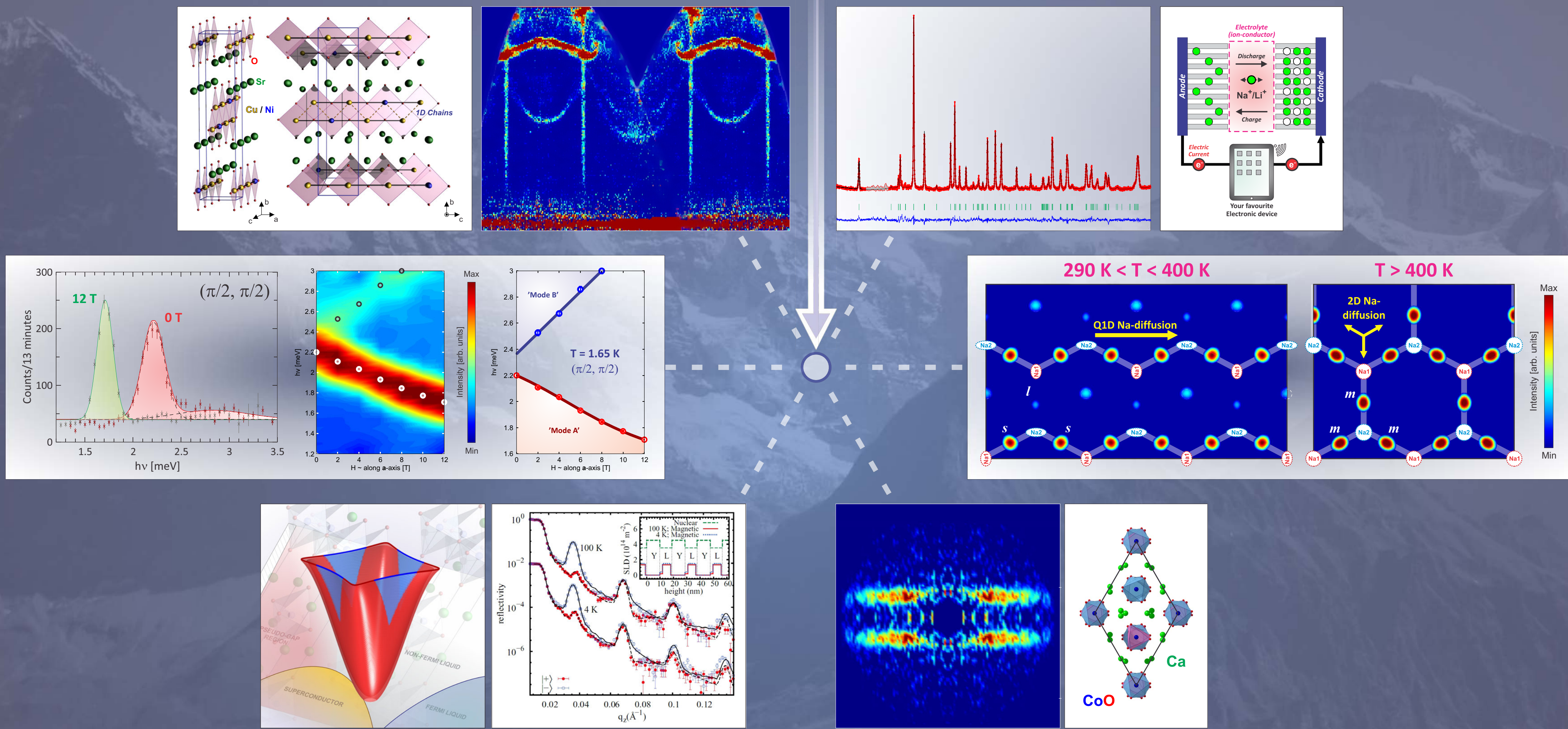
Basic Introduction to Neutron Science



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KTH VETENSKAP OCH KONST

Why Neutron Scattering?

- Neutron scattering is one of the most versatile experimental techniques and is a useful tool for a broad range of scientific fields (materials science, cond. mat. physics, chemistry, biology, engineering, energy...)

- Many material properties can not be measured in any other way and modern condensed matter physics would in principle not exist without NS (magnetic structures, spin-fluctuations in superconductors, quantum magnetism etc.)

- Today's high-tech industry and our everyday electronic devices are using more complex materials and NS is an invaluable tool for future applications (spintronics, energy cells, medical implants, catalysis, engineering...)

- Sweden/Lund will host the state-of-the-art European Spallation Source (ESS), which will be the absolute leading neutron source in the world.

- From 2019 there will be excellent national possi-bilities for young Swedish neutron scatterers to do cutting-edge science.

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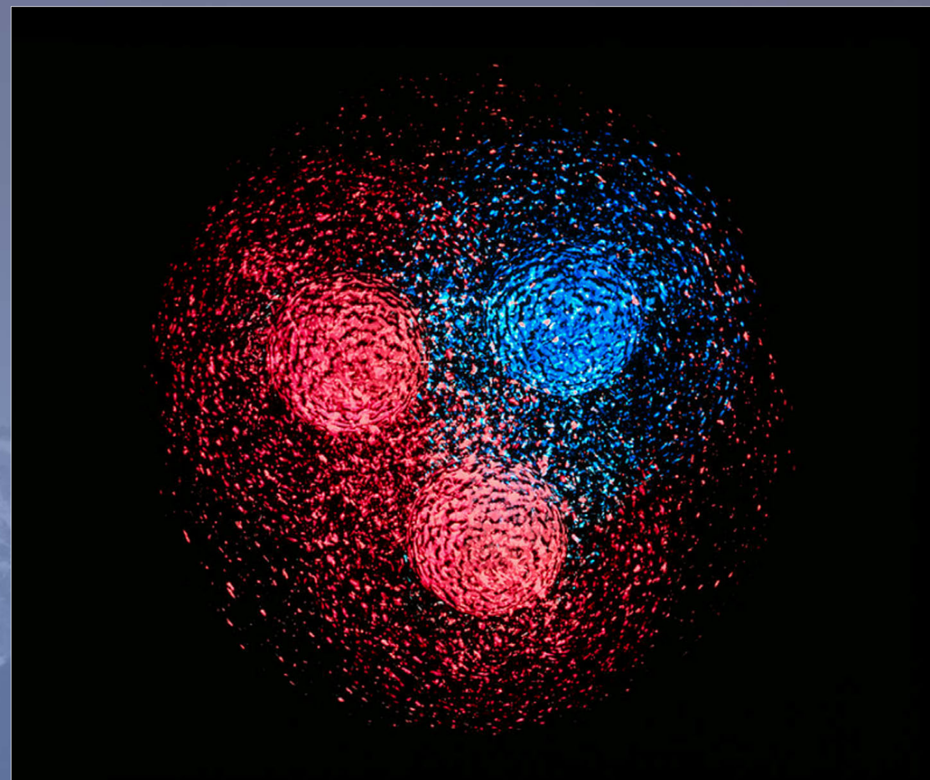
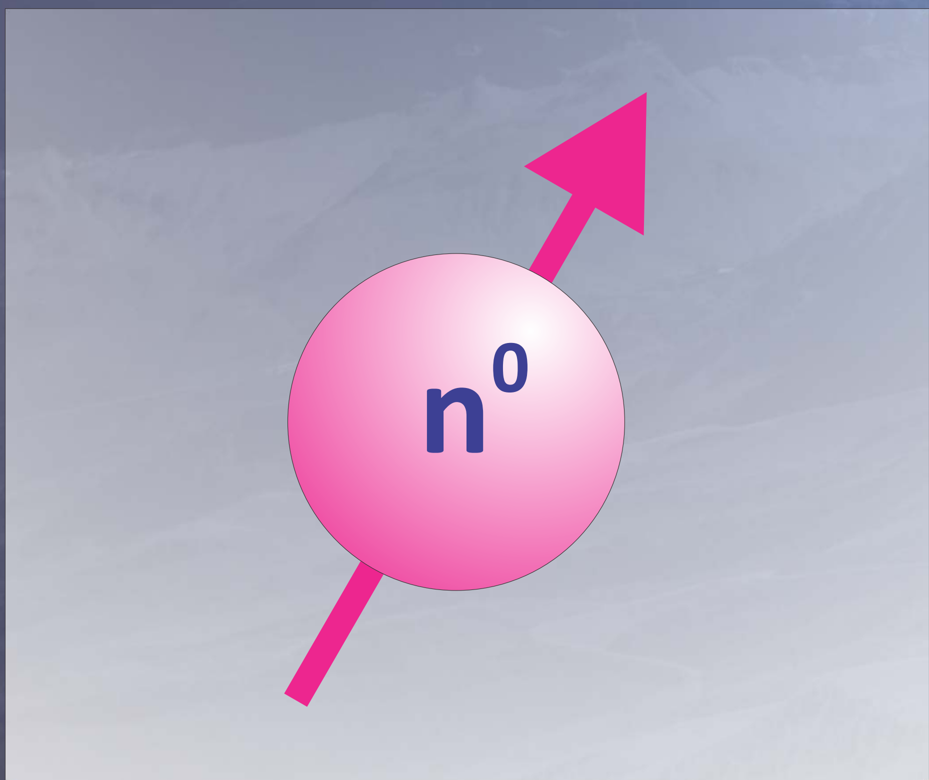
What is a Neutron (n^0)?

For particle physicists:

- A subatomic baryon particle of the hadron family.
- Consists of three quarks (2 down & 1 up) of different flavours held together by gluons.





For neutron scatterers:

- A neutral S = ½ particle used as an optimal tool to investigate microscopic material properties.
- "Can show where atoms are and what they do" + magnetism

Neutron Properties

NEUTRAL

Charge = 0 $\rightarrow$ Very small dipole moment, neutrons do not see charge!

HAS A SPIN

S = ½ $\rightarrow$ Initial state can be polarized & polariz. of final state can be analyzed!

HAS A MAGNETIC MOMENT

$\mu_{n0} = -1.913\ \mu_{Nuc}$ $\rightarrow$ neutrons can see magnetism !!!

RATHER STABLE

β-decays but lifetime τ = 881.5 seconds (enough to survive the experiment!)

VERY SMALL

Confinement radius $R = 7 \times 10^{-14}$ m $\rightarrow$ All interactions are point-like!

'IDEAL' MASS

$m_{n0} = 1.675 \times 10^{-24}$ kg $\approx m_{p+} \approx 184 \times m_{e-}$

PARTICLE- & WAVE-LIKE PROPERTIES

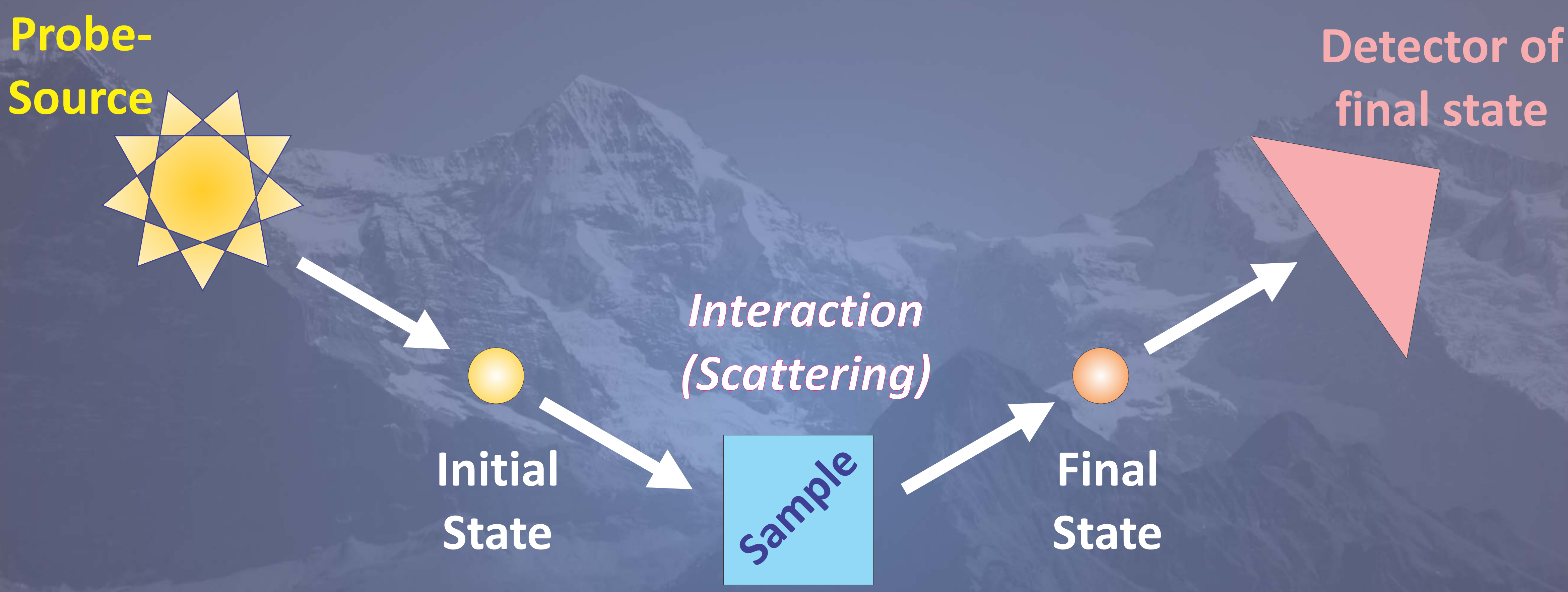
Dispersion relation: $E = \hbar \mathbf{k}^2 / 2m \rightarrow \ldots$

λ = 5 Å $\rightarrow$ E = 3.3 meV

'Lingo'	E [meV]	λ [nm]
Cold	0.1–5	3–0.4
Thermal	5–100	0.4–0.1
Hot	100–500	0.1–0.04

Neutron wavelengths/energies are perfect for studying microscopic material properties and condensed matter physics !!!

