Magnetism in metallic glasses - a clear need for PDF

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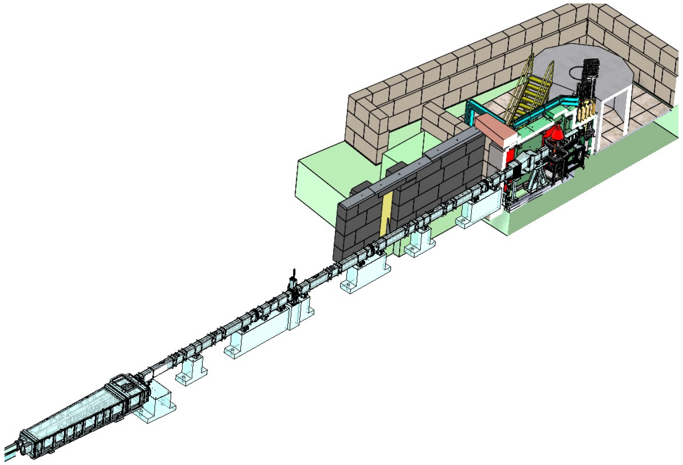
and

Neil Cowlam
University of Sheffield

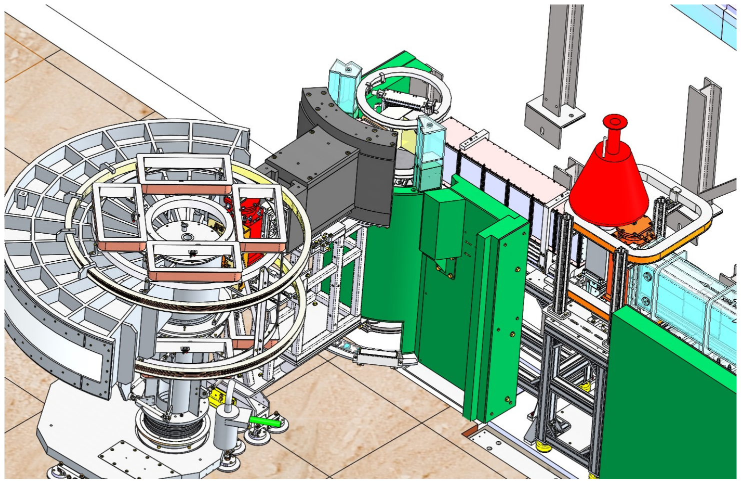
D007

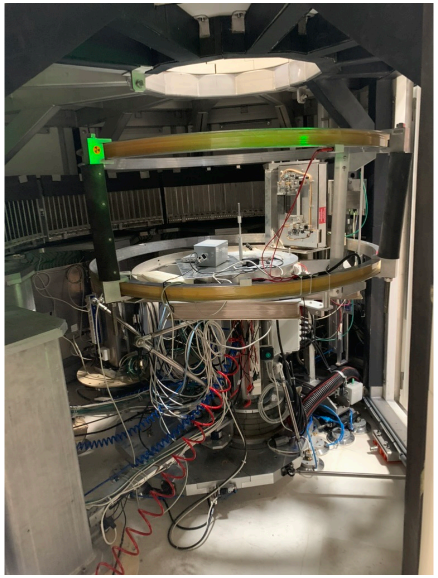
G. J. Nilsen *et al.*, NIMA **951** (2020) 162990



Neutron diffuse scattering spectrometer

- Incident wavelength: $3 < \lambda < 6$ Å
- Q-range: $0.1 \lesssim Q \lesssim 4$ Å^{-1}
- Permanent polarization analysis

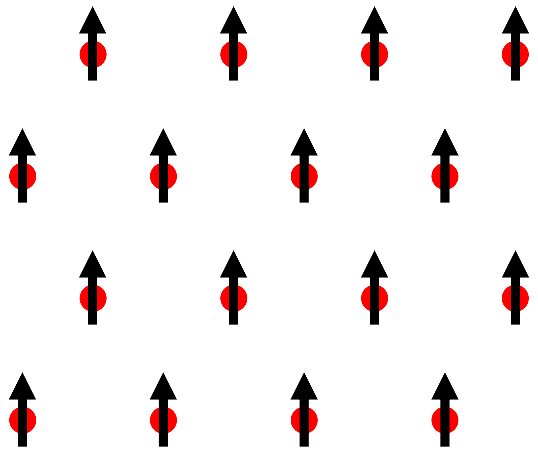




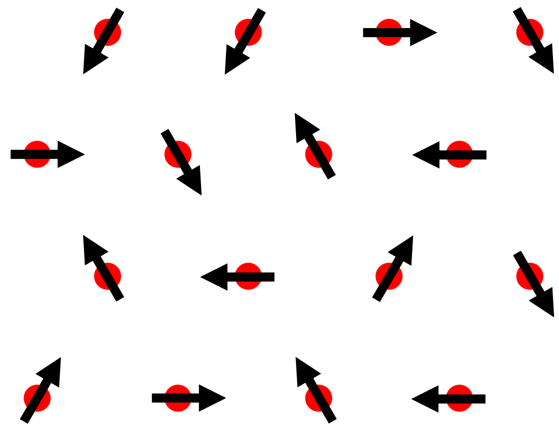
Q-range: $0.1 \lesssim Q \lesssim 4$ Å^{-1}

D007: Built to study short-ranged order
Mostly used for magnetic materials

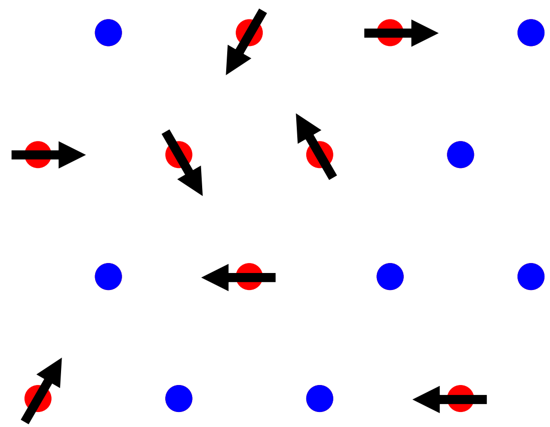
Long-ranged order



Geometric frustration

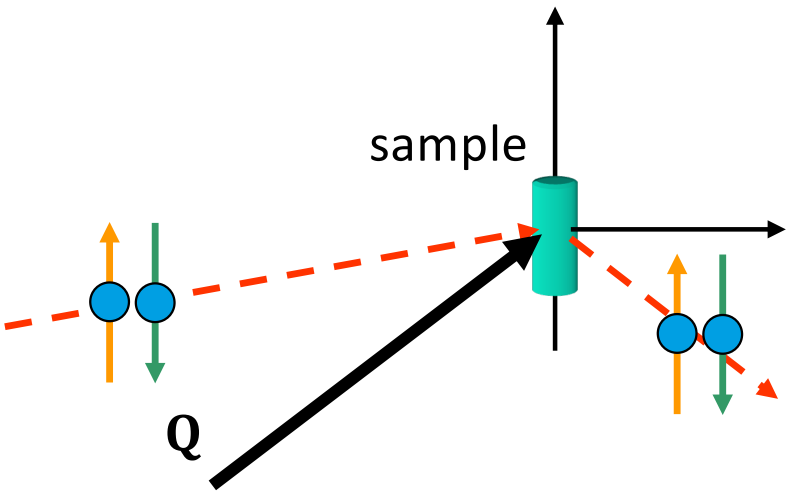


Site/Composition disorder



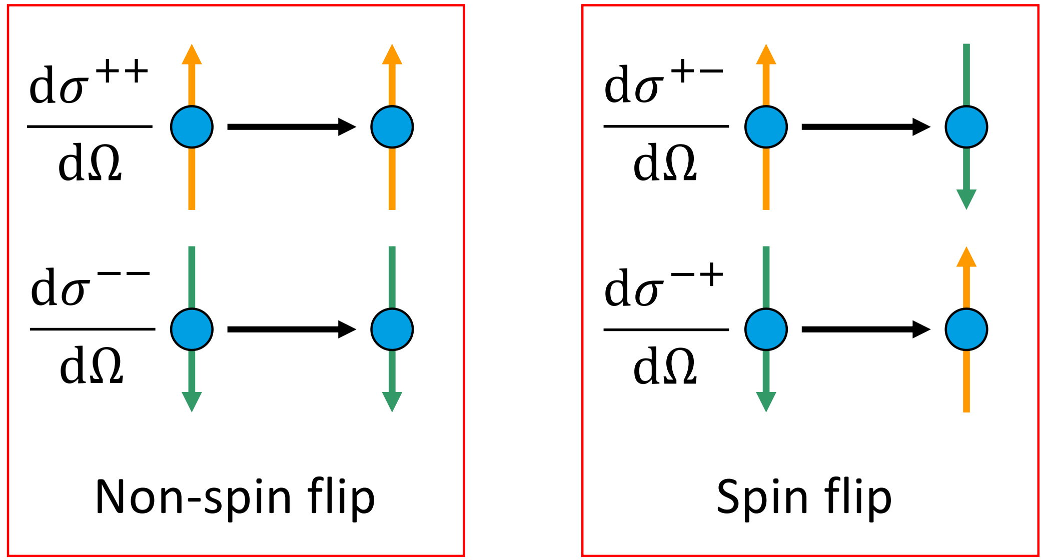
Uniaxial polarization analysis

The neutron scattering potential: $\hat{V} = \frac{2\pi\hbar^2}{m_n}\left(b_c + B\hat{\mathbf{I}}\cdot\hat{\boldsymbol{\sigma}}\right) - \gamma\mu_N\hat{\boldsymbol{\sigma}}\cdot\mathbf{B}$



