Diffraction instrumentation at ESS

IKON 15

12th September 2018

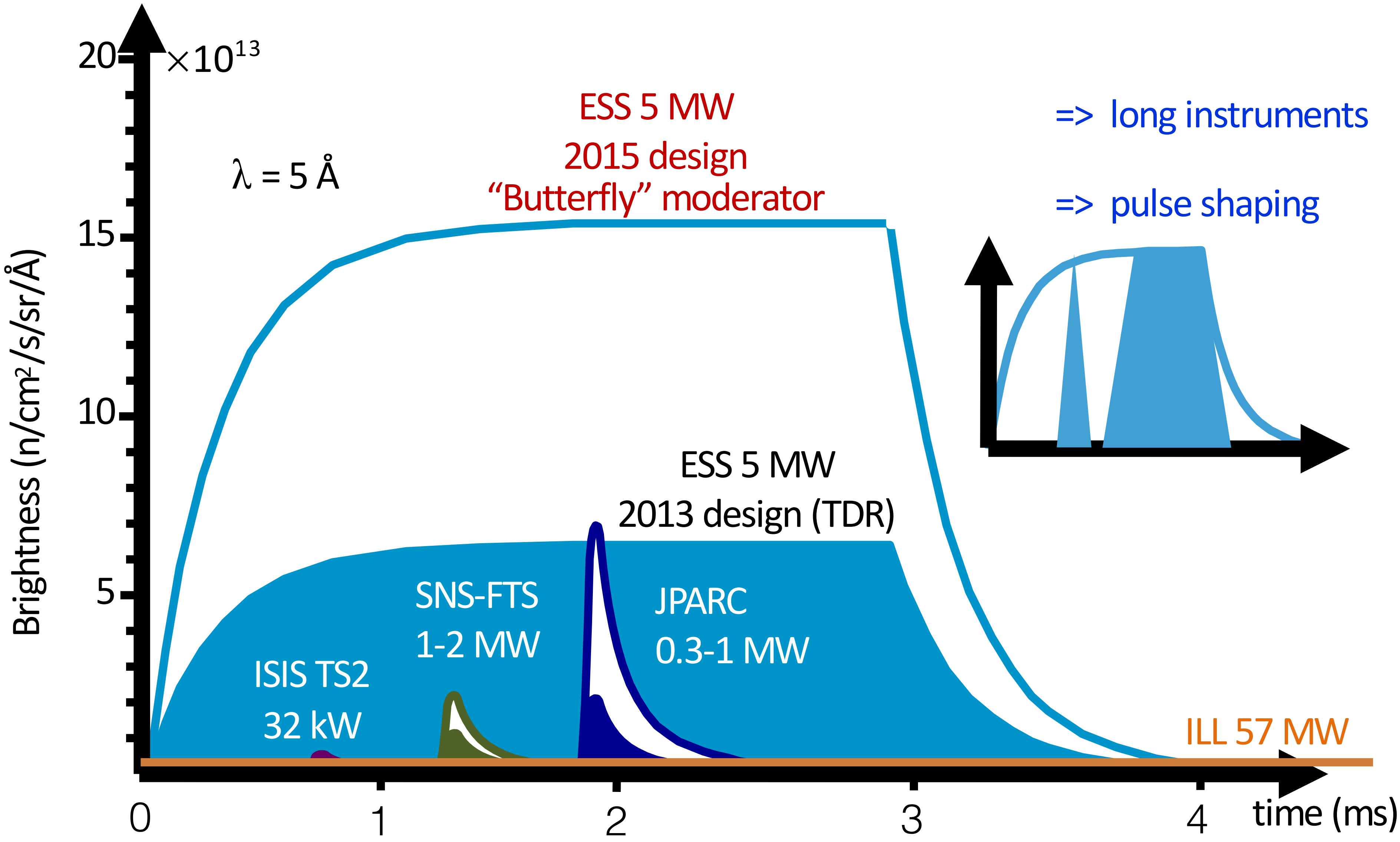
Werner Schweika, Neutron Instruments Division, European Spallation Source ERIC

