-induced DMI

JOURNAL OF APPLIED PHYSICS VOL. 34, NO. 4 (PART 2) APRIL 1963

Dzialoshinski–Moriya Interactions About Defects in Antiferromagnetic and Ferromagnetic Materials

ANTHONY ARROTT

Scientific Laboratory, Ford Motor Company, Dearborn, Michigan

$$H_{DMI} = \sum_{i,j} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

- **DMI is operative at defect sites due to the local breaking of structural inversion symmetry; relevant for disordered polycrystalline magnets and spin glasses (Fert and Levy, PRL 1980; Plakhty, Fedorov et al., PRB 2001; Grigoriev et al., PRL 2008)**

- **local chiral DMI couplings, present even in highly symmetric lattices**

Defect-induced DMI: SANS Theory

$$\frac{d\Sigma^{\pm}}{d\Omega} \sim |\widetilde{N}|^2 + |\widetilde{M}_x|^2 + |\widetilde{M}_y|^2 \cos^2\theta + |\widetilde{M}_z|^2 \sin^2\theta - (\widetilde{M}_y \widetilde{M}_z^* + \widetilde{M}_y^* \widetilde{M}_z) \sin\theta\cos\theta$$

polarization-independent

$$\mp(\widetilde{N}\widetilde{M}_z^* + \widetilde{N}^*\widetilde{M}_z)\sin^2\theta \mp \imath\chi$$

polarization-dependent

$$\Delta\Sigma = \frac{d\Sigma^-}{d\Omega} - \frac{d\Sigma^+}{d\Omega} \sim 2(\widetilde{N}\widetilde{M}_z^* + \widetilde{N}^*\widetilde{M}_z)\sin^2\theta + 2\imath\chi$$

Chiral function

$$\chi(\mathbf{q}) = \left(\widetilde{M}_x \widetilde{M}_y^* - \widetilde{M}_x^* \widetilde{M}_y\right)\cos^2\theta - \left(\widetilde{M}_x \widetilde{M}_z^* - \widetilde{M}_x^* \widetilde{M}_z\right)\sin\theta\cos\theta$$

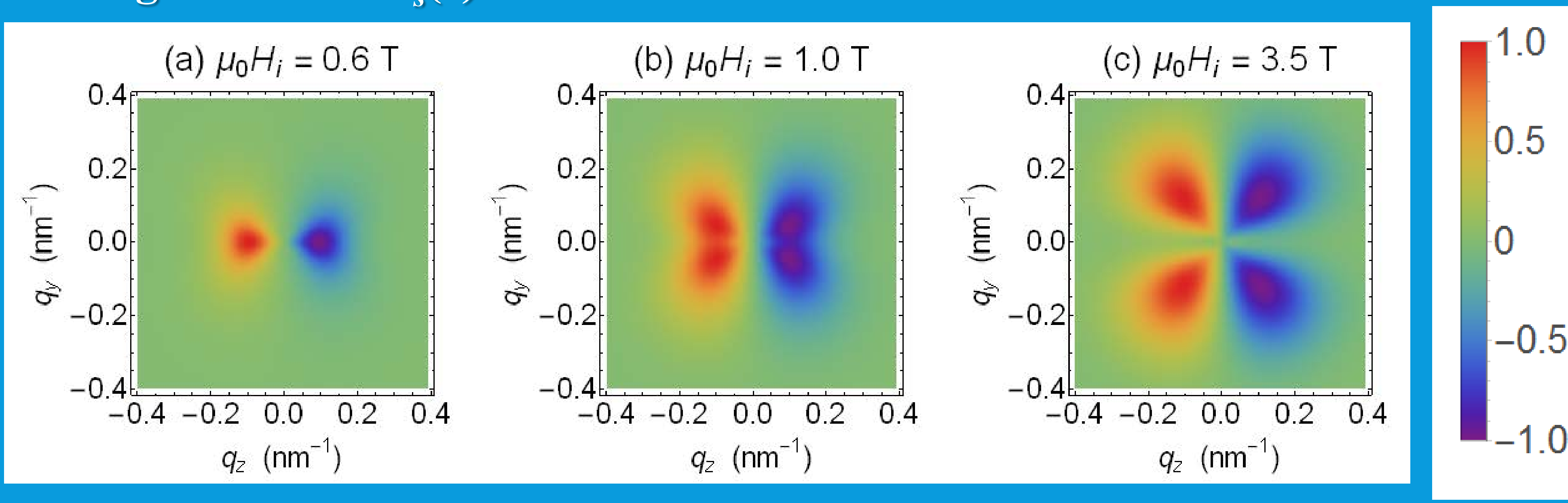
Defect-induced DMI: SANS Theory

Chiral function

$$2\imath\chi(\mathbf{q}) = -\frac{2\widetilde{H}_p^2 p^3 \left(2 + p\sin^2\theta\right) l_D q \cos^3\theta + 4\widetilde{M}_z^2 p(1+p)^2 l_D q \sin^2\theta\cos\theta}{\left(1 + p\sin^2\theta - p^2 l_D^2 q^2 \cos^2\theta\right)^2}$$

$\widetilde{H}_p(\mathbf{q})$: Fourier transform of magnetic anisotropy field $H_p(\mathbf{r})$