Define Z as the polarization axis

Four possibilities:



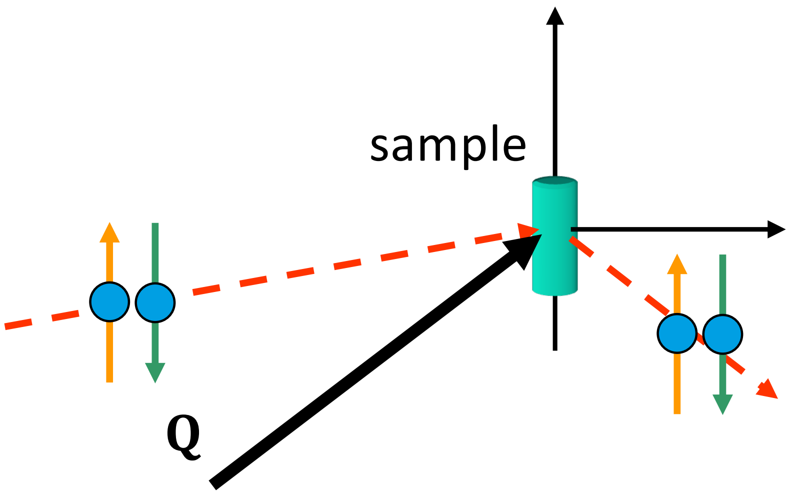
$U^{++} = b_c + BI_z - M_{\perp z}$

$U^{--} = b_c - BI_z + M_{\perp z}$

$U^{+-} = B\left(I_x + iI_y\right) - \left(M_{\perp x} + iM_{\perp y}\right)$

$U^{-+} = B\left(I_x - iI_y\right) - \left(M_{\perp x} - iM_{\perp y}\right)$

Uniaxial polarization analysis



For paramagnetic-like scattering:

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{nuclear-coherent} + \left(\frac{d\sigma}{d\Omega}\right)_{isotope-incoherent} + \left(\frac{d\sigma}{d\Omega}\right)_{nuclear-spin-incoherent} + \left(\frac{d\sigma}{d\Omega}\right)_{magnetic}$$

NSF cross-sections are equivalent, $\frac{d\sigma^{++}}{d\Omega} = \frac{d\sigma^{--}}{d\Omega}$

SF cross-sections are equivalent, $\frac{d\sigma^{+-}}{d\Omega} = \frac{d\sigma^{-+}}{d\Omega}$

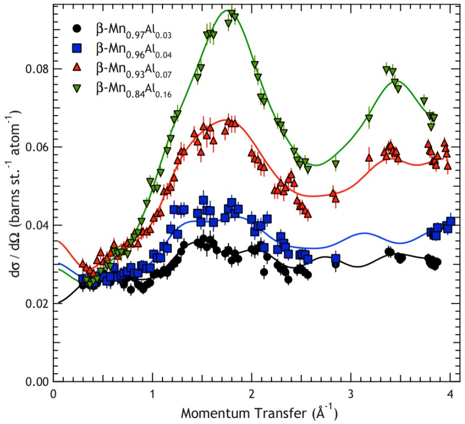
Measure NSF and SF for different polarization directions,
Separate the different contributions to the scattering