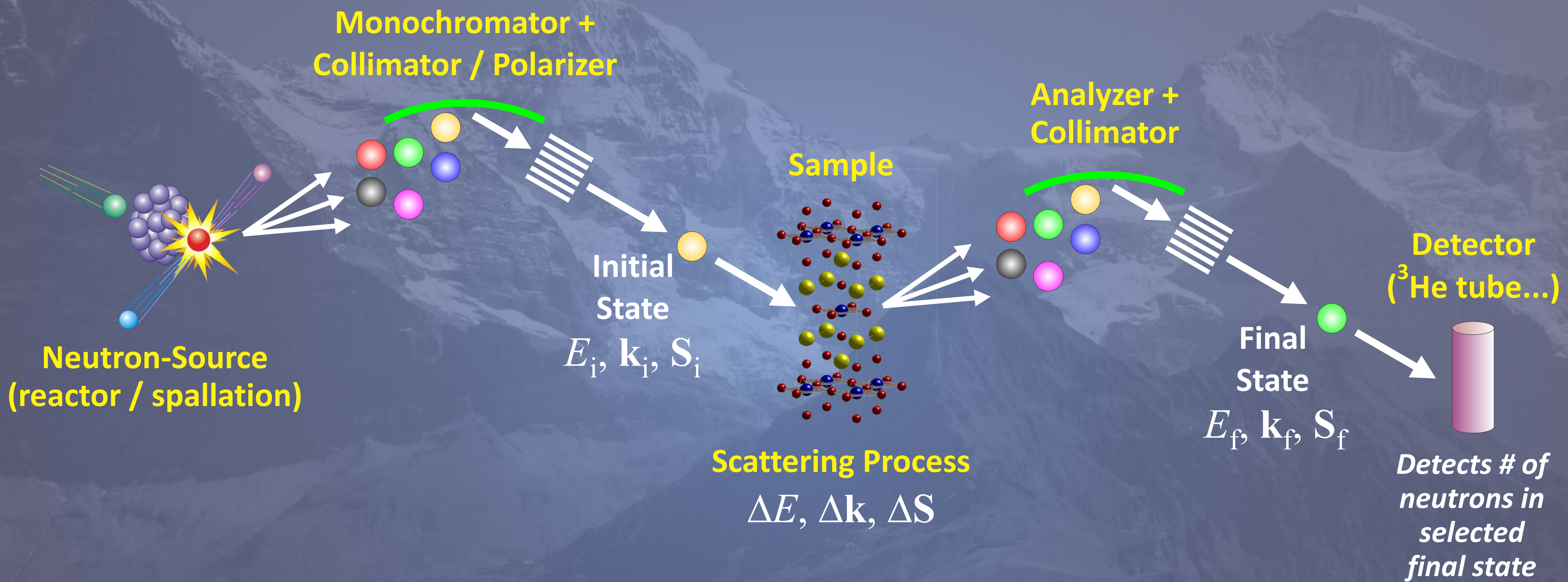
A Scattering Experiment



Remember that scattering methods provide statistically averaged information on structures rather than real-space pictures of particular instances !!!

A Neutron Scattering Experiment

- **Two problems:** **#1**: Can not easily manipulate initial state
  #2: Final state can not be measured directly
- **Solution:** Use 'filters' *e.g.* monochromator, collimators and analyzer



Unfortunately, most neutrons are wasted... twice → ESS !!!

- **Traditionally (continuos sources), many experiments were performed by fixing initial state and scanning the selected final state.** (TIME DEMANDING!)
- **Modern pulsed sources with multi-detectors allow to measure 'everything' in one measurement.**

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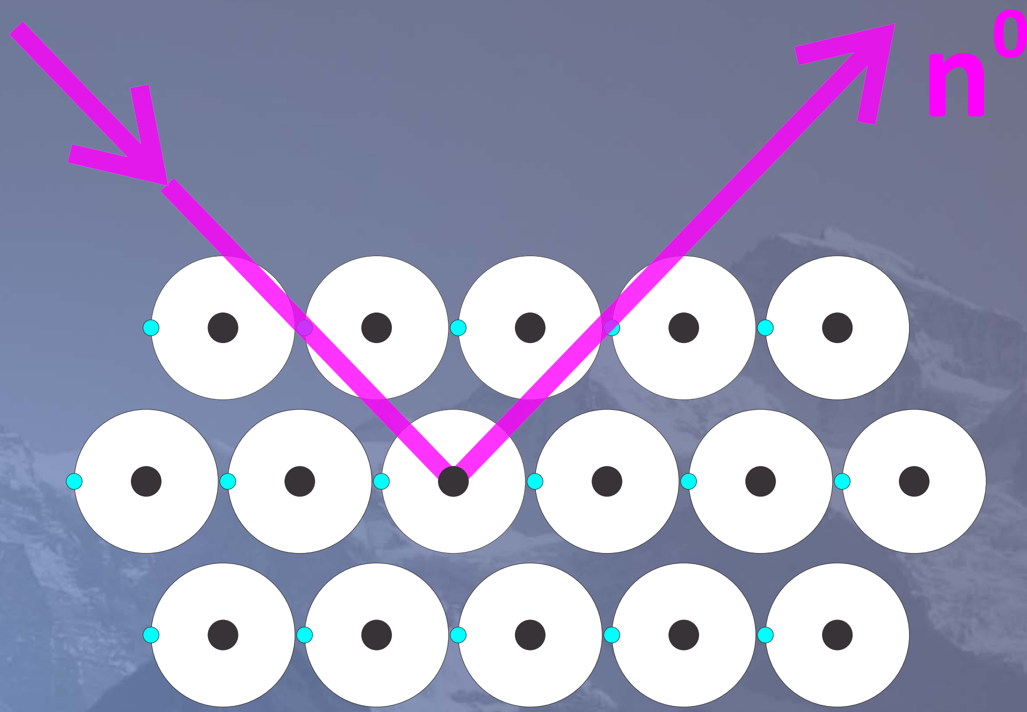
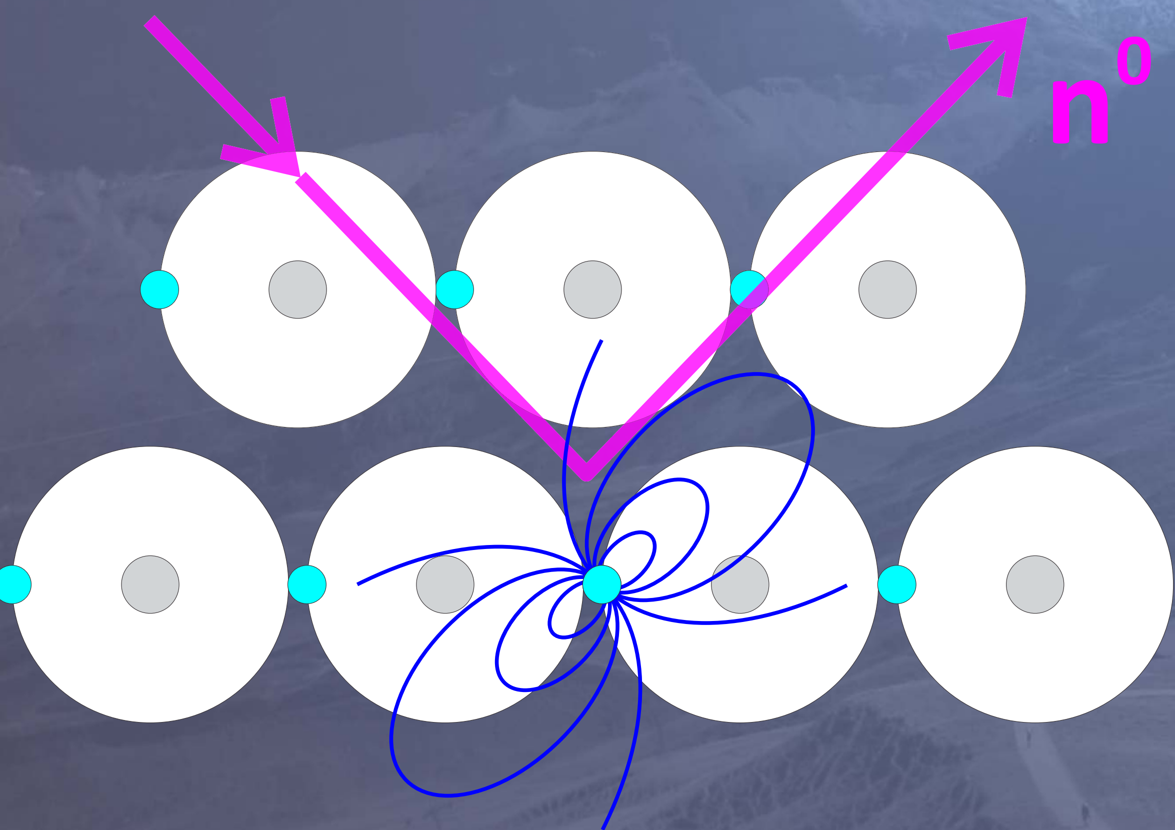
Neutron Interaction with Matter

- Neutrons interact strongly with atomic nuclei on a very short length scale (fm).
- Neutrons see crystal structure, density correlations & excitations (*e.g.* lattice vibrations).
- *“Show where atoms are and how they move”*





- Neutrons also interact with un-paired electrons via a weaker magnetic dipole interaction.
- Neutrons see magnetic struc-tures, spin waves and other magnetic excitations.
- *“Show how spins align and what they do”*

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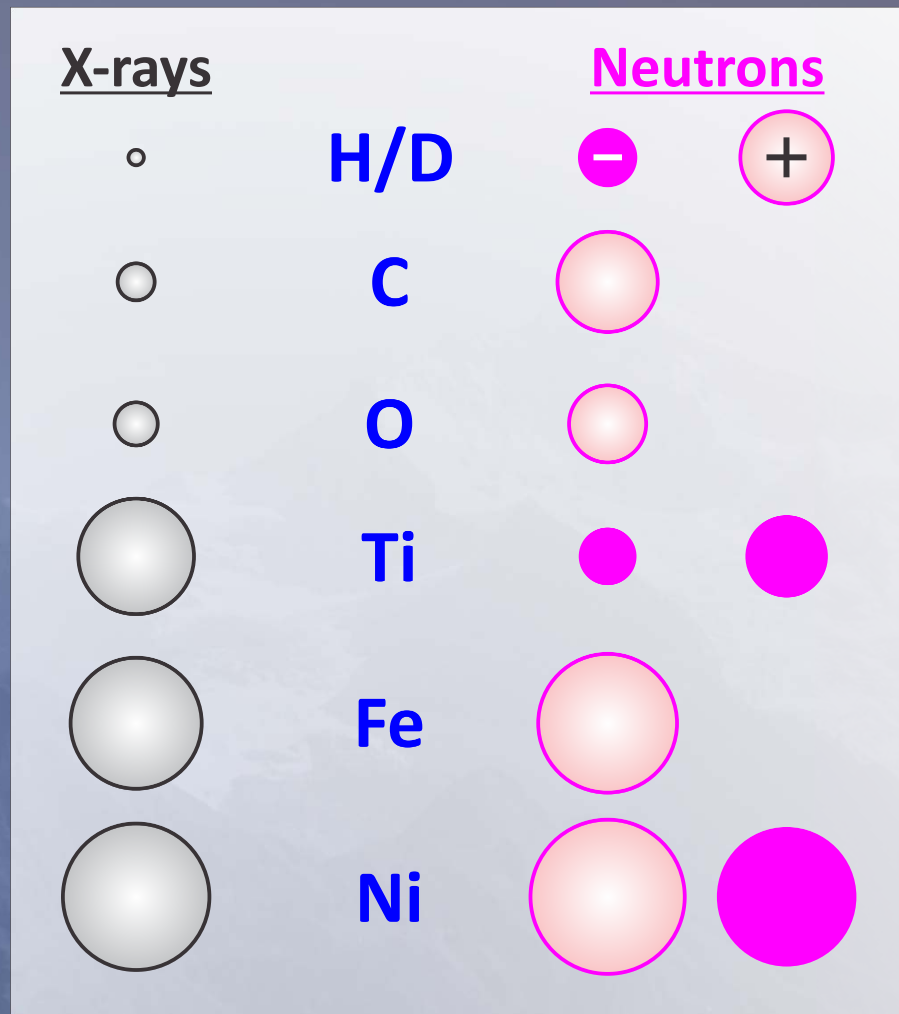
Why is NS *Optimal for Probing Materials?*

- Point-interaction with nuclei (not only e^-) → possible to investigate also light elements + Q-independent form-factor (c.f. x-rays!)
- Isotopic sensitivity → contrast variation. Special case H/D with -/+ scattering lengths i.e. 180° out of phase !!! (very useful)
- Probe bulk properties & buried structures
- Wavelength similar to interatomic distances
- Energy similar to thermal energies (elementary excitations) in matter
- Strong nuclear <u>and</u> magnetic scattering

