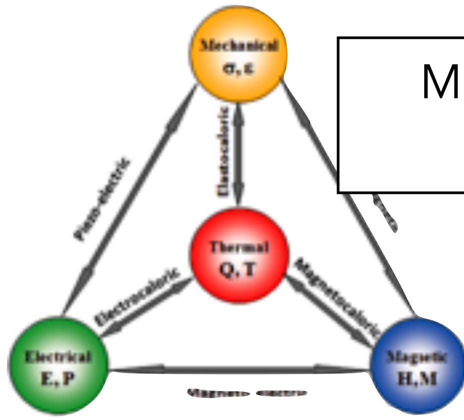
# MAGiC: polarized single crystal diffractometer

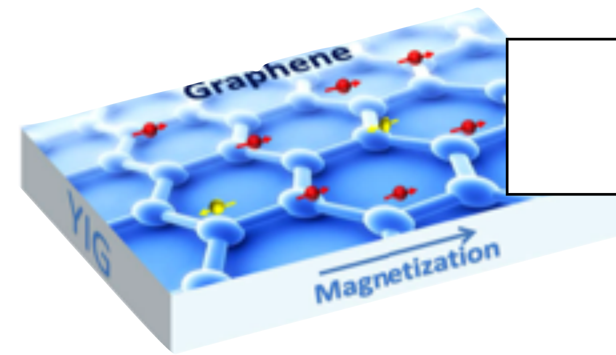
Data management

# The science behind MAGiC

Multi-functional materials

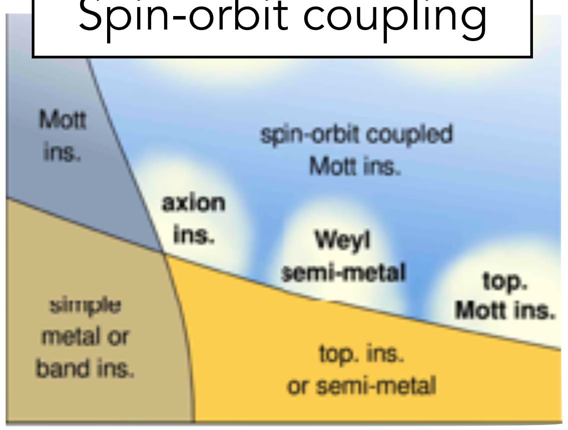



Magnetism at interfaces
Thin films



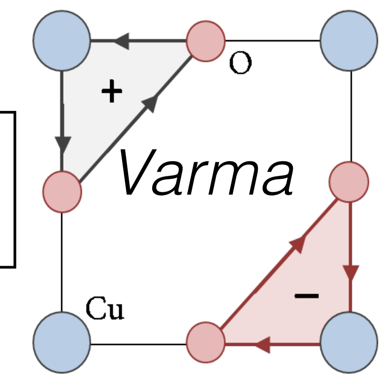

*Phys. Rev. Lett.* **114**, 016603

Spin-orbit coupling

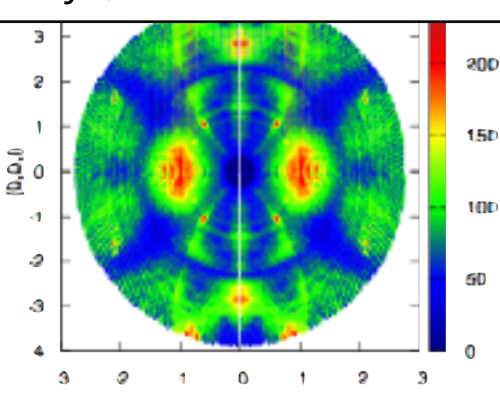



*arXiv*:1305.2193v2

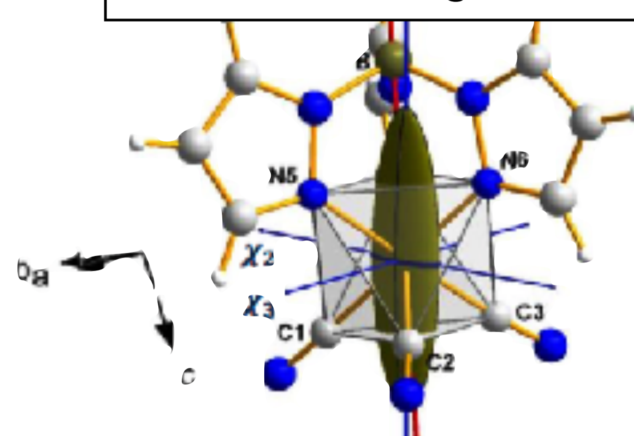
Superconductivity and magnetism




Fundamental magnetism and theory (Coulomb, Kitaev, …)

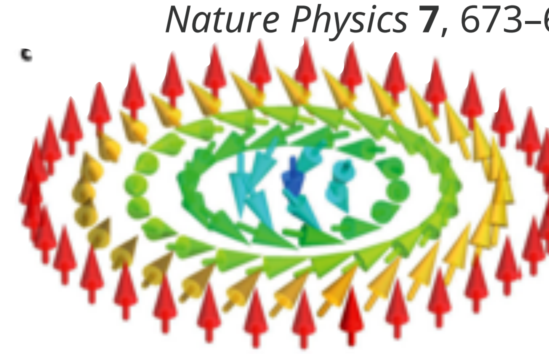


Molecular magnetism



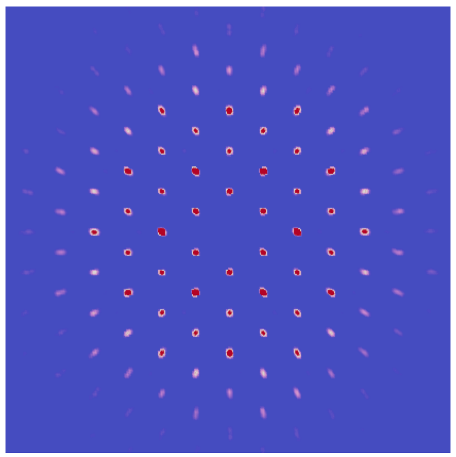

Long range magnetic states (skyrmions, multiferroics, …)

*Nature Physics* **7**, 673–674 (2011)

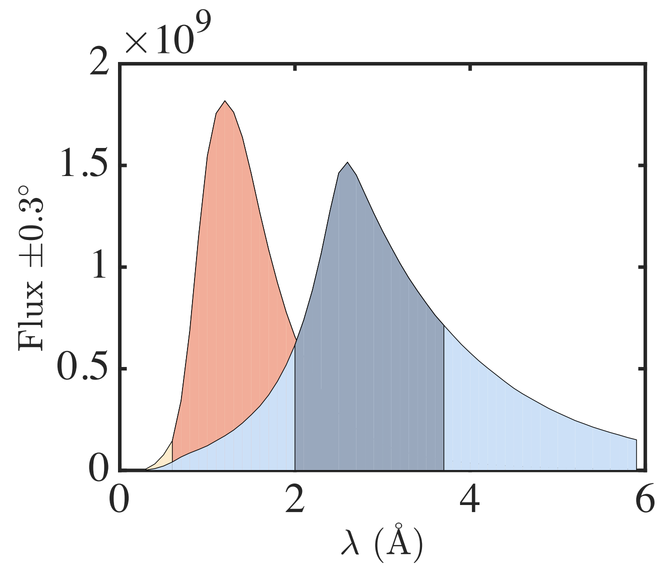


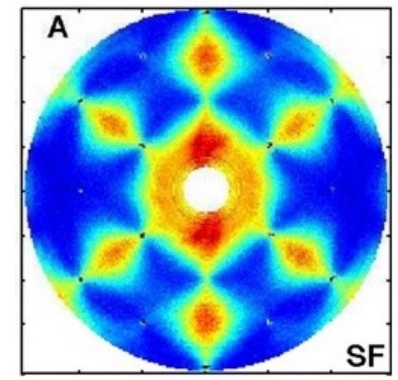
# Requirements

**Spectrum:** thermal & cold



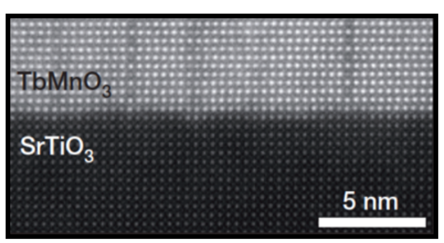
Crystal & magnetic structures
Spin-lattice coupling