Short-range order in β-Mn alloys

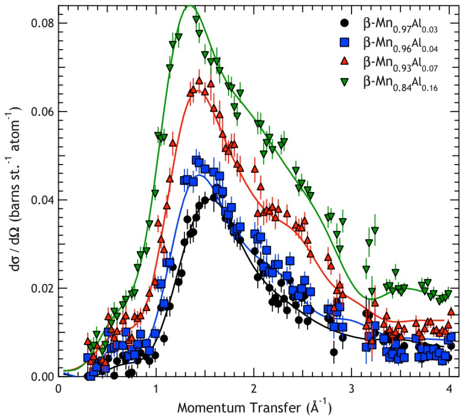
Ross Stewart

Q-range: $0.1 \lesssim Q \lesssim 4$ Å^{-1}

Nuclear diffuse

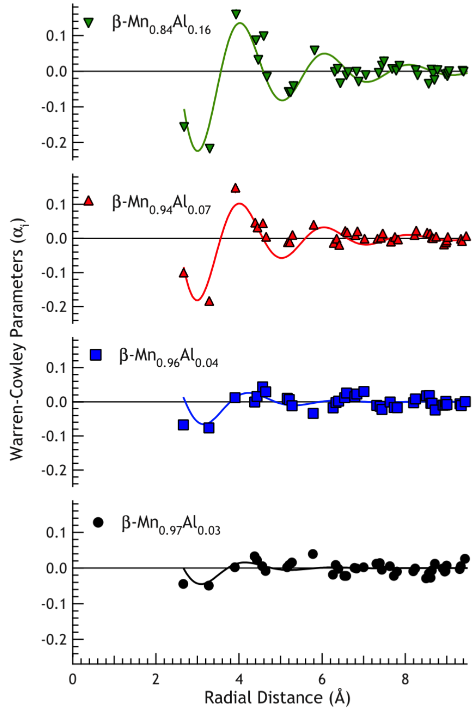


Magnetic diffuse

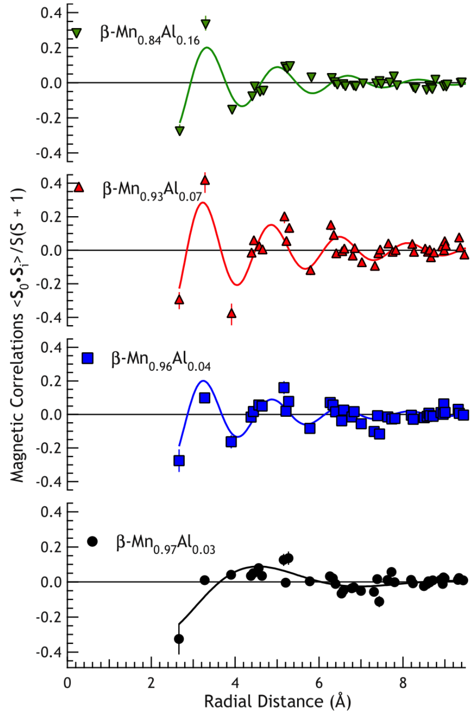


Reverse Monte-Carlo

Nuclear: α_i



Magnetic: $\langle S(0) \cdot S(r) \rangle$



J. R. Stewart *et al.*, Phys. Rev. B **78** (2008) 014428

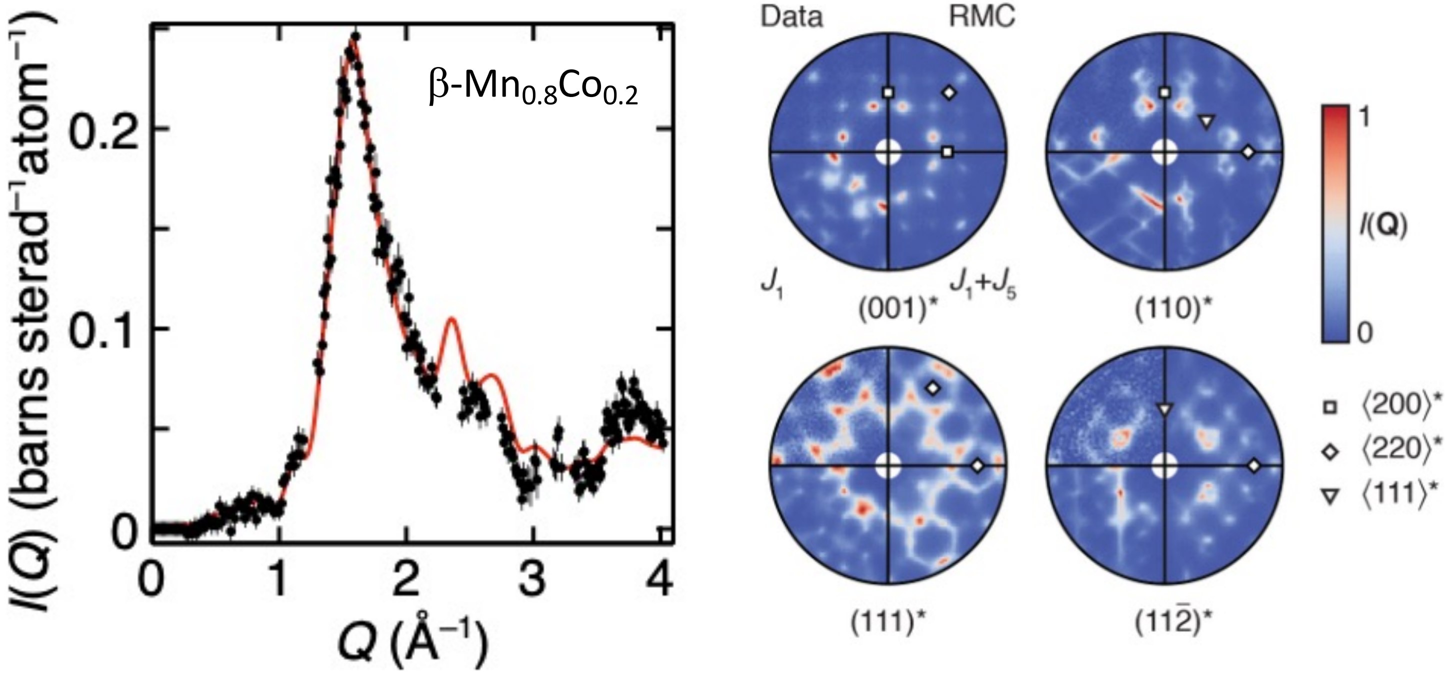
Short-range order in β-Mn alloys

Ross Stewart

Joe Paddison

Polycrystal

Single crystal



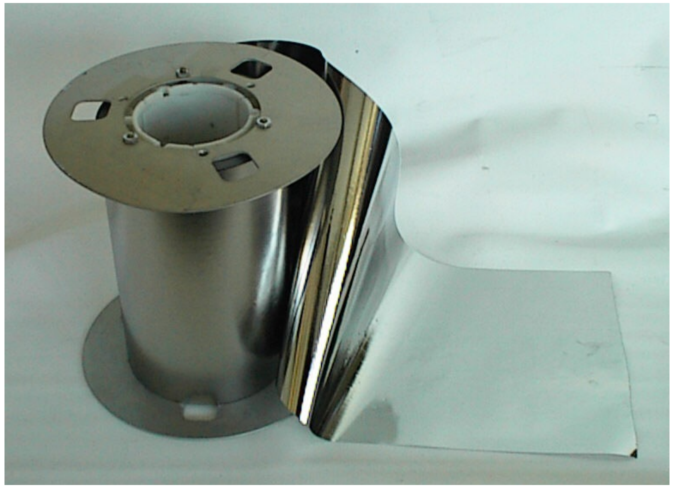
J. R. Stewart *et al.*, J. Phys.: Condens. Matter **21** (2009) 124216

J. A. M. Paddison *et al.*, Phys. Rev. Lett. **110** (2013) 267207

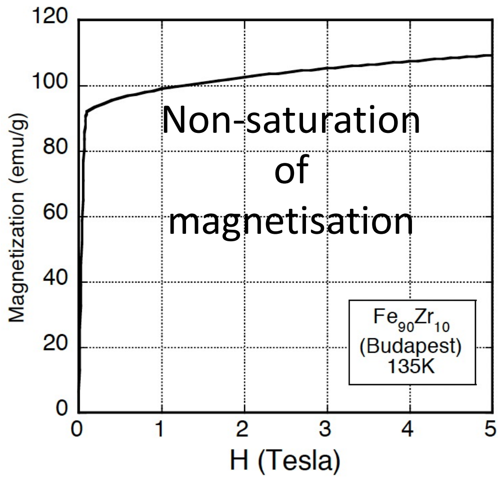
Reverse Monte-Carlo works very well!

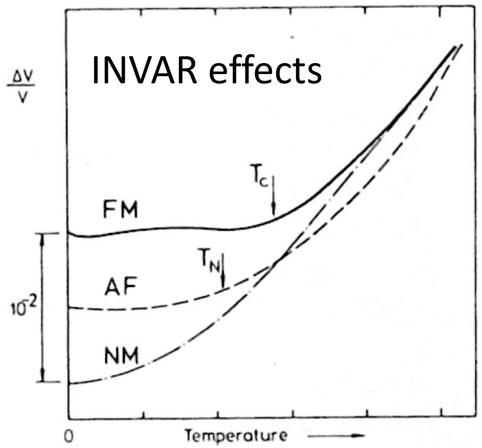
Metallic glasses and non-collinear ferromagnetism

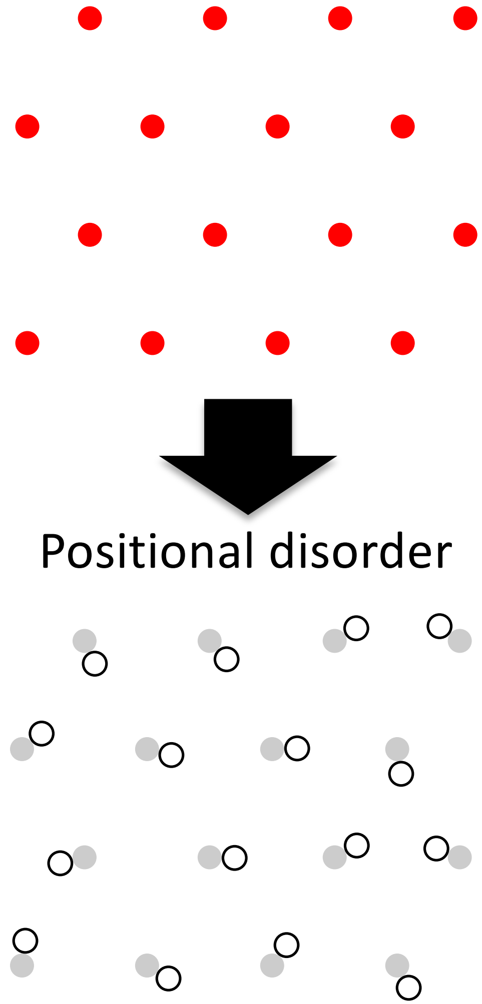
METGLAS© 2605 ($Fe_{78}B_{13}Si_9$)



A huge range of commercial applications
- Transformers
- Springs
- Security tags
- Bimetallic strips
- Surge absorbers







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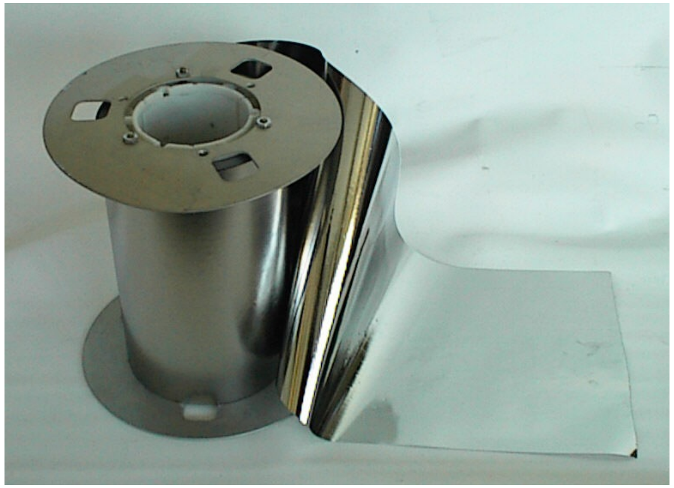

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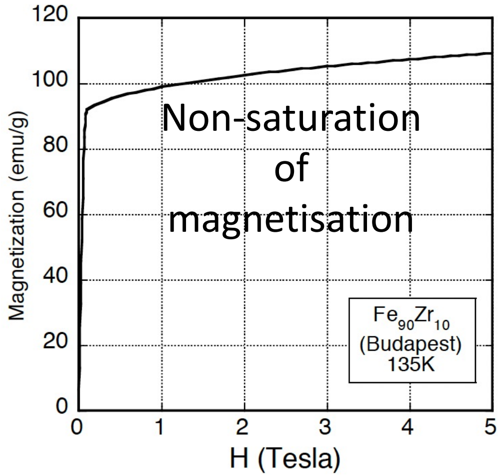
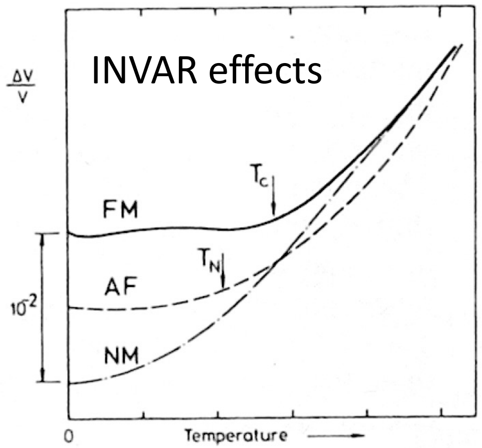
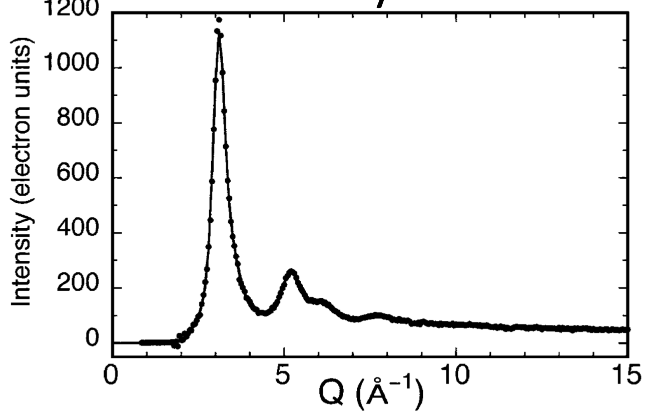
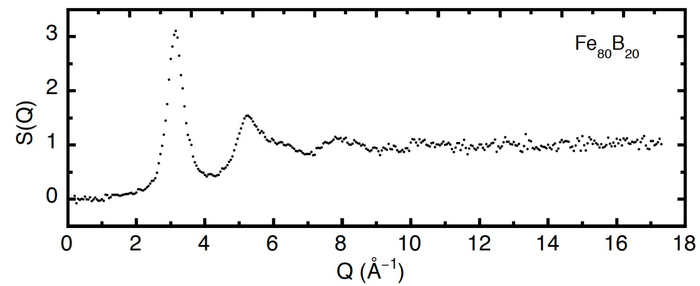