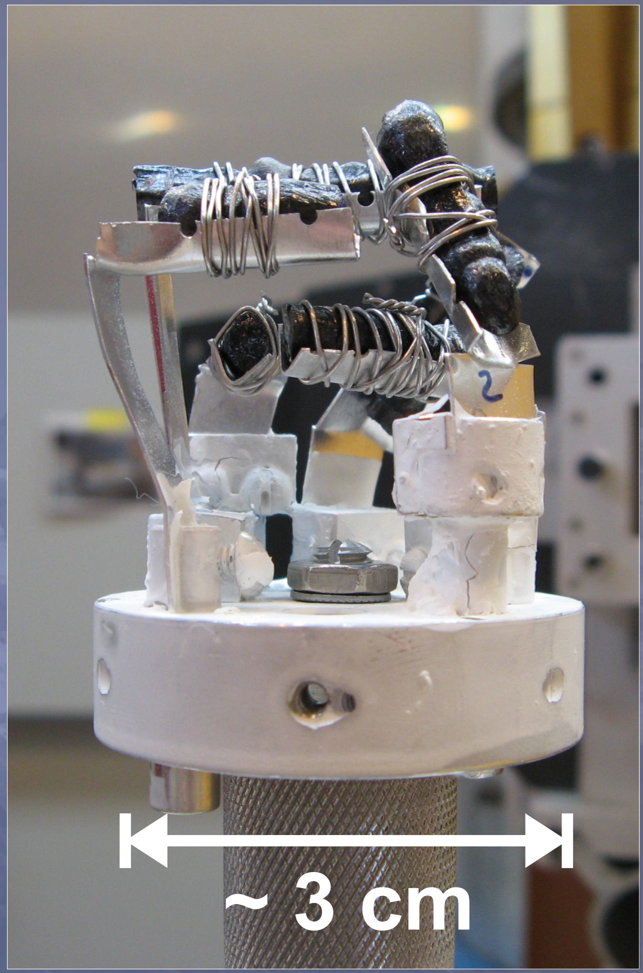


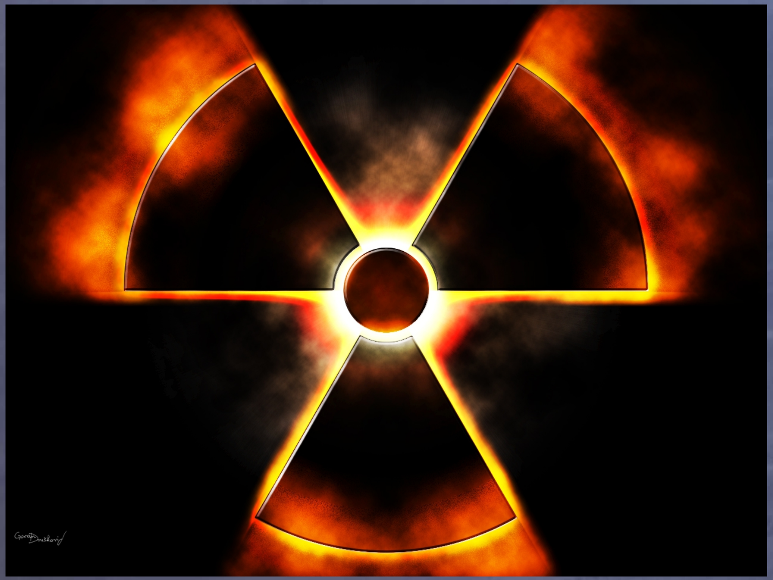
Scattering Strengths

- Some materials (*e.g.* Aluminium) are ‘transparent’ for neutrons → easy to make sample holders/containers for the experiment and...
- Measurements under extreme conditions: low (T = 10 mK) and high (1500 K) temperatures, high pressures (P = 100 kbar) and magnetic fields (H = 20 T).
- Provides statistical averaged data → simple/straightforward fitting and modeling in ideal cases.

Drawbacks of Neutron Scattering

- Rather slow method, high-brilliance neutron sources are needed (ESS) for *e.g.* INS/QENS.
- LARGE-scale facilities are needed to produce neutrons → very expensive and limited amount of experimental beamtime.
- Usually large samples are needed (several grams), which is a problem for *e.g.* single crystal samples.
- Some elements strongly absorbs neutrons (Eu, Cd).
- Neutral particle → technically hard to manipulate particle beam (focus, bend, accelerate and detect).





- Kinematic restrictions on Q for large energy transfers → Difficult to study excitations at higher (eV) energies (...RIXS !!!)
- Some samples gets highly activated in the neutron beam, which is hazardous and sometimes not 'practical'.

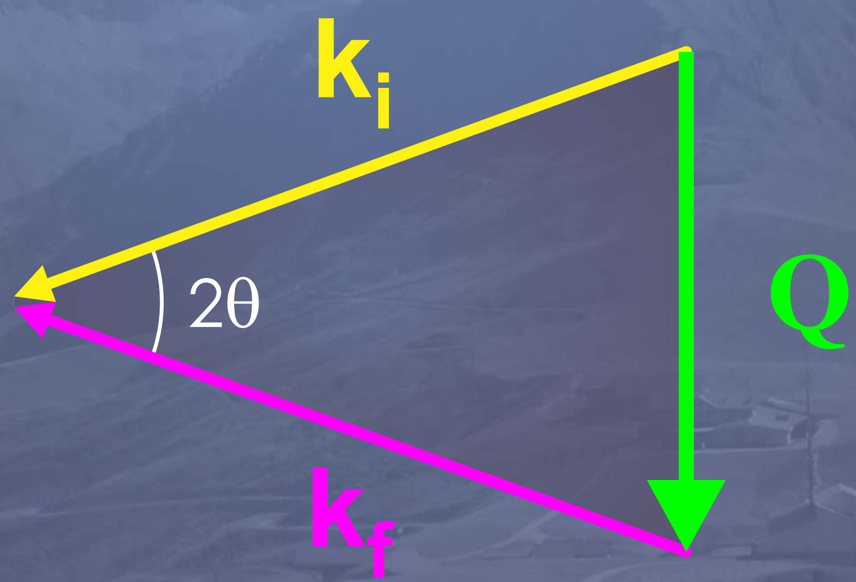
Elastic Neutron Scattering

- The aim of a NS experiment is to determine the probability that an initial neutron of wavevector k_i is scattered into a final state k_f .
- Intensity of the scattered neutrons is measured as a function of momentum transfer (Q) and energy transfer (*E*):

$$\mathbf{Q} = (\mathbf{k}_i - \mathbf{k}_f)$$

$$E = \hbar\omega = \hbar^2(\mathbf{k}_i^{\,2} - \mathbf{k}_f^{\,2}) / 2m$$

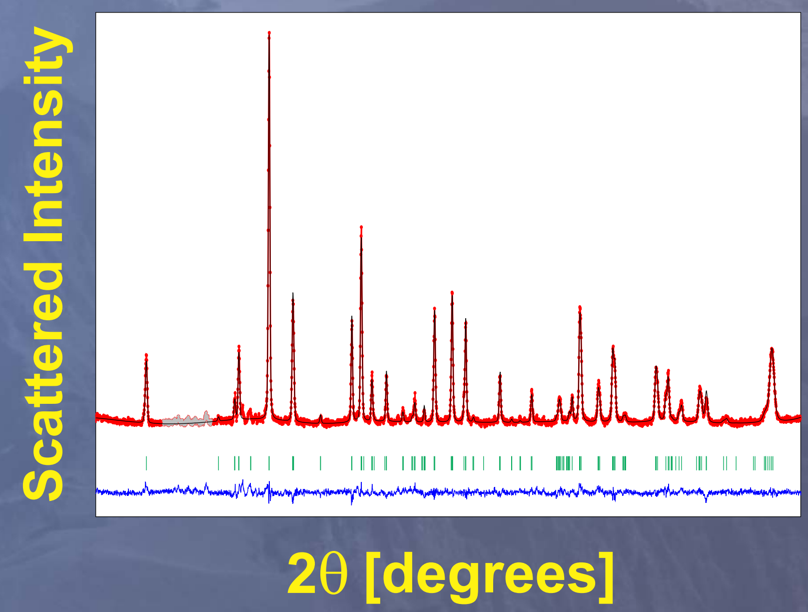
- These two equations describe the momentum and energy conservation of the neutron scattering process !!!
- If the scattering occurs without any loss of neutron energy ($E = 0$ i.e. $|\mathbf{k}_i| = |\mathbf{k}_f|$) this is called Elastic Neutron Scattering:



Tells us about where atoms are and how spins align

Neutron Diffraction

- If the scattering vector $\mathbf{Q} = \tau$ where τ is a reciprocal lattice vector for a nuclear and/or magnetic lattice we obtain coherent elastic scattering.
- As for a normal XRD experiment this is done by performing θ / 2θ scans (2-axis instrument) using fixed & monochromatic incident neutron energy.
- According to the (hopefully) familiar Bragg's law, ($\lambda = 2d_{hkl} \sin\theta$) where θ allows $\mathbf{Q} = \tau$, a coherent Bragg peak appears in the diffraction pattern.



- By collecting large number of Bragg peaks combined with advanced data-analysis it is possible to very accurately refine the structure of a material
- Can be performed for both powder samples as well as single crystals.
- Compared to XRD sample mass is larger (order of a gram) and the measurement is slower [hour(s)].

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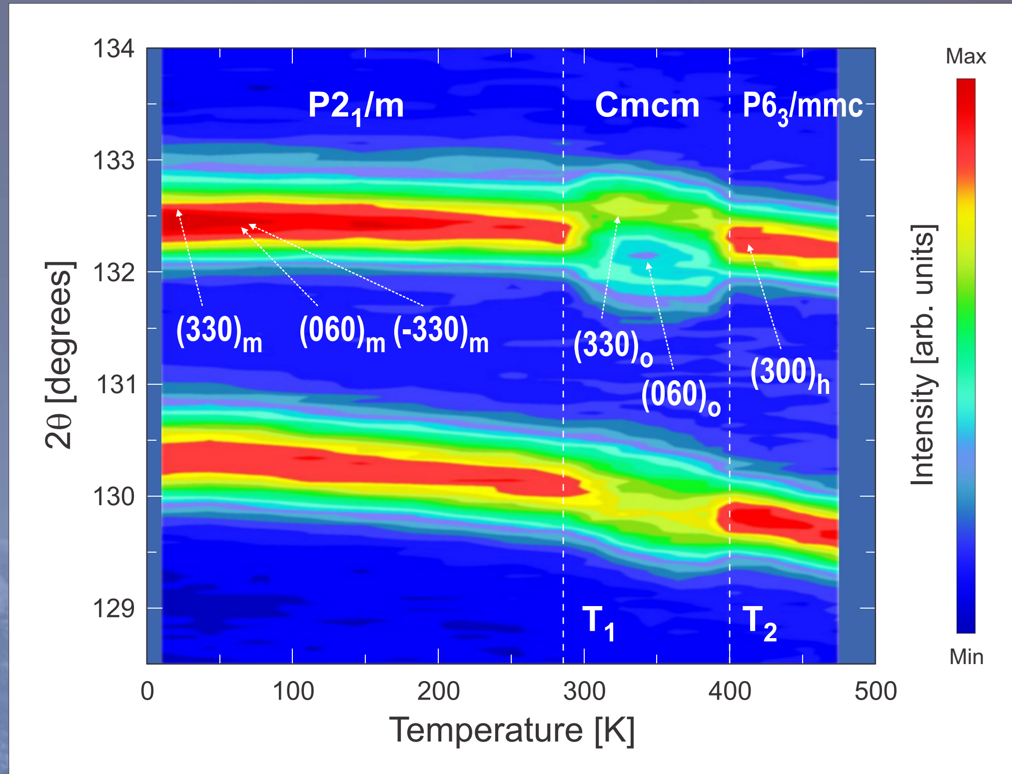
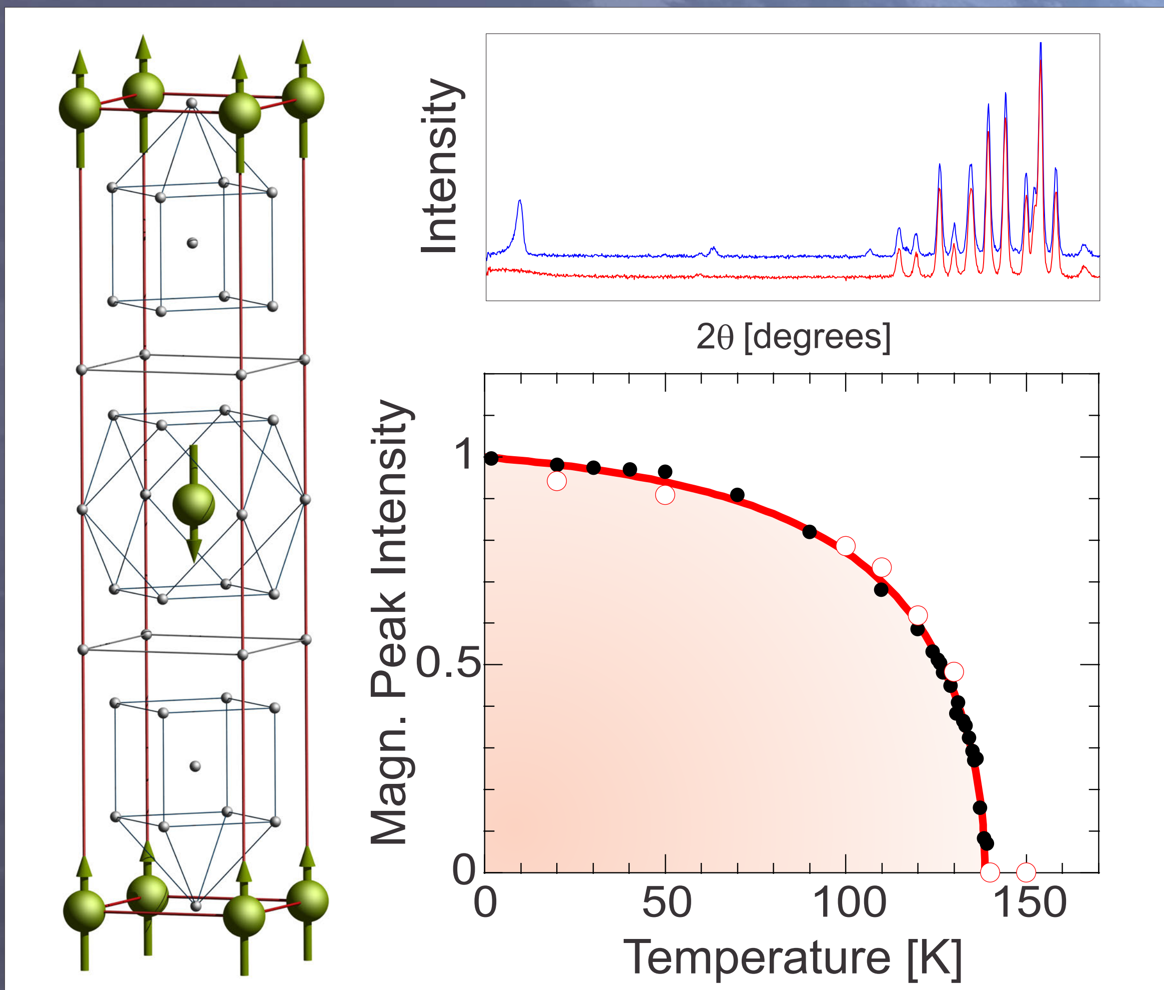
Neutron Diffraction - Examples