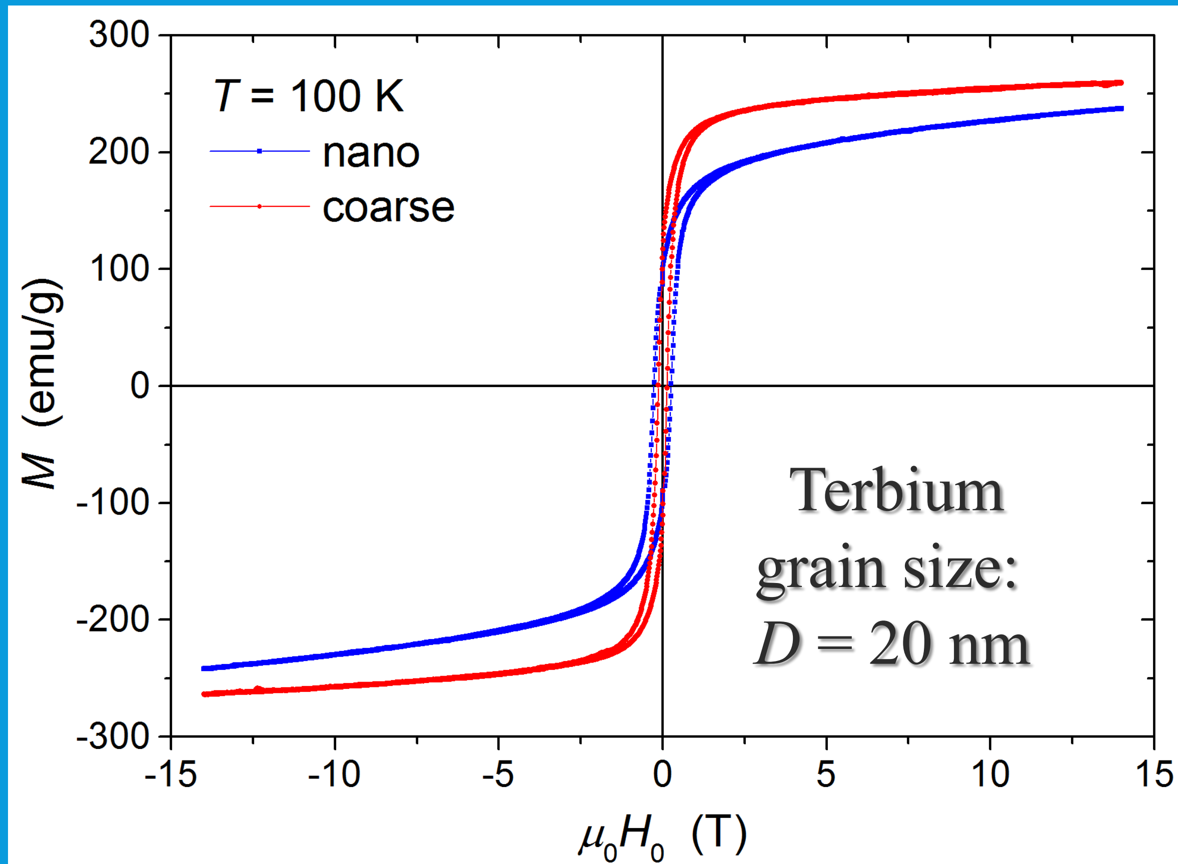
$\widetilde{M}_s(\mathbf{q})$: Fourier transform of spatially-dependent local saturation magnetization $M_s(\mathbf{r})$



A. Michels *et al.*, PRB 94, 054424 (2016).

Defect-induced DMI in nanomagnets

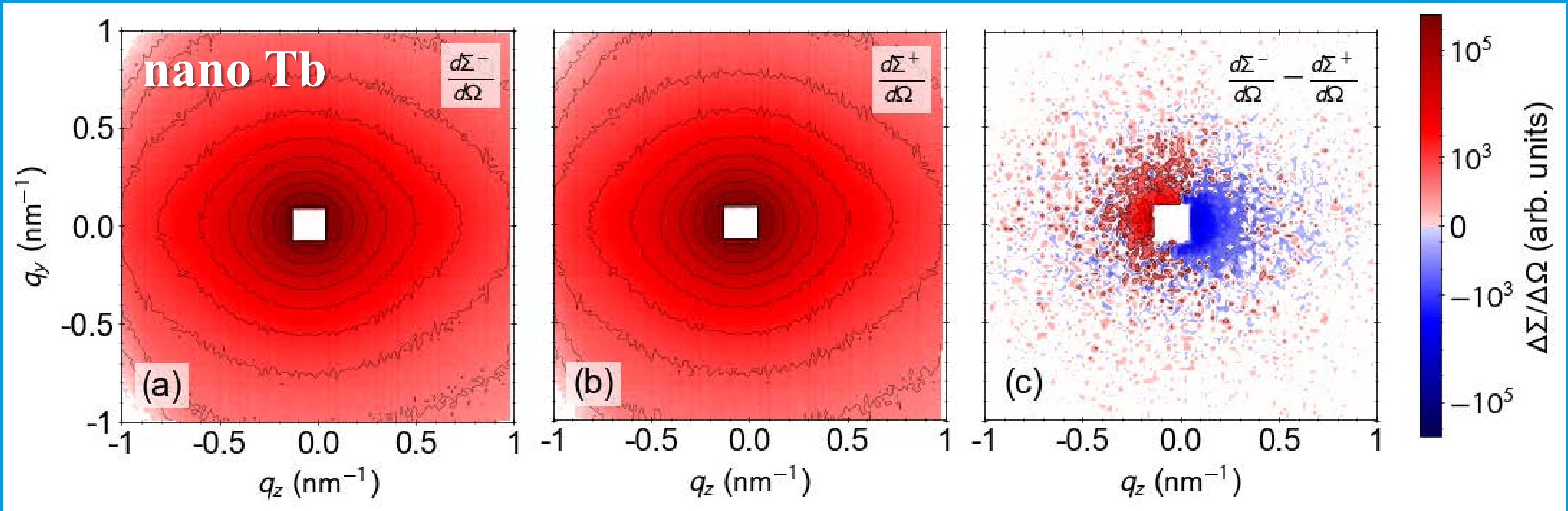
❖ **Nanocrystalline Terbium (large grain-boundary density $\propto 1/D$)**