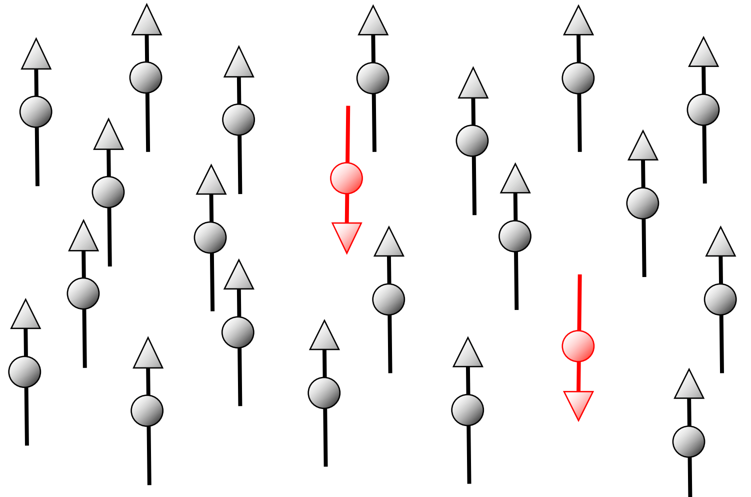
X-rays



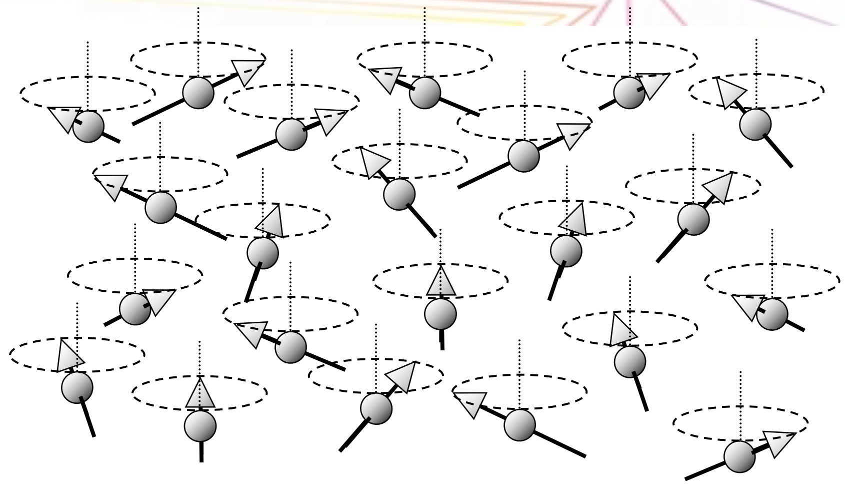
Unpolarized neutrons



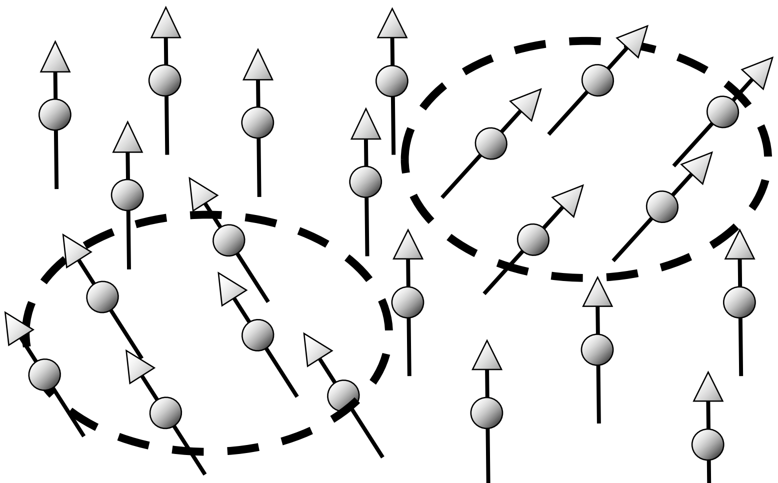
Proposed magnetic structures for Fe-based metallic glasses



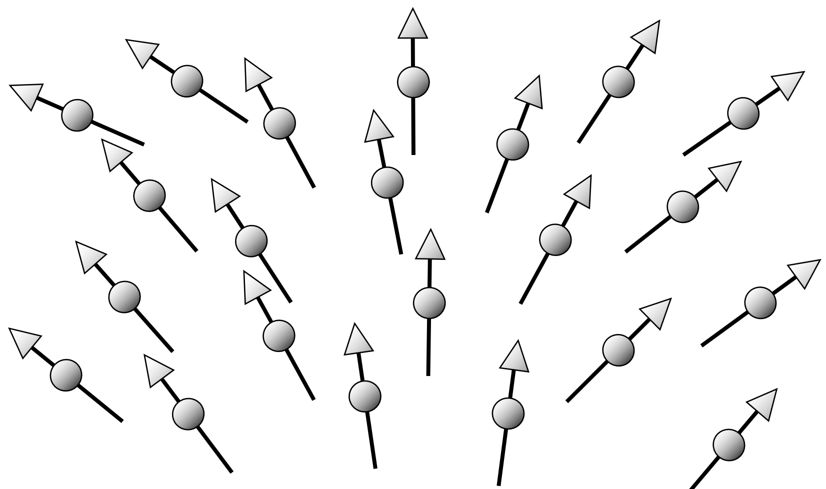
Saito *et al.*, *J. Phys. F.: Metal Phys* **16** (1986) 911



