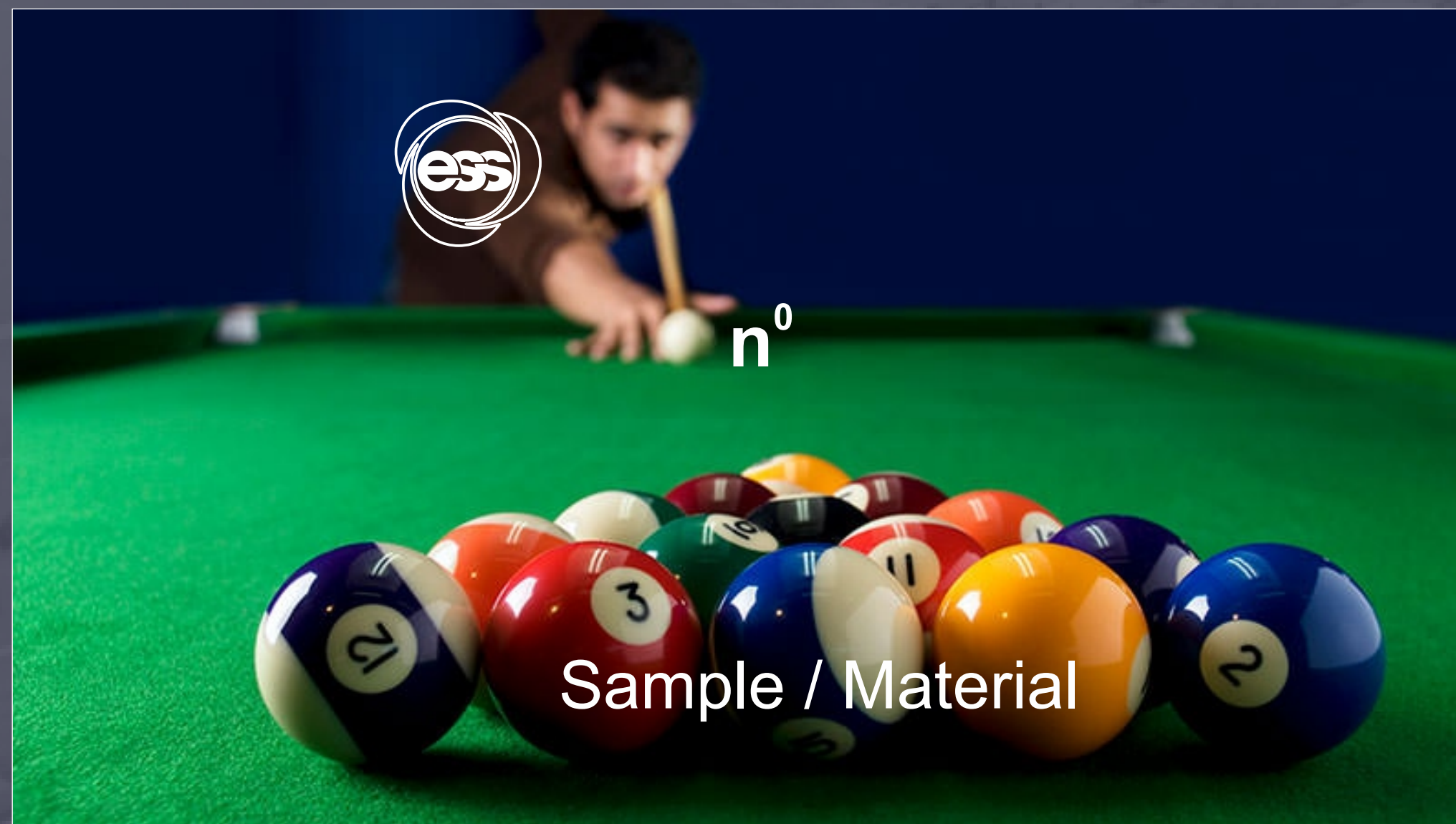


Basic Introduction to Neutron Scattering



Prof. Martin Månsson
Director of Studies, SwedNess

Department of Applied Physics
KTH Royal Institute of Technology
Stockholm, Sweden



Why Learn Neutron Scattering?

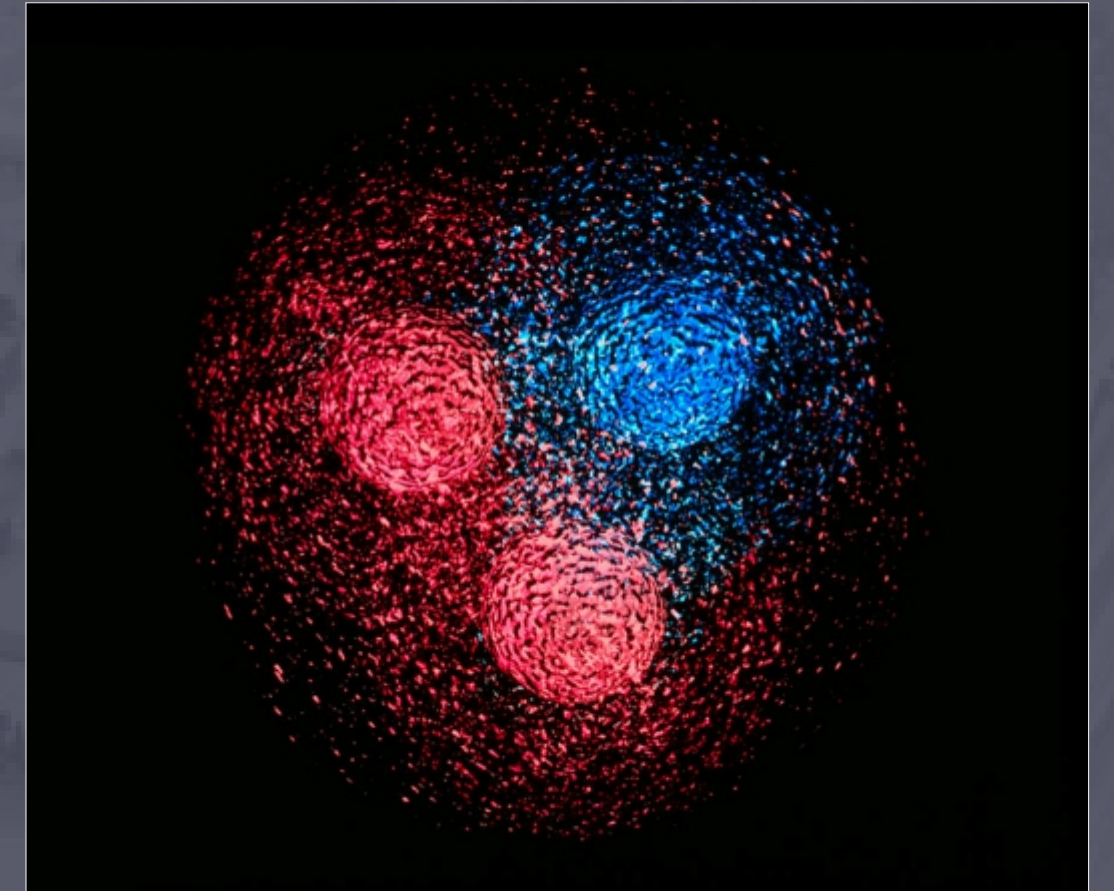
- Neutron scattering is one of the most **versatile experimental techniques** and is a useful tool for a broad range of scientific fields (materials science, condensed matter physics, chemistry, biology, engineering, energy, ...)
- Many **material properties** can not be measured in any other way and 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 everyday devices are using more complex materials i.e. NS is an invaluable tool for future applications (spintronics, green construction materials, energy cells, medical implants, catalysis...)
- Sweden hosts the state-of-the-art **European Spallation Source (ESS)**, which will be the leading neutron source in the world.
- From ~2025 there will be excellent **possibilities** for young scientists & industry to perform world-leading science & developments.



What is a Neutron (n^0)?

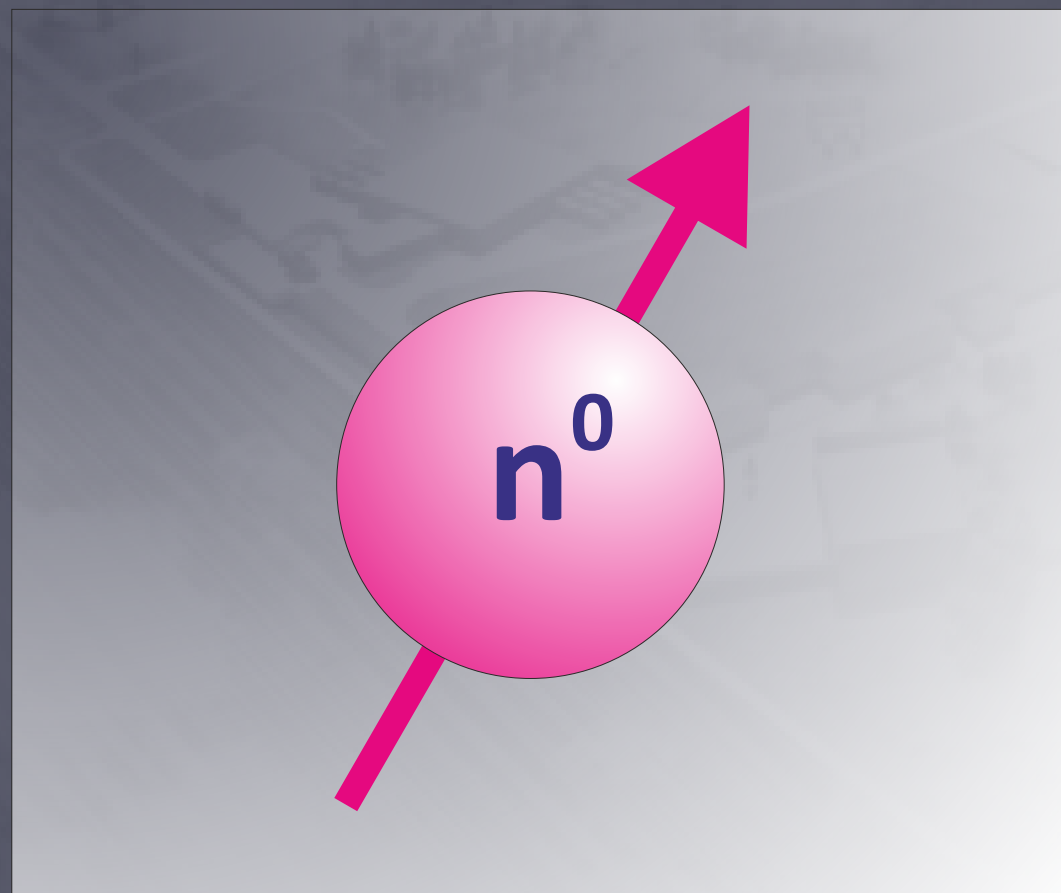
For particle physicists:

- 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 $S = \frac{1}{2}$ particle used as an optimal tool to investigate microscopic / macroscopic materials / device properties.
- “Can show where atoms are and what they do” + **magnetism**



Neutron Properties

NEUTRAL

Charge = 0 → infinitely small electronic dipole moment, neutrons do not see charge!

HAS A SPIN

$S = 1/2$ → Initial state can be polarized & polarization of the final state can be analyzed!

HAS A MAGNETIC MOMENT

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

RATHER STABLE

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

VERY SMALL

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

'IDEAL' MASS

$m_{n0} = 1.675 \times 10^{-27}$ kg $\approx m_{p+} \approx 1840 \times m_{e-}$

PARTICLE- & WAVE-LIKE PROPERTIES

Dispersion relation: $E = \hbar^2 k^2 / 2m \rightarrow \dots$
 $\lambda = 5 \text{ \AA} \rightarrow E = 3.3 \text{ meV}$

'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 i.e. condensed matter physics !!!