Medarde, Phys. Rev. Lett. 110, 266401 (2013)

Nuclear Diffraction

- Determination of and changes in atomic structure when a sublattice contains light atoms or under extreme conditions *e.g.*
  - Li/Na ions in battery materials
  - Hydrogen lattice sites in H-storage materials
  - High-P / low-T induced structural changes
  - Structure of organic materials





Magnetic Diffraction

- Only available tool (!!!) to <u>directly</u> study magnetic order:
  - Determine complex spin-structures and size + direction of magnetic moment for spintronics, storage, novel materials...
  - Magnetic order parameters as a function of T/H to understand formation of spin order *e.g.* frustrated/quantum magnets.
  - Polarized diffraction allow to study AF + FM order

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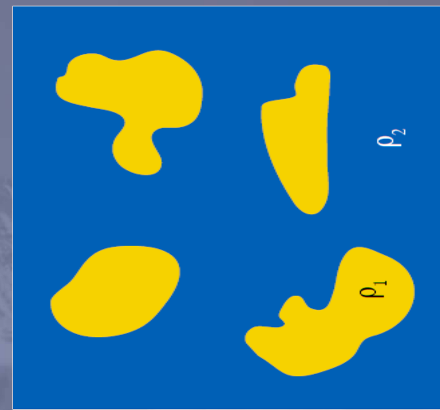
Small-Angle Neutron Scattering (SANS)

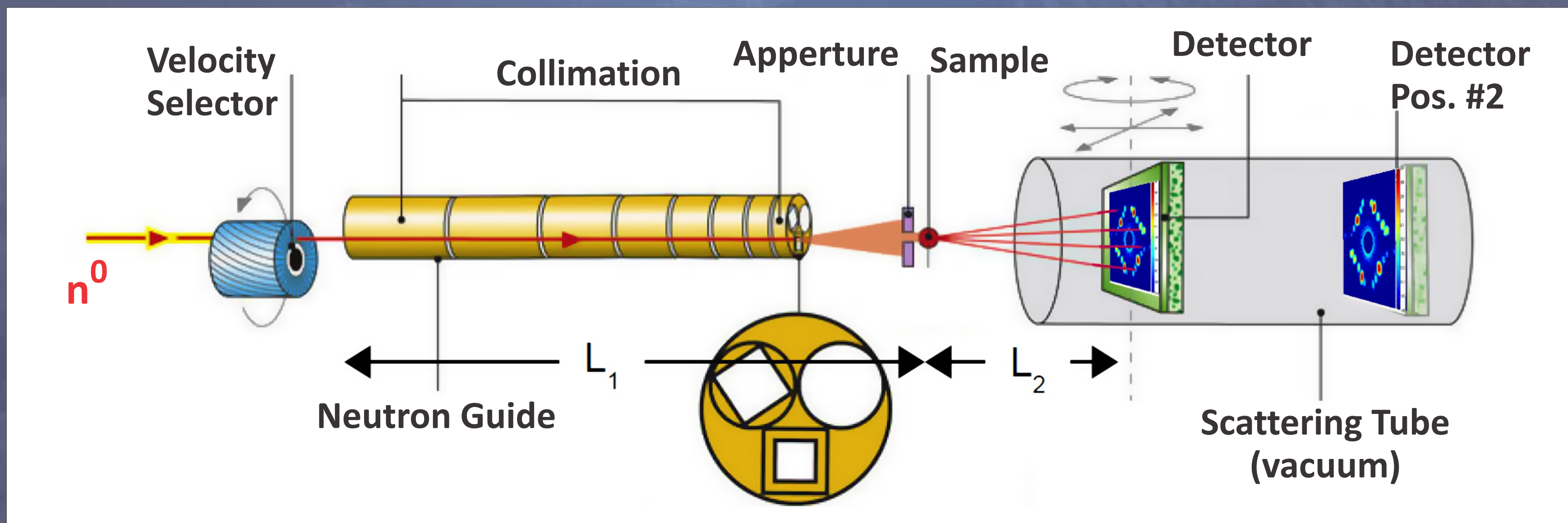
- ‘Large’ scales (> atomic distance) in real space 1 nm – 4 μm ⇔
  Low scattering vectors (small scattering angles) $0.5 - 6{\cdot}10^{-4}$ Å^{-1}

- ‘Sees’ inhomogeneities & correlations of the scattering length density (nuclear/magnetic) ≈ nano-/micro-sized ‘defects’. (Can use isotopic contrast variation!)



- Info on size-distribution, volume fractions & correlation effects of mesoscopic structural and/or magnetic objects.

- Neutrons of selected energy are shot through the sample (<≈ 2 mm thick) that can be powder, single crystal, liquid, particles in solution etc. The result is a 2D (Q_x vs. Q_y) scattering-intensity pattern.



- Good resolution for small scattering angles → good collimation + large spectrometers (L = 10-50 m, H = 2-5 m) with adjustable detector distance.

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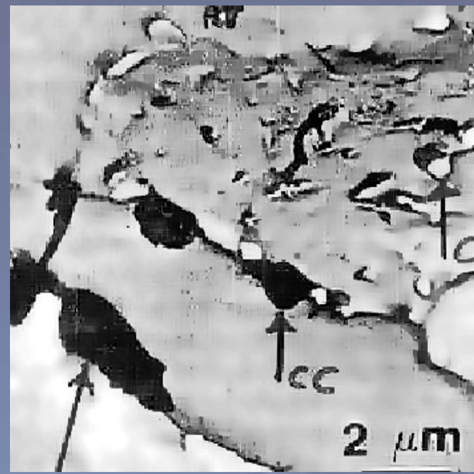
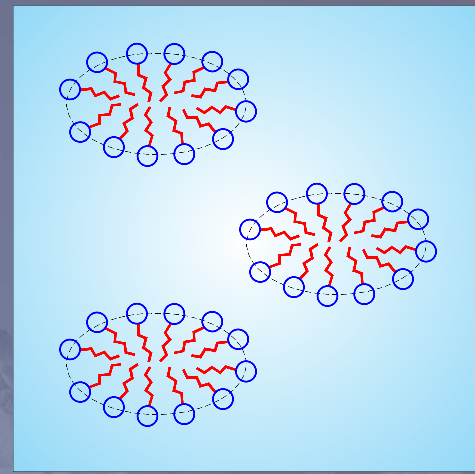
SANS - Examples

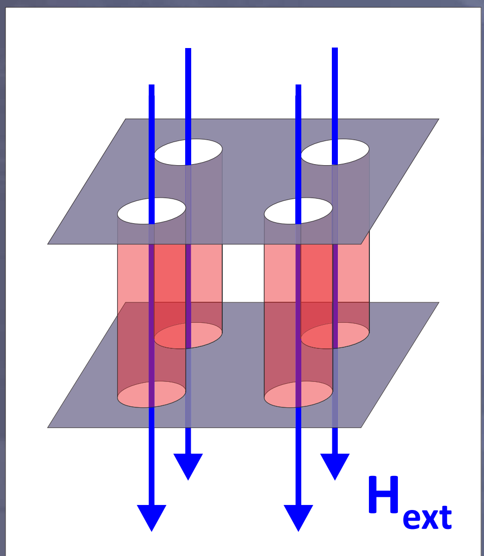
'LARGE' STRUCTURES

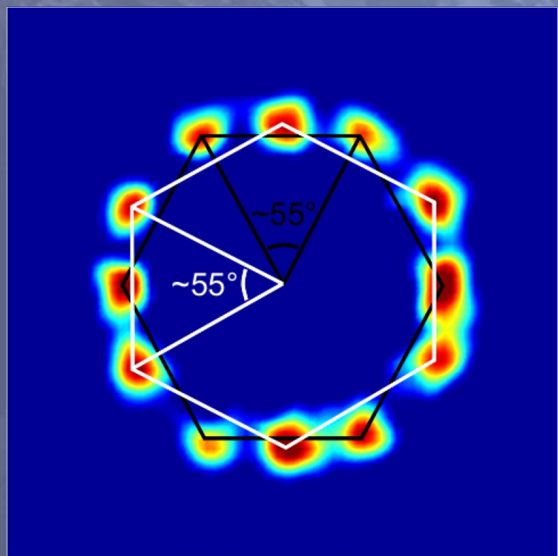
- Metallurgy: creep cavitation damage in steel at high T where volume fraction and size distribution of cavities is obtained.
- 'Soft' matter: size, shape and interaction of particles *e.g.* proteins/micelles in solution or nano-phases in polymers. [H vs. D!]





H. Kawano-Furukawa, Phys. Rev. B 84, 024507 (2011)





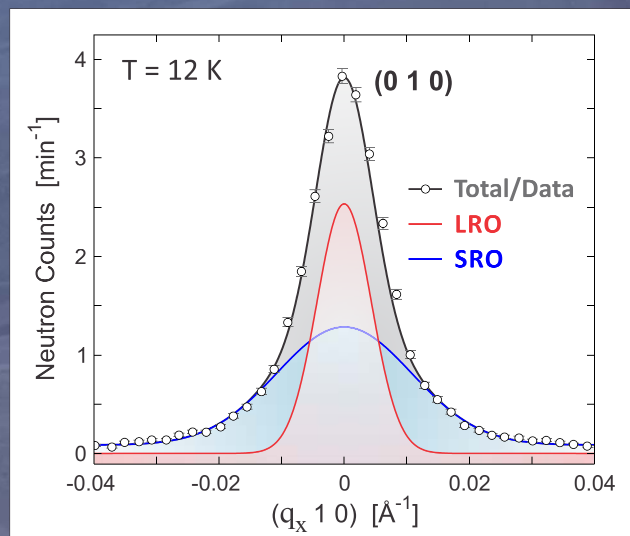
HIGH-TEMPERATURE SUPERCONDUCTIVITY

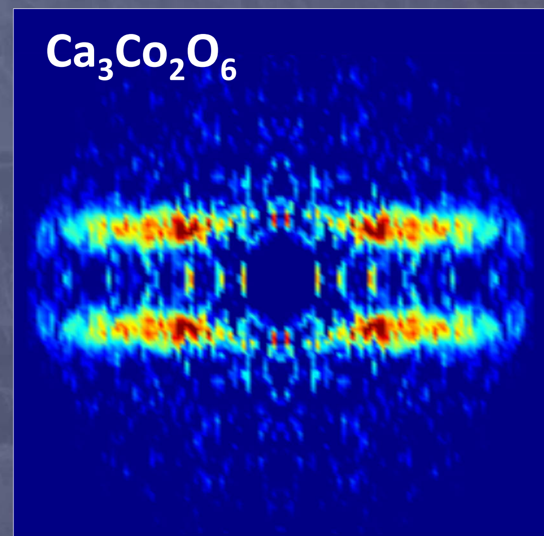
- Vortex lattices in TYPE-II superconductors created by externally applied magn. field.
- The size, distribution and elasticity tells a lot about the underlying physics, FS/OP symmetry and transport properties.

MAGNETISM

- Low-dimensional FiM micro-phases stabilized within a AF long-range order ('magnetic noodle-soup').
- Combining diffraction and SANS gives a complete picture.