Impressions from the construction site
User operation will start end of 2023

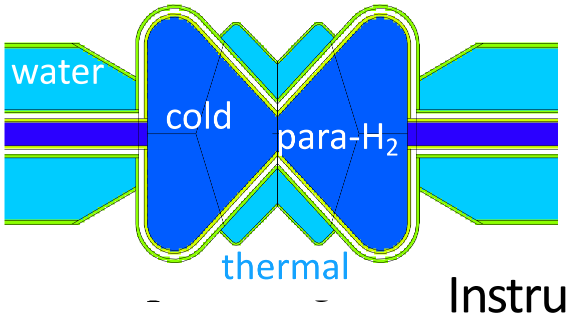
EUROPEAN SPALLATION SOURCE

ESS: long-pulse 14Hz

superior flux & brightness

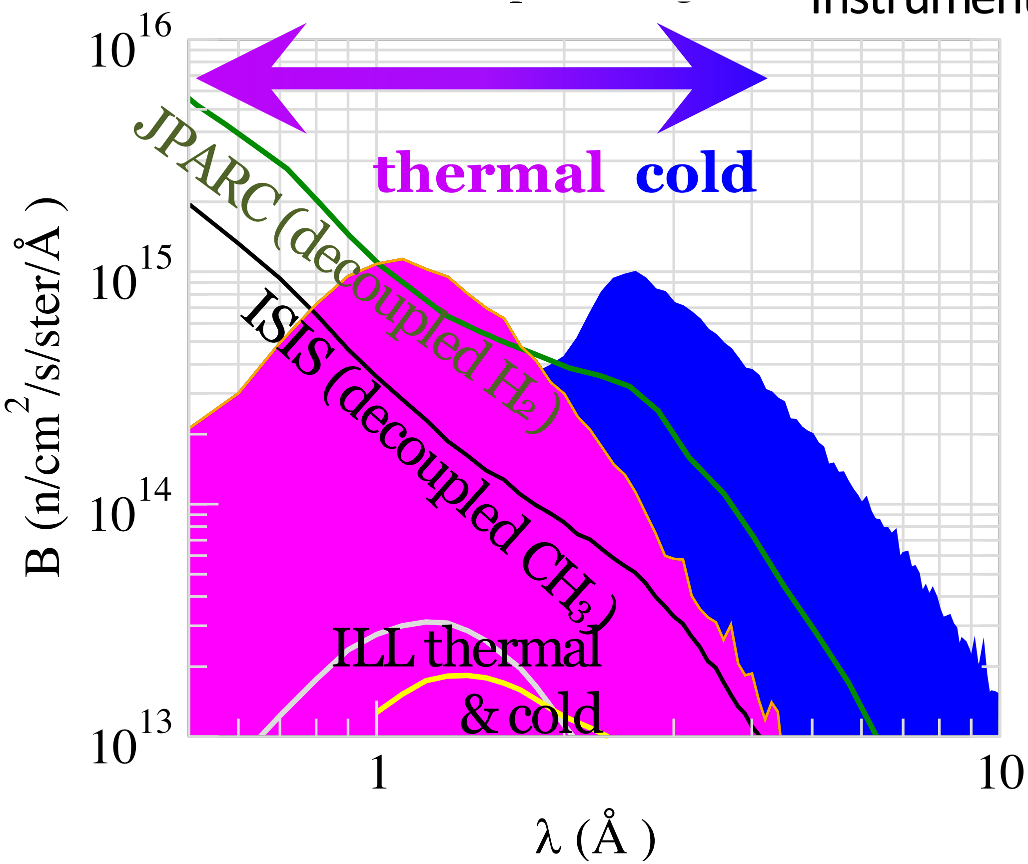


ESS “Butterfly” Moderator



height reduced
to 3 cm

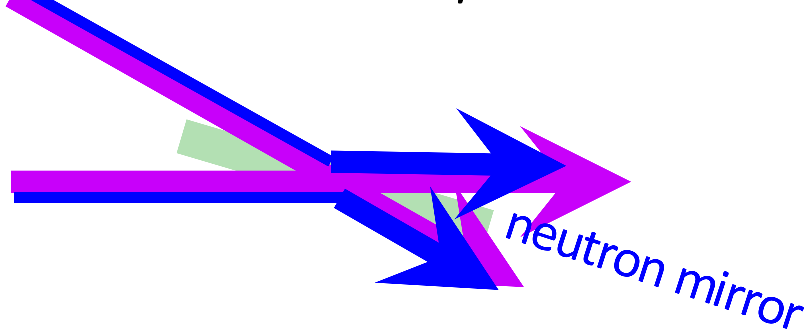
peak
brightness



Instruments can choose thermal or cold moderator

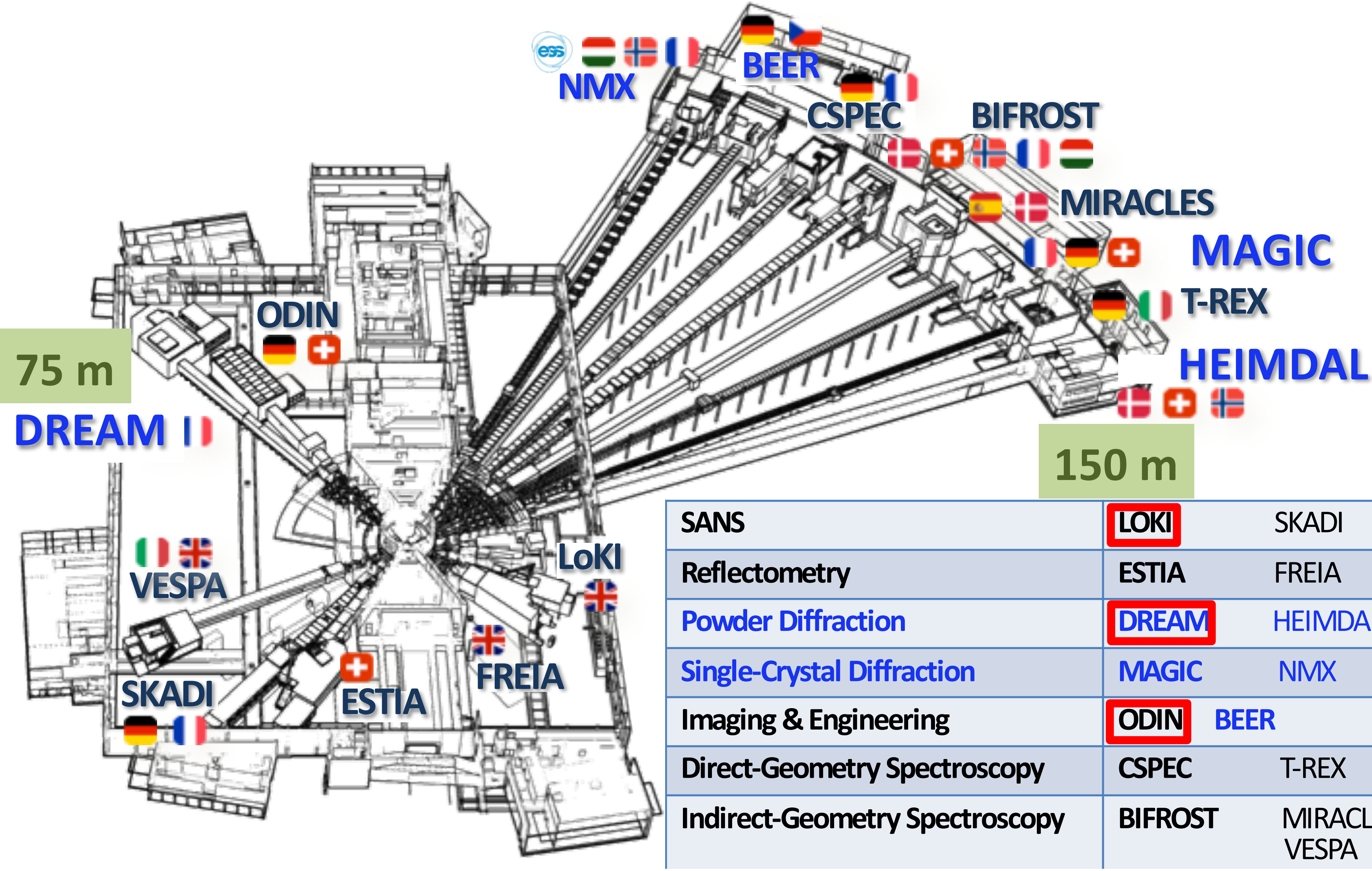
viewing simultaneously
the peak flux of both

the trick is a “bi-spectral switch”



ESS instruments / diffractometers
are very flexible

Instrument Suite

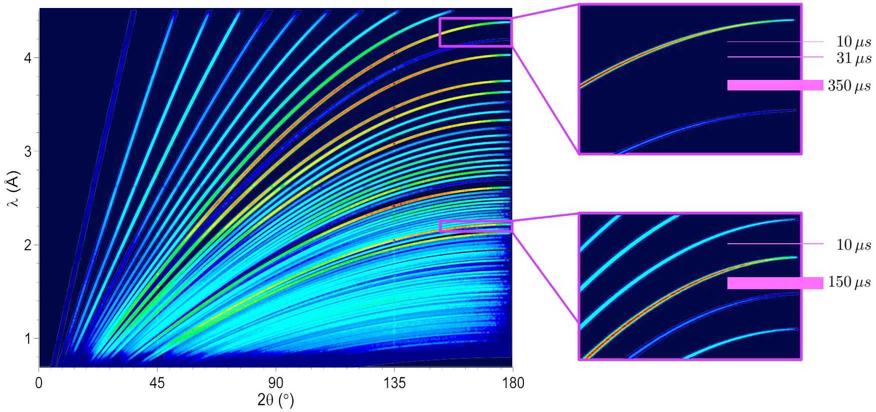


SANS	LOKI	SKADI
Reflectometry	ESTIA	FREIA
Powder Diffraction	DREAM	HEIMDAL
Single-Crystal Diffraction	MAGIC	NMX
Imaging & Engineering	ODIN	BEER
Direct-Geometry Spectroscopy	CSPEC	T-REX
Indirect-Geometry Spectroscopy	BIFROST	MIRACLES VESPA

powder diffraction

very high intensity compared to existing instruments
very flexible resolution due to pulse shaping