A Scattering Experiment

Probe-
Source

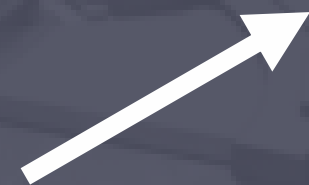


Initial
State

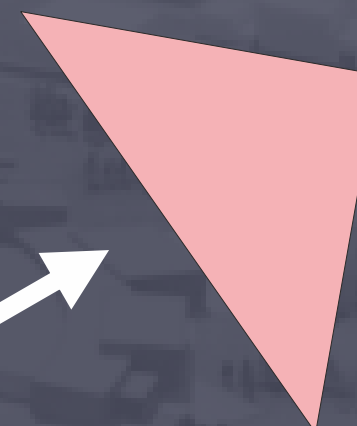
*Interaction
(Scattering)*



Final
State



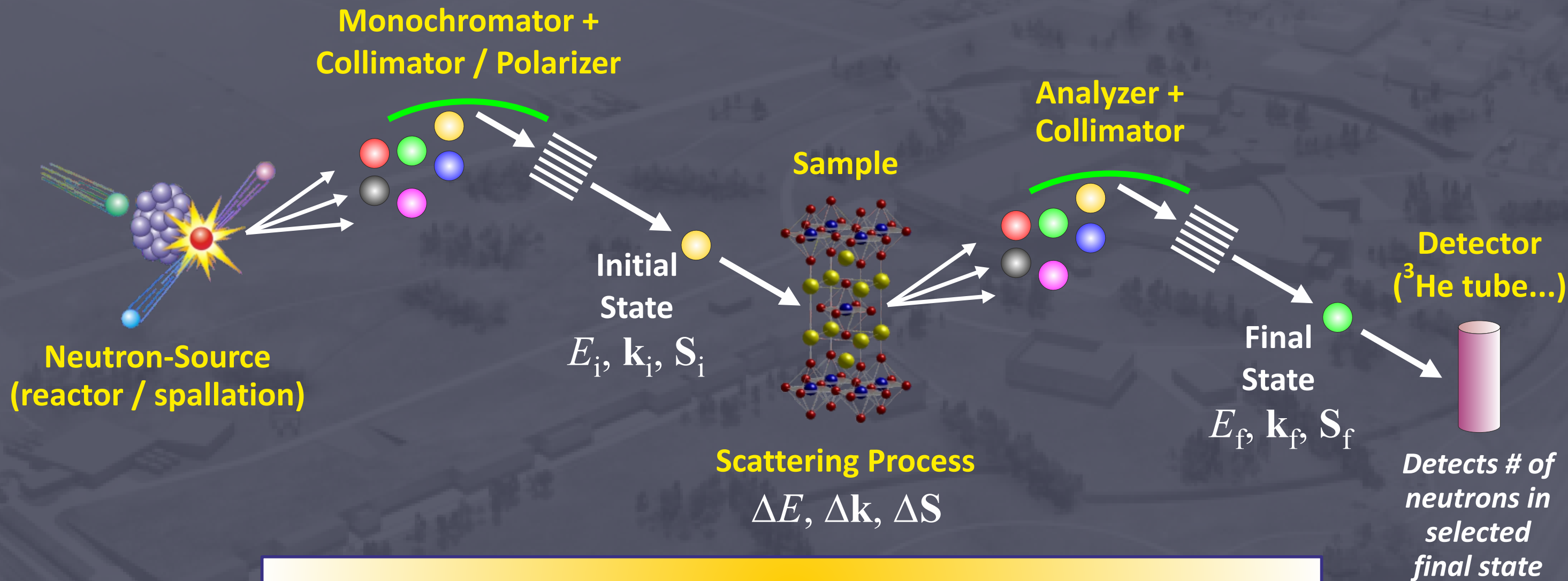
Detector of
final state



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

The 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



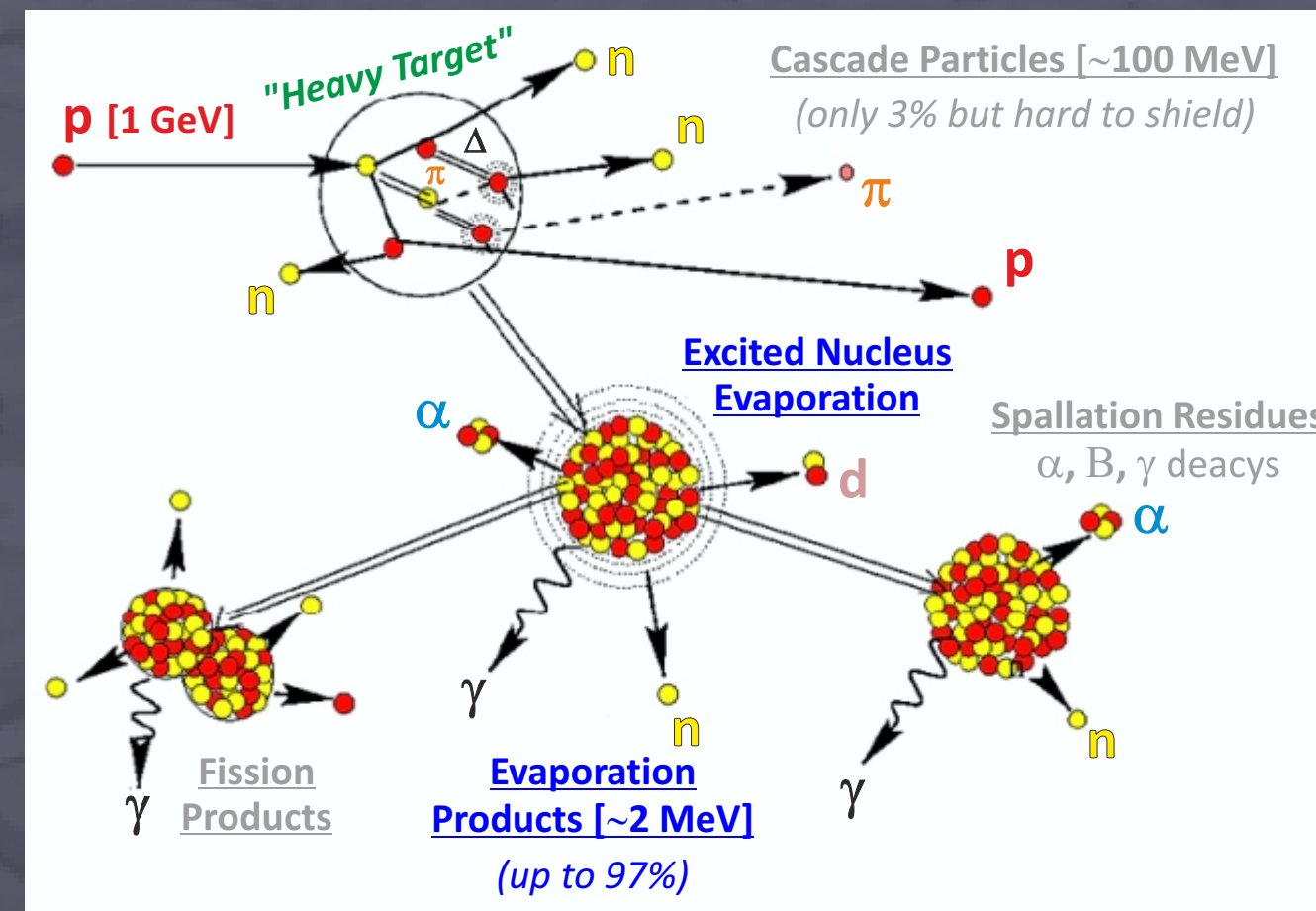
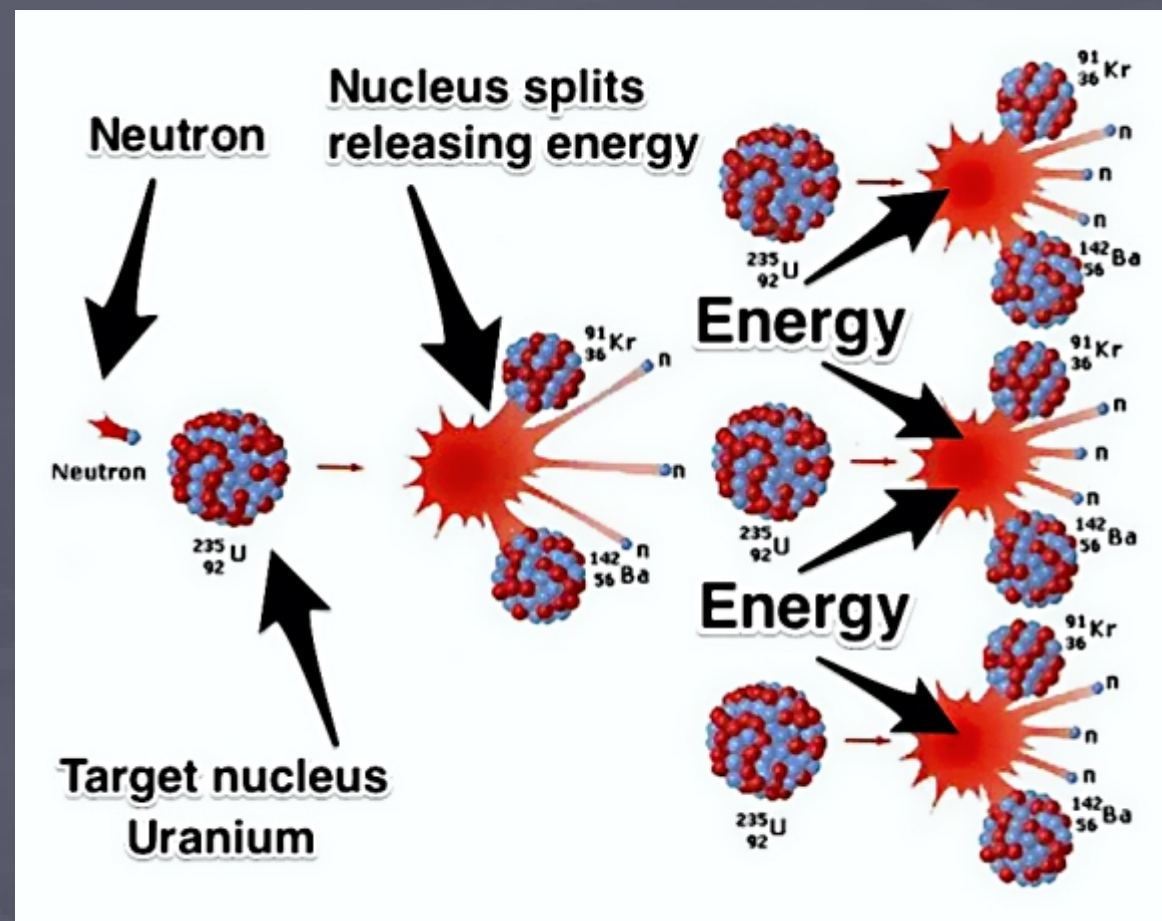
Unfortunately, most neutrons are wasted... twice → ESS !!!

- Traditionally (continuous 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.