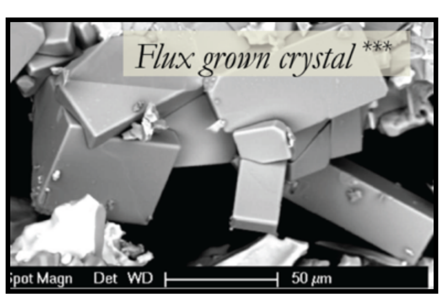


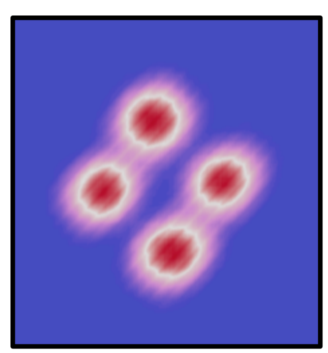

Fundamental magnetism
Diffuse scattering

## Focusing



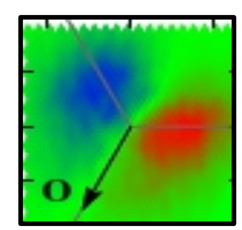




## Flexible Q-resolution

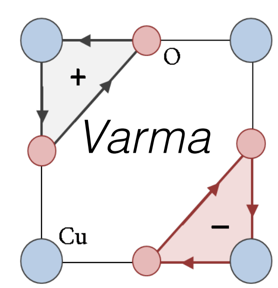


$\Delta Q \sim 10^{-2} ... 10^{-3}\text{Å}^{-1}$

## Polarised




Vector properties
Chirality

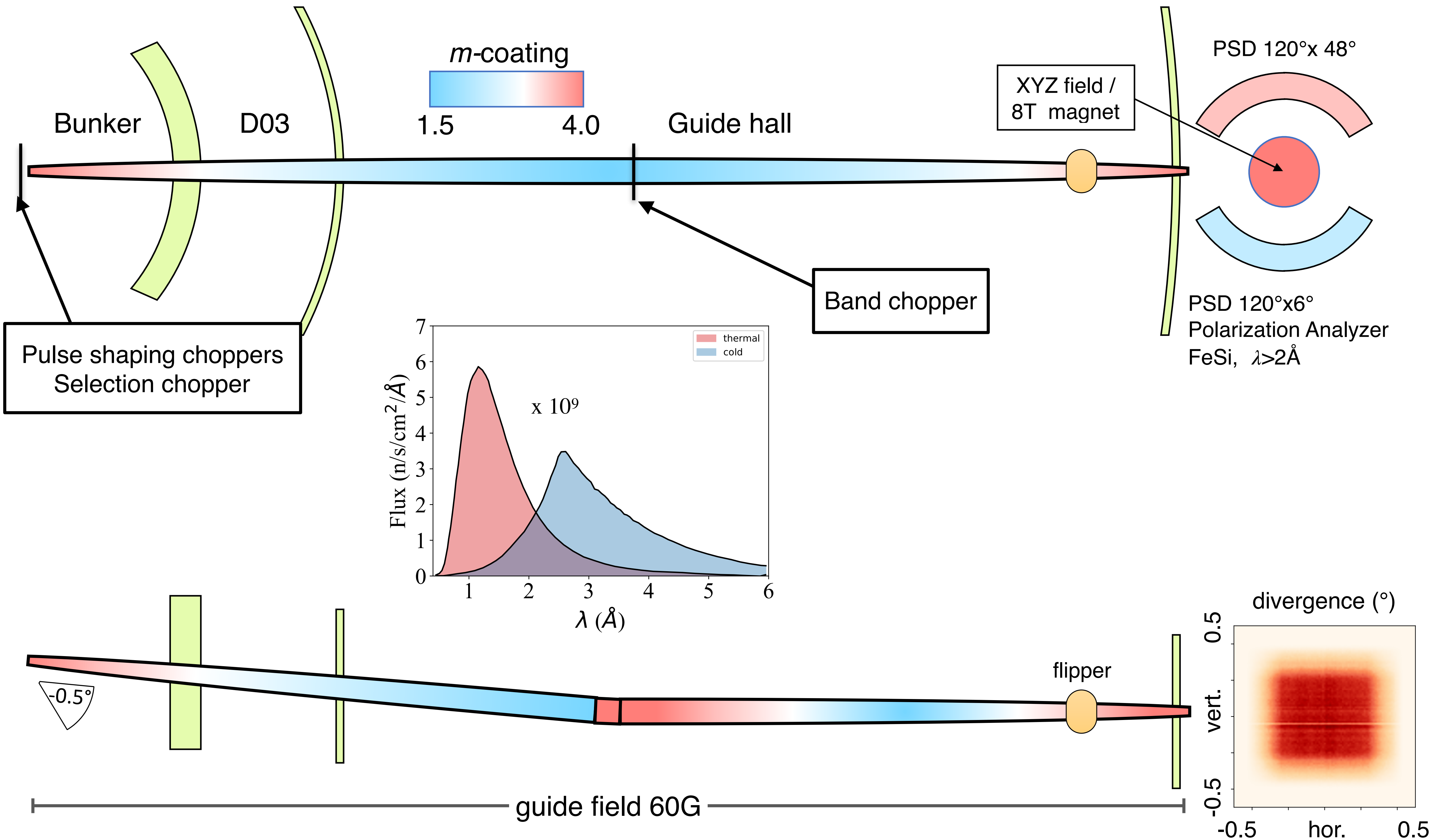



Separation of weak
Magnetic from nuclear
contributions

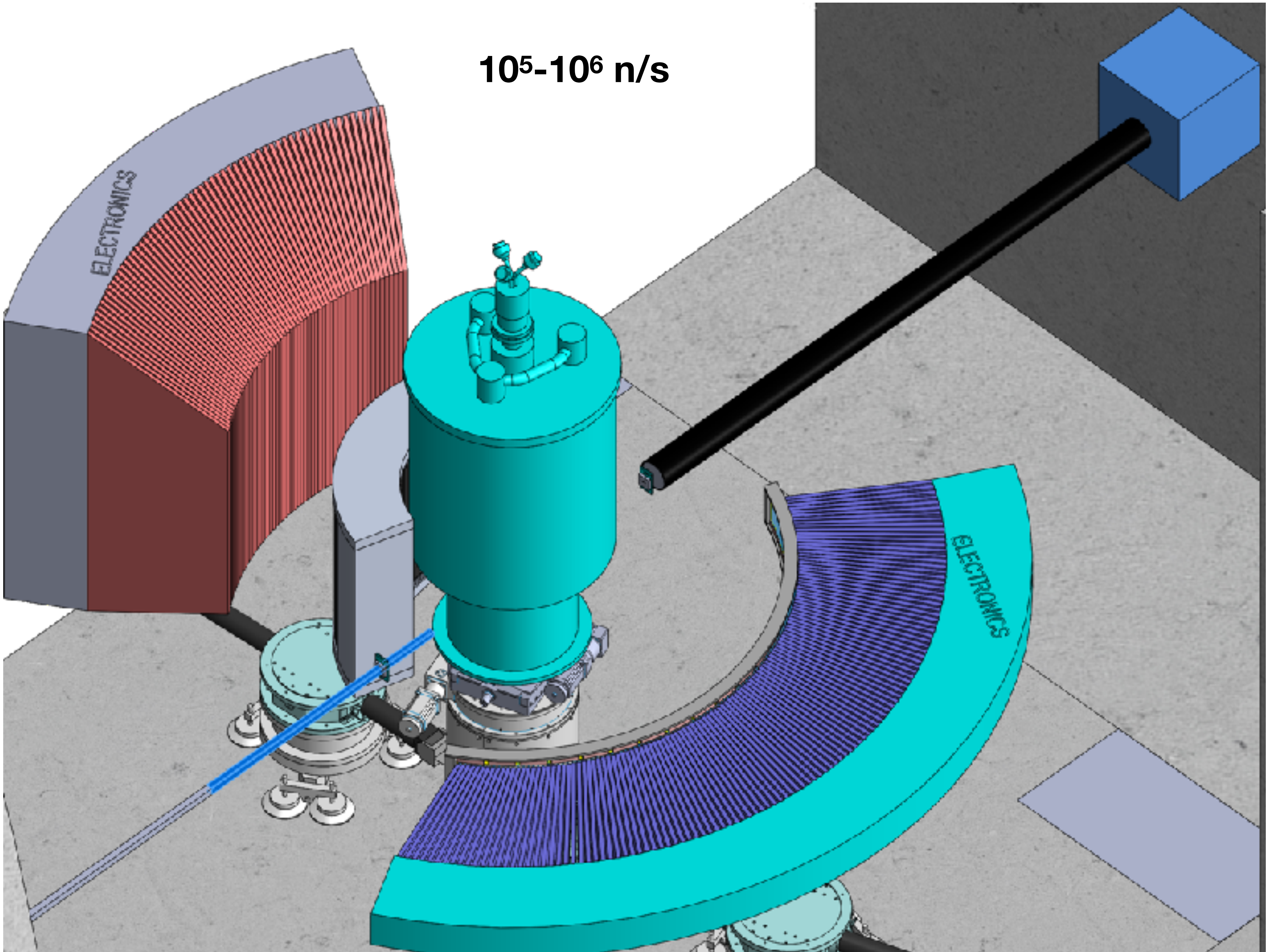
# The instrument

| Quick Facts | |
|---|---|
| Instrument length | 160 m |
| Commissioning/Operation | 2022/2024 |
| Moderator | Cold & Thermal |
| Q-Range | 0.1 – 20 Å-1 |
| Spin-Polarization/-Analysis | yes/yes |
| Wavelength Band | 1.7 Å |
| Wavelength Range | 0.6 – 6 Å |
| Momentum Resolution | ΔQ/Q= 2-10 % |
| Detector half-polarized<br>Resolution | 10B 60°x48°<br>h=0.11°, v=0.3° |
| Detector PA<br>Resolution | 10B 120°x6°<br>h=0.11°, v=0.3° |