DREAM thermal and cold (+ nm-SANS)

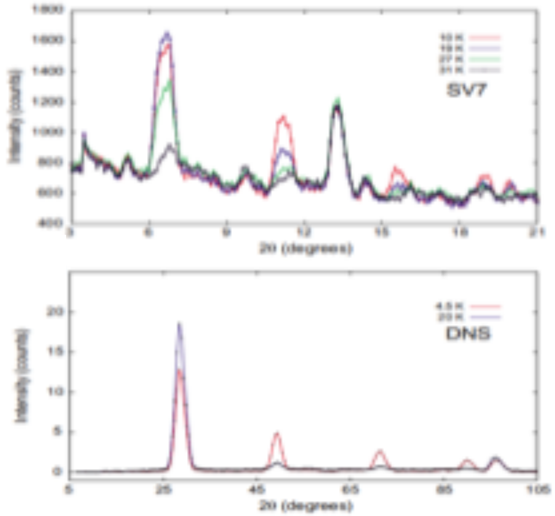


HEIMDAL thermal (+SANS)
multiple length scales

MAGIC polarized

separating
magnetic neutron scattering
… and incoherent H …

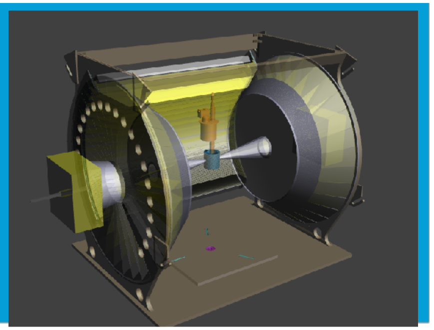
These instruments have new ^{10}B - detectors
* high efficiency and
* count rate capability
- **2D (3D) resolution**
  single crystal diffraction
  texture