Neutron Production

Soon to be the past
Reactors (fission)

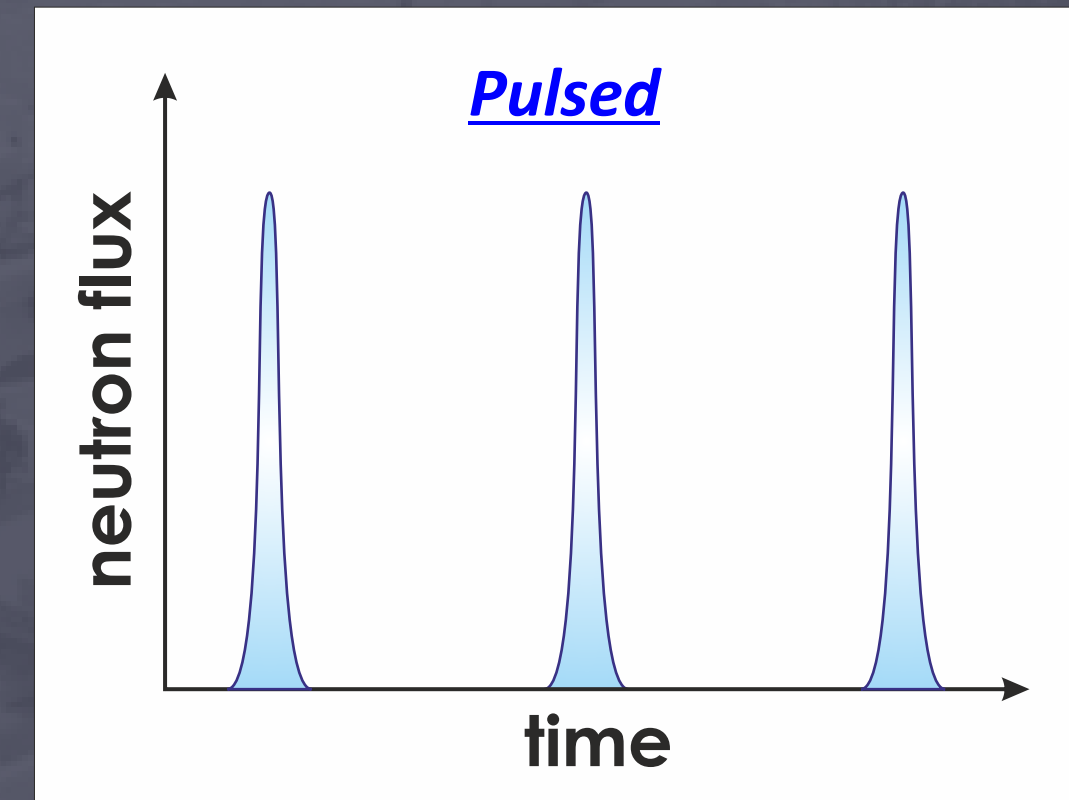
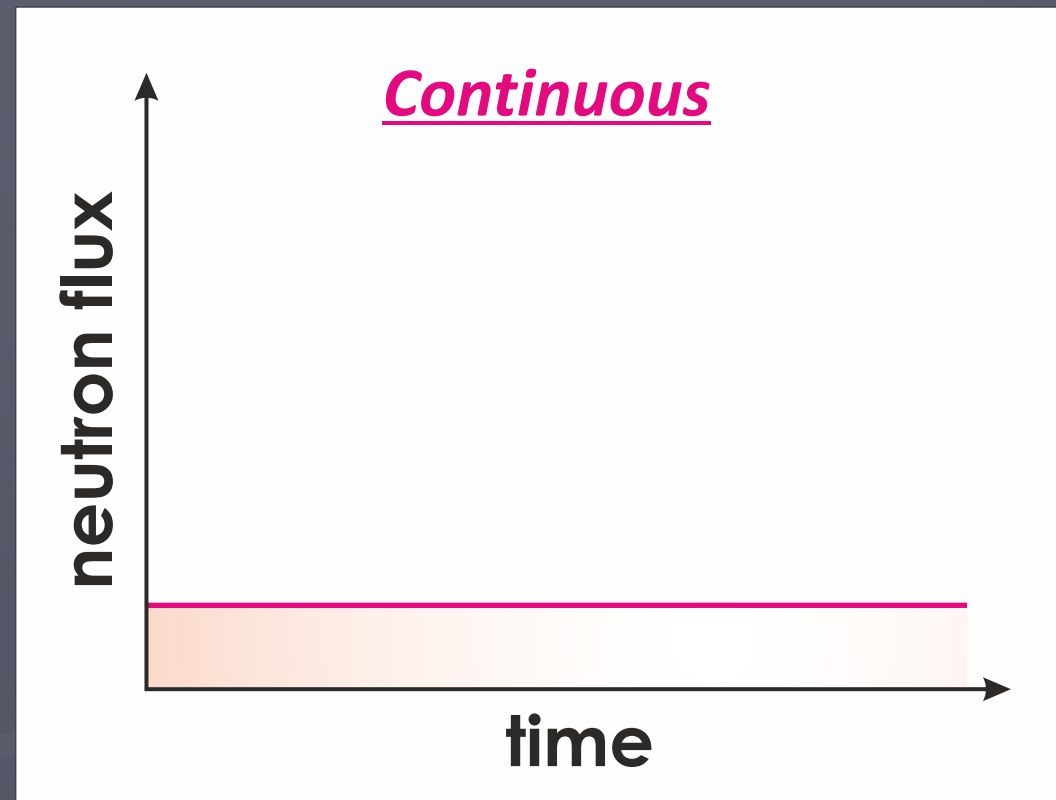
Future already here
Spallation Sources



- Energy per neutron ~180 MeV
- High and continuous flux
- Waste a lot of neutrons in ToF
- Rare beam down, but if...
- Safety / Politics complicated

- Energy per neutron ~20 MeV
- 10 times higher brightness / unit heat
- "External power source" needed
- Beam dumps but quicker recovery (?)
- Safety / Politics much easier

Continuous vs. Pulsed Sources

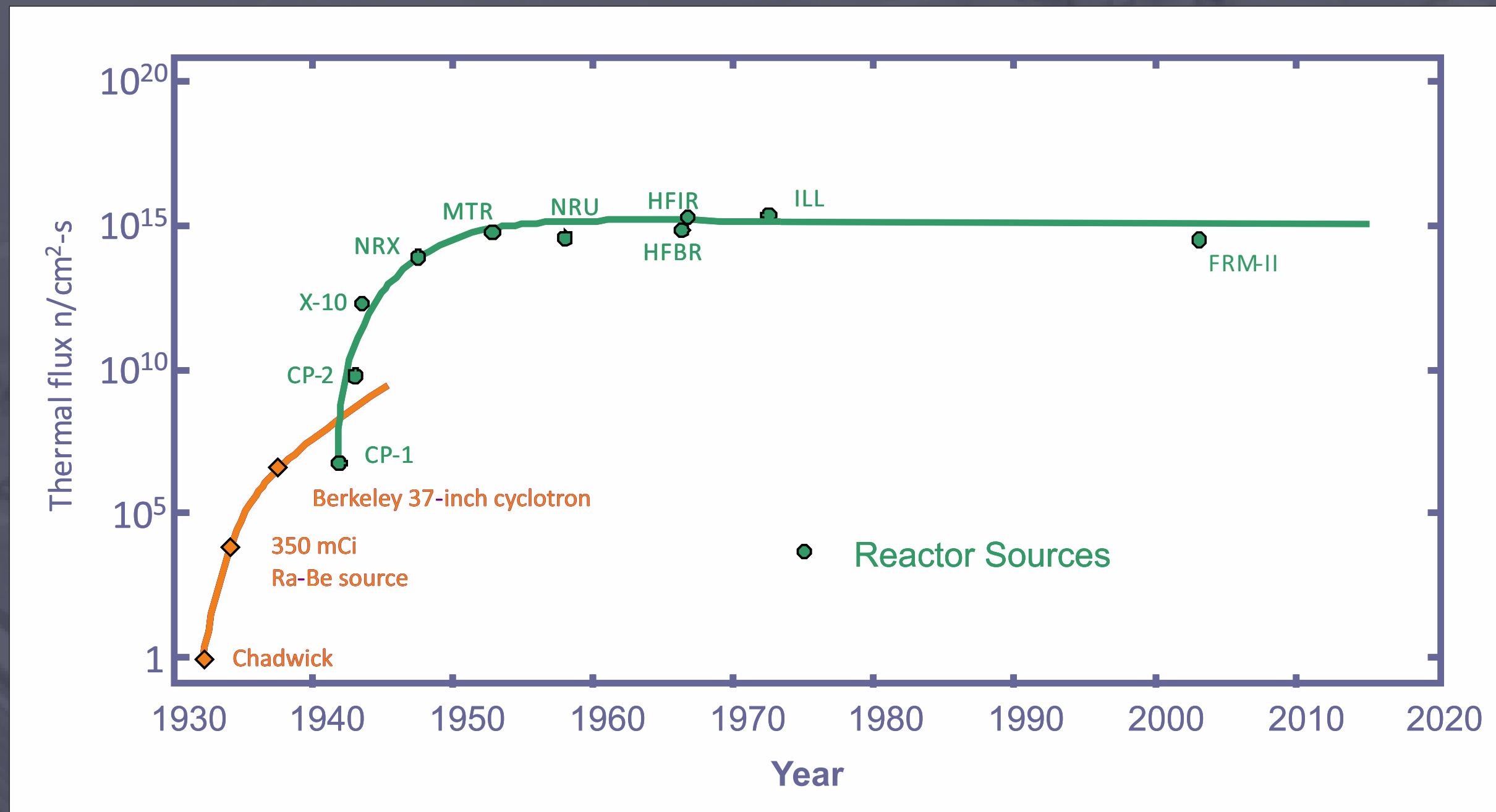


- Optimized for average flux
- Good enough for most applications
- Fission neutrons easier to shield
- Easy to build compact and simple instruments
- Simple electronics / data
- **Tried and tested ('Old School')**

- Optimized for peak flux and pulse shaping
- Better for most applications
- Cascade neutrons hard to shield
- Instruments long, advanced and expensive
- Very fast electronics and huge data sets
- **Still developing ('The Future')**