➢ **Defects (e.g., interfaces, dislocations) reduce magnetization**

A. Michels *et al.*, PRB 99, 014416 (2019).

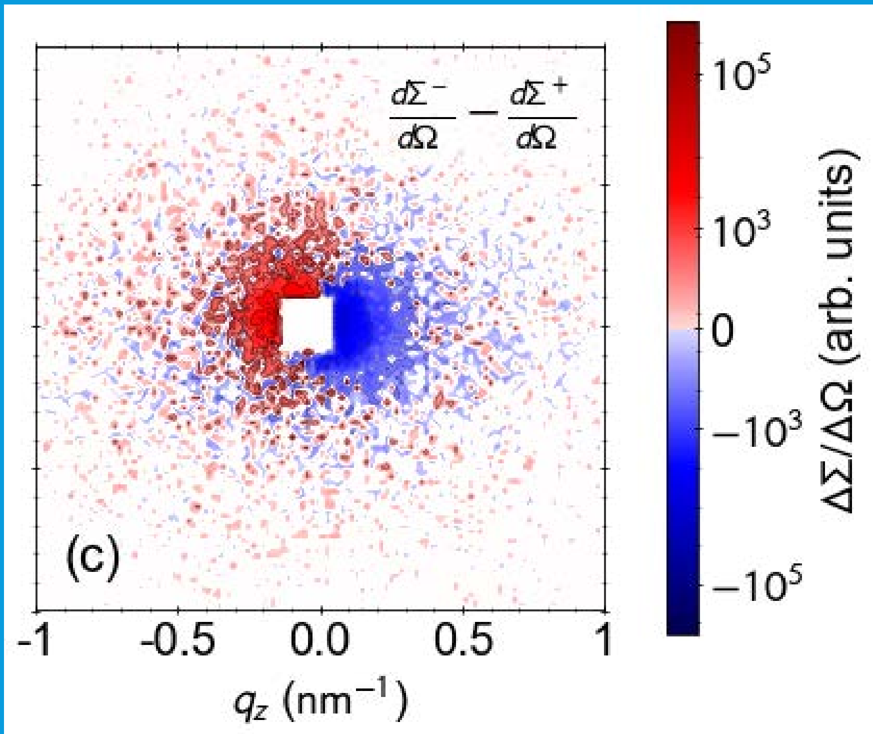
Defect-induced DMI: Experiment

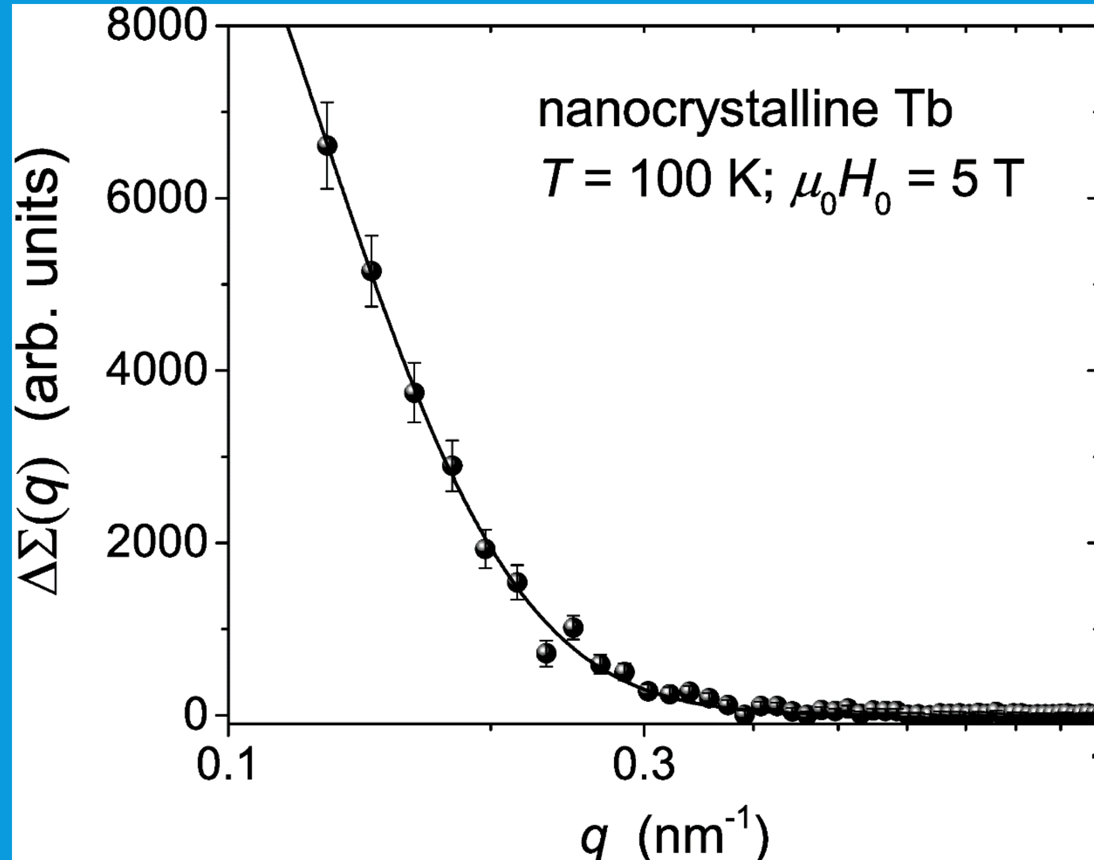


$$\Delta\Sigma = \frac{d\Sigma^-}{d\Omega} - \frac{d\Sigma^+}{d\Omega} \sim 2(\widetilde{N}\widetilde{M}_z^* + \widetilde{N}^*\widetilde{M}_z)\sin^2\theta + 2\imath\chi$$