Krott et al, PRB 80 (2009), 024117

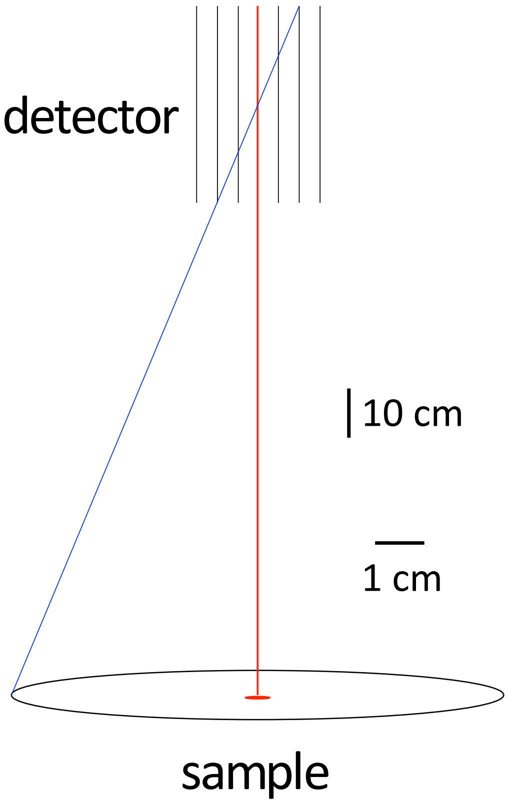
Using 2D and 3D detector information

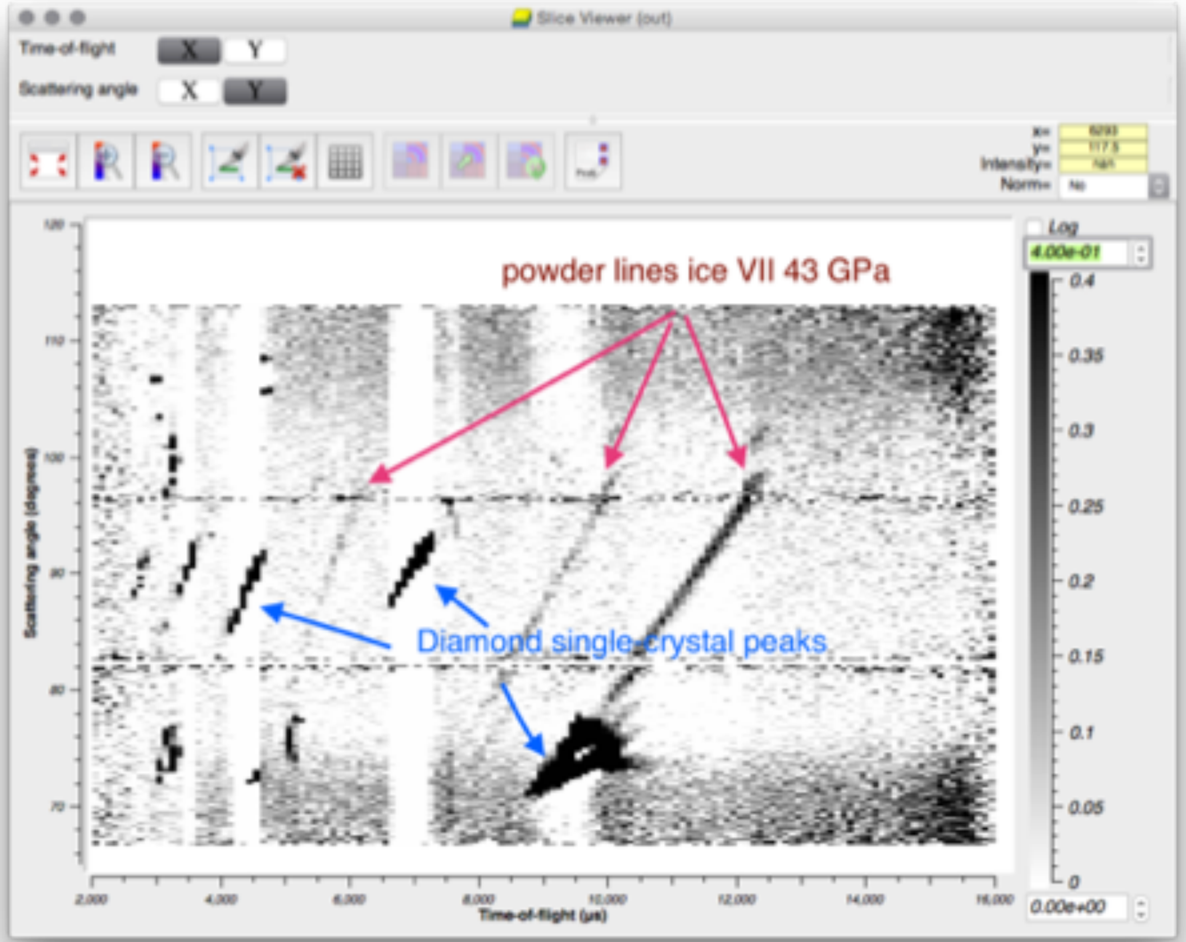
High pressure – very small samples



a great help for identifying **weak signals** in large background

intrinsic collimation
& back-tracing





Courtesy of Malcolm Guthrie

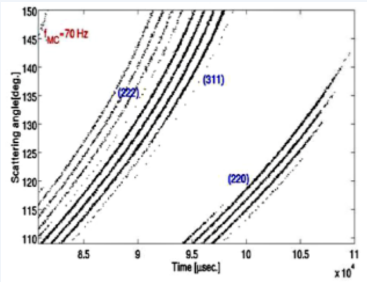
powder & texture

Engineering Diffractometer

BEER thermal and cold

Materials under stress

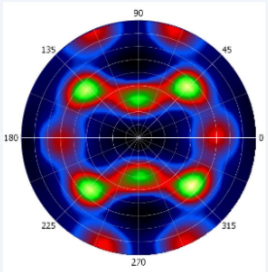
in-situ in operando



modulation technique

TOF

Powder diffraction



Texture measurements

Imaging & SANS **in future**

J. Fenske (HZG, Germany) P. Beran (NPI, Czech Republic)

TOF Laue diffraction => 3d Q space

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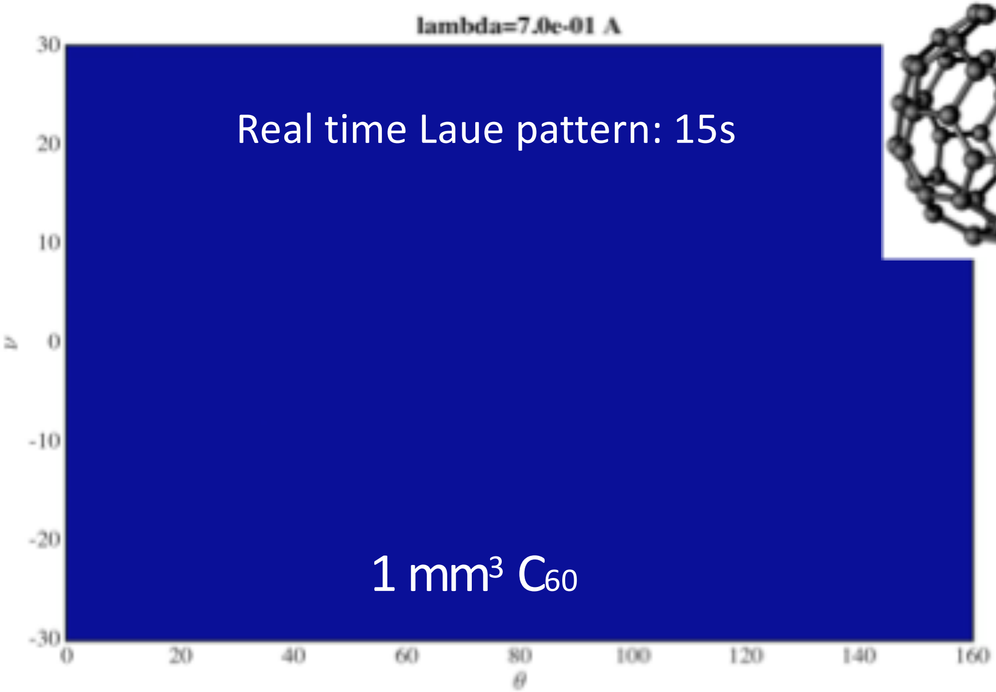
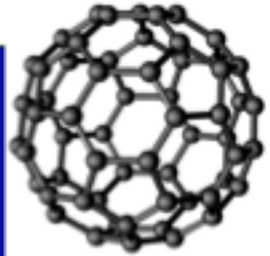
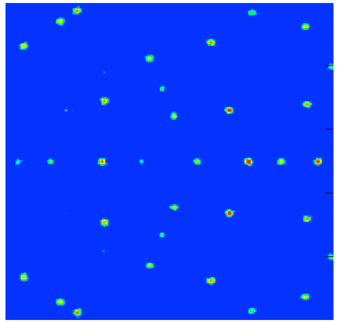
Instruments for single crystal diffraction

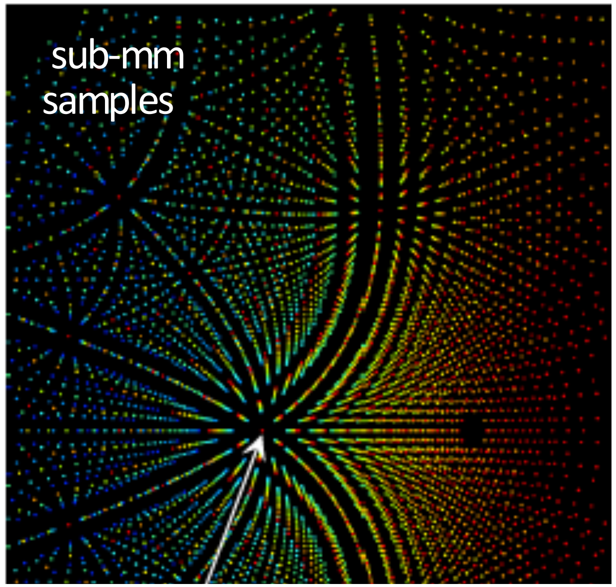
MAGIC dedicated for magnetism - **polarized**

DREAM unpolarized / higher resolution / 3D PDF (HEIMDAL)







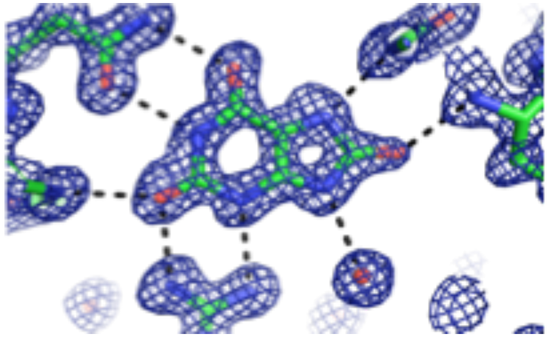


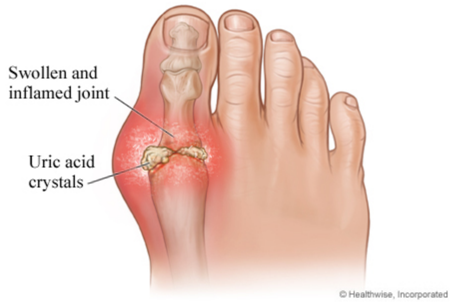
Hydrogen positions

NMX for macromolecular crystallography
Esko Oksanen

Neutron Macromolecular Crystallography

Neutrons see Hydrogen
relates to bonding and function



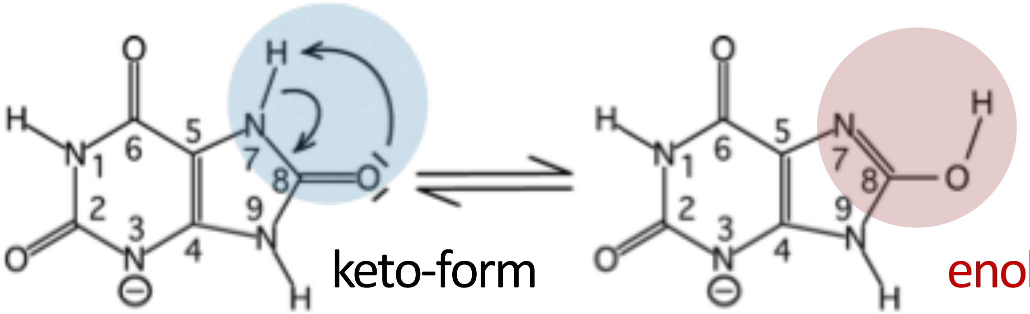


Enzyme mechanisms

Protein-ligand interactions

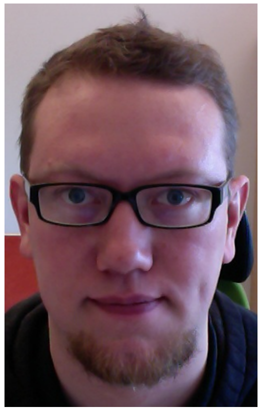
Proton transport across membranes

urate oxidase transforms uric acid - how?