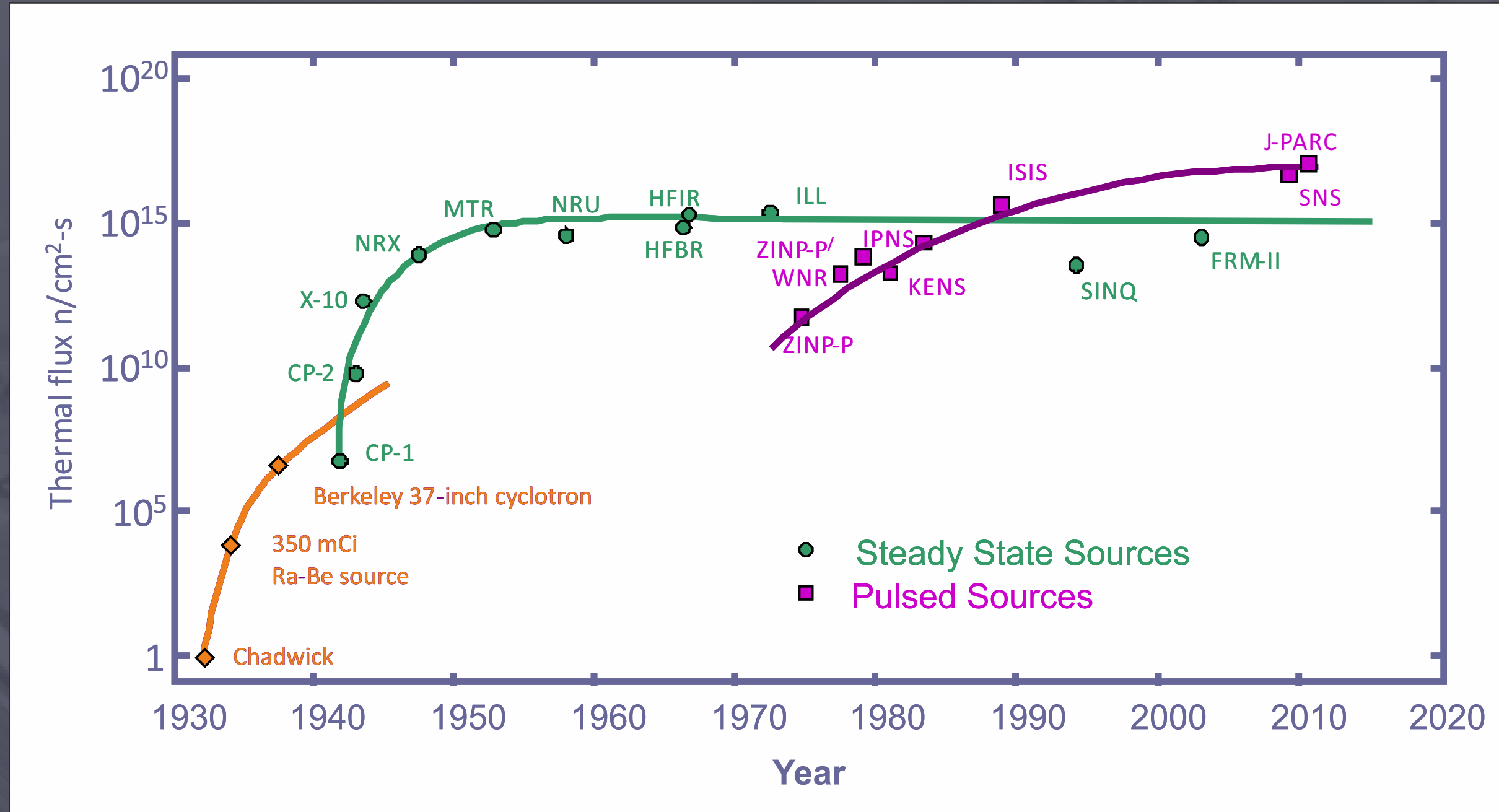
Historical Source Development

- Traditional reactor sources have reached a plateau since many years



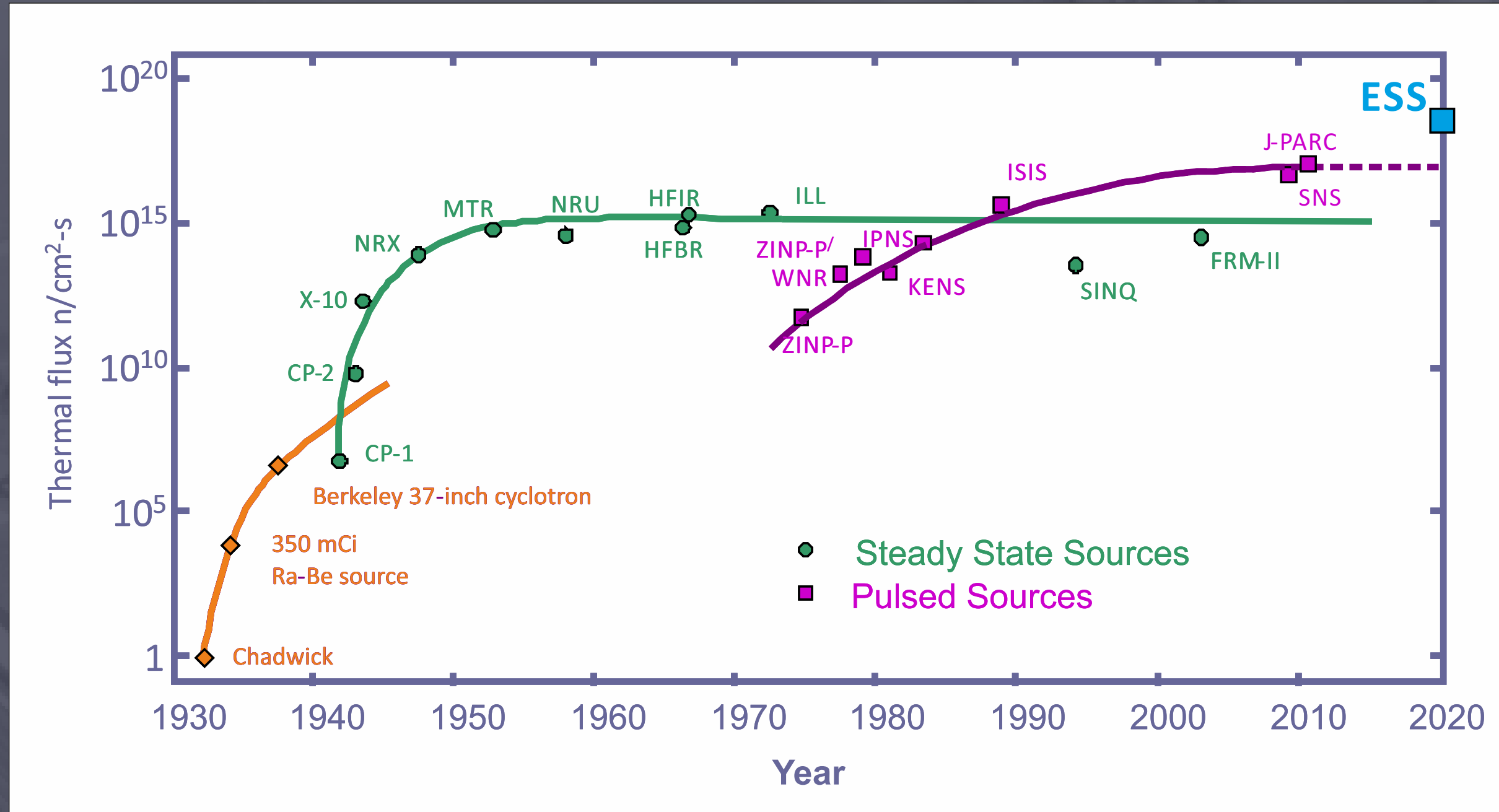
Historical Source Development

- Traditional reactor sources have reached a plateau since many years
- Also pulsed spallation sources have had the same development



Historical Source Development

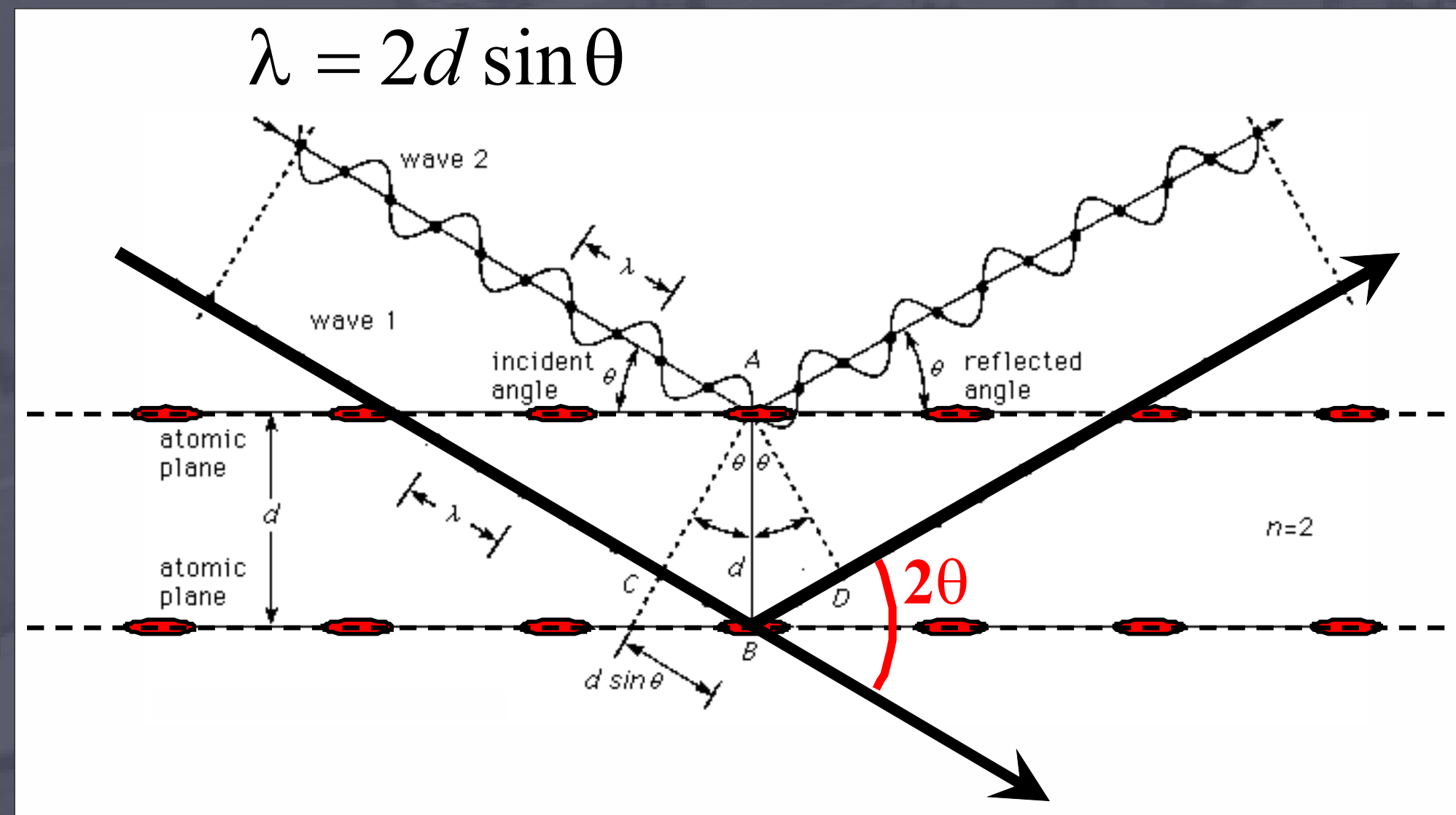
- Traditional reactor sources have reached a plateau since many years
- Also pulsed spallation sources have had the same development



- Hope surpass such trend with new technological developments at ESS !!!

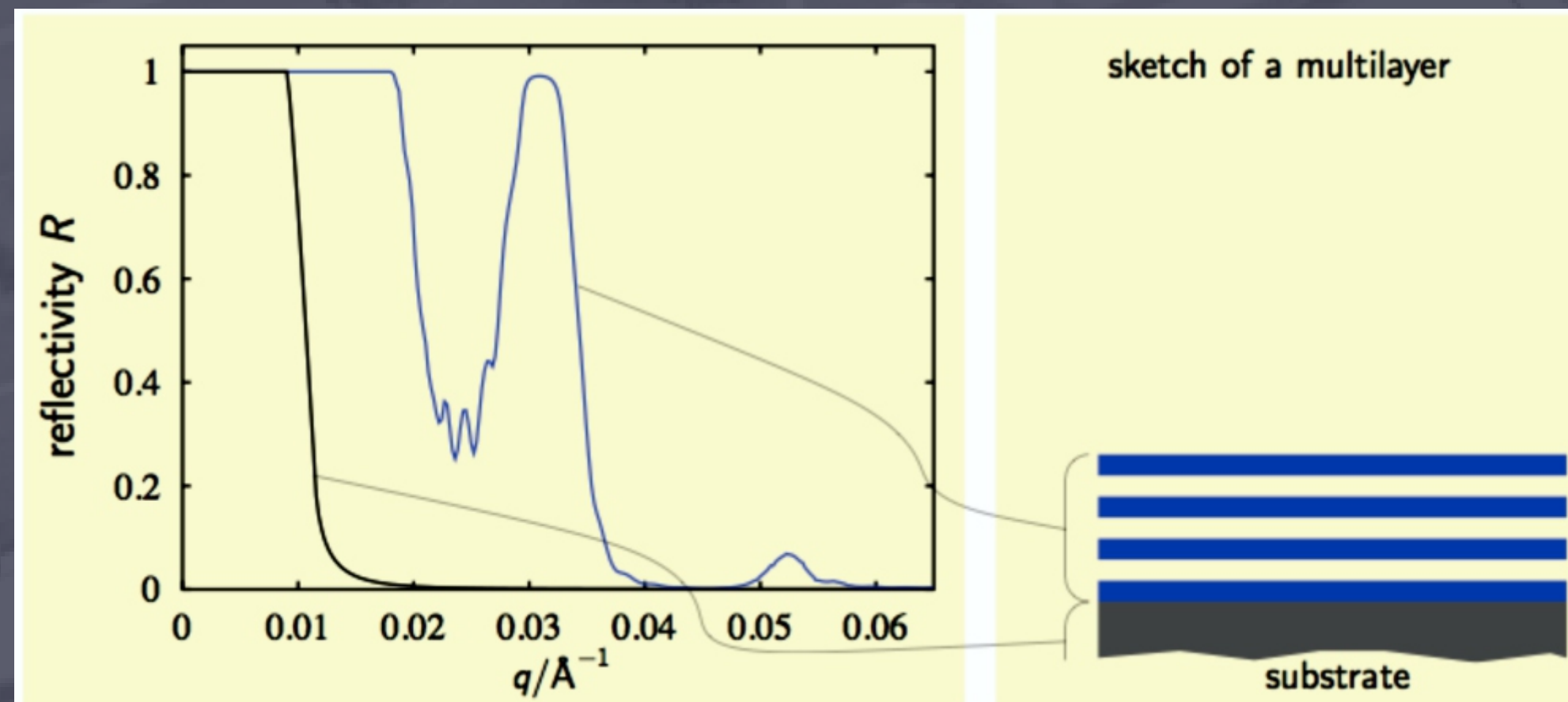
Neutron Guides

- Neutrons are neutral i.e. they are hard to manipulate
- However, neutrons can scatter e.g. on atomic planes (**Bragg's Law**)