➢ **Difference between "spin up" and "spin down" cross sections: only polarization-dependent terms survive**

Defect-induced DMI: Experiment





average along horizontal direction

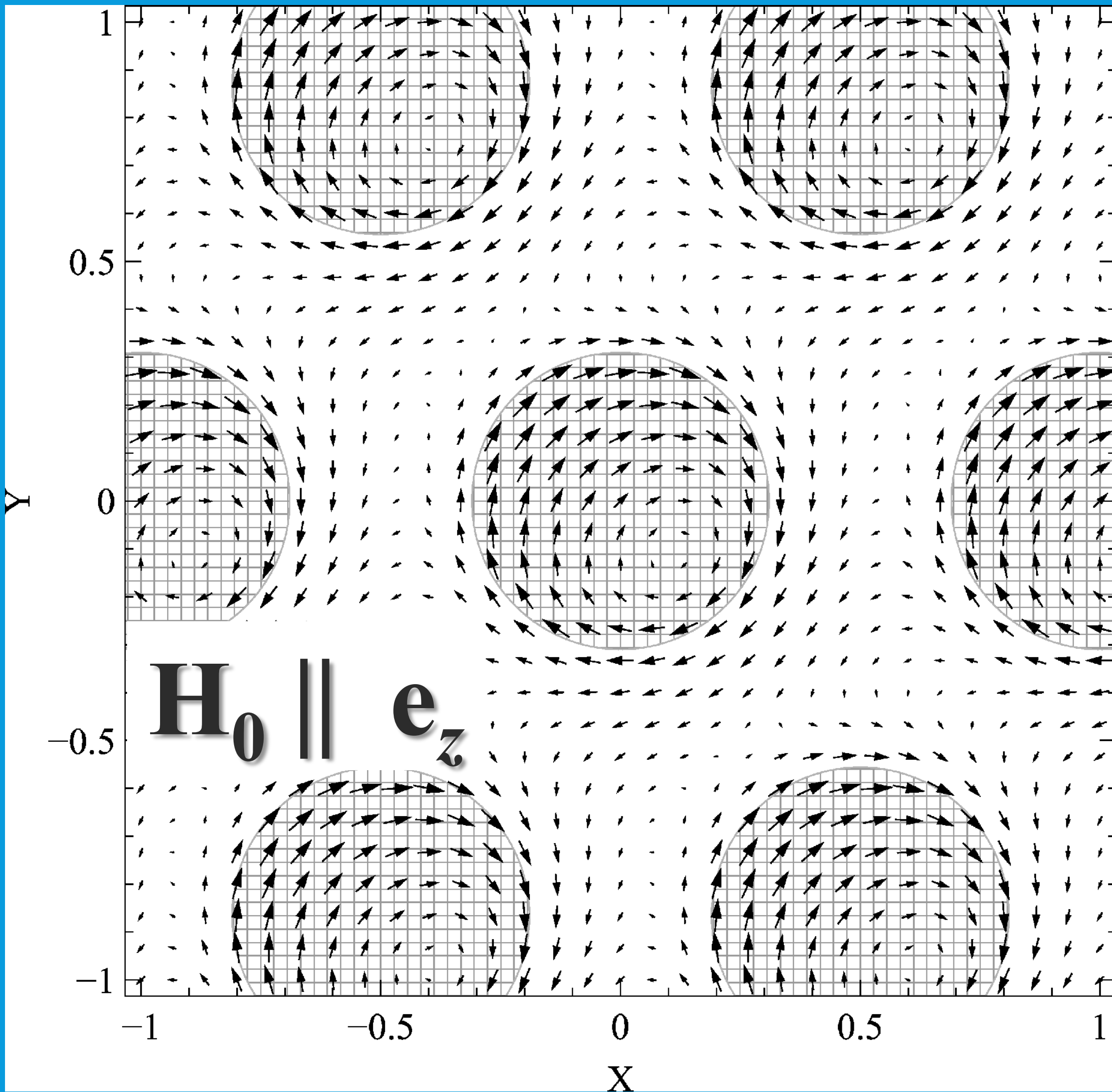
$$2\imath\chi(q, H_i) = \mp \frac{4\widetilde{H}_p^2 p^3 l_D q}{\left(1 - p^2 l_D^2 q^2\right)^2}$$