enol-form

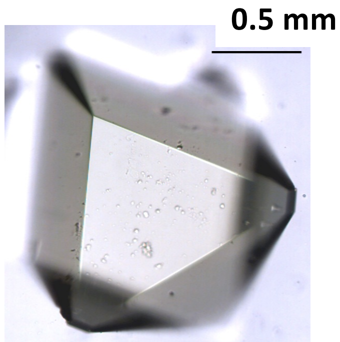
neutrons see

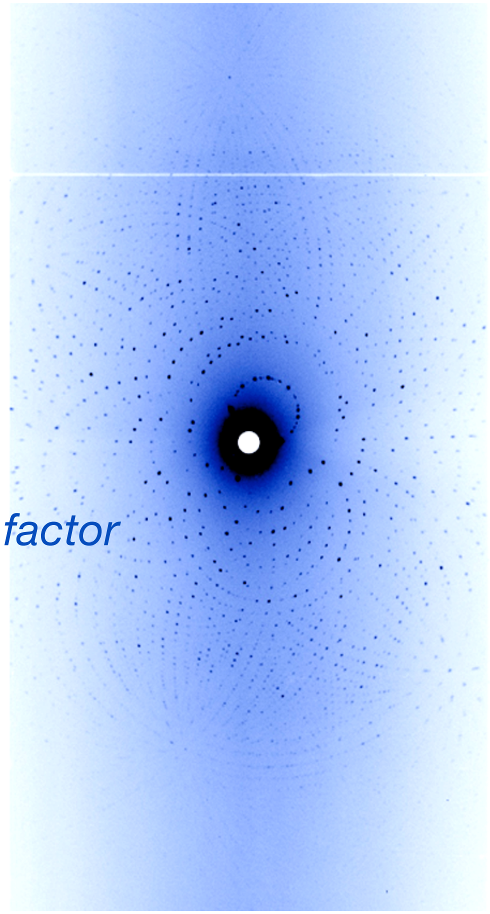


Esko Oksanen
ESS

J. R. Soc. Interface **2009,** *PLoS ONE* **2014**

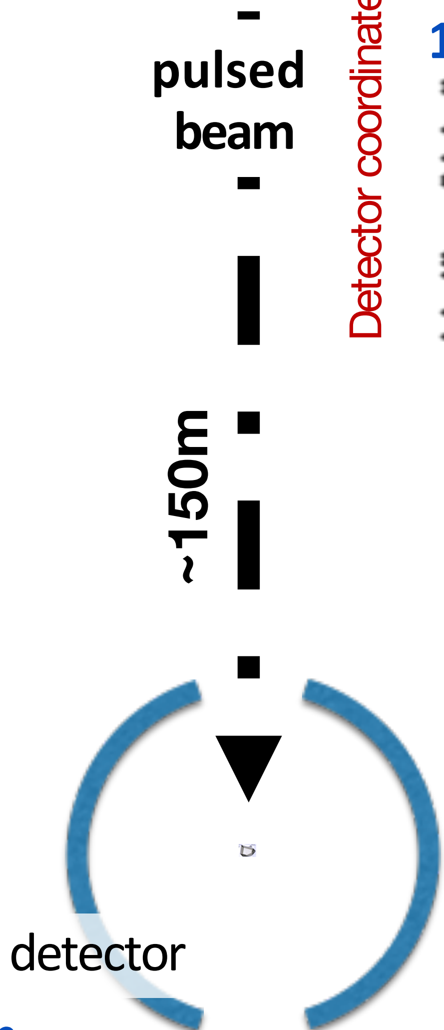
Time-of-flight Neutron Laue Diffraction



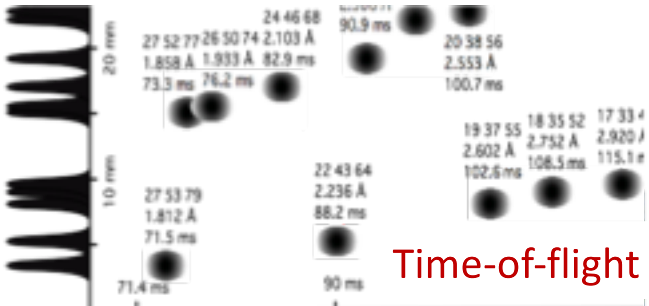


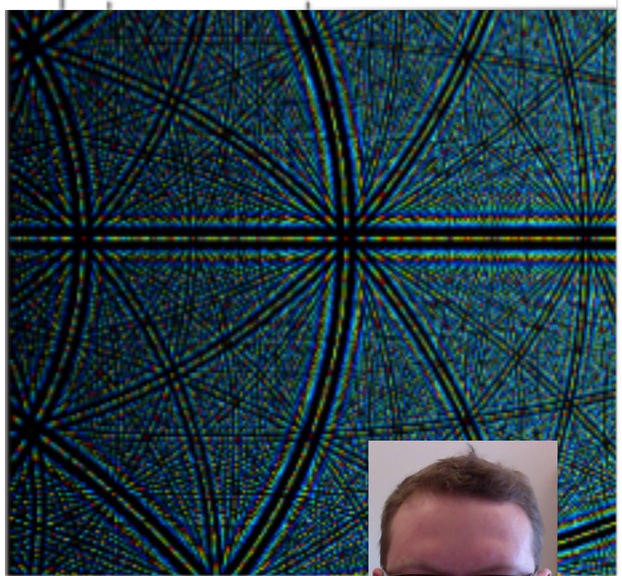
need for “large“
single crystals
often is a limiting factor