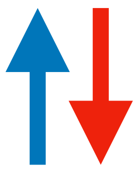
# The instrument

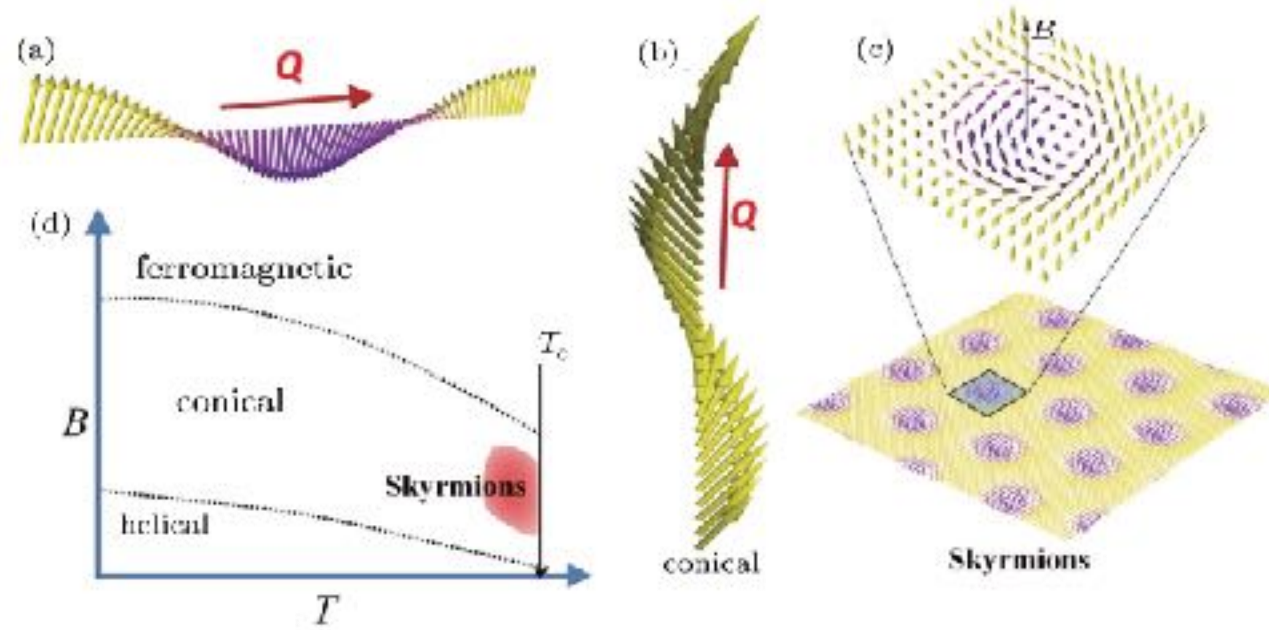


# The detectors



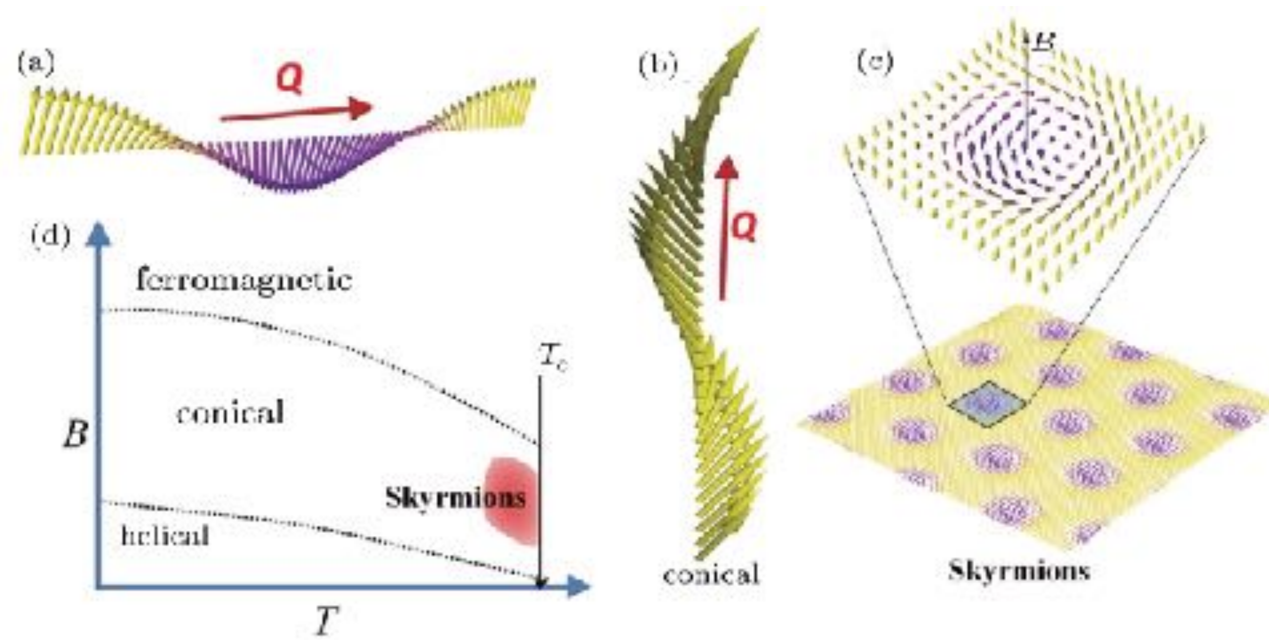
# Unpolarized mode





# Unpolarized mode

$$I(Q) = F_N^2(Q) + F_M^2(Q)$$



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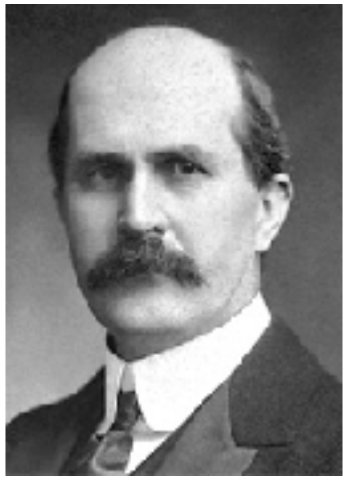
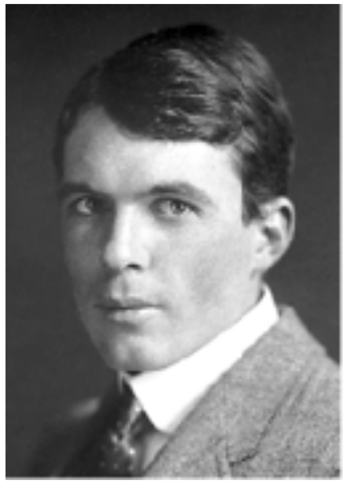
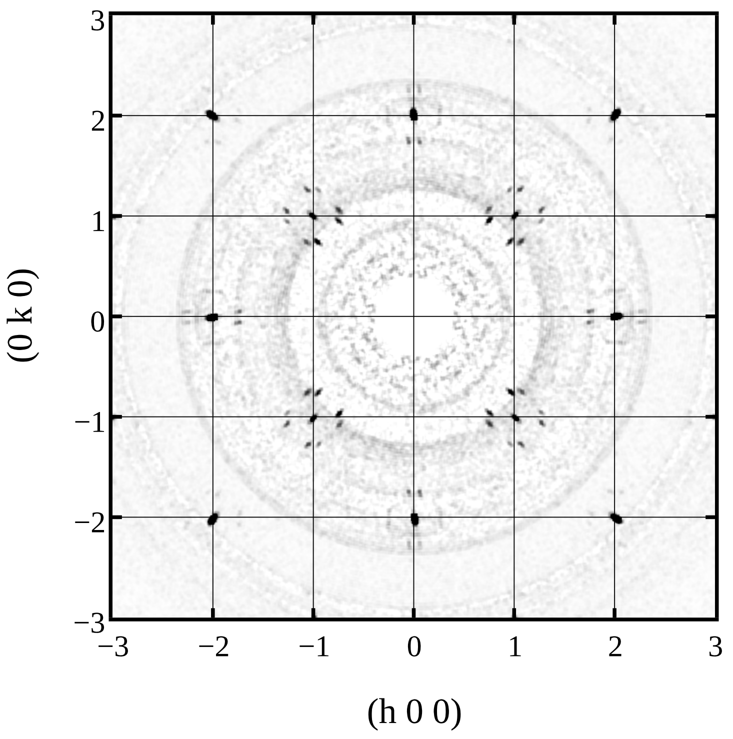
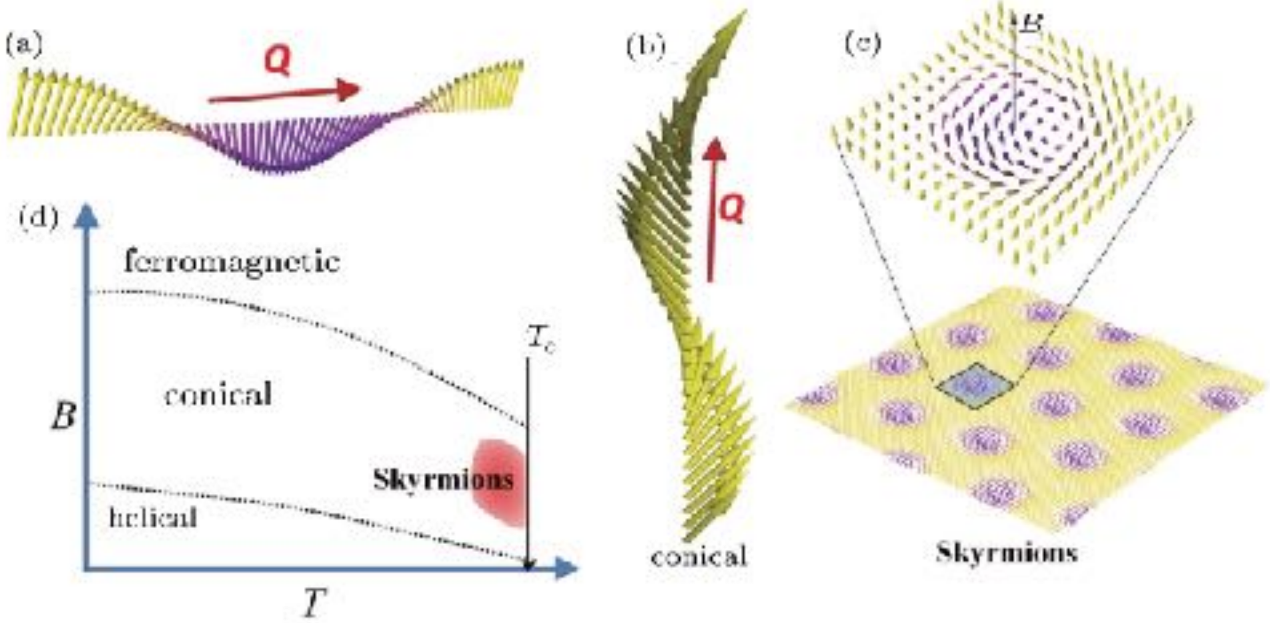