Karlsson *et al.*, *J. Phys.: Condens. Matter* **11** (1999) 9249



Kaul, *J. Phys. F.: Metal Phys* **18** (1988) 2089

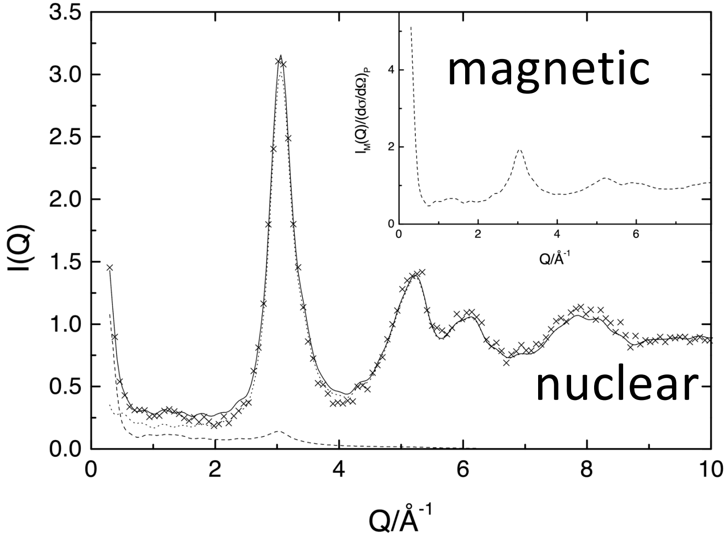


Ryan *et al.*, *Phys. Rev.* B **35** (1987) 8630

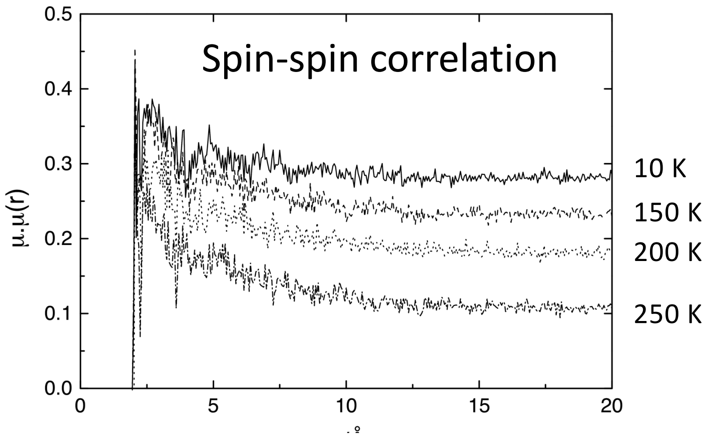
RMC on a magnetic metallic glass

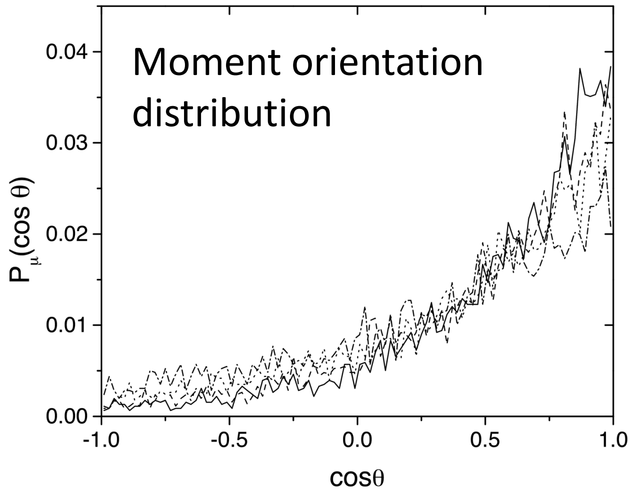
Robert McGreevy

$Fe_{90}Zr_{10}$ glass
Unpolarized neutrons



R. L. McGreevy, JPCM **13** (2001) R877
L. Karlsson *et al.*, JPCM **11** (1999) 9249





Uniaxial polarization analysis

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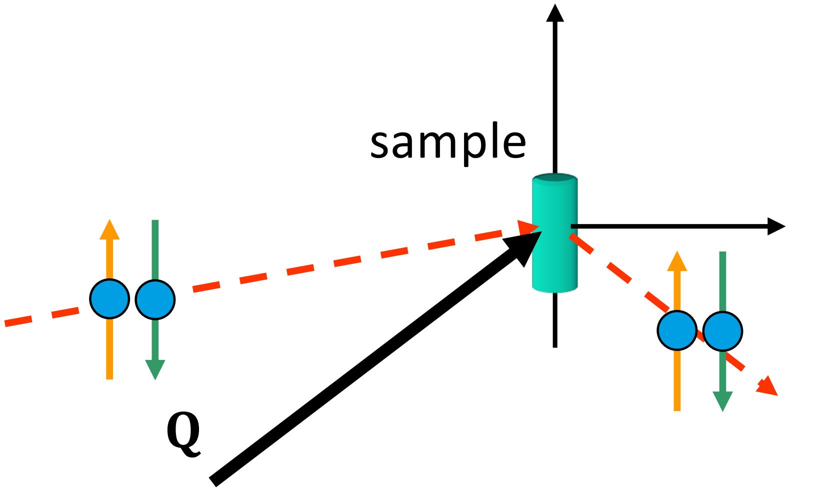
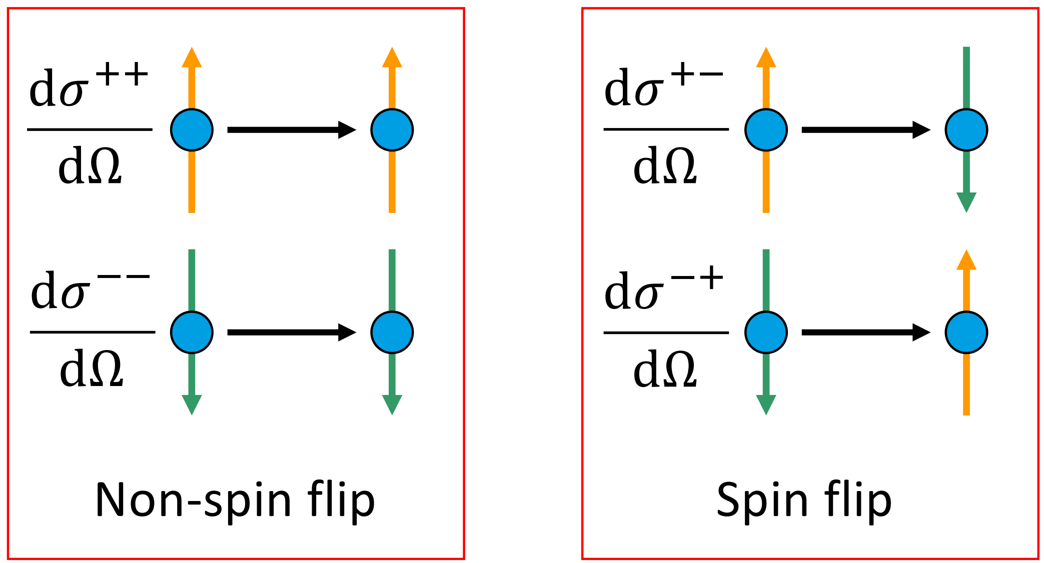


Define Z as the polarization axis

Four possibilities:



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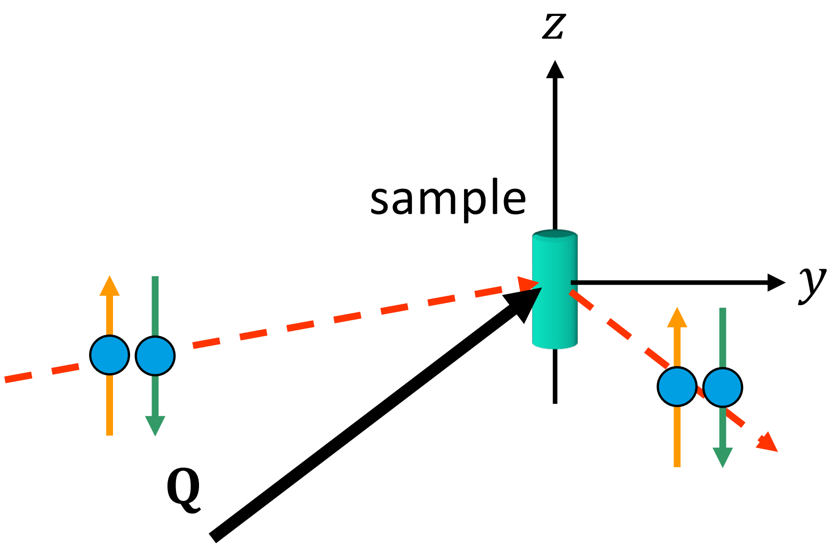

Define a horizontal scattering plane

Define a vertical polarization axis, $\mathbf{P}$

$$\mathbf{P} \perp \mathbf{Q}$$

NSF

$$\frac{d\sigma^{++}}{d\Omega} \propto \left| \int \big(b(\mathbf{r}) - M_{\perp z}(\mathbf{r})\big) e^{i\mathbf{Q}\cdot\mathbf{r}} d\mathbf{r} \right|^2$$

$$\frac{d\sigma^{--}}{d\Omega} \propto \left| \int \big(b(\mathbf{r}) + M_{\perp z}(\mathbf{r})\big) e^{i\mathbf{Q}\cdot\mathbf{r}} d\mathbf{r} \right|^2$$

Not equivalent!

SF

$$\frac{d\sigma^{\pm\mp}}{d\Omega} \propto \left| \int M_{\perp y}(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d\mathbf{r} \right|^2$$

Moment component separation

Metallic glasses and non-collinear ferromagnetism

Polarized neutrons, “saturating” vertical field

P ⊥ Q

$$\frac{d\sigma^{\pm\pm}}{d\Omega} = \left| \int \left(b(\mathbf{r}) \mp M_{\perp z}(\mathbf{r}) \right) e^{i\mathbf{Q}\cdot\mathbf{r}} d\mathbf{r} \right|^2$$

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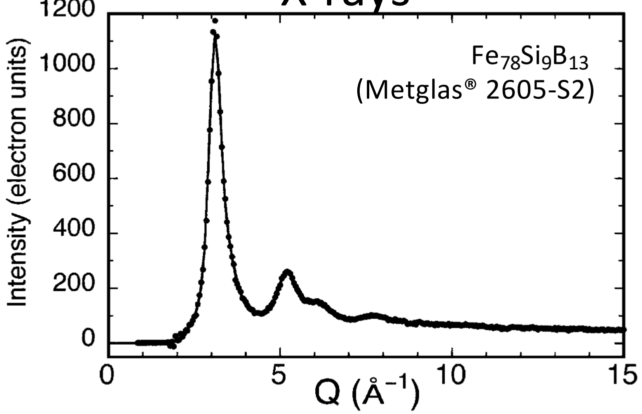
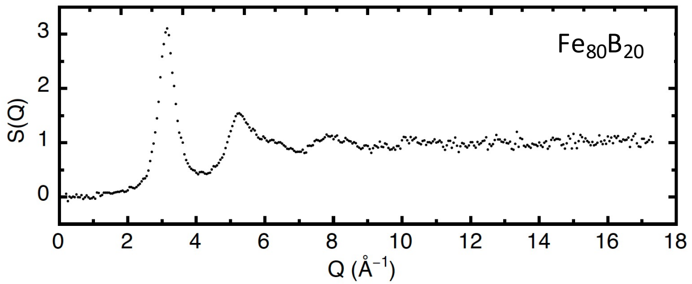
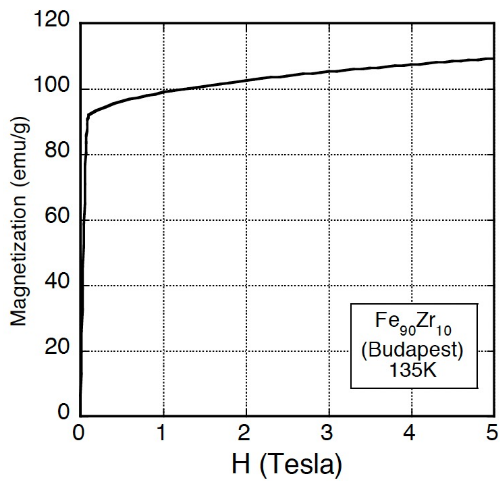


Unpolarized neutrons





A. R. Wildes *et al.*, Europhys. Lett. **68** (2004) 582

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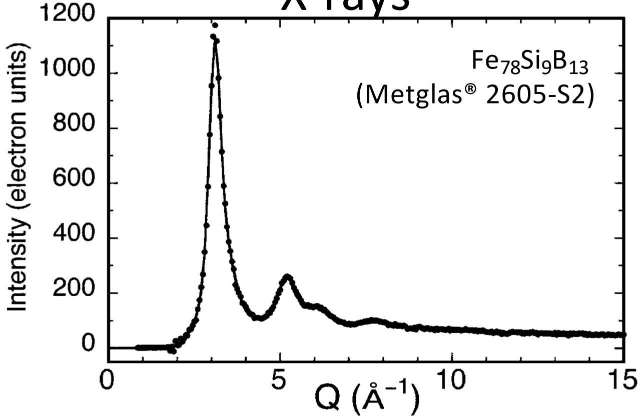