$D = 0.45 \pm 0.07$ mJ/m^2

A. Michels *et al.*, PRB 99, 014416 (2019).

Defect-induced DMI: Real-space structure

Result of micromagnetic theory

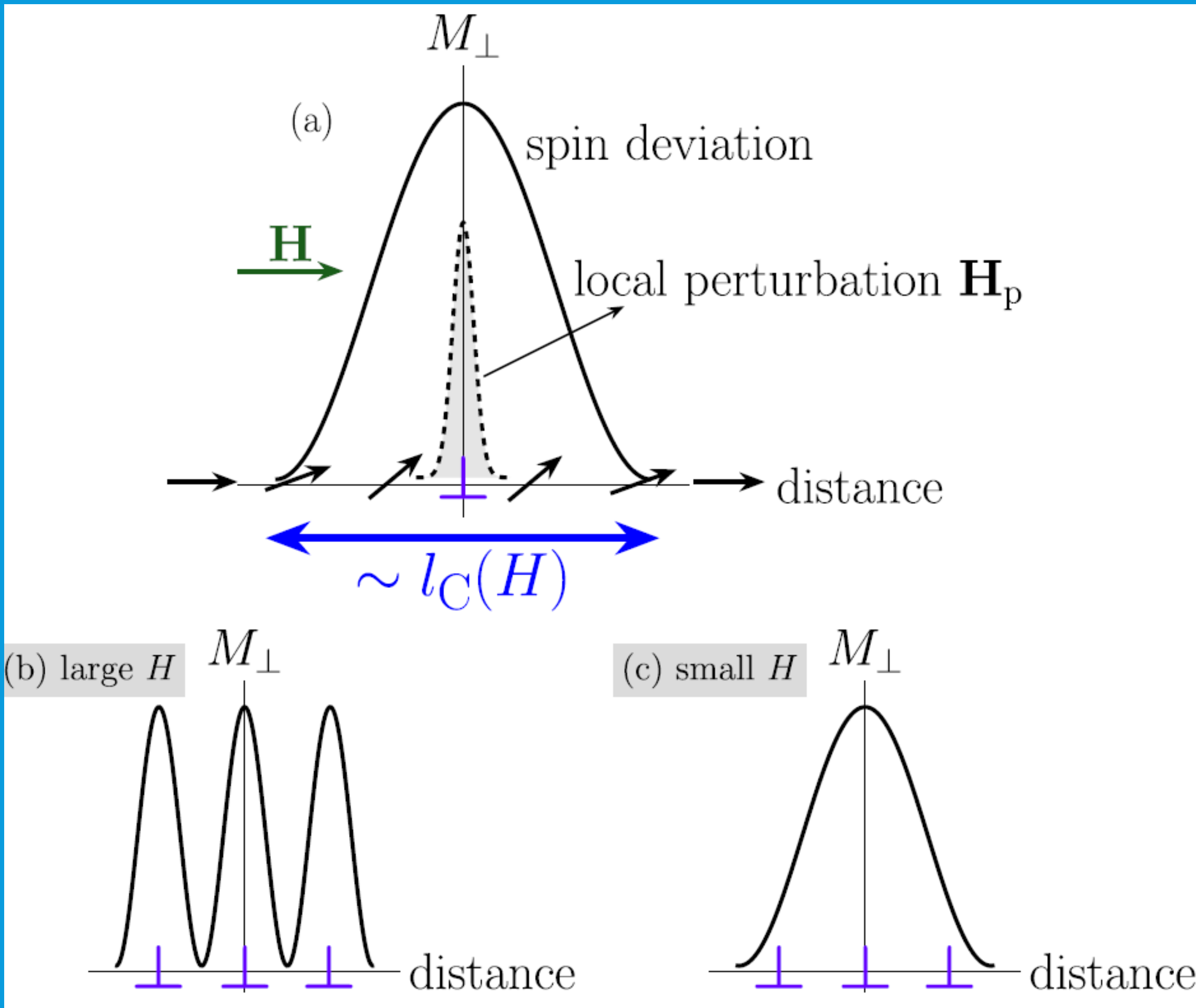


- Shaded circular areas: defect sites with different M_s and anisotropy field
- **M**(**r**) is asymmetric wrt the center of the defect
- Result of DMI, which introduces chiraltity into the sample
- Largest gradients in spin distribution near/at defect sites (interfaces)
- *D*-value from SANS experiment reflects emerging DMI strength at interfaces