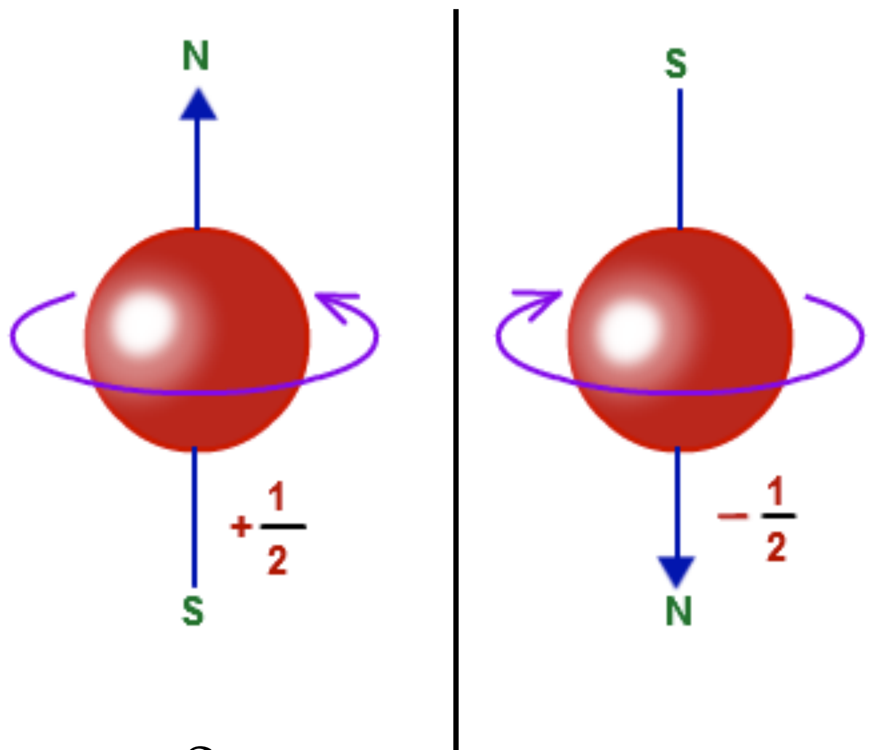
$$\lambda = 2d\sin(\theta)$$



# Half-polarized mode

$$I^{\pm} = (F_N \pm F_M)^2$$

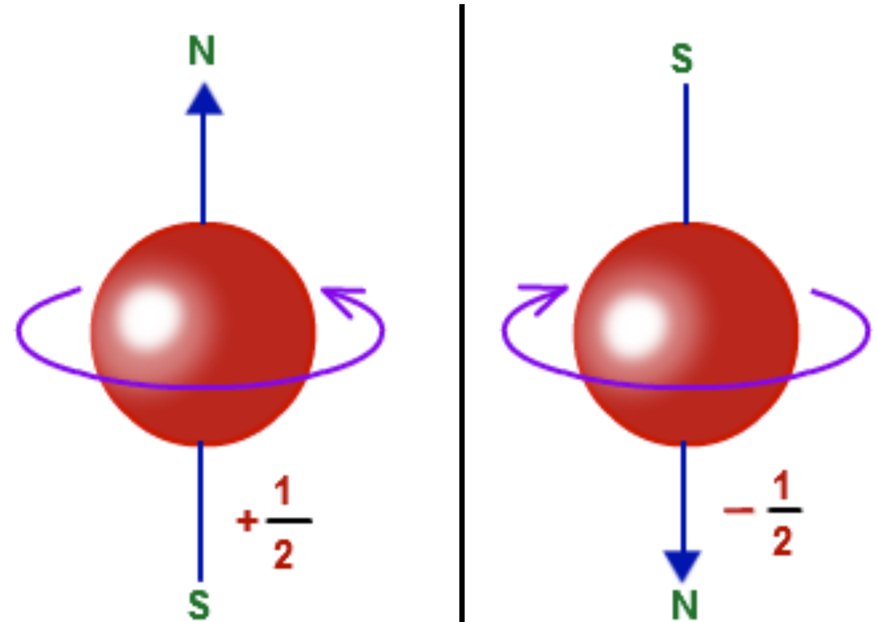



$$I^{+} + I^{-} \;\alpha\; F_N^2 + F_M^2$$

$$I^{+} - I^{-} \;\alpha\; 4F_N F_M$$

# Half-polarized mode

$$I^{\pm} = (F_N \pm F_M)^2$$




$$I^+ + I^- \ \alpha \ F_N^2 + F_M^2$$

$$I^+ - I^- \ \alpha \ 4F_N F_M$$

$$F_N = 1 \qquad F_M = 0.1$$

$$I^+ = 1.21 \qquad I^- = 0.81$$

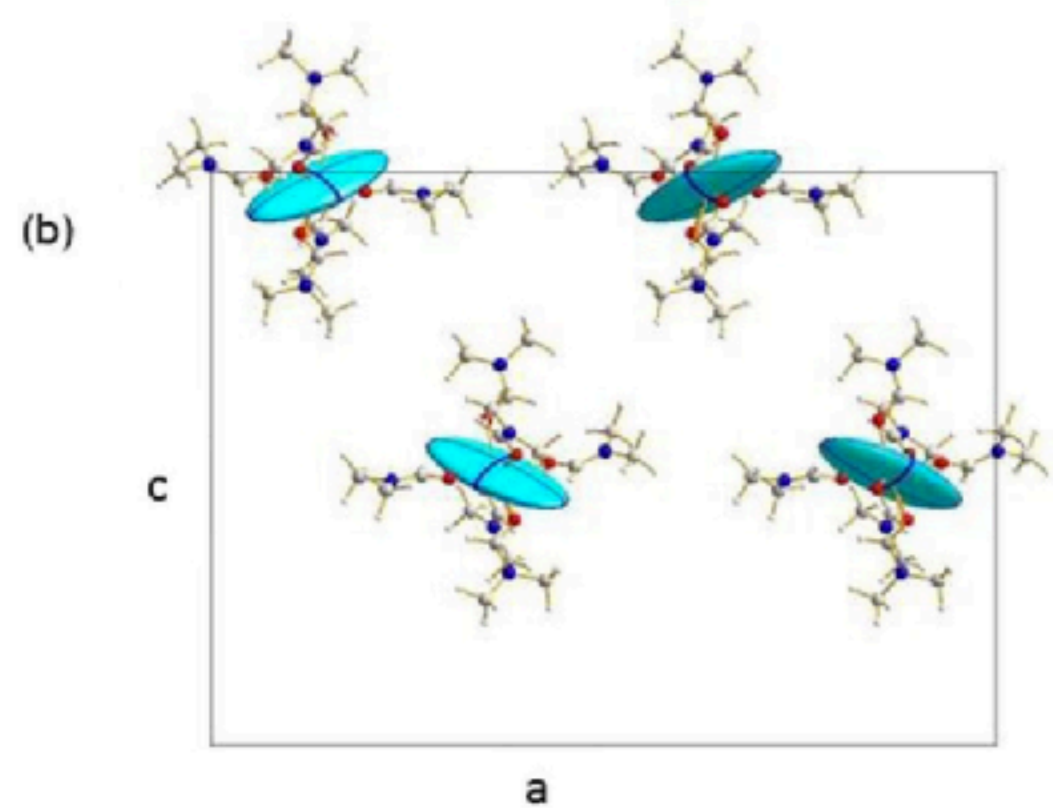
$$FR = 1.49$$

High sensitivity to weak magnetic contributions

# Half-polarized mode

**Local anisotropy = local SQUID**

**Spin density**




$Cu_2(NC_9H_{13})_4(N_3)_2(ClO_4)_2$