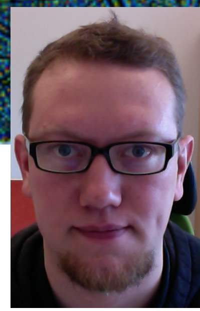
Neutron Laue diffraction
LADI at ILL, Grenoble



intensity gain ~10^2
1 extra dimension



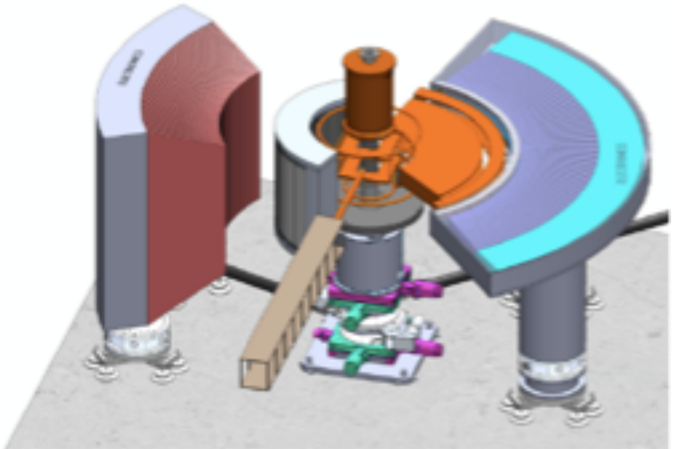


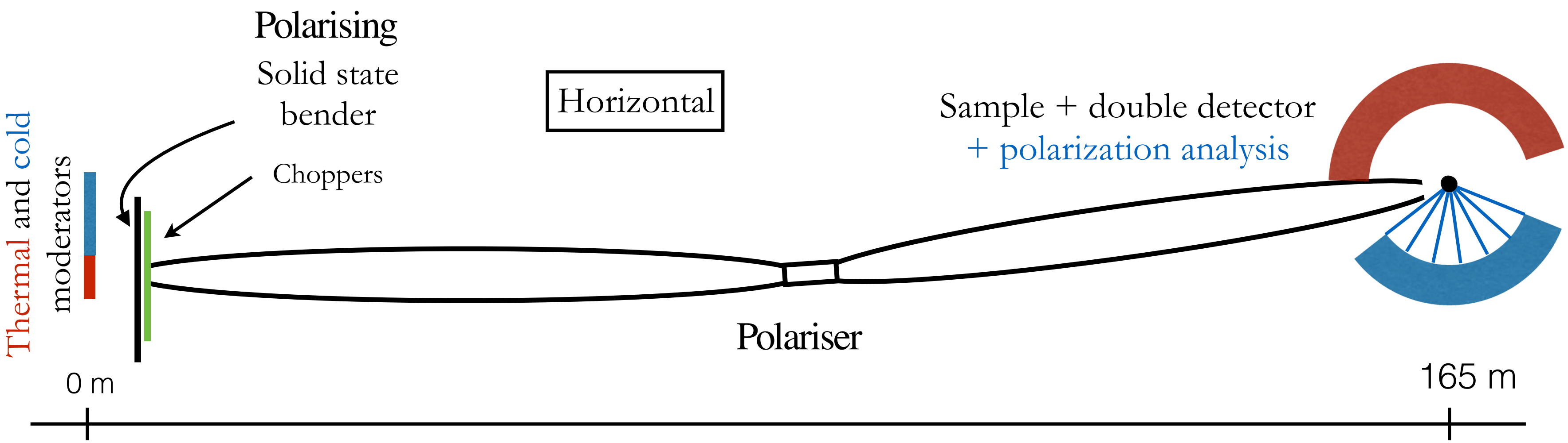


NMX at ESS

MAGIC
Polarized single crystal diffractometer for magnetism

Magnetic structures
Spin densities & Local susceptibilities
Frustrated magnetism - Diffuse scattering





Blume – Maleyev (1963)
general theory for polarized neutron scattering

… yields two expressions

for **scattering intensity**

$$\sigma_{\mathbf{Q}} = |N_{\mathbf{Q}}|^2 + \sigma^{\mathbf{N}}_{\mathbf{Q},\text{isotope-inc}} + \sigma^{\mathbf{N}}_{\mathbf{Q},\text{spin-inc}}$$

$$+ |\mathbf{M}^{\perp}_{\mathbf{Q}}|^2 + \mathbf{P}(N_{-\mathbf{Q}}\mathbf{M}^{\perp}_{\mathbf{Q}} + \mathbf{M}^{\perp}_{-\mathbf{Q}}N_{\mathbf{Q}}) + i\mathbf{P}(\mathbf{M}^{\perp}_{-\mathbf{Q}} \times \mathbf{M}^{\perp}_{\mathbf{Q}})$$

magnetic *magnetic-nuclear interference* *chirality*

and **final polarized intensity**

$$\mathbf{P}'\sigma_{\mathbf{Q}} = \mathbf{P}|N_{\mathbf{Q}}|^2 + \mathbf{P}\sigma^{\mathbf{N}}_{\mathbf{Q},\text{isotop-inc}} - \tfrac{1}{3}\mathbf{P}\sigma^{\mathbf{N}}_{\mathbf{Q},\text{spin-inc}}$$

$$+\mathbf{M}^{\perp}_{\mathbf{Q}}(\mathbf{P}\mathbf{M}^{\perp}_{-\mathbf{Q}}) + \mathbf{M}^{\perp}_{-\mathbf{Q}}(\mathbf{P}\mathbf{M}^{\perp}_{\mathbf{Q}}) - \mathbf{P}\mathbf{M}^{\perp}_{\mathbf{Q}}\mathbf{M}^{\perp}_{-\mathbf{Q}}$$

$$+\mathbf{M}^{\perp}_{\mathbf{Q}}N_{-\mathbf{Q}} + \mathbf{M}^{\perp}_{-\mathbf{Q}}N_{\mathbf{Q}} + i(\mathbf{M}^{\perp}_{\mathbf{Q}}N_{-\mathbf{Q}} - \mathbf{M}^{\perp}_{-\mathbf{Q}}N_{\mathbf{Q}}) \times \mathbf{P} + i\mathbf{M}^{\perp}_{\mathbf{Q}} \times \mathbf{M}^{\perp}_{-\mathbf{Q}}$$

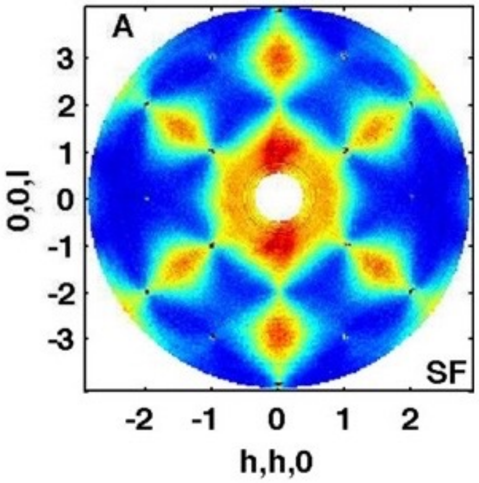
XYZ-polarization analysis for single crystals

Separation of all terms for a multidetector system

W. Schweika 2010 J. Phys.: Conf. Ser. **211** 012026

Polarized $|\mathbf{M}_{\mathbf{Q}}^{\perp}|^2$
Time-of-flight Neutron Laue Diffraction