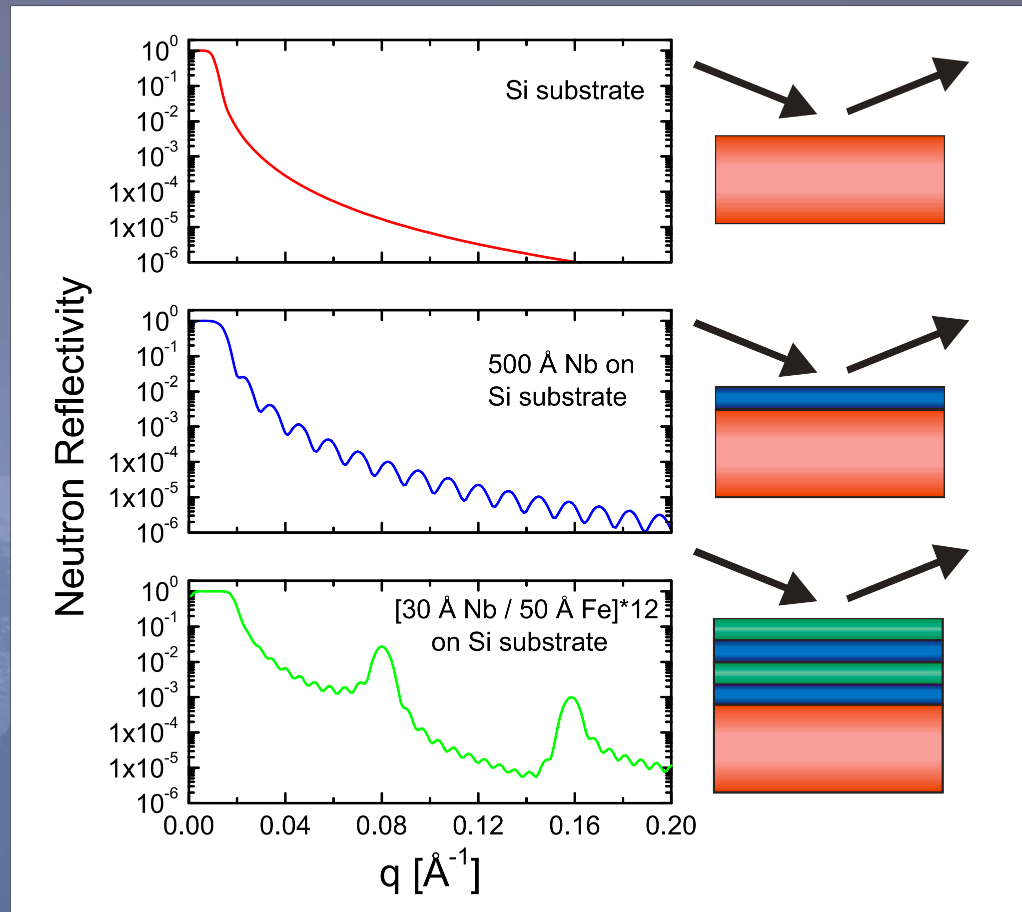
Prsa, arXiv:1404.7398

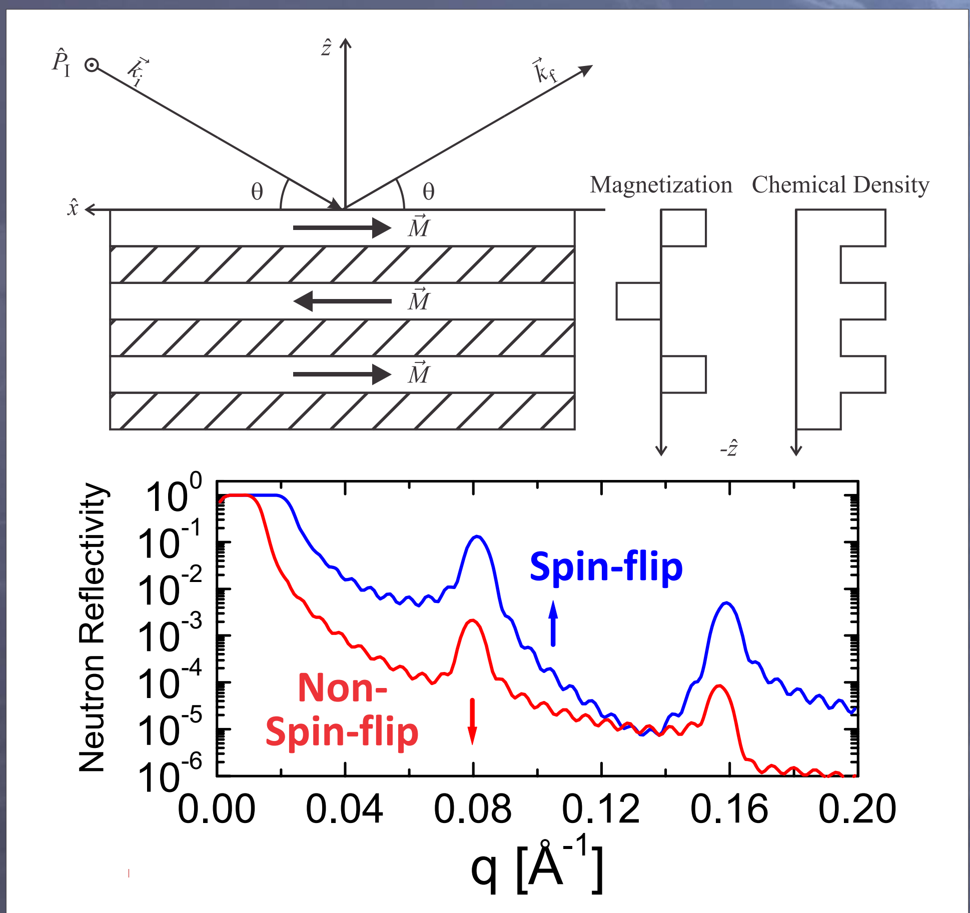




Neutron Reflectometry

- Though neutrons probe bulk properties it is indeed possible to investigate also thin films and surfaces.
- A highly collimated neutron beam is shot onto an flat surface and the intensity of reflected neutrons is measured as a function of angle or wavelength.
- Modeling is clearly a key point for the understanding but...





- ...the exact shape of the reflectivity profile can provide very detailed info about the structure of the surface, including the thickness, density, and roughness of any thin films layered on the substrate.
- If the measurement is done polarized (PNR) it is possible to deduce also the magnetic spin orientation of the film(s) / layer(s).

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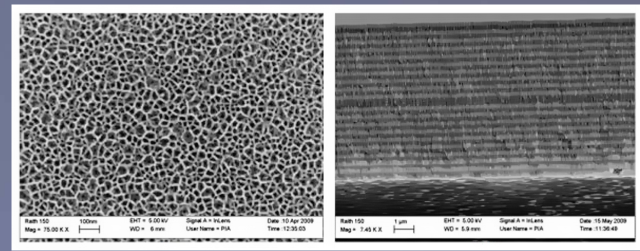
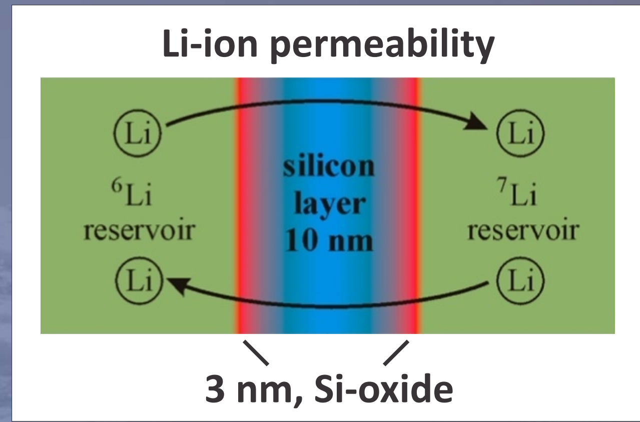
Reflectometry - Examples

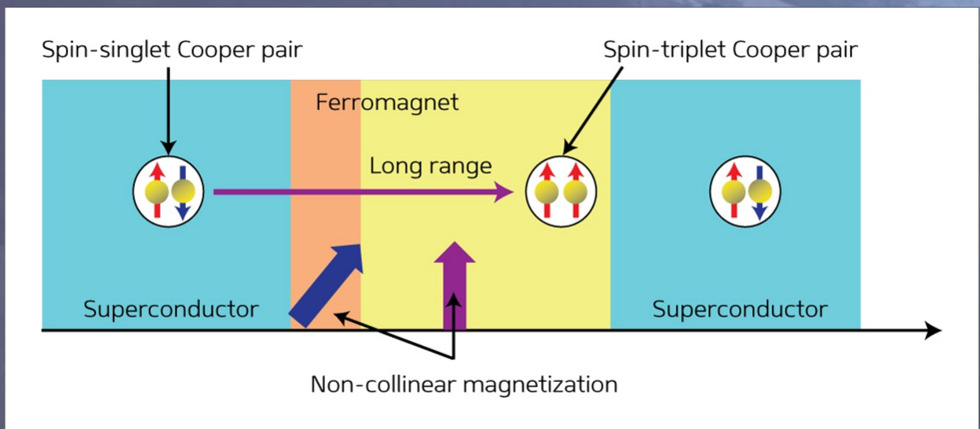
Non-polarized / Structural

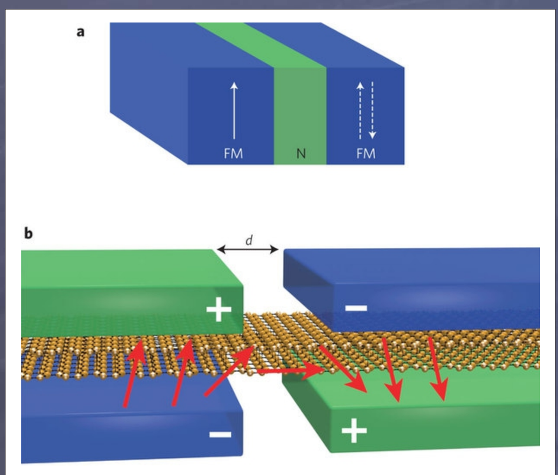
- Determination of film thickness, depth-resolved density profile, roughness and interface properties of multilayers:
  - Spin-coated polymer films (e.g. insulation in electrical motors, solar cells...) and other surface coatings
  - Semiconductor multilayers
  - Liquid adhesion and chemical aggregation at surfaces
  - Ion-diffusion through membrane (contrast)

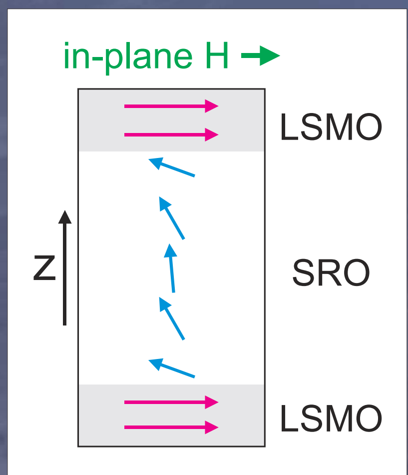




Hüger, Nano Letters 13, 1237 (2013)







Polarized Neutron Reflectometry (PNR)

- Magnetic properties of thin films and bi-/multi-layers:
  - Magnetism in thin films and multilayers (magnetic storage...)
  - Magnetic coupling and 'twisting' in multi-layers (mag. / non-mag. / mag.)
  - Magnetic / Superconducting multi-layers (co-existing of SC and magnetism)
  - Spintronics in *e.g.* graphene and topological insulators

Inelastic Neutron Scattering

- Intensity of the scattered neutrons is measured as a function of momentum transfer (**Q**) and energy transfer (***E***):

$$\mathbf{Q} = (\mathbf{k}_i - \mathbf{k}_f)$$

$$E = \hbar\omega = \hbar^2(\mathbf{k}_i^{\,2} - \mathbf{k}_f^{\,2}) \,/\, 2\mathrm{m}$$

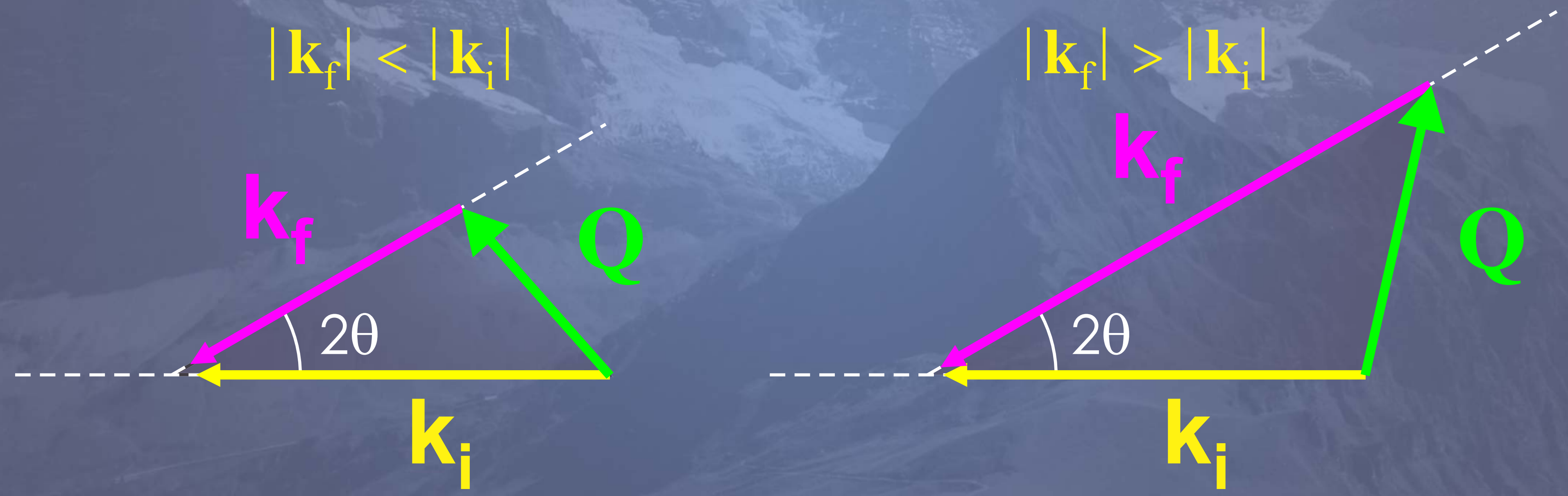
- If the neutrons lose or gain energy in the scattering process ($E \neq 0$ i.e. $|\mathbf{k}_i| \neq |\mathbf{k}_f|$) this is called Inelastic Neutron Scattering (INS):

Neutron Loses Energy

$|\mathbf{k}_f| < |\mathbf{k}_i|$

Neutron Gains Energy

$|\mathbf{k}_f| > |\mathbf{k}_i|$



Tells us what the atoms and electron spins 'do'

- INS intensity is presented as the dynamic structure factor $S(\mathbf{Q},\omega)$, which in case of magnetic scattering equals the dynamic susceptibility $\chi''(\mathbf{Q},\omega)$.