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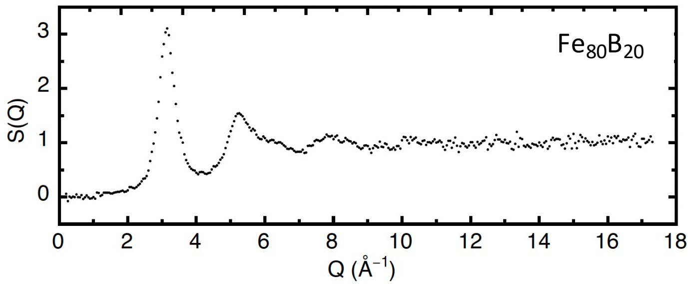
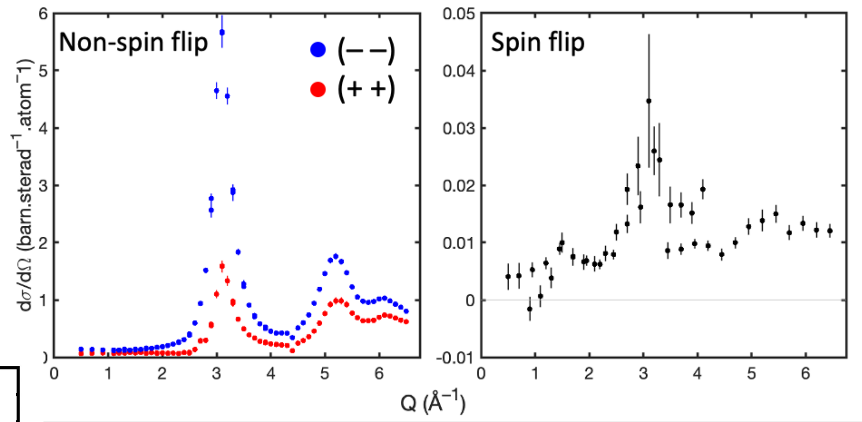
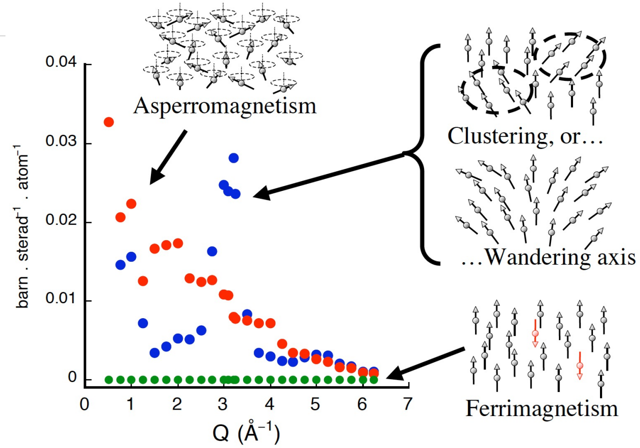


$Fe_{78}Si_9B_{13}$ (Metglas® 2605-S2)





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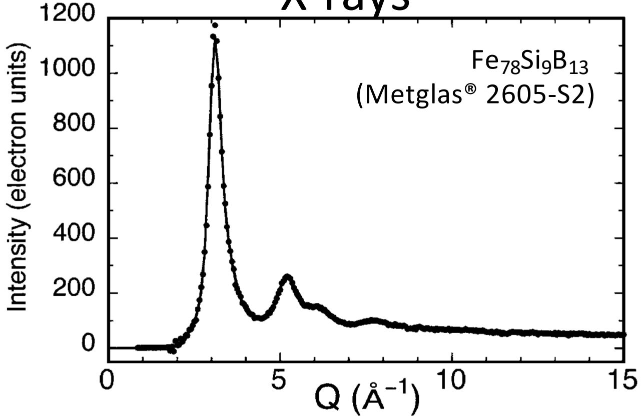

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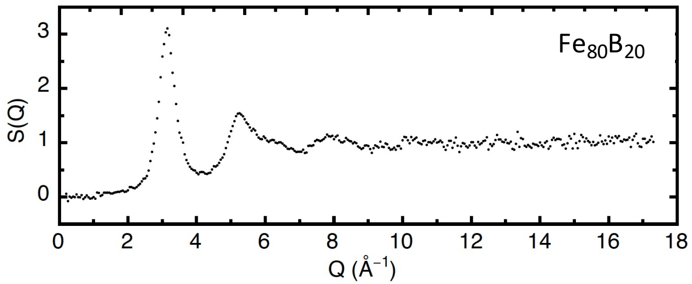

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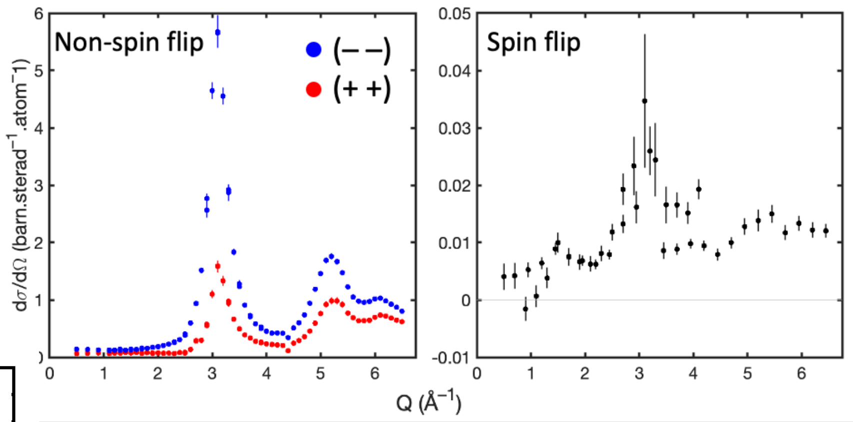

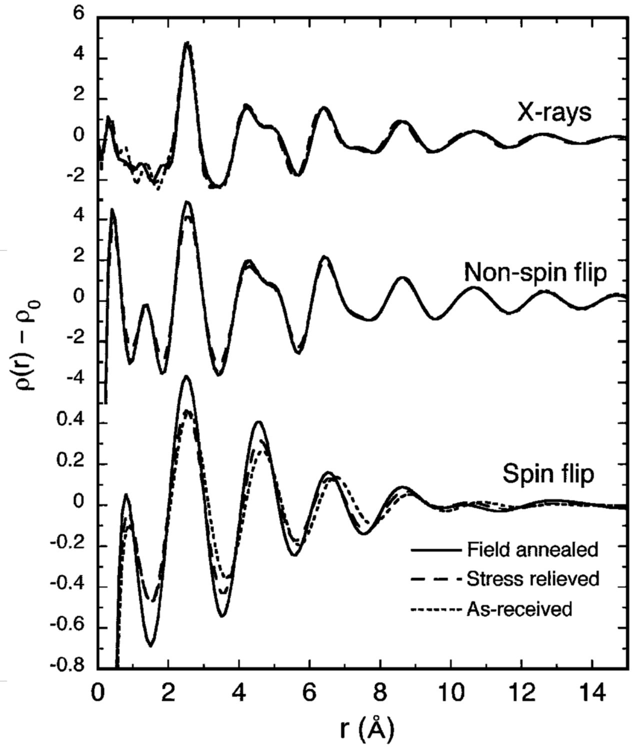

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Diffuse scattering in metallic glasses, $Fe_{64}Er_{19}B_{17}$

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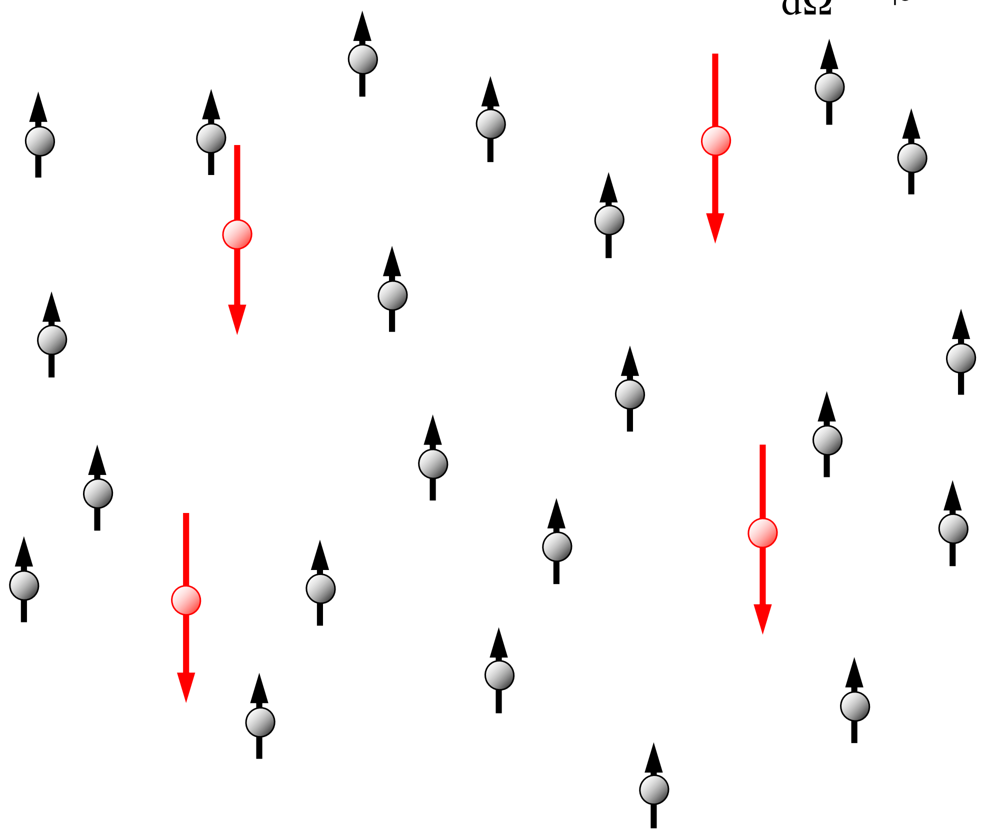