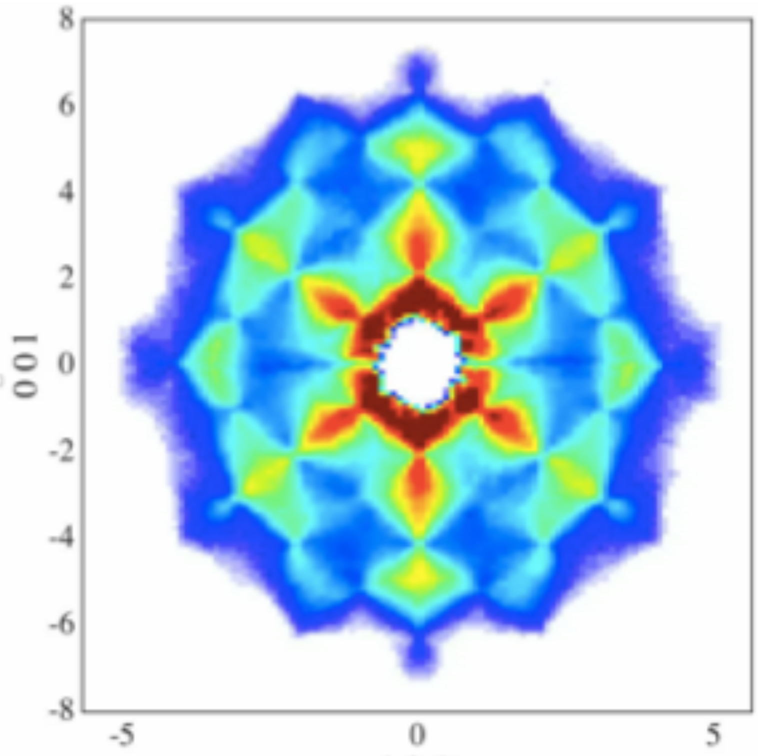
D7: 2x10^6 n/s/cm^2



$Ho_2Ti_2O_7$

T. Fennell *et* al.
Science 2009

seeing topological magnetic monopoles



MAGiC: 2x10$^{\mathbf{9}}$ n/s/cm^2

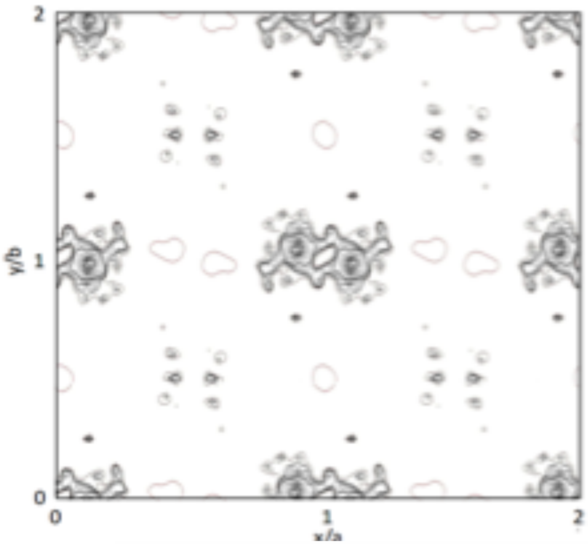
10 min & 10 mm^3

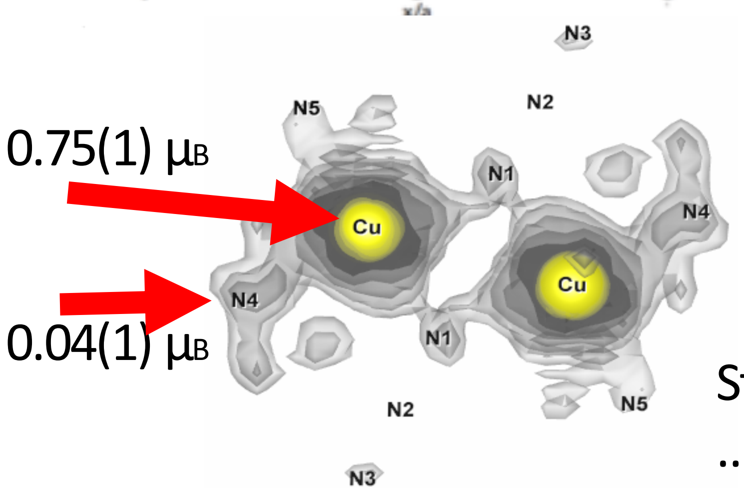
Polarized Time-of-flight Neutron Laue Diffraction

$$\mathbf{P}(N_{-\mathbf{Q}}\mathbf{M}^{\perp}_{\mathbf{Q}} + \mathbf{M}^{\perp}_{-\mathbf{Q}}N_{\mathbf{Q}})$$