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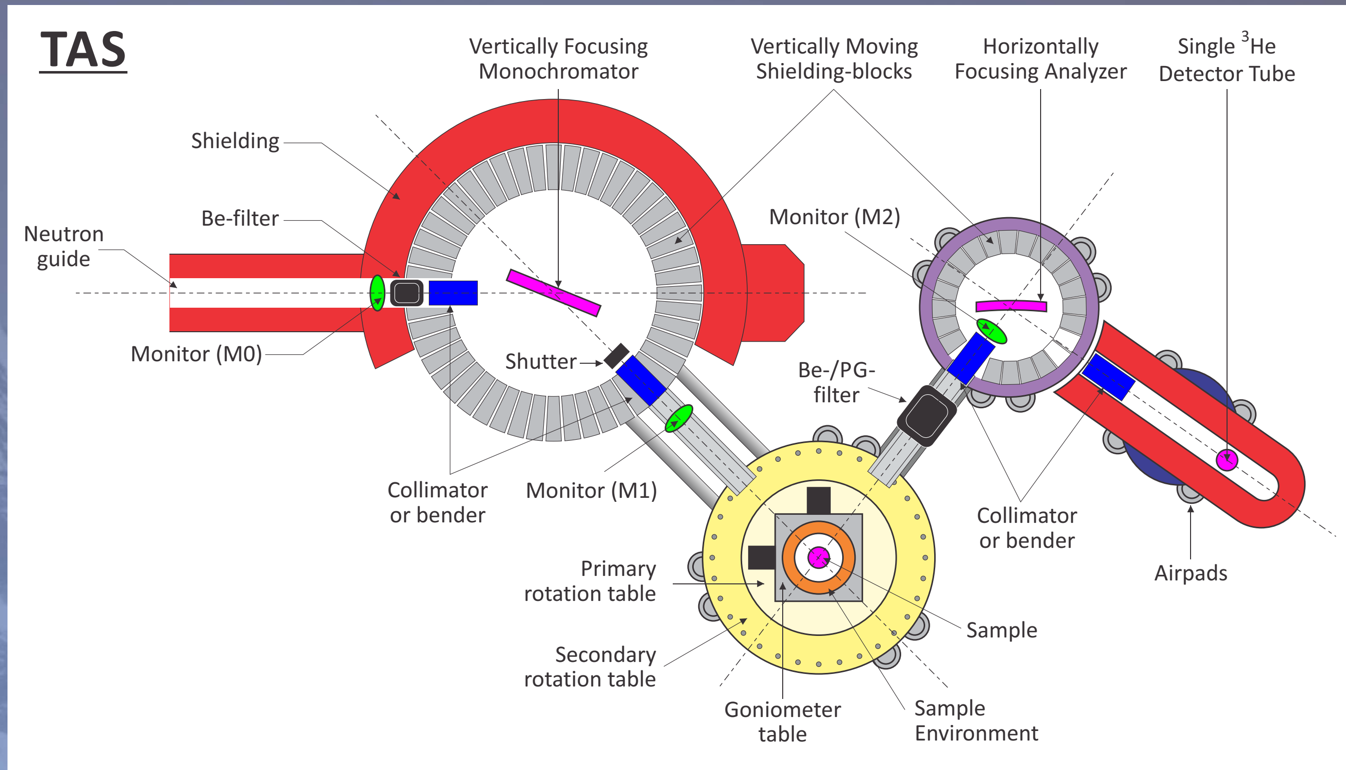
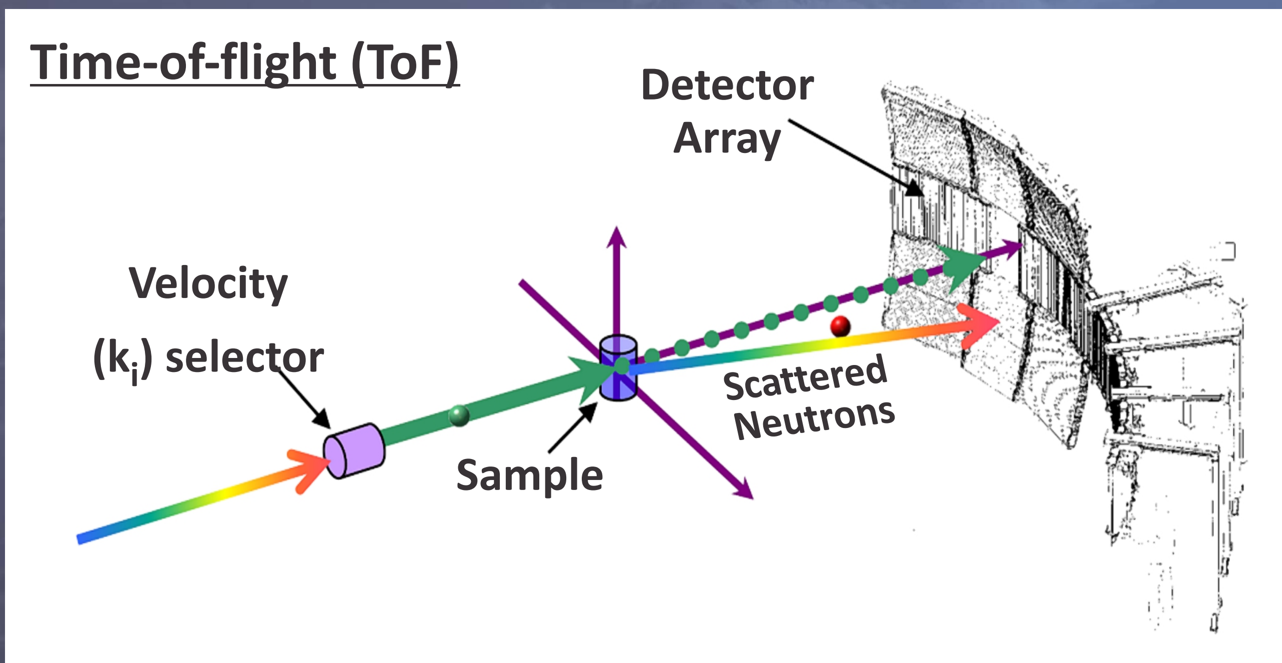
The INS Experiment

- Traditional way is to use a triple axis spectrometer (TAS) where $S(Q, \omega)$ is measured point by point by scanning k_i, k_f, θ, 2θ
- Rather slow but controlled (resolution, background) measurement.
- Large single crystal (mosaic)
- Continuous source is optimal



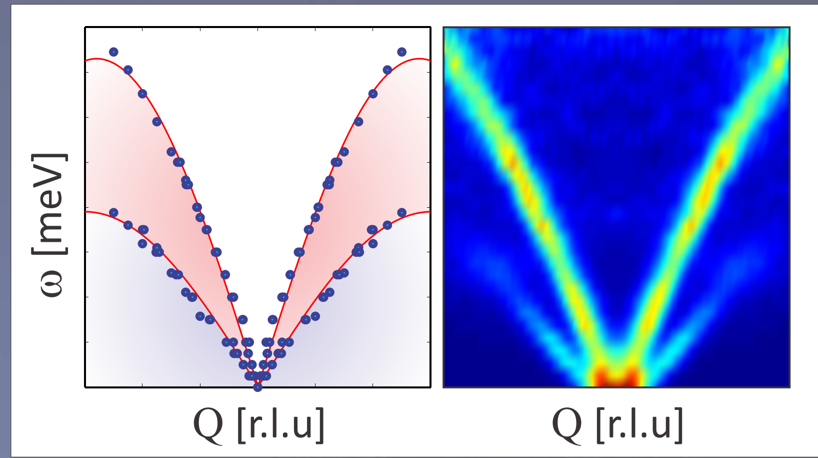


- Modern way is to use a time-of-flight (ToF) spectrometer with selected/fixed k_i and measure the complete 4D $S(Q_{xyz}, \omega)$ set by a multi-detector array.
- Faster but huge data-sets that needs to be analyzed carefully for background and resolution after the experiment
- Needs a (short-)pulsed source

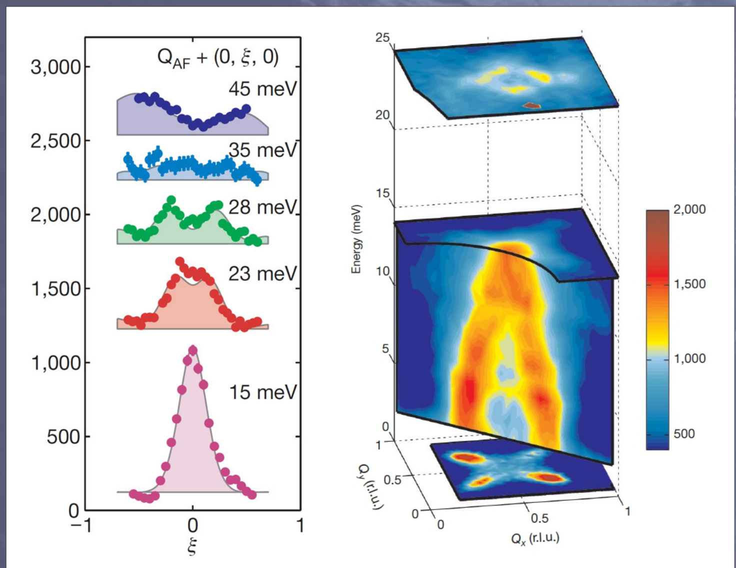
INS - Examples

NUCLEAR EXCITATIONS

- Lattice vibrations i.e. phonons have traditionally been extensively investigated (*e.g.* cooper-pair formation in conventional superconductors)
- Mostly done by thermal neutrons (10's of meV)



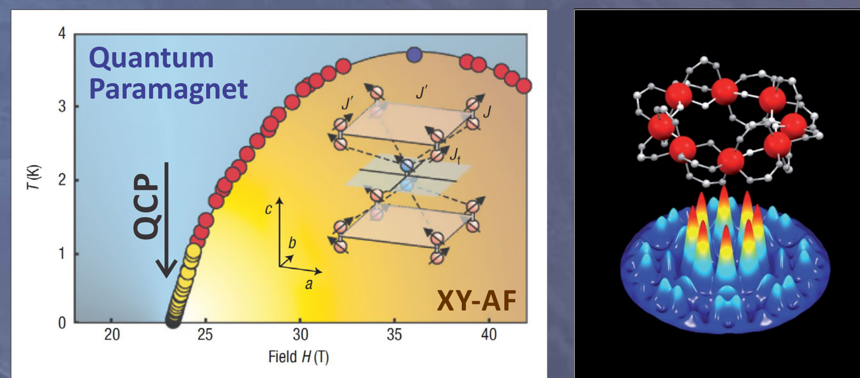
Boothroyd, Nature 471, 341 (2011)



HIGH-TEMPERATURE SUPERCONDUCTIVITY

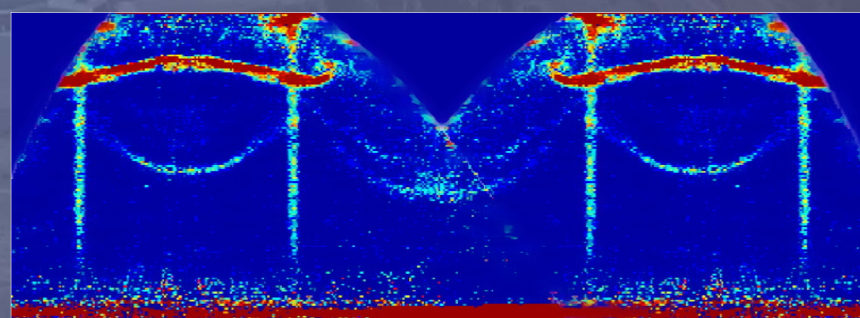
- HTSC emerges from AF parent compounds. INS has shown that spin excitations remain even in the SC phase.
- INS in combination with diffraction are currently trying to understand the connection between spin excitations & 'stripe' phases (1D spin/ charge order)

GIAMARCHI, Nature Physics 4, 198 (2008)



MAGNETISM

- Spin-wave/magnon mapping in exotic magnets (triangular frustration, square lattice AF etc.)
- Induce magnetic order by pressure, external field (Bose Einstein Condensation and QCP in quantum/molecular magnets).
- Destroy magnetism by *e.g.* creating disorder (defects,doping) → opening of a spin gap.