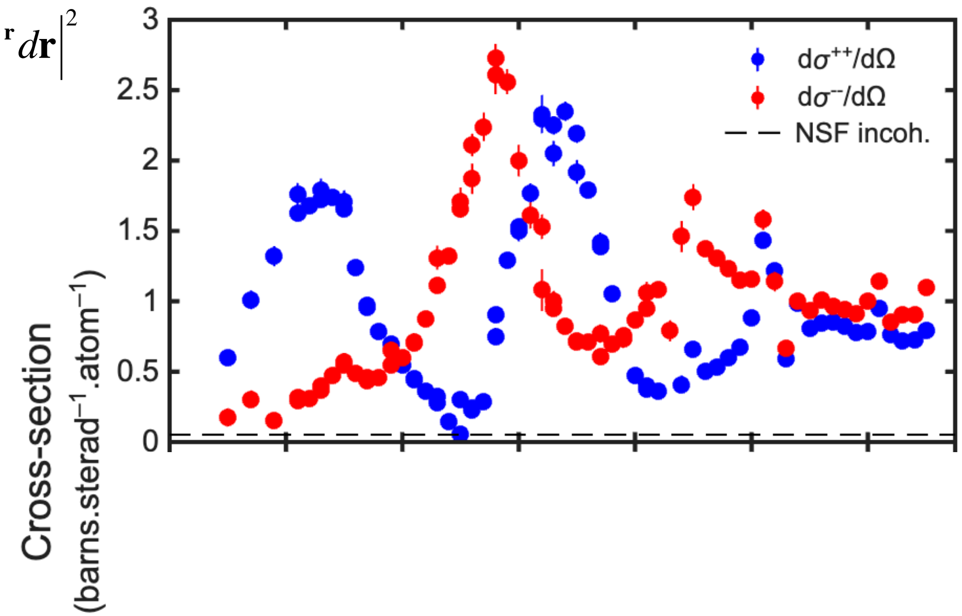

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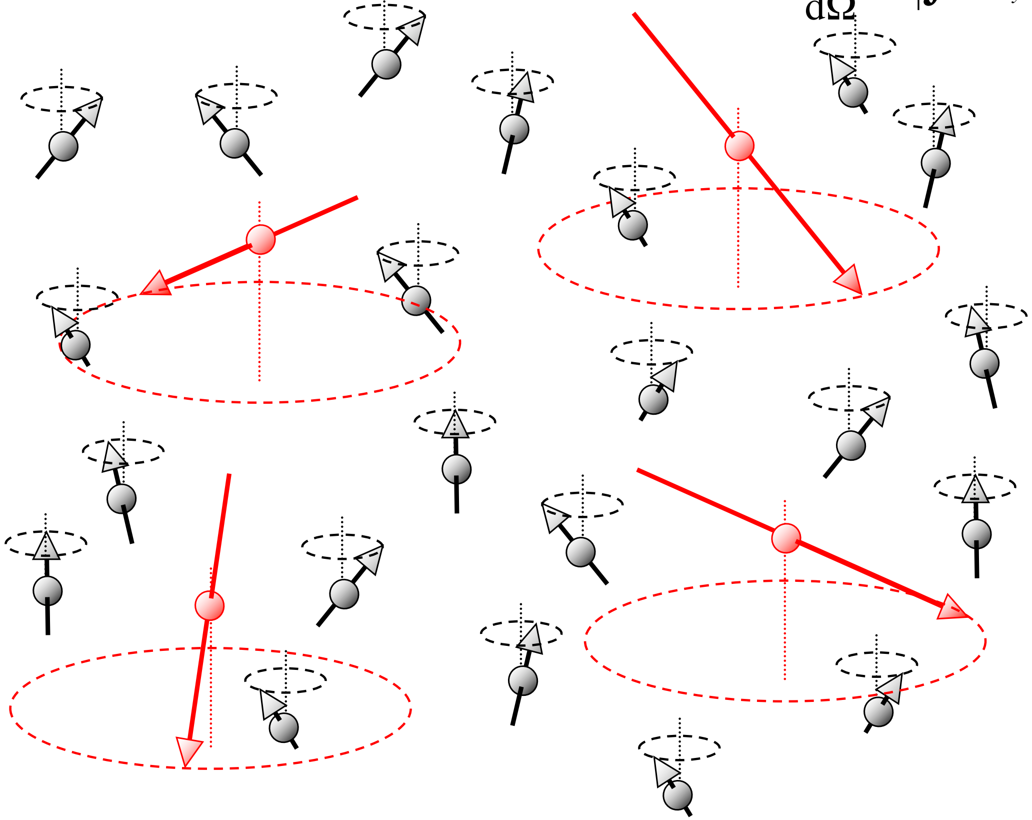