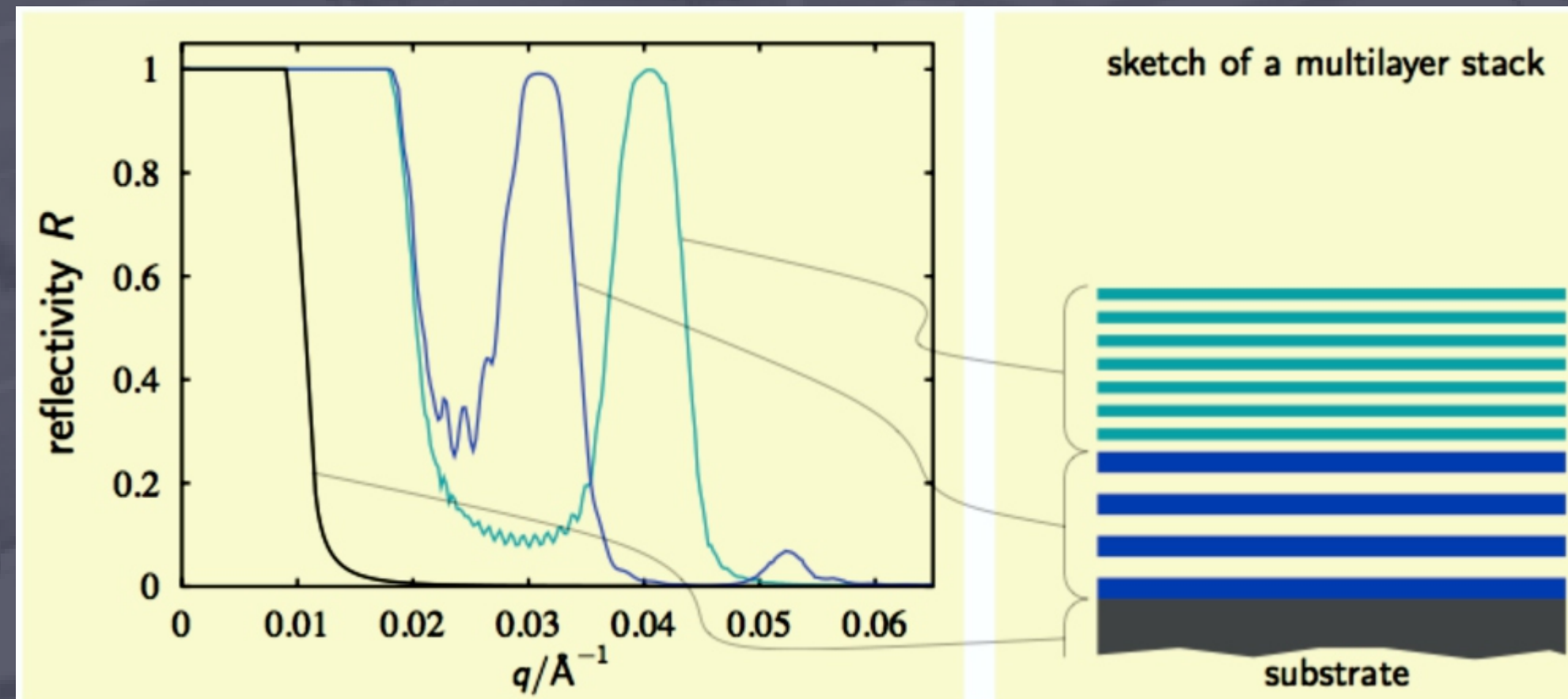
Neutron Super Mirrors

- Use "artificial atomic planes" i.e. grow thin film multi-layers in order to guide the neutrons.
- Alternating layers of "transparent" (Ti) and reflecting (Ni) materials
- One set of multi-layers only scatter (reflect) a certain range of neutrons.



Neutron Super Mirrors

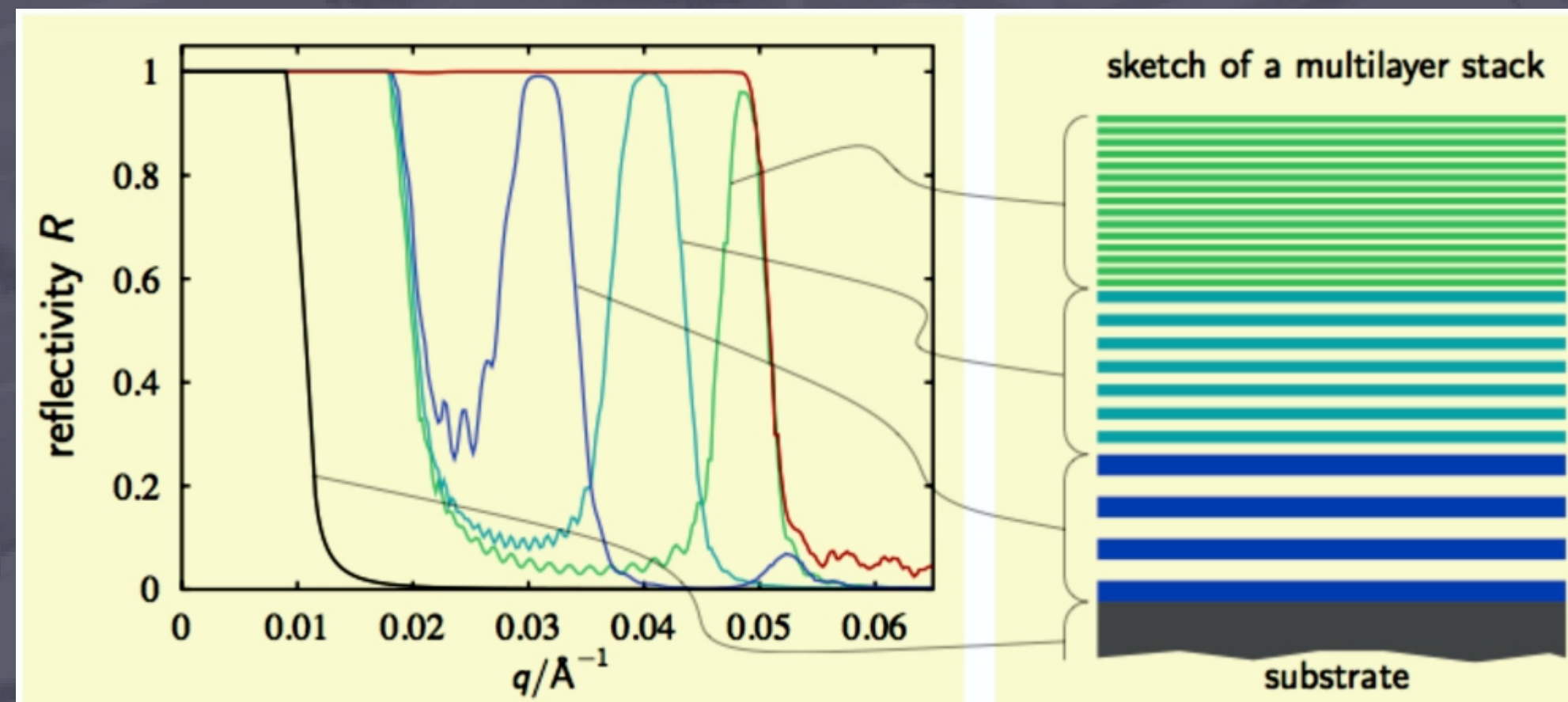
- Use "artificial atomic planes" i.e. grow thin film multi-layers in order to guide the neutrons.
- Alternating layers of "transparent" (Ti) and reflecting (Ni) materials
- One set of multi-layers only scatter (reflect) a certain range of neutrons.



- So we grow several different multi-layers on top of each other in order to guide a broader band-width of neutrons.

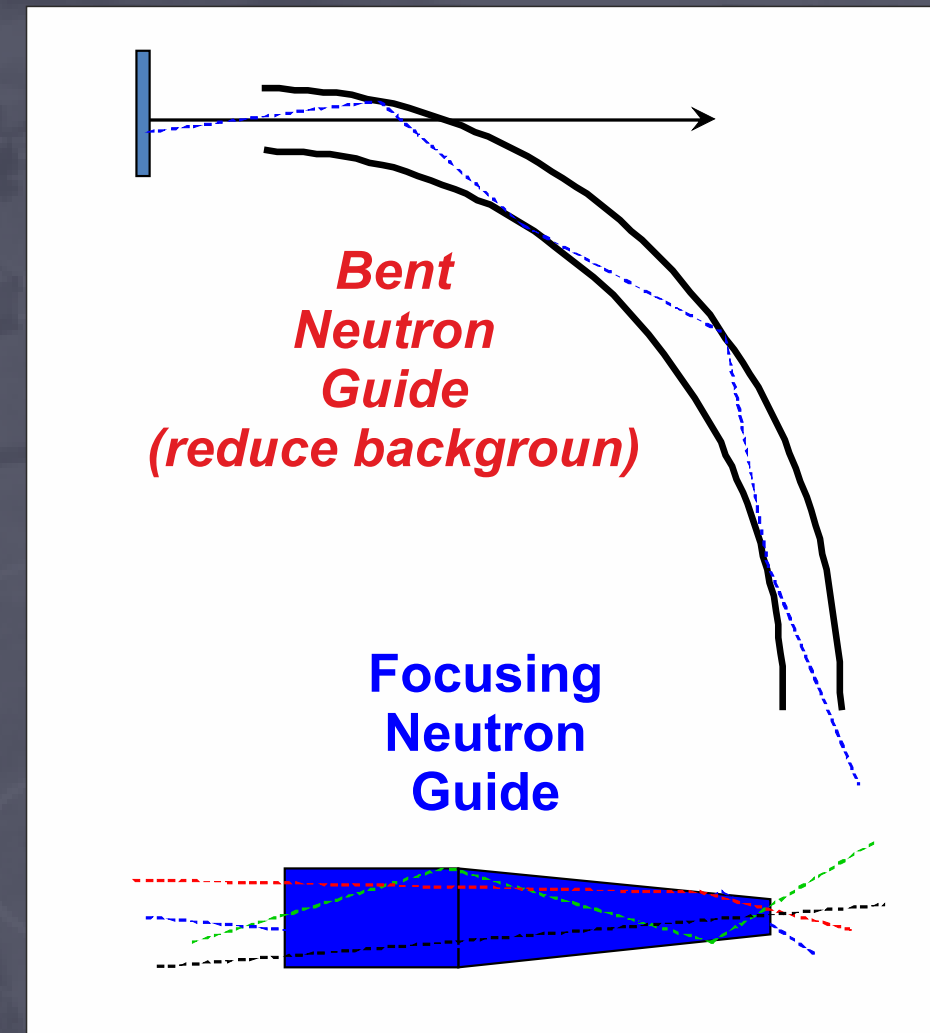
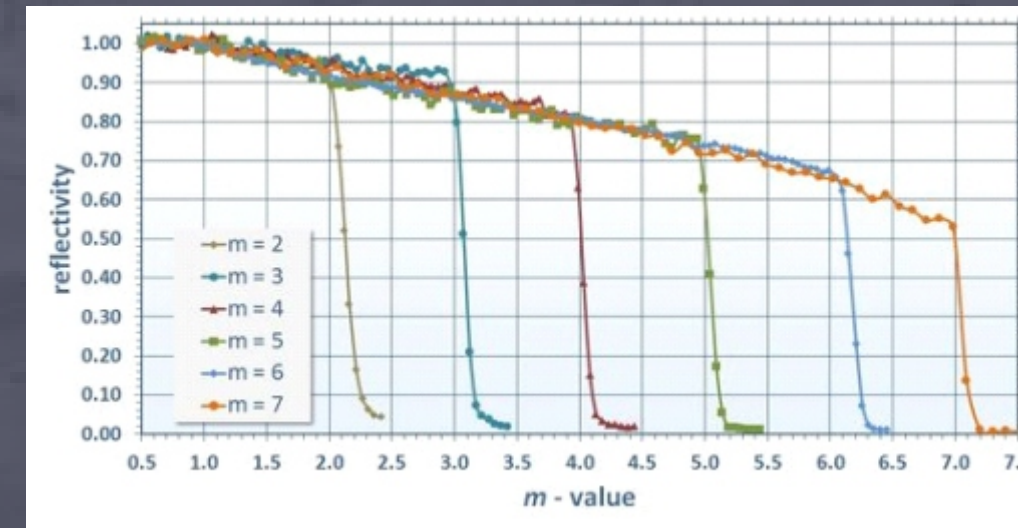
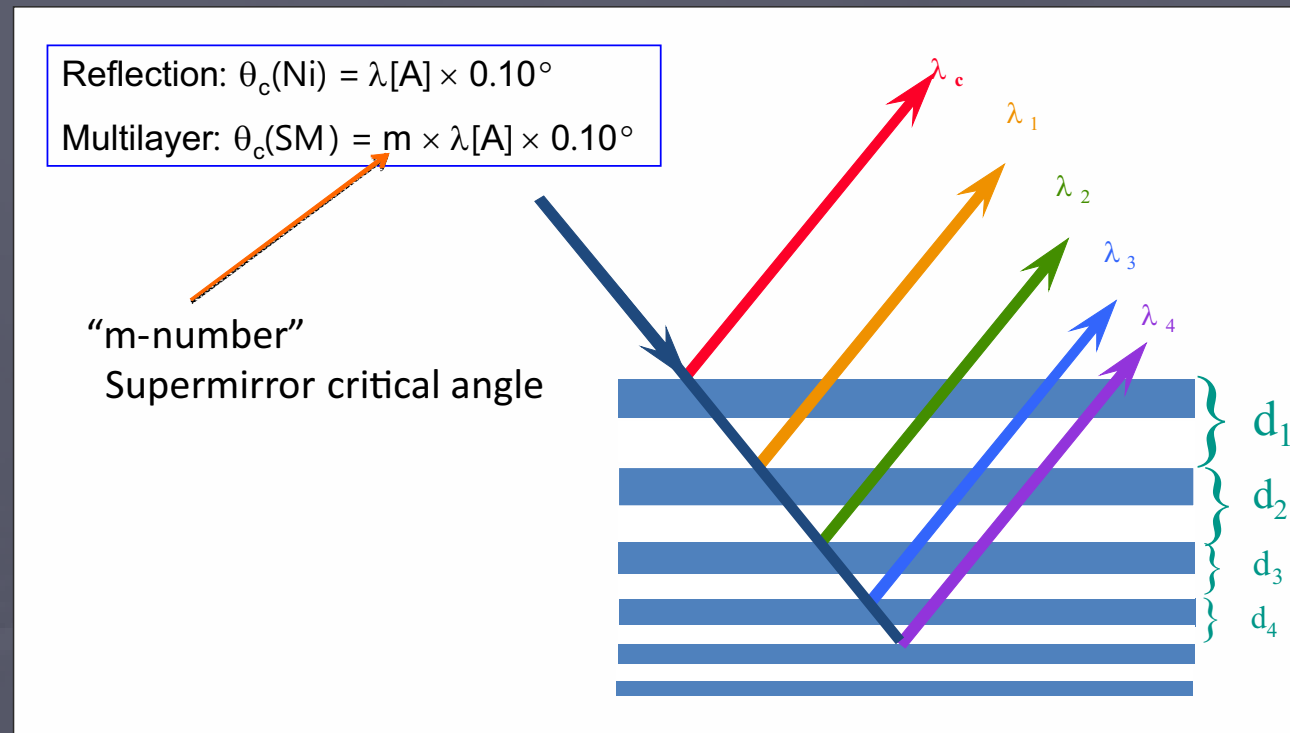
Neutron Super Mirrors