A. Michels *et al.*, PRB 99, 014416 (2019).

➢ Scaling in magnetic SANS

Scaling in magnetic SANS



- $l_\mathrm{C}(H)$ is a measure for size of inhomogeneously magnetized regions around defects
- magnetization response similar at different fields H
- existence of scaling?
- Ansatz

defect size

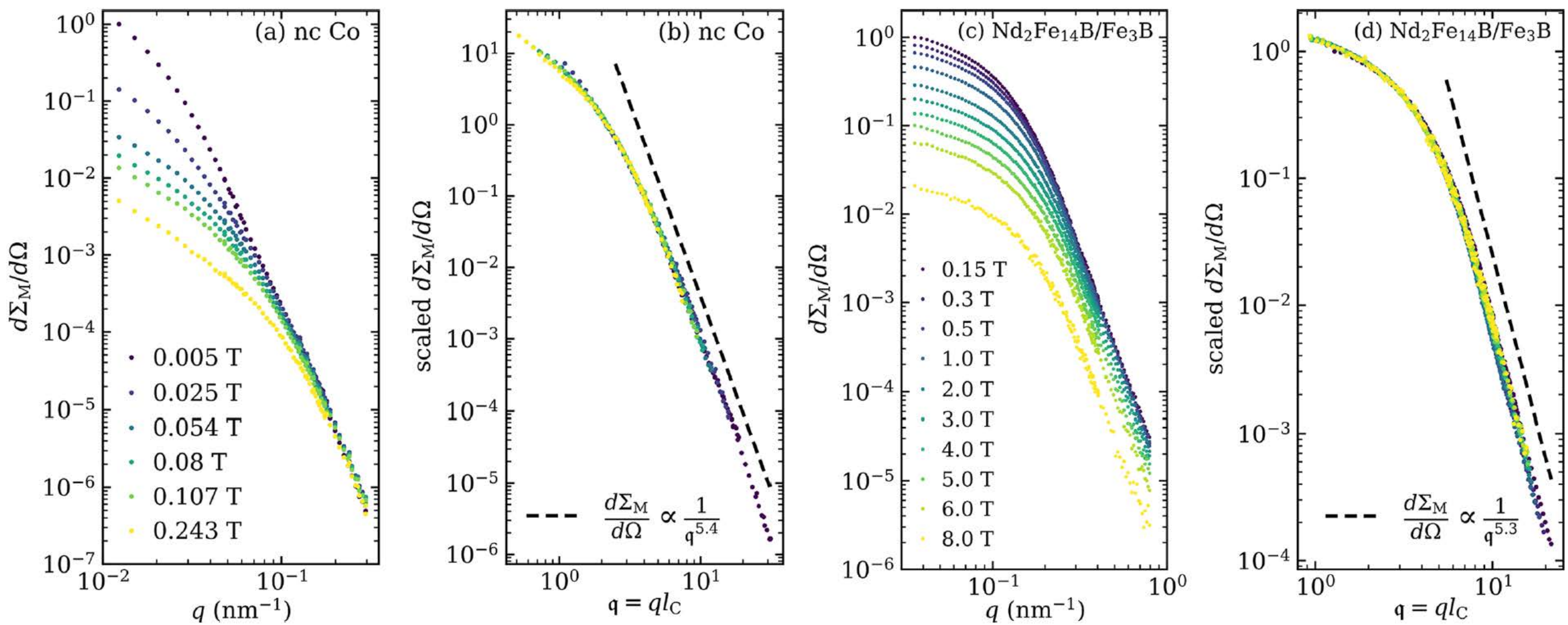
$$l_\mathrm{C}(H) = D + l_\mathrm{H}(H)$$