**Magnetism Studies** |*Hot Paper*|

**Polarized Neutron Diffraction as a Tool for Mapping Molecular Magnetic Anisotropy: Local Susceptibility Tensors in Co$^{II}$ Complexes**

Karl Ridier,[a, f] Béatrice Gillon,*[a] Arsen Gukasov,[a] Grégory Chaboussant,[a] Alain Cousson,[a] Dominique Luneau,*[b] Ana Borta,[b, g] Jean-François Jacquot,[c] Ruben Checa,[b] Yukako Chiba,[d] Hiroshi Sakiyama,[d] and Masahiro Mikuriya[e]

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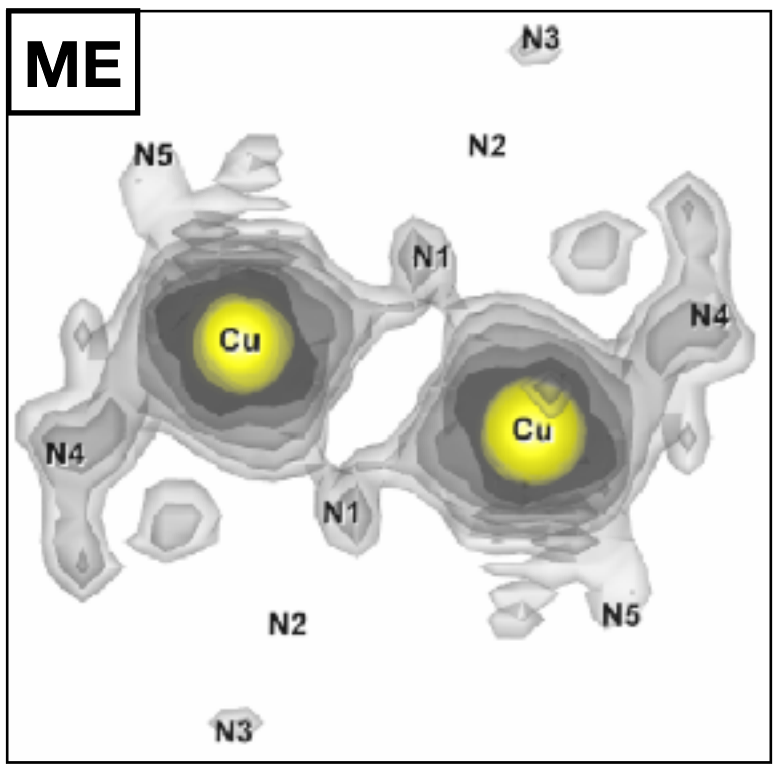


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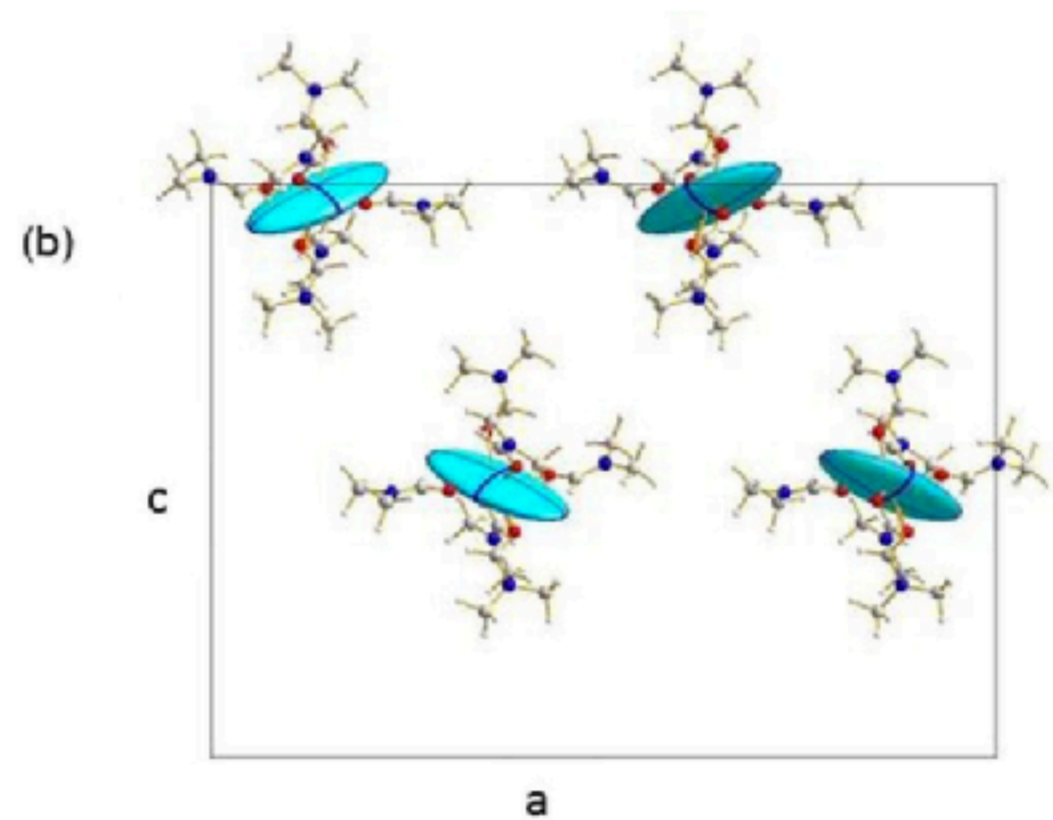