- Use "artificial atomic planes" i.e. grow thin film multi-layers in order to guide the neutrons.
- Alternating layers of "transparent" (Ti) and reflecting (Ni) materials
- One set of multi-layers only scatter (reflect) a certain range of neutrons.



- So we grow several different multi-layers on top of each other in order to guide a broader band-width of neutrons.

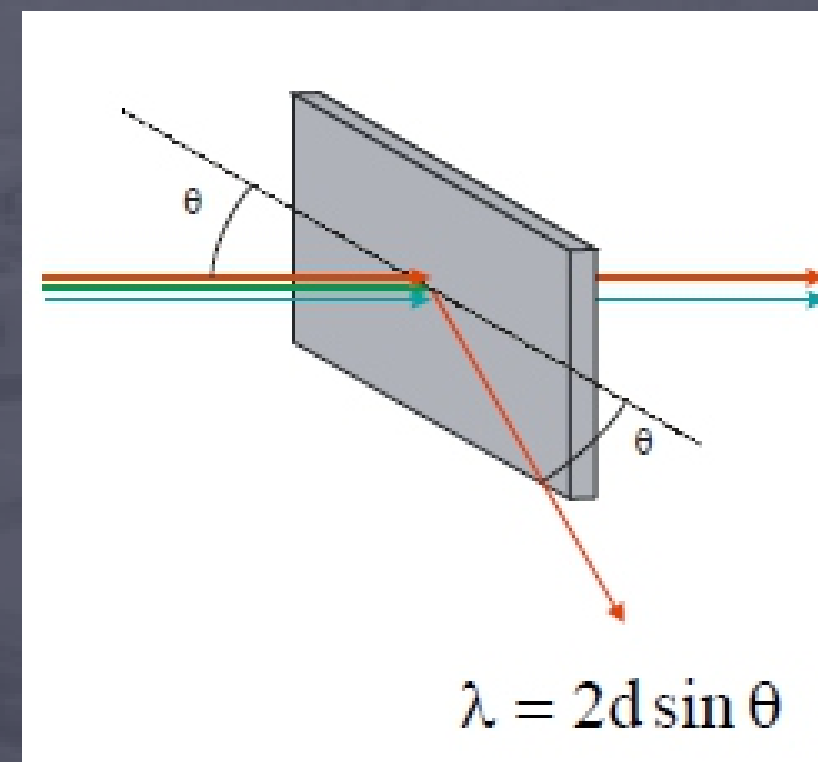
Neutron Super Mirrors



- Neutron guides can also be focusing, "bending" (to reduce background) or even polarizing!

Defining E: Crystal Monochromators

- Same idea as supermirrors but use single crystals of pure materials.
- Several very careful co-aligned crystals are put together into a monochromator.
- Angle and crystal type selects the outgoing neutron energy
- Can be made to also focus the beam.

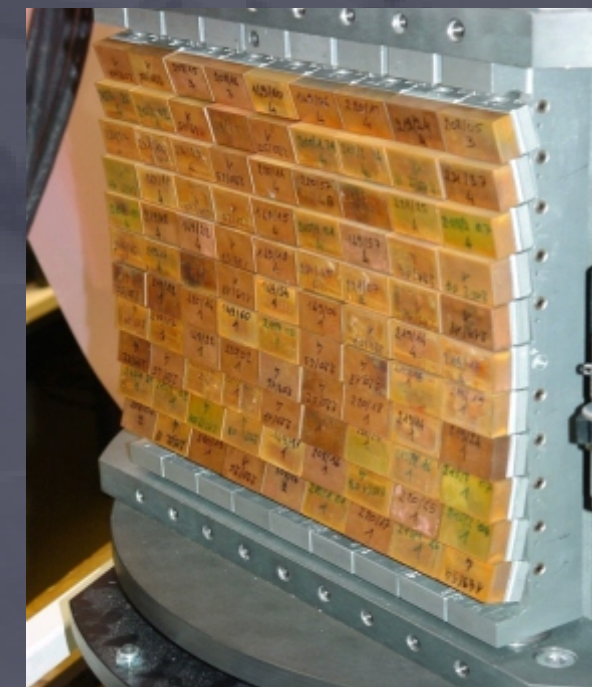


Material	d-spacing
Ge [333]	1.089 Å
Be	1.79 Å
Cu [200]	1.807 Å
Si [111]	3.14 Å
Graphite/PG [002]	3.355 Å
Mica [002]	9.98 Å

Graphite [002]



Copper [200]



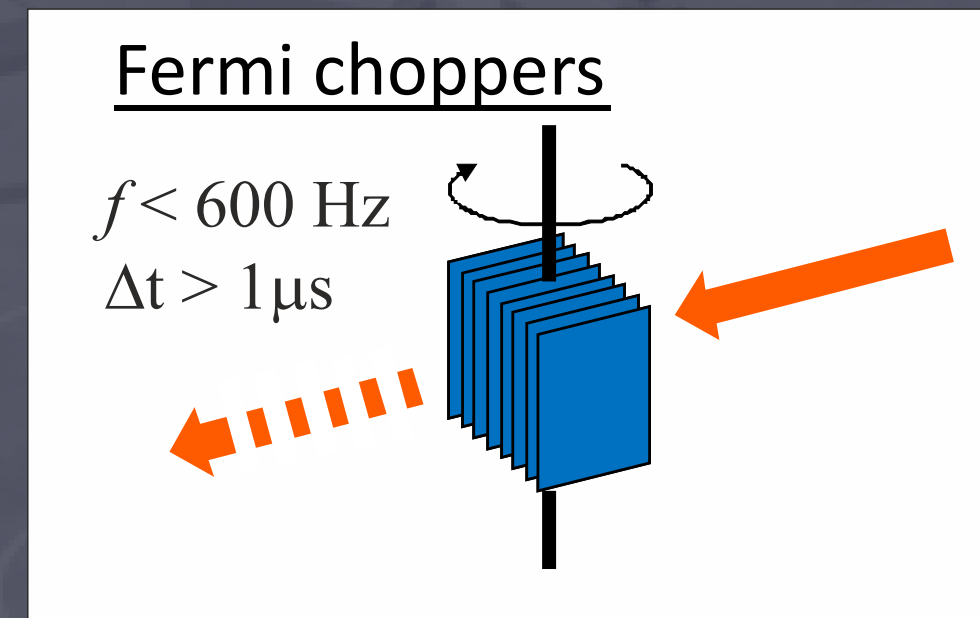
- Mainly used in the "old type" of reactor/continuous neutron sources.

Defining E/t : Neutron Choppers

- Another way to select neutron energy is to use so-called **choppers**.
- Simplest form is a spinning disc made out of a neutron absorbing material with a gap that works as a velocity selector.

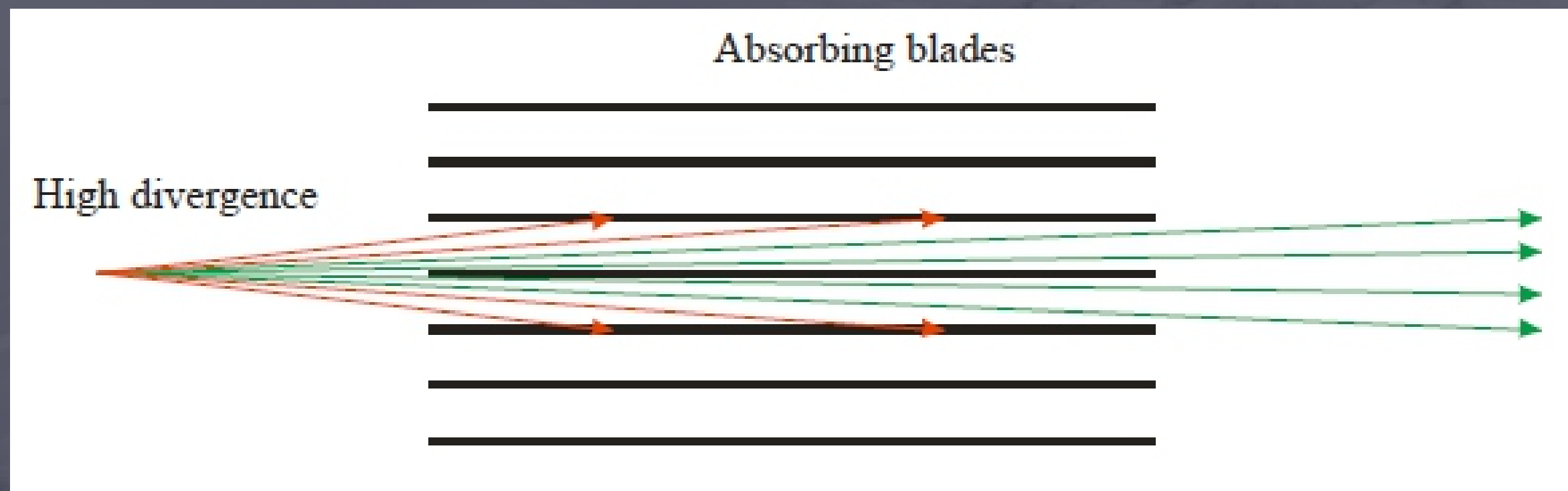
Choppers =  velocity selector

- Combining several choppers and controlling both their individual speed and phases allow to choose a narrow energy range (or several overtones)
- There are several other more complex chopper designs allowing to "shape" the neutron beam even more carefully.
- Can be used at any type of source but of course much more efficient for pulsed sources where "time = energy is used"
- ESS will have MANY MANY MANY choppers installed... will explain why a bit later in this lecture...