exchange length

$$l_\mathrm{H}(H) = \sqrt{\frac{2A}{\mu_0 M_0 H}}$$

V. Rai and A. Michels, PRB 112, 144403 (2025).

Scaling in magnetic SANS



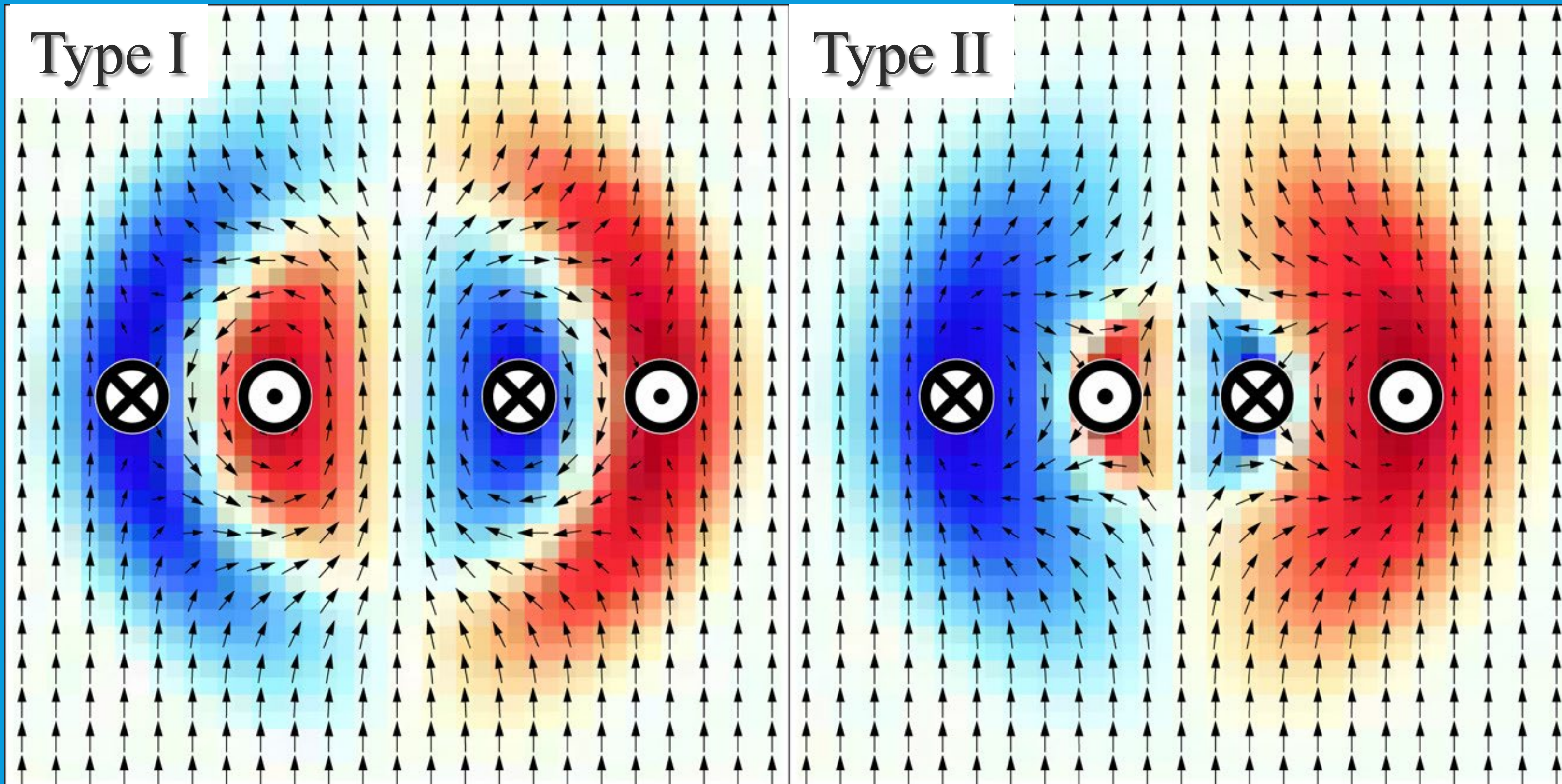
- horizontal scaling

$$\boxed{\mathfrak{q}(H) = q\, l_C(H)}$$

- ❑ l_C describes scaling behavior in the mesoscopic magnetic microstructure of bulk ferromagnets

➢ Signatures of hopfions

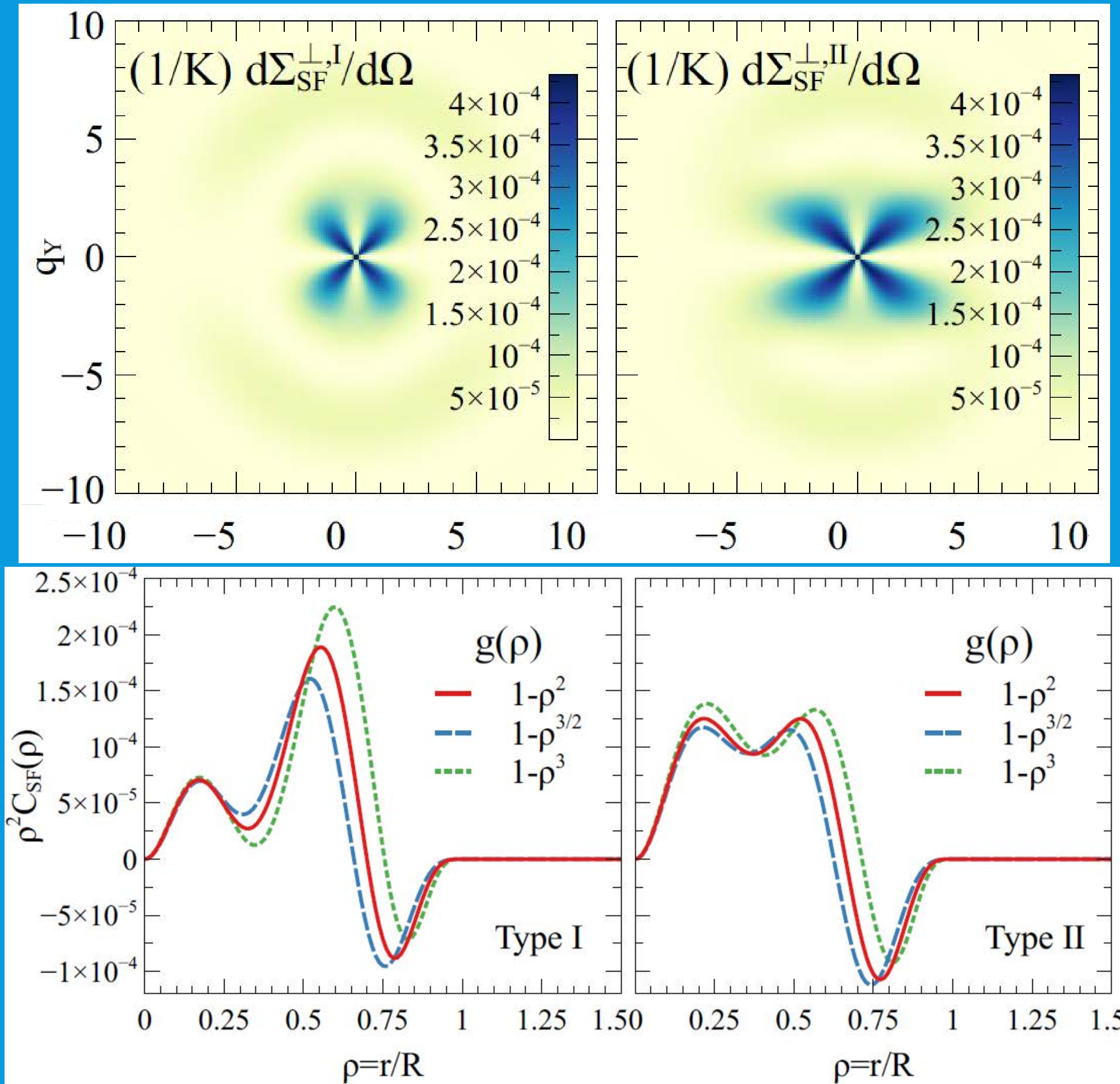
SANS signature of hopfions



- ❖ Localized 3D topological object in an unbounded bulk magnet
- ❖ Contain a circular outer antivortex tube wrapped around a circular inner vortex tube (type I), and vice versa for type II