Simutis, Phys. Rev. Lett. 111, 067204 (2013)

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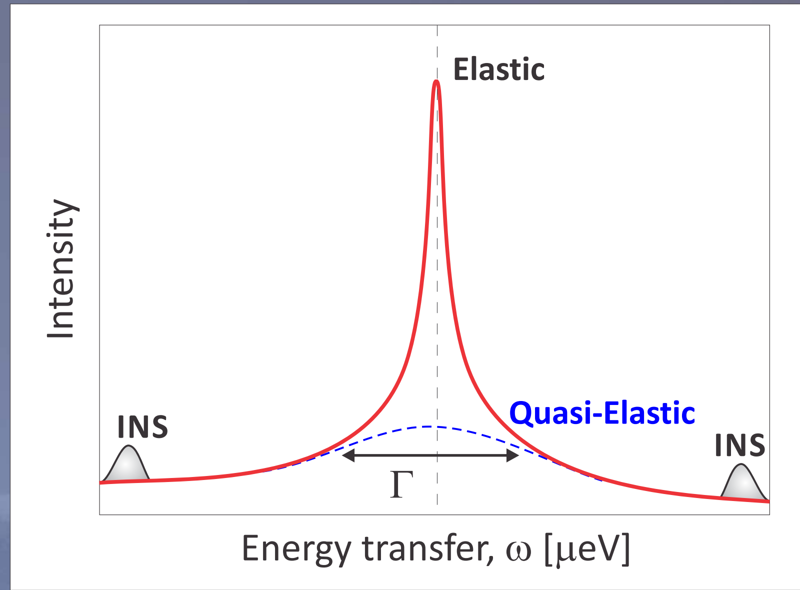
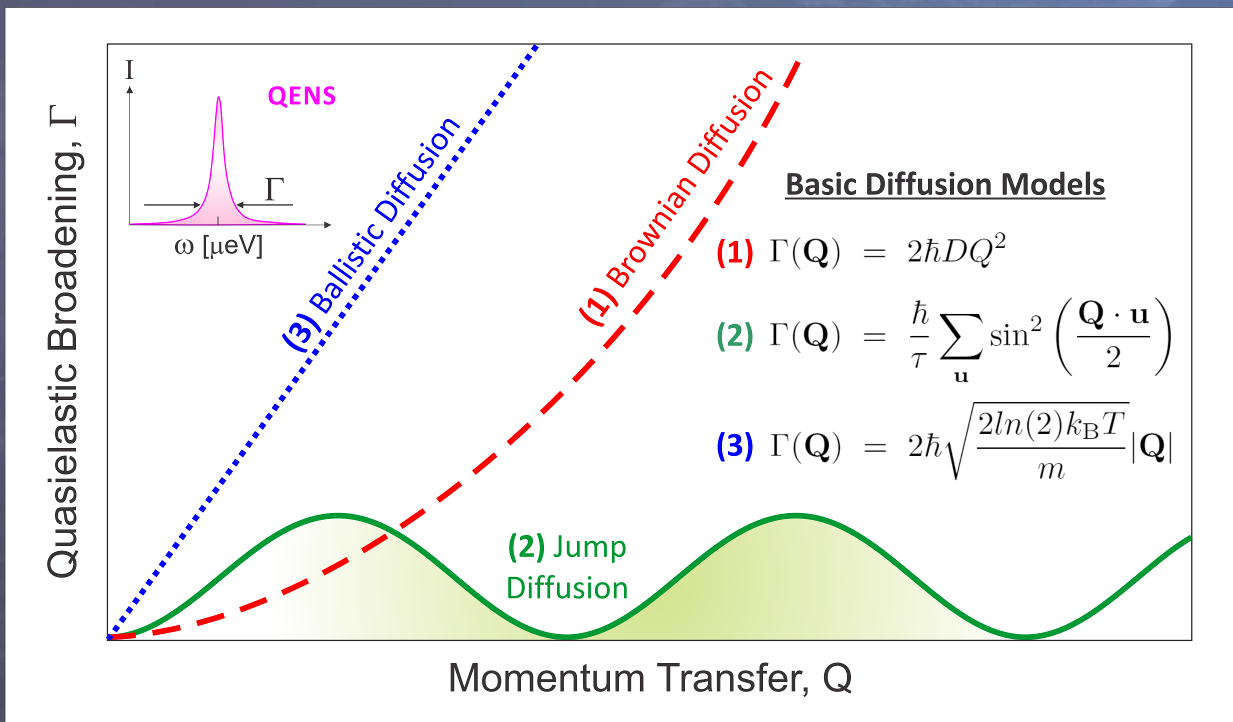
Quasi-Elastic Neutron Scattering (QENS)

- QENS is a ‘sub-genre’ of INS and deals with $\omega_{max} \approx \pm 2$ meV using high-resolution [μeV]
- QENS, however, deals mostly with **incoherent** scattering that gives information on **single particles** due to a distribution in scattering lengths due to presence of several isotopes and/or dynamics (c.f. coherent = spatial correlations and collective motions)



- The QENS signal and its line-width (Γ) supply info on particle/ion/molecular diffusion and/or dynamics on a 0.1–100 nm & ps–ns scale.



- Temperature dependence can give the activation energy (E_a).
- By looking at the Q-dependence of the elastic incoherent signal (structure factor) and Γ(Q) it is possible to deduce the geometry of the diffusion process by fitting (continuous, jump, rotation...).
- Very slow (high-resolution!) → need large (10 grams) samples

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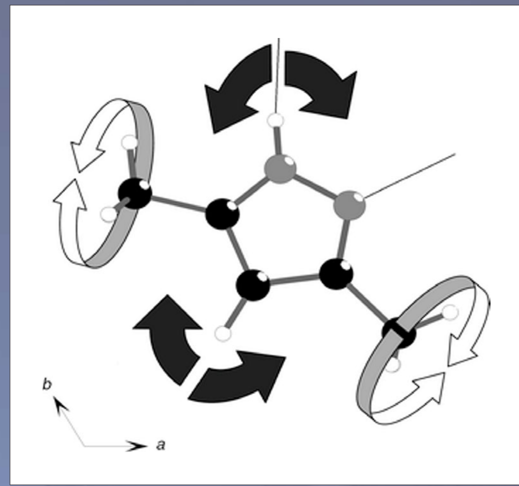
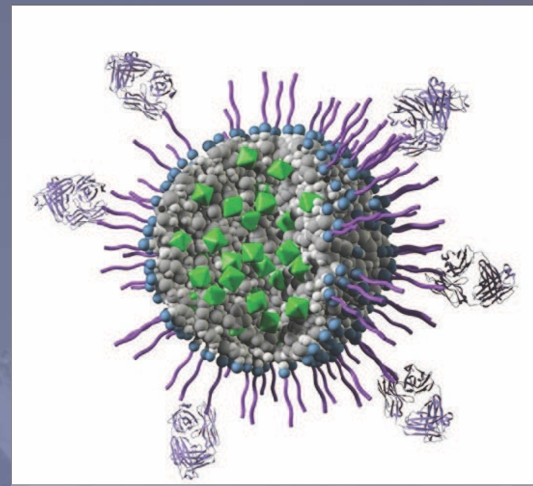
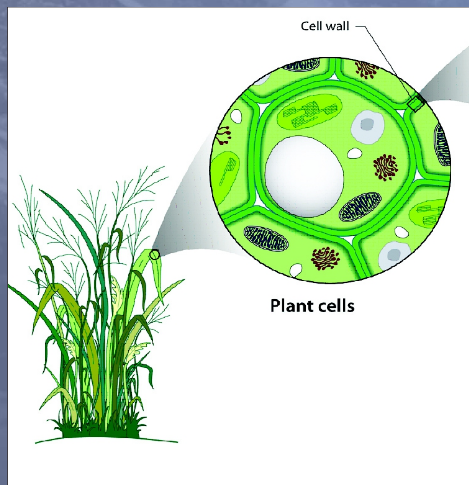
QENS - Examples

- **Molecular dynamics (bond rotations...):**
  - Self-organizing or annealing of polymers
  - Drug delivery systems (confined molecules)
  - Dynamic transitions in proteins

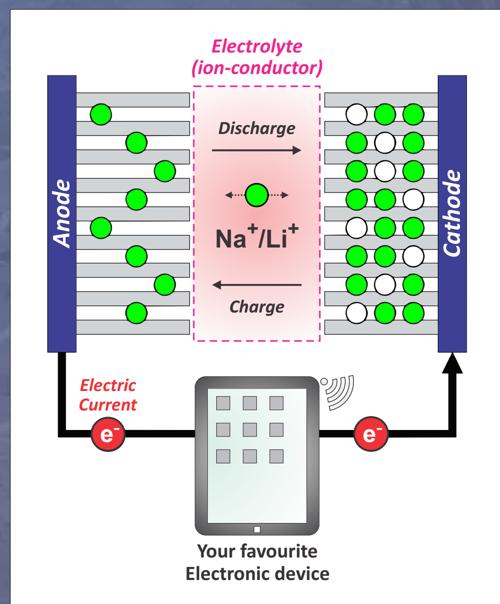


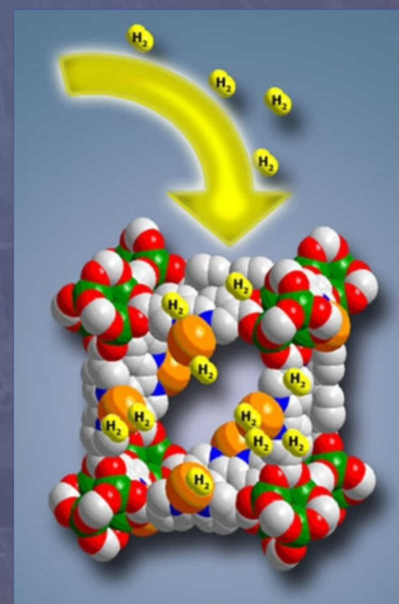




- **Fluid dynamics:**
  - Confined liquid *e.g.* water in wood/plants
  - Complex liquids and clays
  - Melting processes (*e.g* ice/water)

- **Energy materials:**
  - Li/Na diffusion in rechargeable batteries
  - Ion-diffusion in solid electrolytes (fuel-cells)
  - Hydrogen ad-/de-sorpion for H-storage
  - Catalysis reactions





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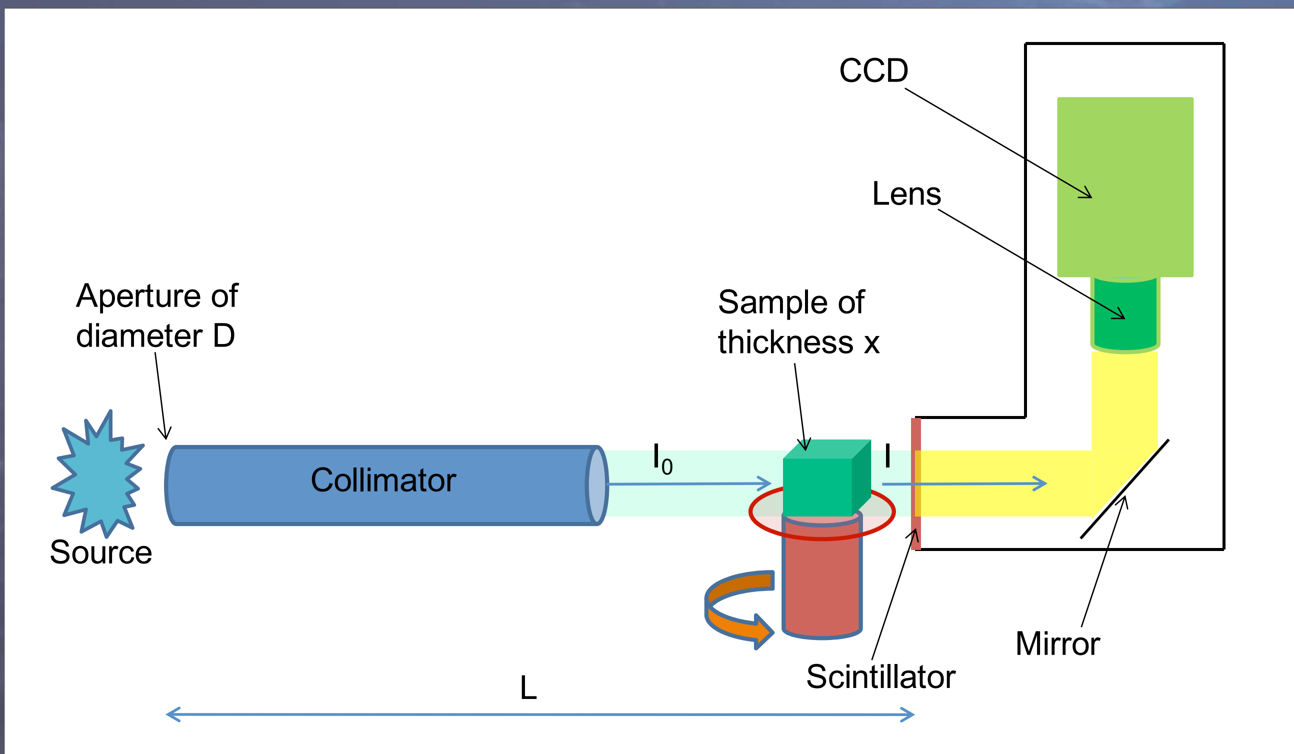
Neutron Imaging

- Similar to an X-ray radiography but technically not a scattering technique
- The resulting image is based on the neutron attenuation properties of the different parts of the imaged object.
- Provide information about the composition and the amount of structure in the sample and changes in them (defects, pores, cracks or inclusions).
- Due to the different interaction mechanism of neutrons and X-rays with matter, neutrons delivers complementary information
- Neutrons provide high contrast for light elements (H, Li, B...) and allow better (than X-rays) penetration of metallic materials.



- Modern CCD cameras allow high-resolution on μm scale
- Stroboscopic measurements allow to study slow dynamics
- Possible to make tomography to obtain a 3D image of the object's internal structure
- Non-destructive testing of large objects!