Defining "direction": Collimators

- Slit collimators: of Al-plates with neutron absorbing coatings e.g. Gd



- Defined how accurate they are by 'minutes' (lower is better but more neutrons are lost = **no free lunch!**)
- Previously changed by hand, but now often controlled by motors/mechanics
- Also have radial collimators to avoid scattering from cylindrical sample environment (cryostats, magnets...)

Detecting the Neutrons

- Neutral particle = hard to detect \Rightarrow Need nuclear reaction.
- Two "old" technologies (^3He is most common):

^3He Tubes



> 1mm resolution

High Efficiency

Low gamma sensitivity

Supply/cost problem!!!



Scintillators

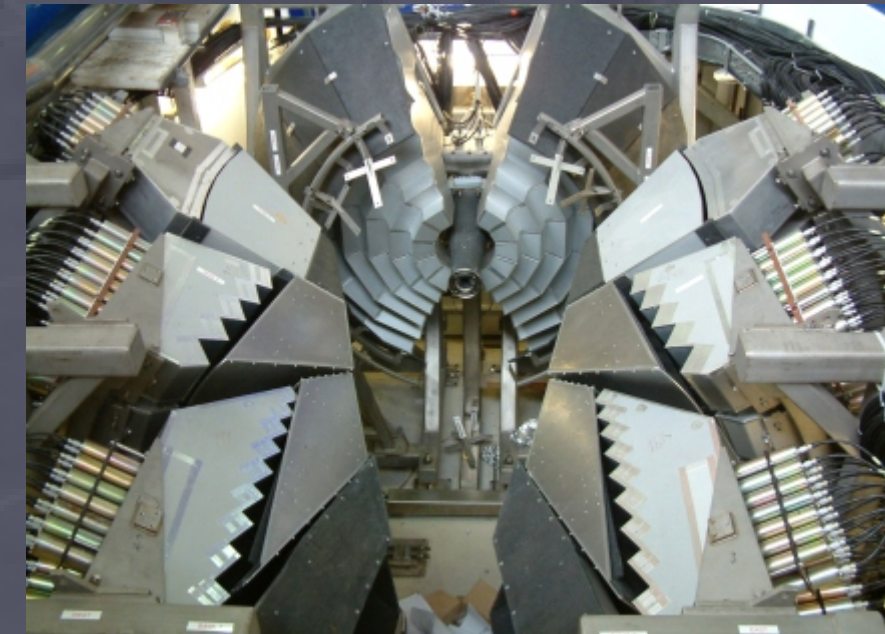


< 1mm resolution

Medium Efficiency

Some gamma sensitivity

Magnetic Field Sensitive!



- ESS would need about 25 000 liters of ^3He (2000 USD/liter = 500 MSEK!)

Detecting the Neutrons

- New technology under development based on ^{10}B :

^{10}B Detectors



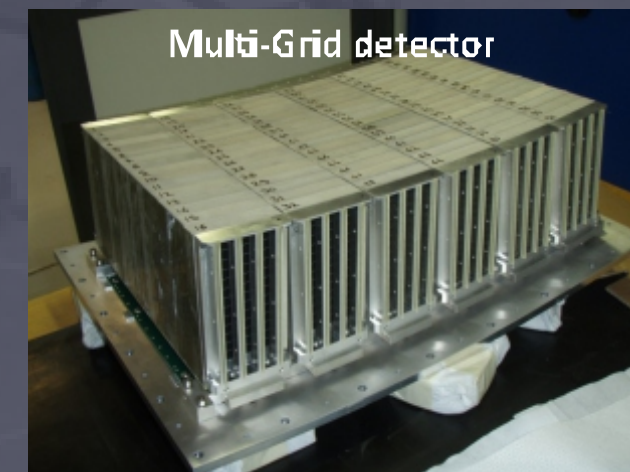
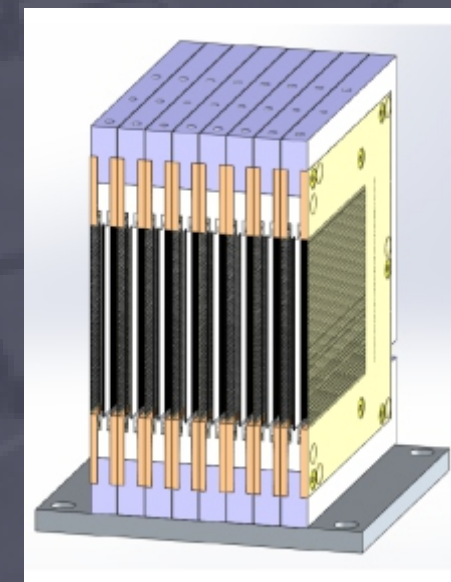
<<< 1mm resolution

70% Efficiency of ^3He

^{10}B is abundant (20% of natural B)

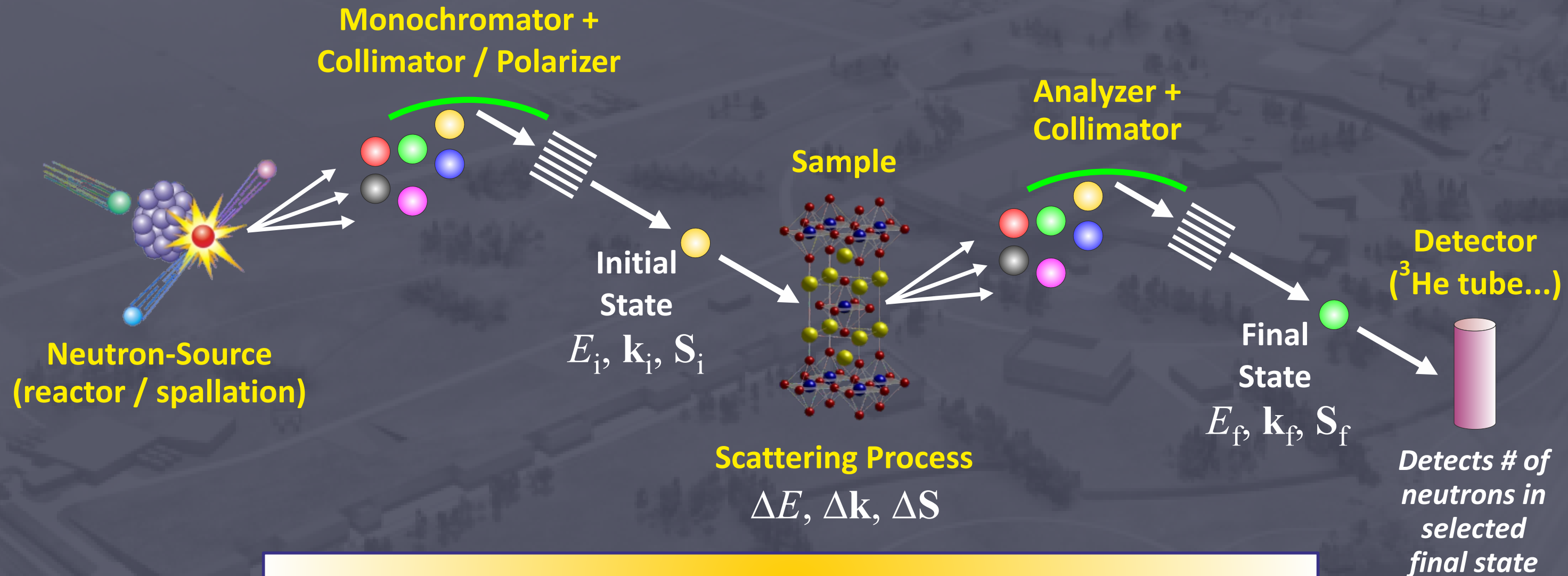
New Technology under development!!!

- $\sim 1 \mu\text{m}$ thin solid ^{10}B -containing layer (α and ^7Li need to exit) \Rightarrow only 5% efficiency \Rightarrow multi-layers and multisegment / blades
- Use $^{10}\text{B}_4\text{C}$ since it is mechanically, chemically & thermally very stable
- Big development program and production at LiU for ESS



The 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

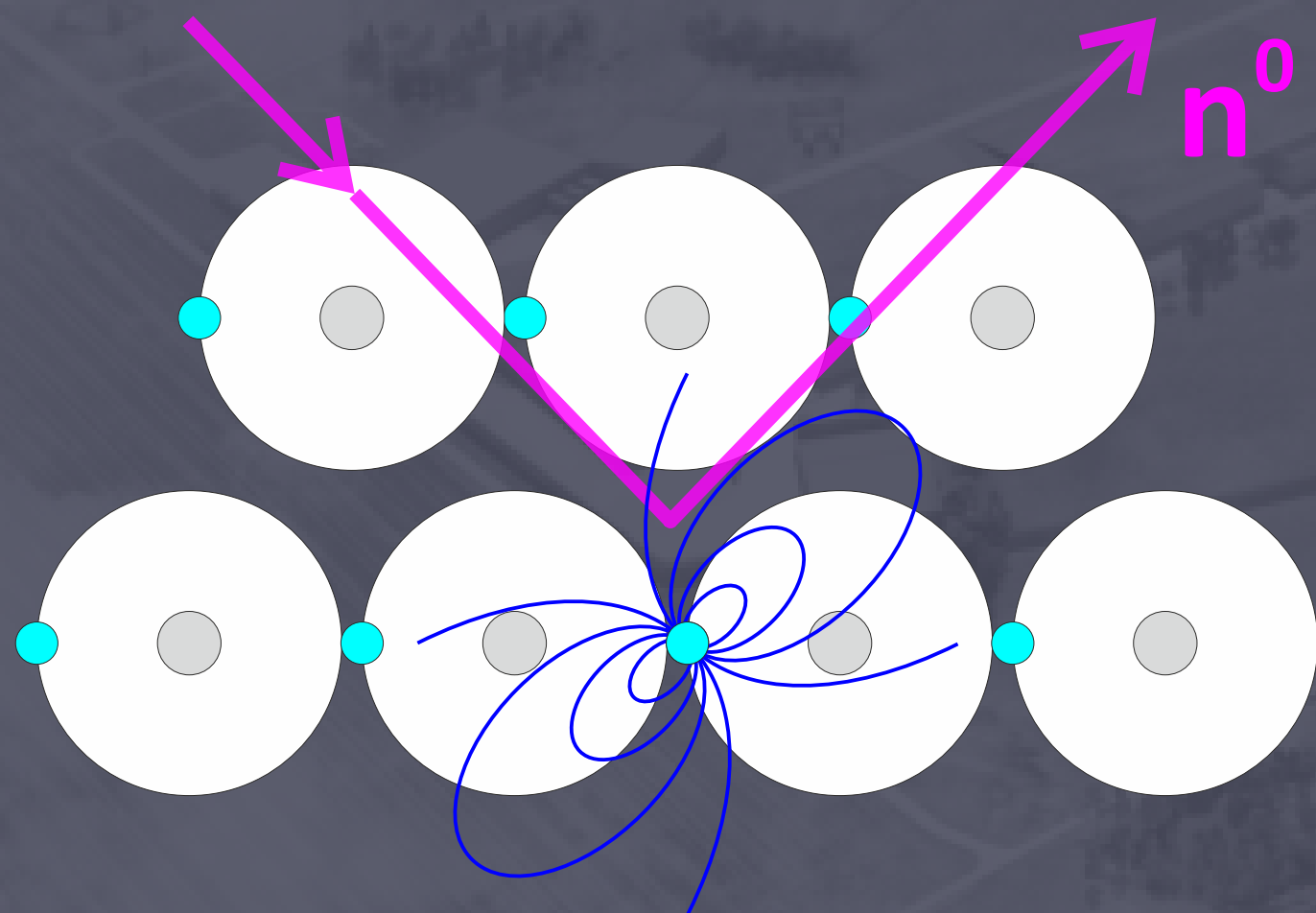
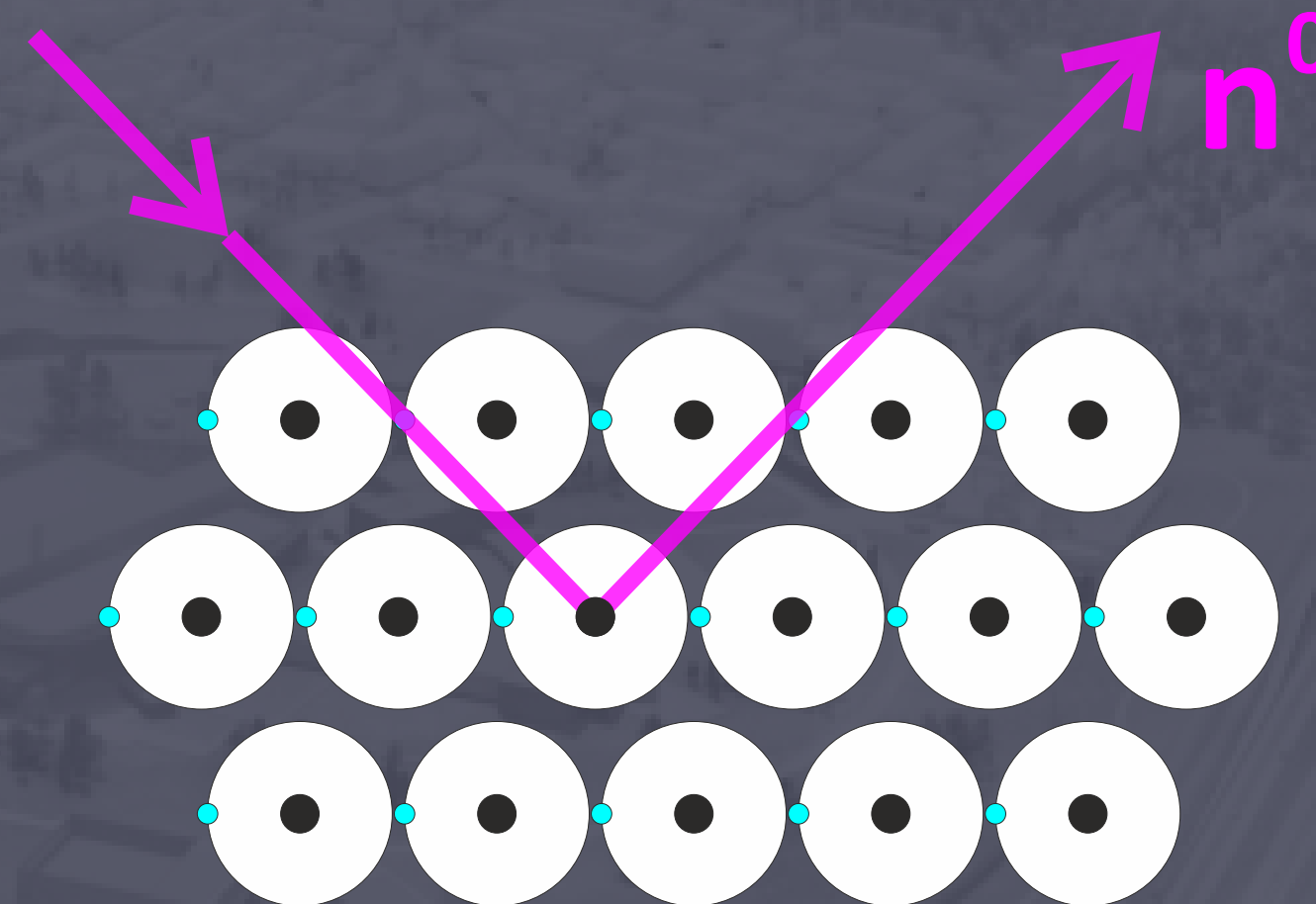