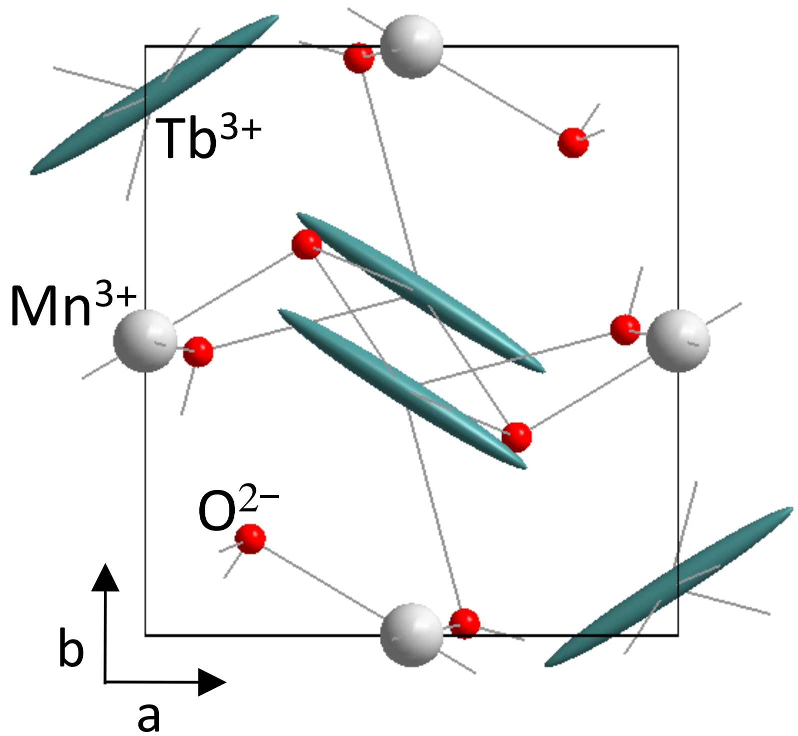
EUROPEAN SPALLATION SOURCE

Spin densities in molecular magnets





Local susceptibilities anisotropies



State-of-the art single crystal measurements in magnetic field

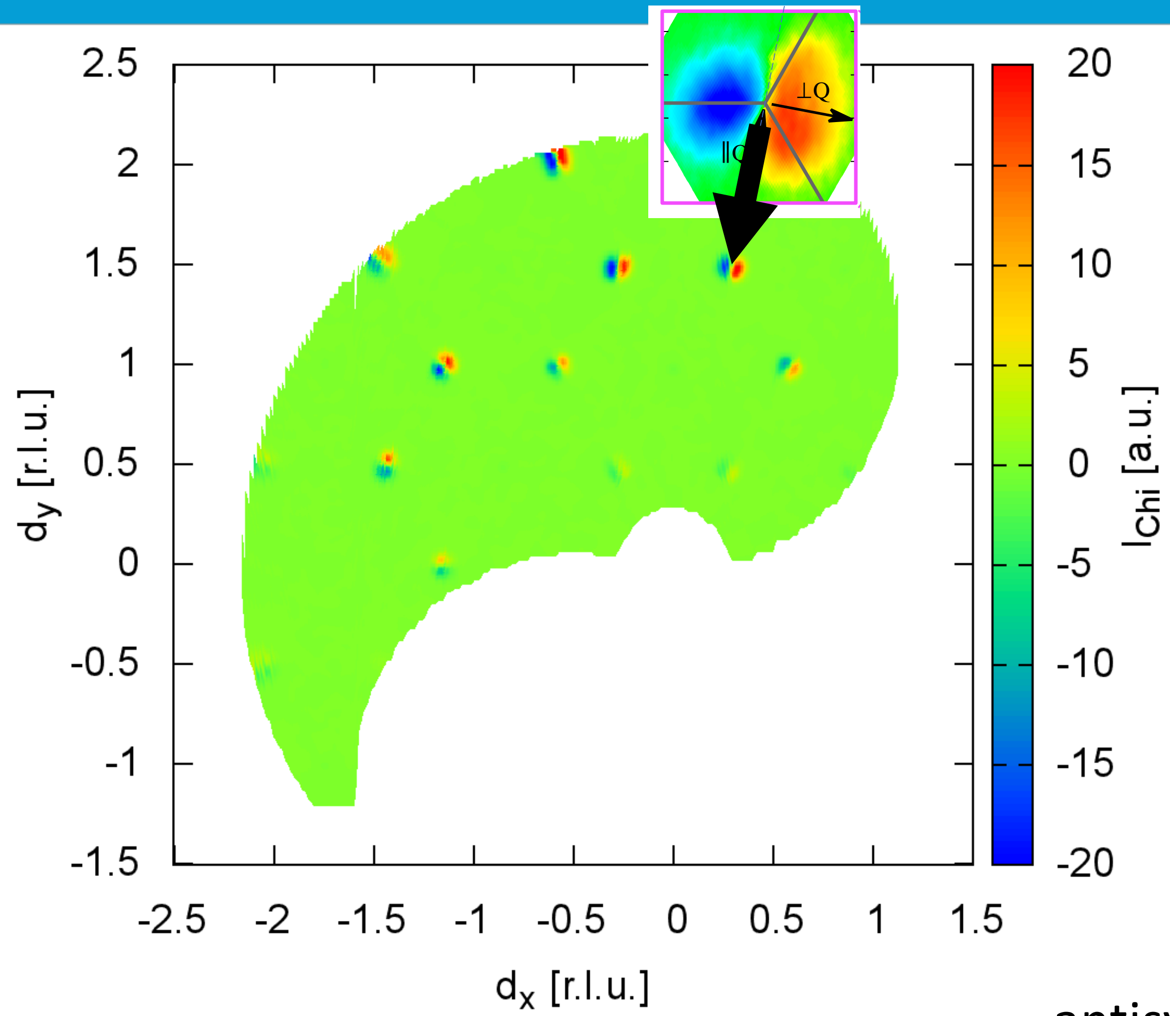
... Do it with powders !

Polarized
Time-of-flight Neutron Laue Diffraction

$$i\mathbf{P}(\mathbf{M}^{\perp}_{-\mathbf{Q}} \times \mathbf{M}^{\perp}_{\mathbf{Q}})$$

chirality

J. Reim et al, PRB 2018

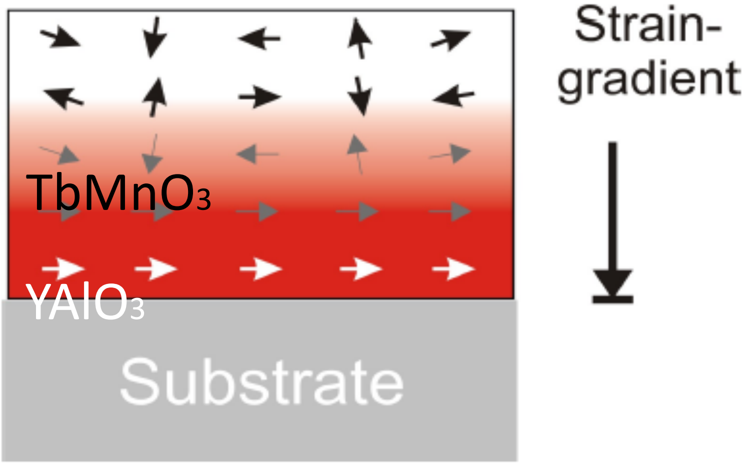


antisymmetric
$\mathbf{C} \perp$ propagation

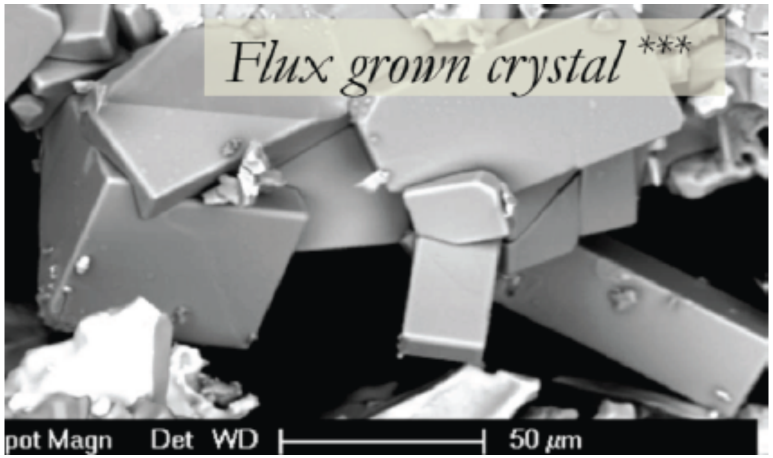
=> cycloid

Future at ESS
Small moments, small samples or heterostructures

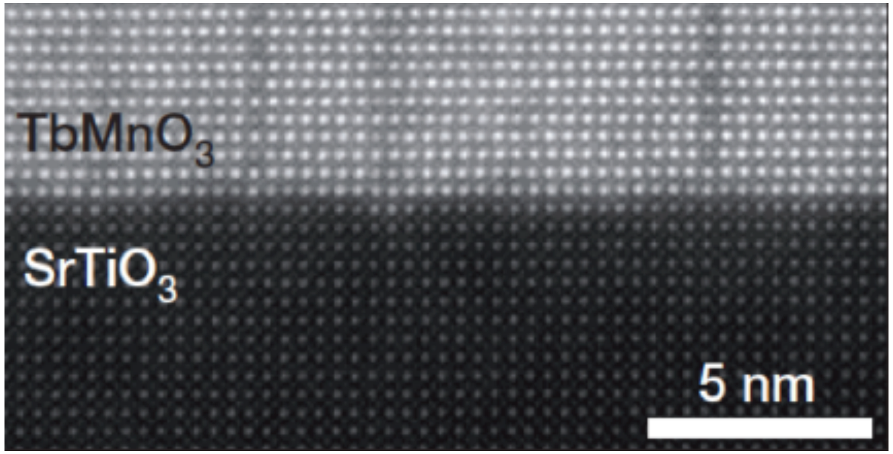
Many single crystalline materials are only available in very small quantities



Adapted from J. White et al., Phys. Rev. Lett. **111**, 037201 (2013)



Courtesy Dr. M. Valldor



S. Farokhipoor et al, Nature Materials **515** , 379 (2015)