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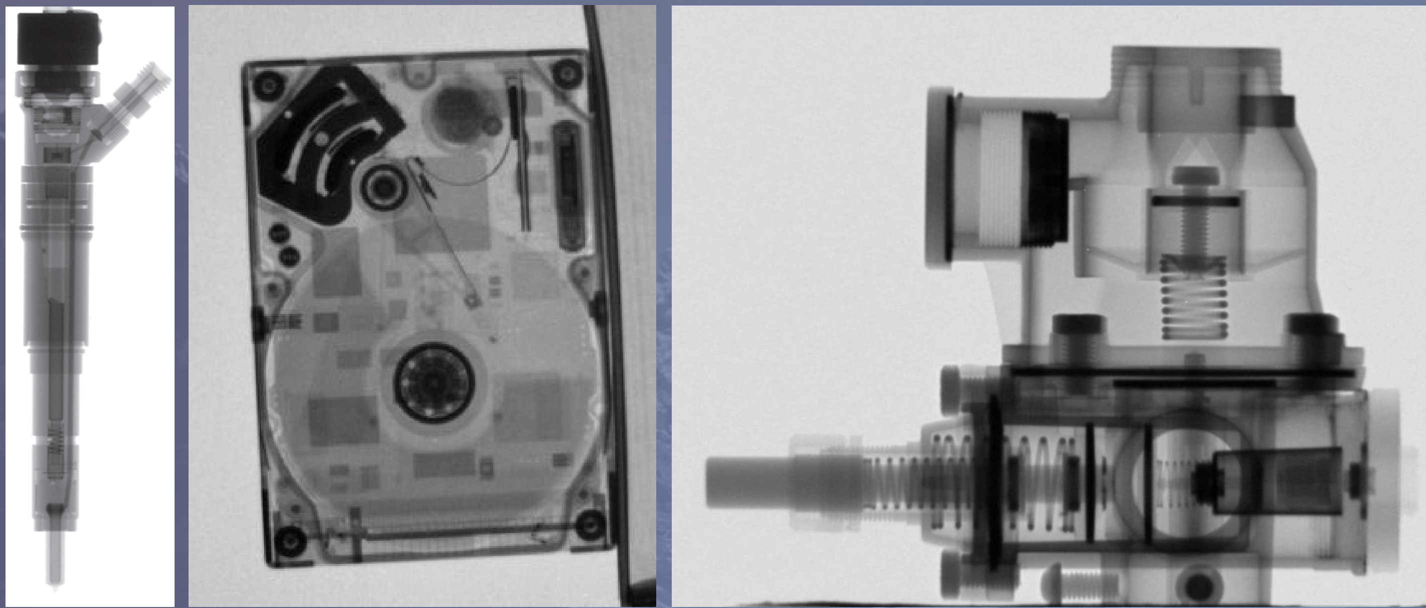
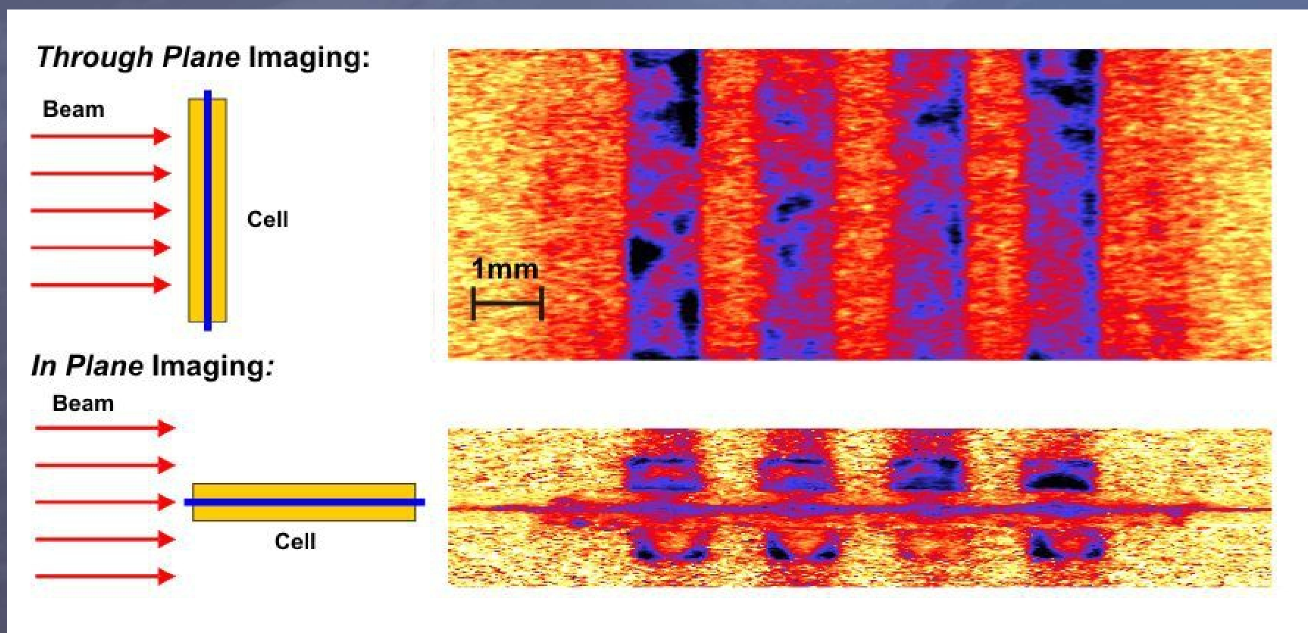
Neutron Imaging - Examples

Non-destructive testing of mechanical components

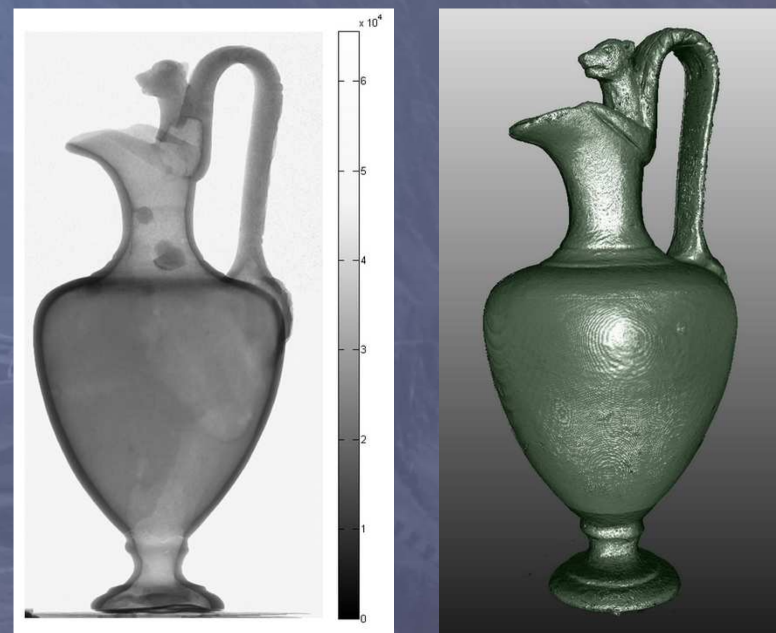


Root-system of plants

Stroboscopic measurement of water distribution in a stacked hydrogen PEM fuel-cell



Radiography / Tomography of archeological artefacts



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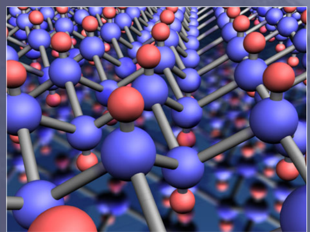
Neutrons & X-rays

- Neutron and X-ray scattering techniques are complementary to each other.
- Together they create a very powerful experimental tool-box for a wide range of research fields.



- Deduce complex crystallographic structures that contains atoms visible/unvisible by X-rays and neutrons, respectively.
- Connection between changes in magnetic spin structure and very subtle structural transitions.
- Contrast variation in imaging/tomography techniques.
- Covering different inelastic energy ranges for excitation studies using INS and RIXS.

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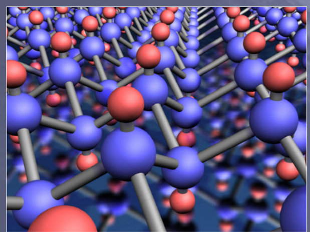

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How to Practically do Neutron Experiments

- Have an idea for how neutrons can help your research
- Talk to an expert (*e.g.* send me an e-mail: condmat@kth.se)
- Consider your sample!!! (available size/mass, crystal/powder/thin film).
- Think about if you sample contains elements with low scattering or high absorption
  http://www.ncnr.nist.gov/resources/n-lengths/
- Select appropriate source and instrument for your experiment (check deadlines!)
- Contact instrument responsible to discuss experiment (before you submit proposal!)
- Write a proposal and apply for beamtime at your selected neutron source/instrument
- Cross your fingers and wait for the review committee + in some cases ”national quota”
- If you obtain beamtime start to prepare your experiments well advance
  (align crystals, manufacture sample holders etc.)
- Check necessary paperwork at source and perform the mandatory ”safety training”
- If you plan to do experiments at different sources with same samples: consider activation of your samples (active sample transport is complicated and expensive!)

Neutron Sources of the World

EUROPE

ILL, Grenoble, France
LLB, Saclay, France (...2019 !!!)
FRM-II
ISIS, Didcot, UK
SINQ, PSI, Switzerland
IFE, Kjeller, Norway
ESS, Lund, Sweden (2019...)

Other Examples

HFIR/SNS, Oak Ridge, USA
J-PARC, Japan
ANSTO, Bragg Institute, Australia

http://www.neutrons.se/

http://www.neutronsources.org/

http://www.ncnr.nist.gov/nsources.html

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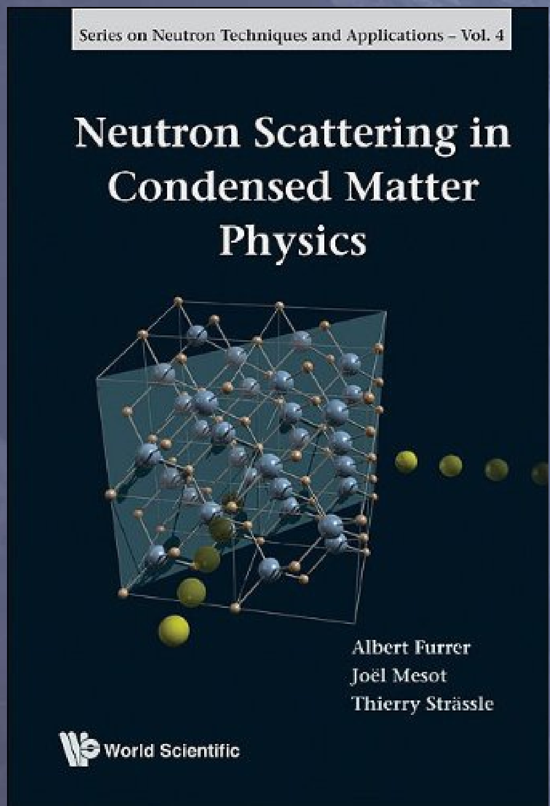
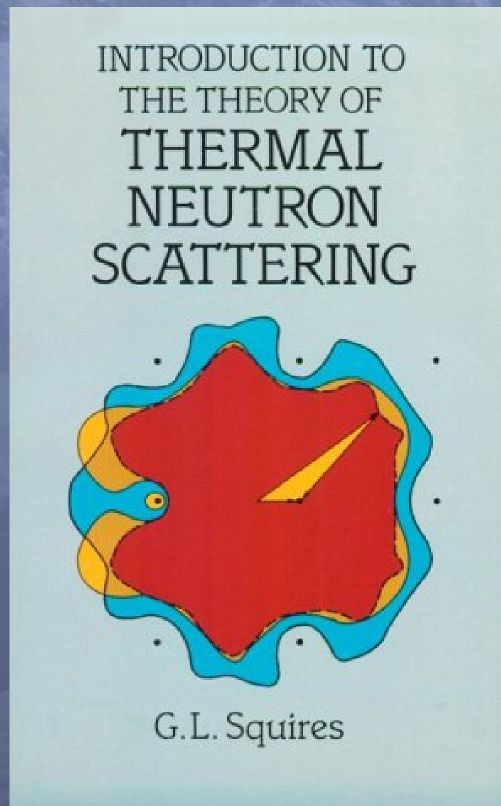
Neutron References

http://www.neutrons.se/

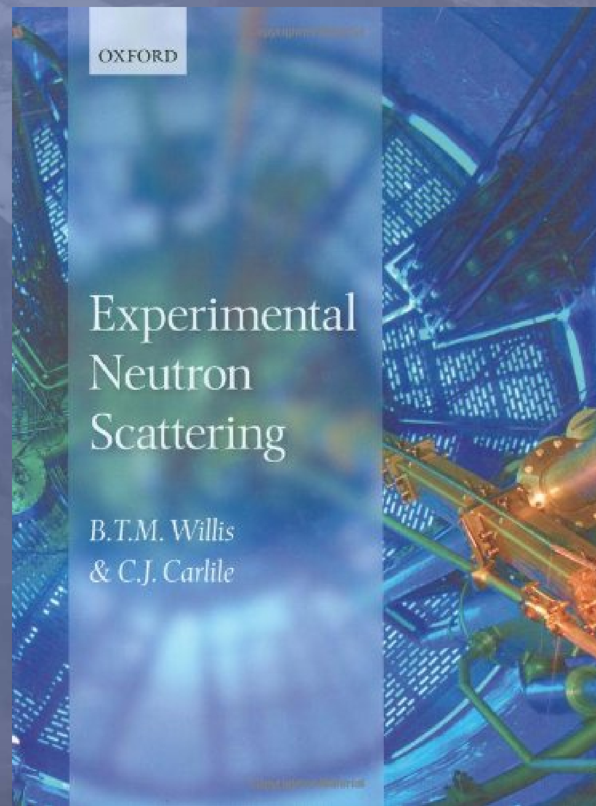
Lecture series given by Prof. Roger Pynn, Indiana University, USA
https://www.indiana.edu/~sesame/WebSite/TeachingResources.html



"Neutron Scattering in Condensed Matter Physics"
A. Furrer, J. Mesot, T. Strässle



"Introduction to the theory of thermal neutron scattering"
G. L. Squires



Experimental Neutron Scattering
Willis and Carlile


Thank You for your attention !!!
:Månsson Design™