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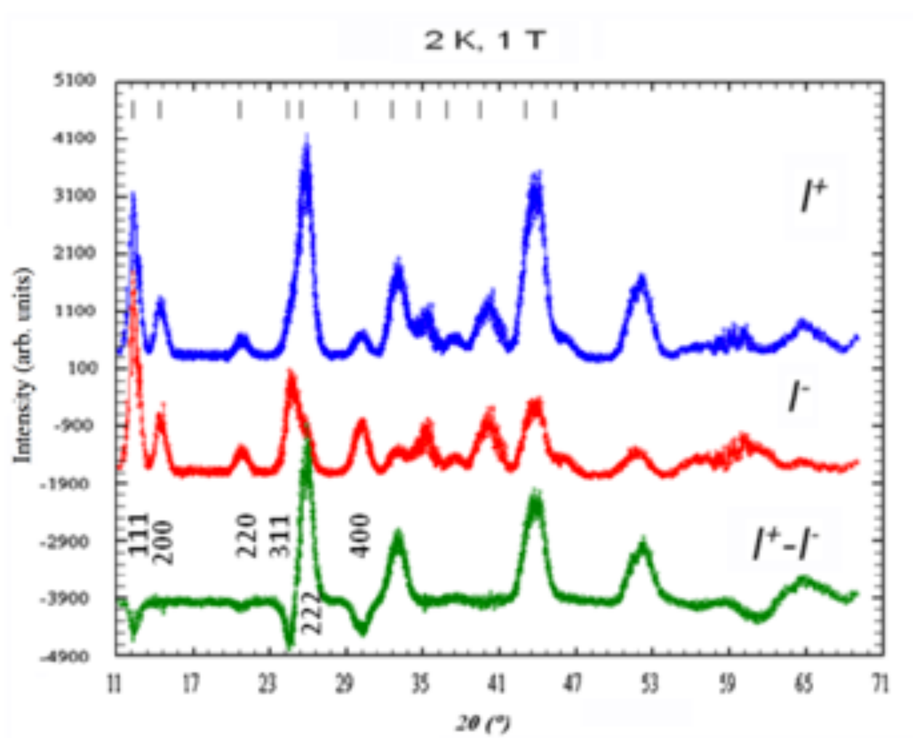
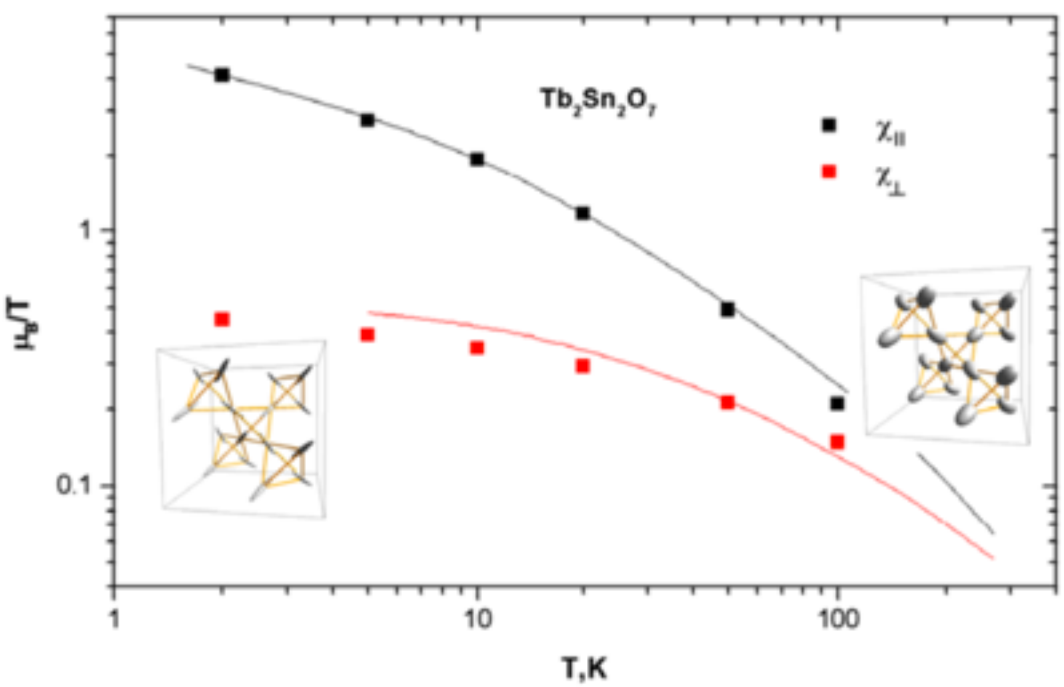
# Half-polarized mode

Spin density **Local anisotropy = local SQUID**

Works on powder sample too




(a)




Molecular

$Co^{II}$

Complexes

Karl Ridier,[a, f] Béatrice Gillon,*[a] Arsen Gukasov,[a] Grégory Chaboussant,[a] Alain Cousson,[a]
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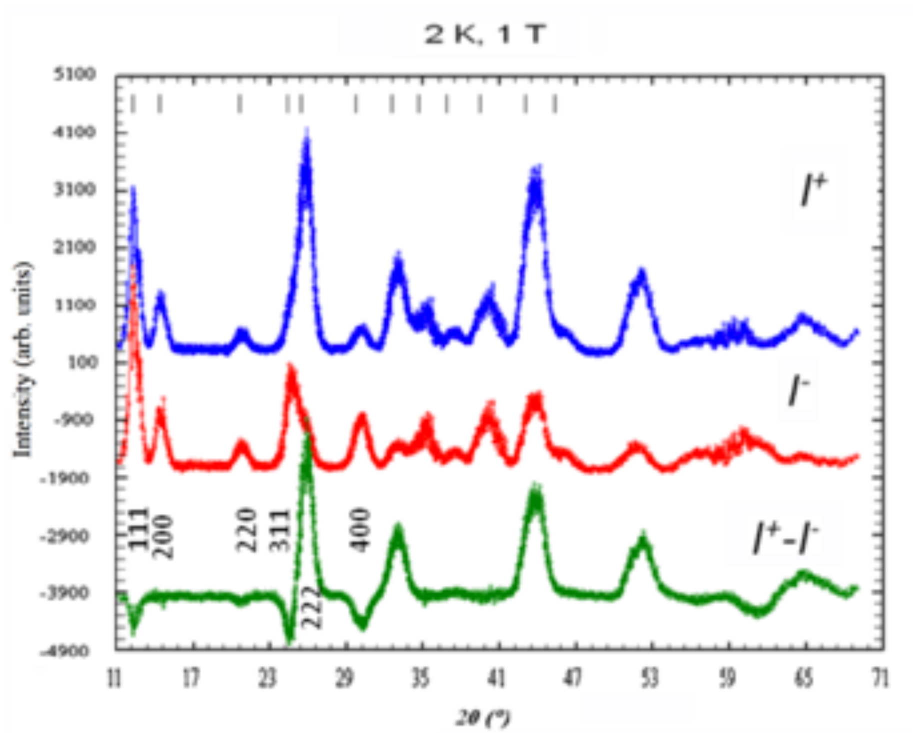
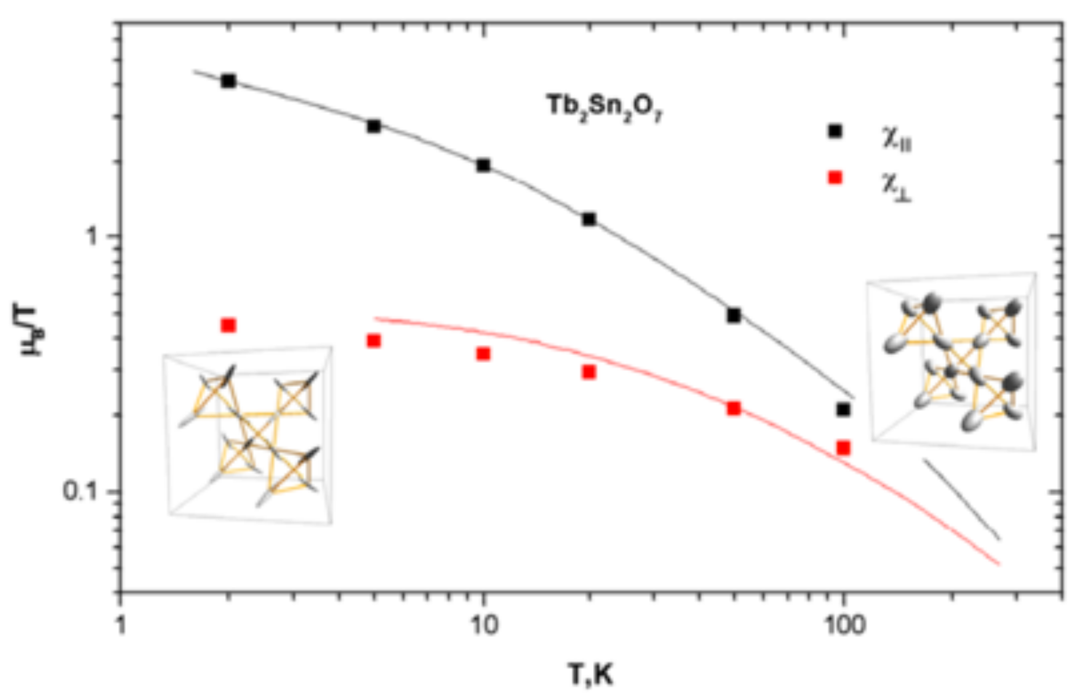