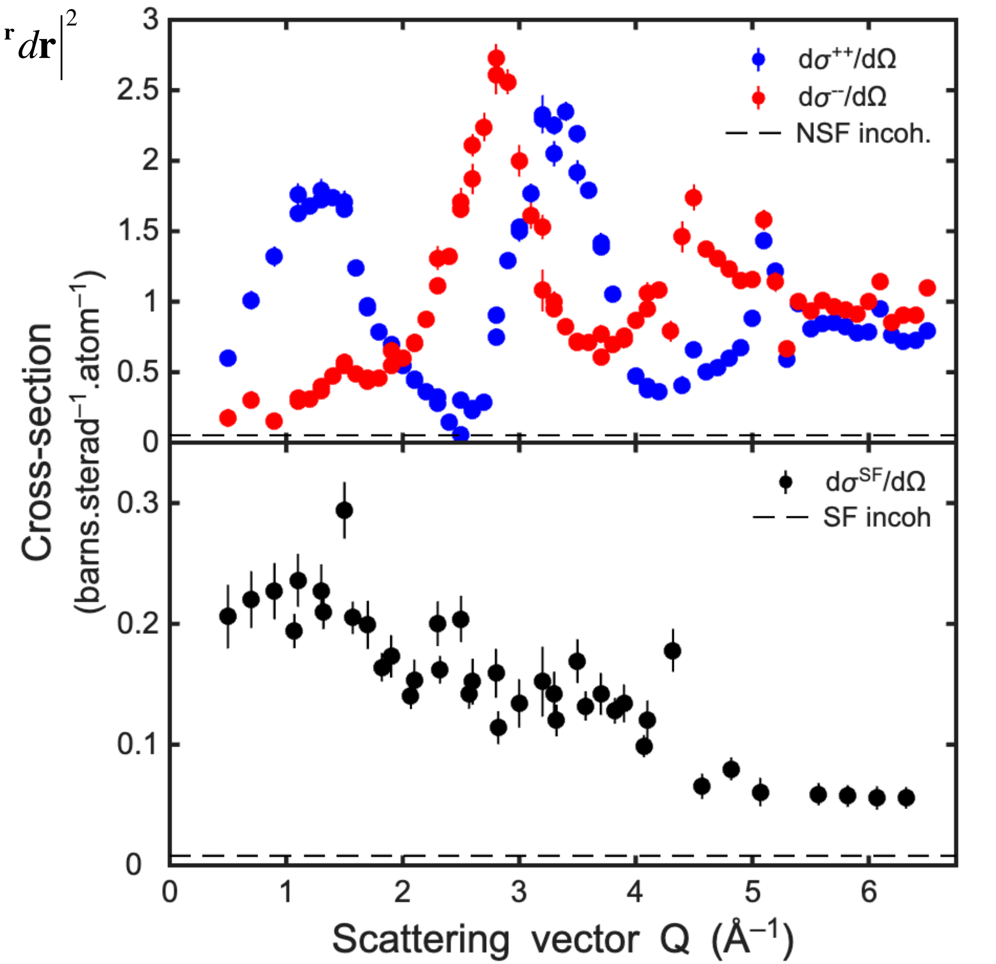

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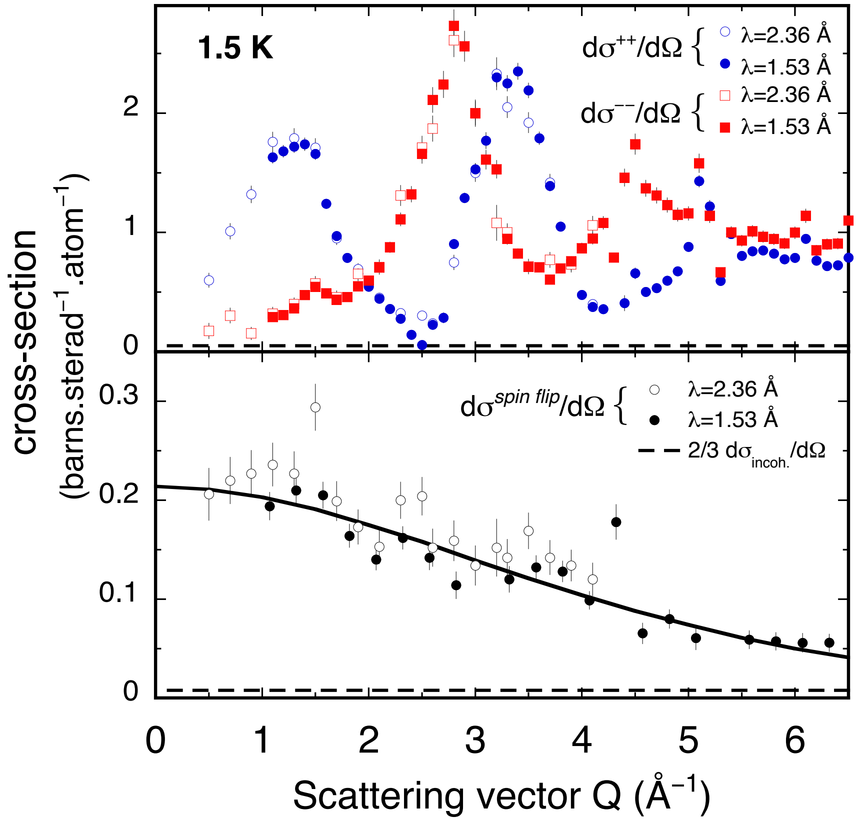
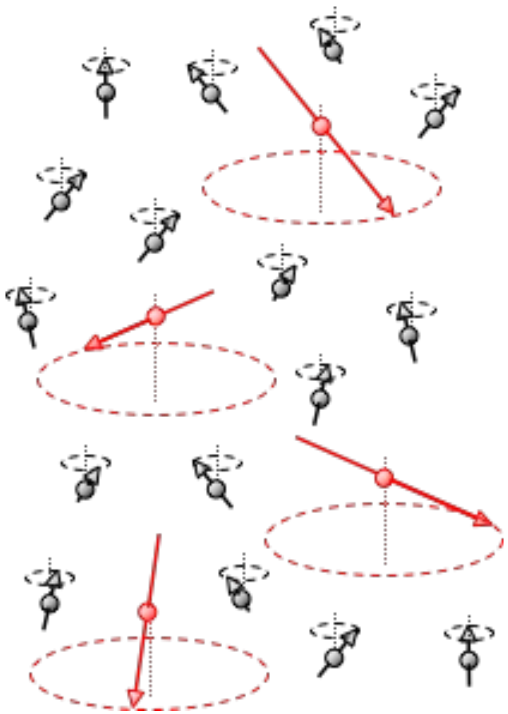
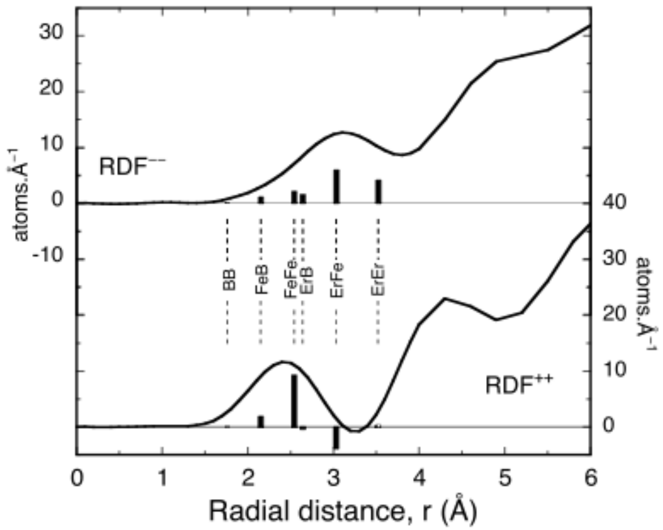


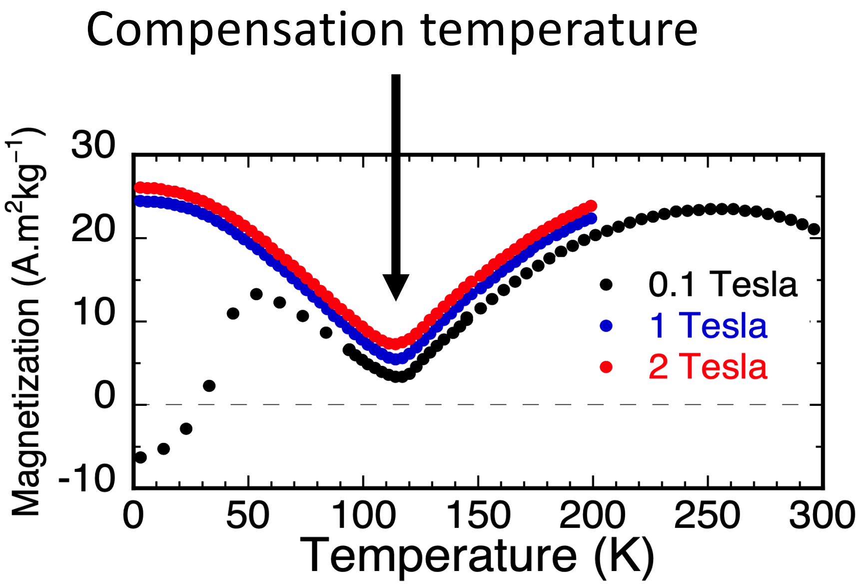


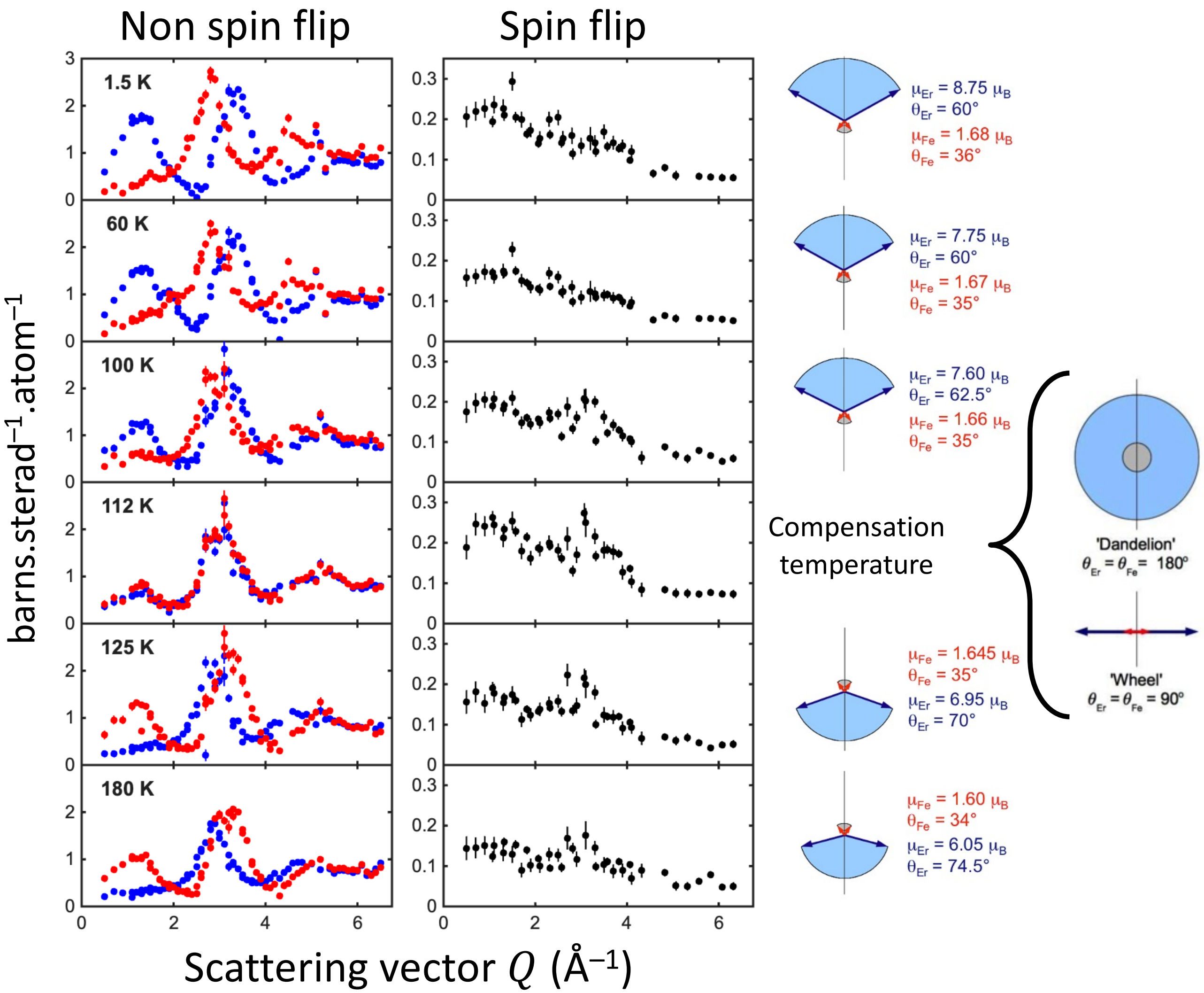
$$RDF(r) = 4\pi r^2 \rho g(r)$$



A. R. Wildes and N. Cowlam, JPCM **23** (2011) 496004
N. Cowlam and A. R. Wildes, JPCM **23** (2011) 496005

Diffuse scattering in metallic glasses, $Fe_{64}Er_{19}B_{17}$





A. R. Wildes and N. Cowlam, JPCM **23** (2011) 496004

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A. R. Wildes *et al.*, J. Kor. Phys. Soc. **63** (2013) 517

Conclusions

Magnetic glasses have a clear need for magnetic PDF methods

- Neutron polarization analysis is a necessity (IMHO)
  - Compositional disorder
  - Positional disorder
  - Collinear and non-collinear moment components
- Numerous datasets must be simultaneously analysed
- Optimised instrumentation would:
  - Measure to large Q
  - Support appropriate sample environments (magnetic fields)
  - Be able to measure all four spin-dependent cross-sections