K.L. Metlov, Physica D 443, 133561 (2023).

Spin-flip SANS and correlation function



- Spin-flip SANS exhibits saturated-spheres-like scattering
- With a double-peak radial correlation function and a zero crossing produced by vortex and antivortex tubes
- Dipolar interaction destabilizes hopfions (MnSi is promising candidate material among skyrmion hosts)

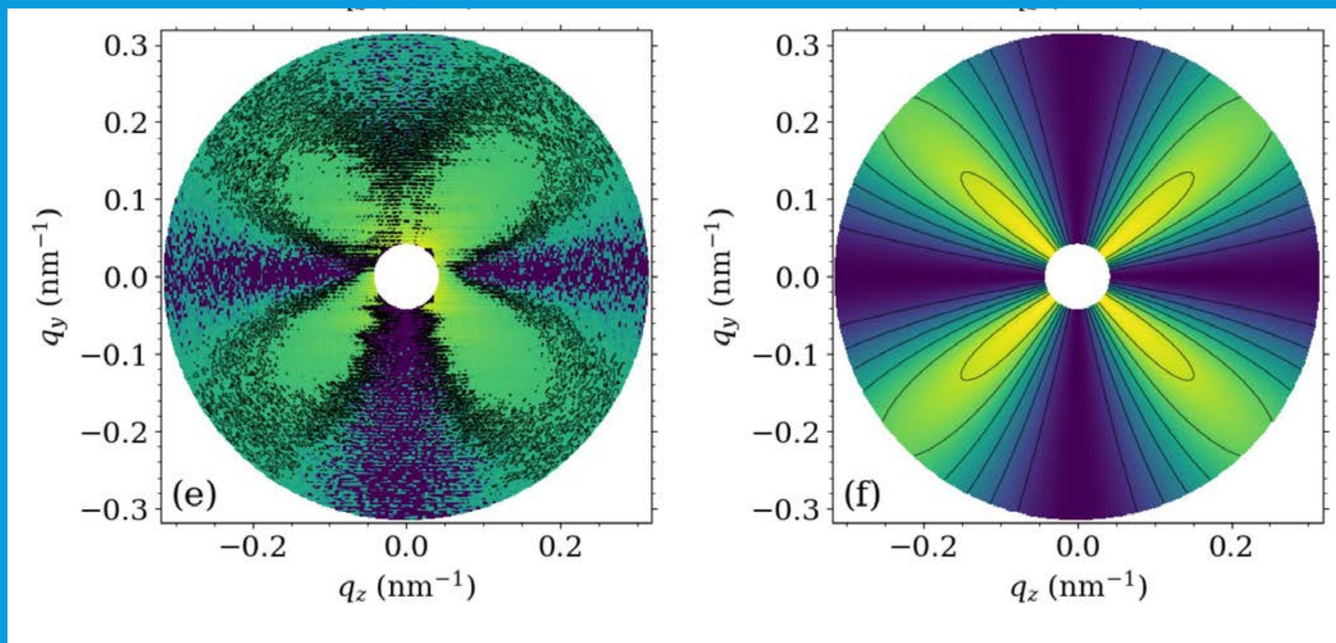
K.L. Metlov and A. Michels, PRB 109, L220408 (2024).
K.L. Metlov, Physica B 695, 416498 (2024).

Spin-disorder-induced anisotropy in polarized SANS

Difference between spin-up and spin-down SANS

$$\Delta\Sigma = K\left[(\widetilde{N}\widetilde{M}_z^* + \widetilde{N}^*\widetilde{M}_z)\sin^2\theta \right.$$
$$\left. \boxed{-(\widetilde{N}\widetilde{M}_y^* + \widetilde{N}^*\widetilde{M}_y)\sin\theta\cos\theta}\right]$$

Experiment Theory



I. Titov *et al.*, Phys. Rev. Lett. **135**, 196706 (2025).

Conclusions

- Magnetic Neutron Scattering is important technique in physics and materials science to study <u>dynamics</u> and <u>structure</u> of magnetic materials

- Magnetic SANS in particular allows one to study <u>mesoscale</u> magnetization structure in the bulk of magnets (resolution range: ~ 1nm-20μm)

- Magnetic SANS + micromagnetic theory is useful tool for <u>quantitative</u> analysis of bulk magnetic materials (exchange constant, magnetic anisotropy and magnetostatic fields, correlation length, ...)

- Dipolar interaction results in angular anisotropies; must be taken into account for fundamental understanding of magnetic SANS

- DMI in defect-rich materials results in asymmetry of polarized SANS; effect is generic to polycrystalline magnets

- Existence of scaling; hopfion signatures