(a)




Molecular
Magnetic Anisotropy: Local Susceptibility Tensors in $Co^{II}$
Complexes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# XYZ polarization

$$\begin{pmatrix} P_{xx} & P_{xy} & P_{xz} \\ P_{yx} & P_{yy} & P_{yz} \\ P_{zx} & P_{zy} & P_{zz} \end{pmatrix}$$

$$\begin{pmatrix} P_{yy} & P_{\bar{y}y} \\ P_{y\bar{y}} & P_{\bar{y}\bar{y}} \end{pmatrix}$$

**36 combinations**

$$\begin{pmatrix} P_{xx} & P_{xy} & P_{xz} \\ P_{yx} & P_{yy} & P_{yz} \\ P_{zx} & P_{zy} & P_{zz} \end{pmatrix}$$

**Longitudinal polarization**
**12 possible terms**

$Q_{//}$, $Q_{\perp}$ and $Q_z$ to extract

Done on a triple axis or single counter instrument

# XYZ polarization analysis

$$
\begin{aligned}
\sigma_x^{++} &= \sigma_x^{nsf} \\
\sigma_x^{+-} &= \sigma_x^{sf} - P_0 M_{ch}
\end{aligned}
$$

$$
\begin{aligned}
\sigma_x^{--} &= \sigma_x^{nsf} \\
\sigma_x^{-+} &= \sigma_x^{sf} + P_0 M_{ch}
\end{aligned}
$$

**Longitudinal polarization**
**12 possible terms**

$$
\begin{aligned}
\sigma_z^{++} &= \sigma_z^{nsf} + P_0 \cdot R_z \\
\sigma_z^{--} &= \sigma_z^{nsf} - P_0 \cdot R_z \\
\sigma_z^{+-} &= \sigma_z^{sf} \\
\sigma_z^{-+} &= \sigma_z^{sf}
\end{aligned}
$$

$$
\begin{aligned}
\sigma_y^{++} &= \sigma_y^{nsf} + P_0 \cdot R_y \\
\sigma_y^{--} &= \sigma_y^{nsf} - P_0 \cdot R_y \\
\sigma_y^{+-} &= \sigma_y^{sf} \\
\sigma_y^{-+} &= \sigma_y^{sf}
\end{aligned}
$$

# XYZ polarization analysis

$$\sigma_N = \sigma_x^{++} = \sigma_x^{--}$$

$$\sigma_M^y = \frac{\sigma_y^{++} + \sigma_y^{--}}{2} - \frac{\sigma_x^{++} + \sigma_x^{--}}{2} = \frac{\sigma_x^{+-} + \sigma_x^{-+}}{2} - \frac{\sigma_y^{+-} + \sigma_y^{-+}}{2}$$

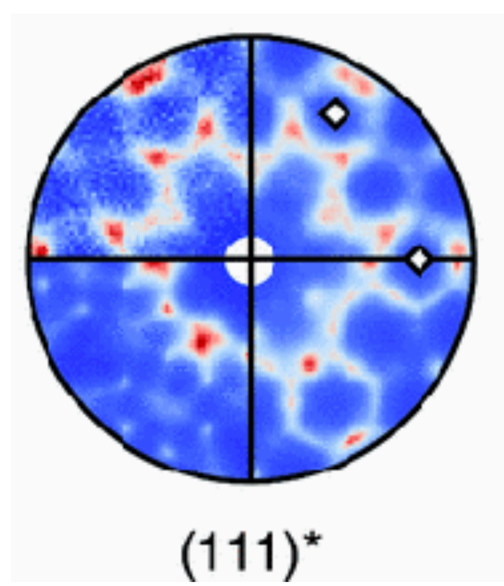
$$\sigma_M^z = \frac{\sigma_z^{++} + \sigma_z^{--}}{2} - \frac{\sigma_x^{++} + \sigma_x^{--}}{2} = \frac{\sigma_x^{+-} + \sigma_x^{-+}}{2} - \frac{\sigma_z^{+-} + \sigma_z^{-+}}{2}$$

$$M_{ch} = \frac{\sigma_x^{-+} - \sigma_x^{+-}}{2P_0}$$

$$R_y = \frac{\sigma_y^{++} - \sigma_y^{--}}{2P_0}$$

$$R_z = \frac{\sigma_z^{++} - \sigma_z^{--}}{2P_0}$$

**Magnetic nuclear separation**
**Chirality**
**Magnetic/nuclear interference**



**magnetic diffuse scattering**

**Co doped β-Mn**
**50 mK**

J.A.M. Paddison *et al*

# What is needed

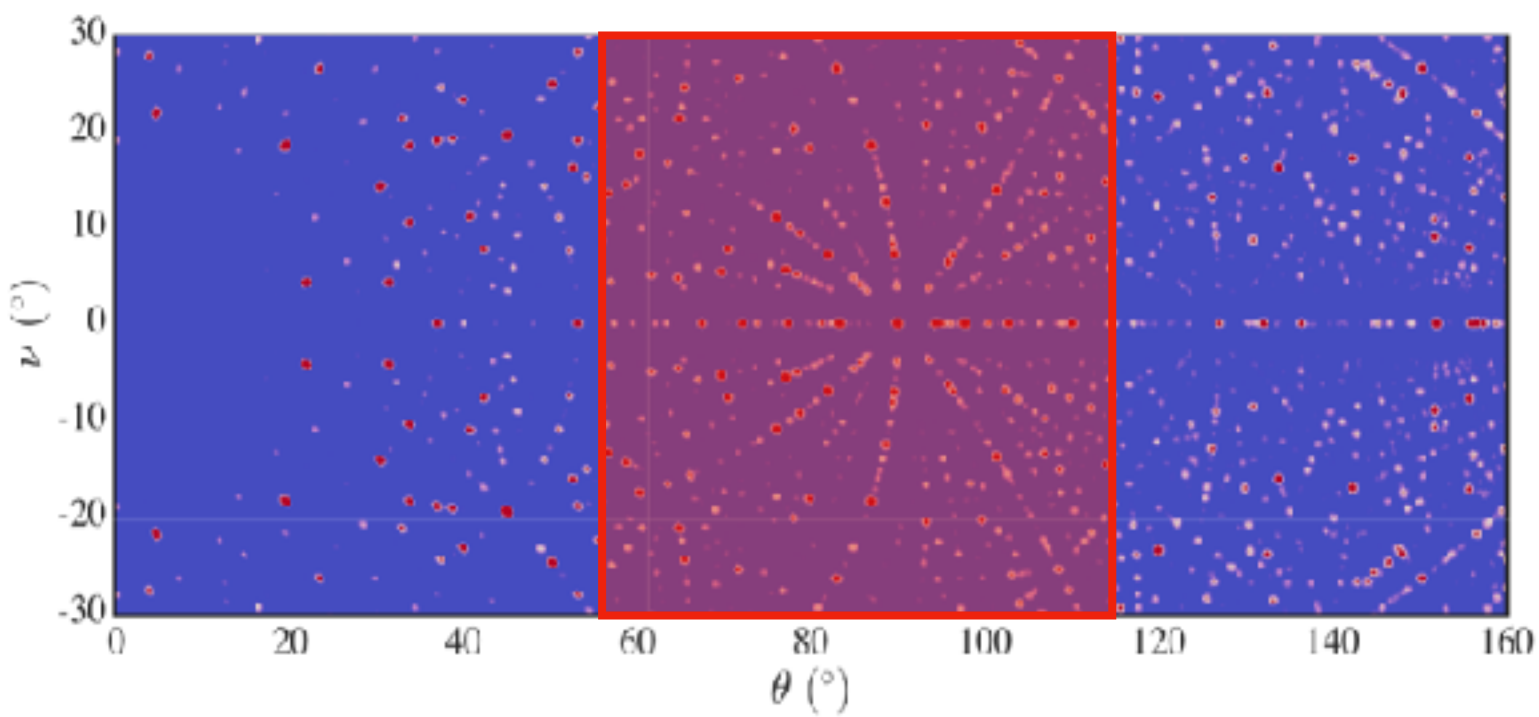
- Data reduction
  - Events mode
  - Histograms
  - Peak detection
  - UB matrix definition
  - Peak integration in Q-space
  - Export to dedicated software in ascii mode

**Keep polarization information**
**Keep sample orientation information**

**Allow for incommensurate magnetic peaks integration based on a given/detected k vector**

# What is needed

- Data visualization
  - Detector data (in instrument space)
  - Q-space 3D volume in Q and hkl space
  - oriented 2D slices in Q and hkl space
  - 1D line (peak profile, resolution)



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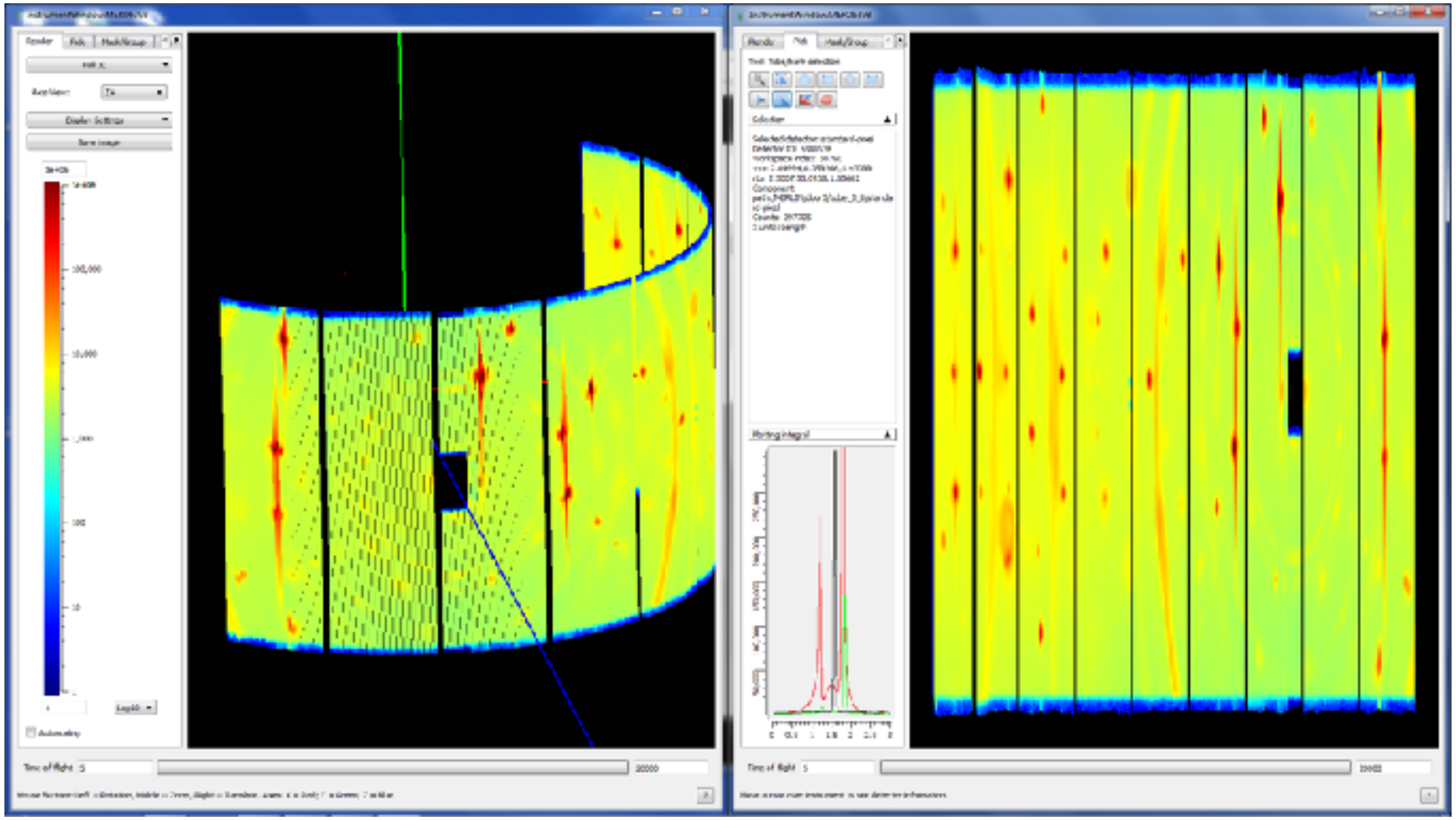

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- Data visualization
  - Detector data (in instrument space)
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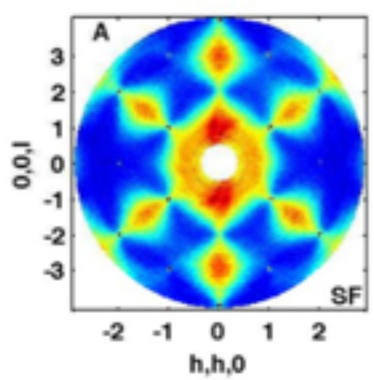
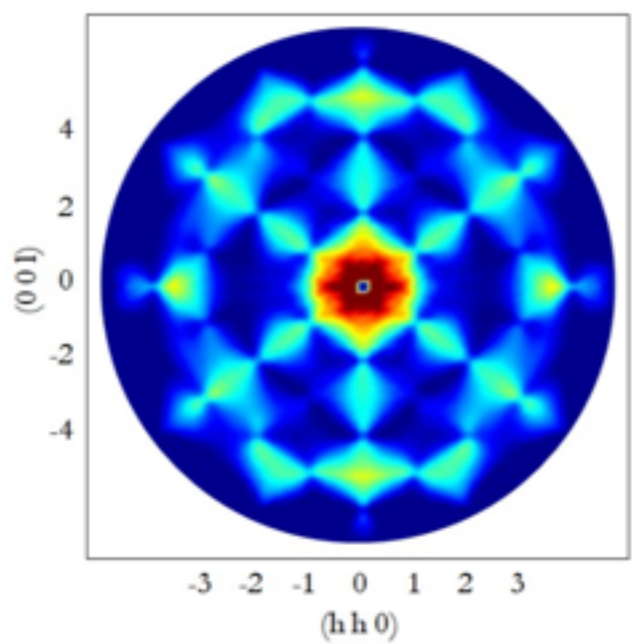
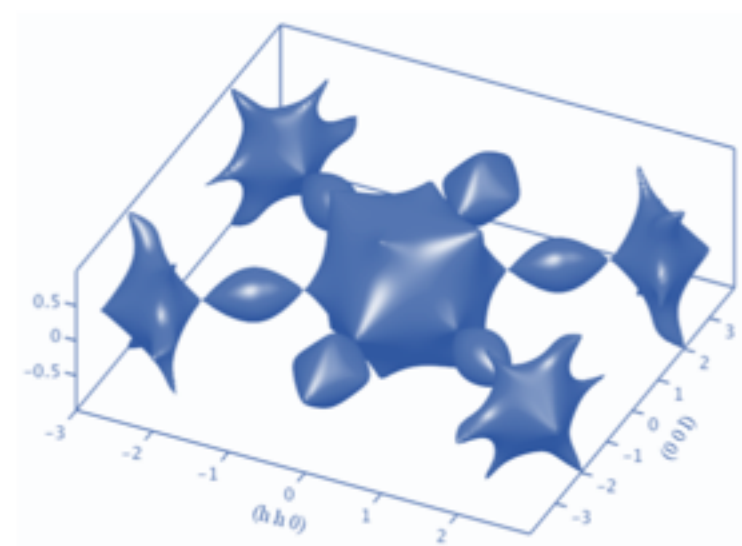
  - oriented 2D slices in Q and hkl space
  - 1D line (peak profile, resolution)
  - Nuclear-magnetic separation








**Polarization in XYZ instrument space**
**Projection on sample Q-space (UB matrix)**
**Reconstruction of Q//, Qperp and Qz information**

# When do we need it

- Instrument control: Q2/2021
  - Cold commissionning

- Data visualization: Q2/2022
  - First neutrons on the instrument in 07/2022

- Data reduction: Q3/2022
  - Beam and detectors commissionned in 12/2022
  - First experiments in unpolarized mode