Unfortunately, most neutrons are wasted... twice → ESS !!!

- Traditionally (continuous 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.

Neutron Interaction with Matter

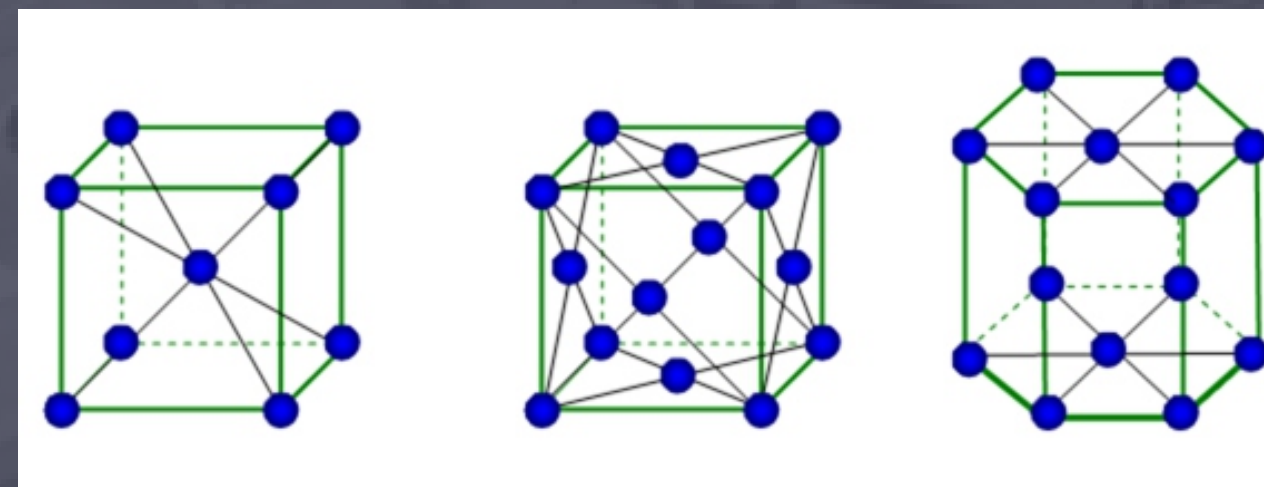
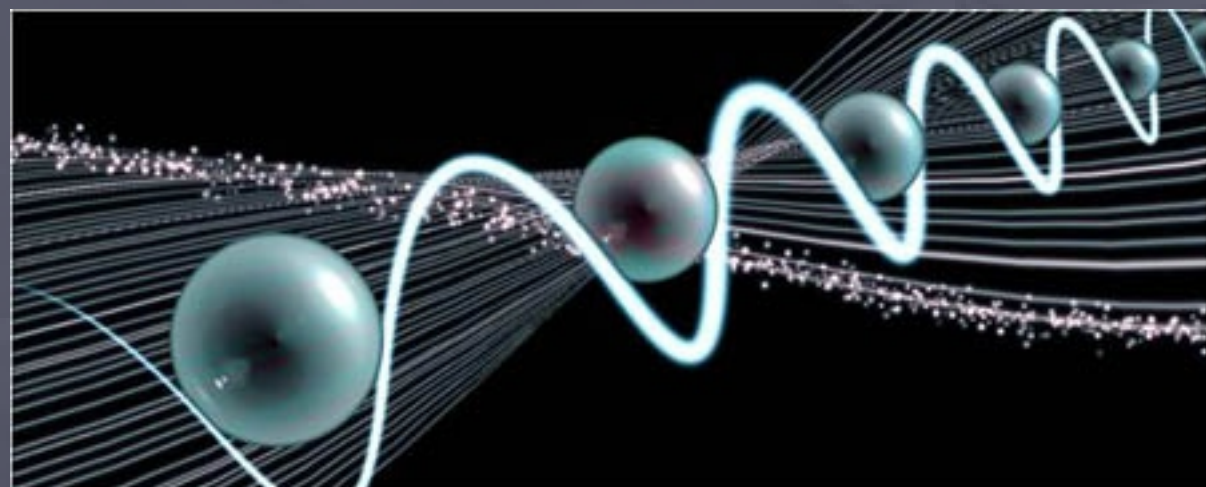
- Neutrons interact strongly with atomic nuclei on a very short length scale (fm) = "point-like" interaction
- Neutrons see crystal structure, density correlations & excitations (e.g. lattice vibrations).
- *"Show us where atoms are and how they move"*



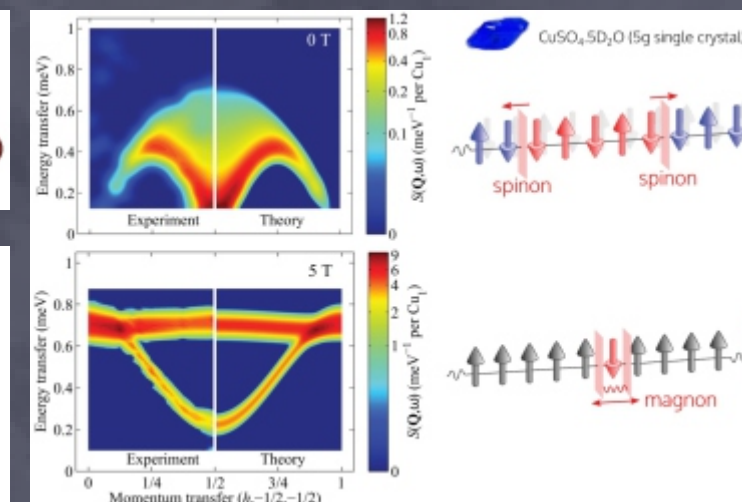
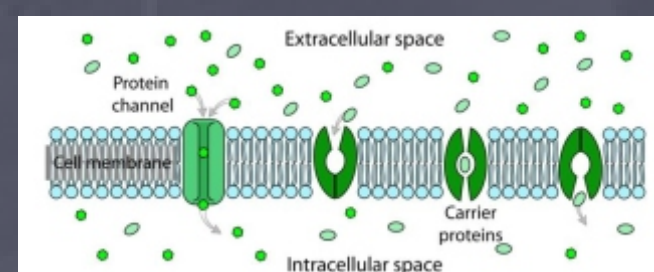
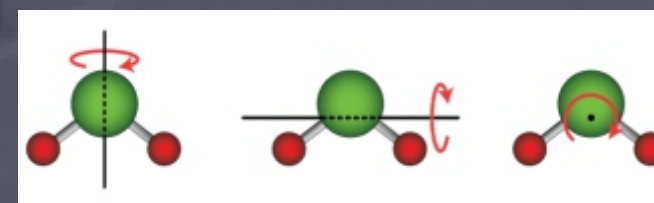
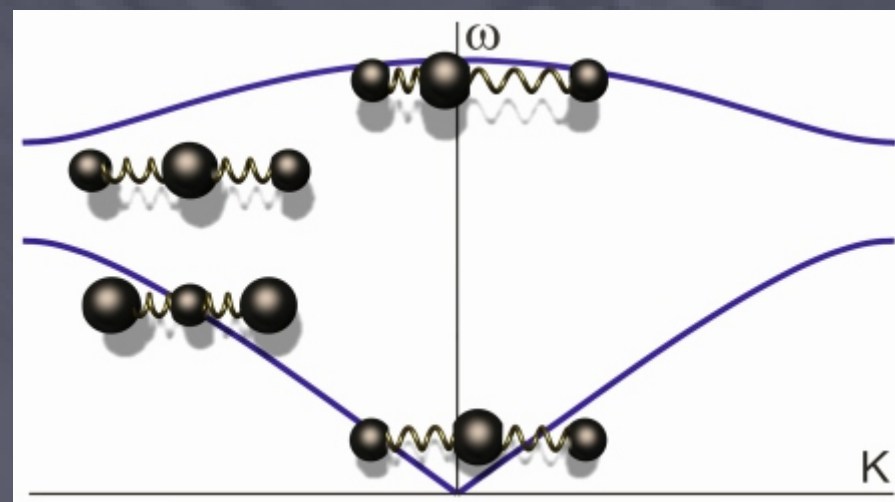
- Neutrons also interact with unpaired electrons via a weaker magnetic dipole interaction.
- Neutrons see magnetic structures, spin waves and other magnetic excitations.
- *"Show us how spins align and what they do"*

Why is NS Optimal for Probing Materials (I) ?

- Strong nuclear scattering AND magnetic scattering
- Neutron wave-length is approximately "a few Ångström" (~1-30 Å)
- Same length-scale as interatomic distances = ideal probe for atomic lattices, molecules & spin-order!

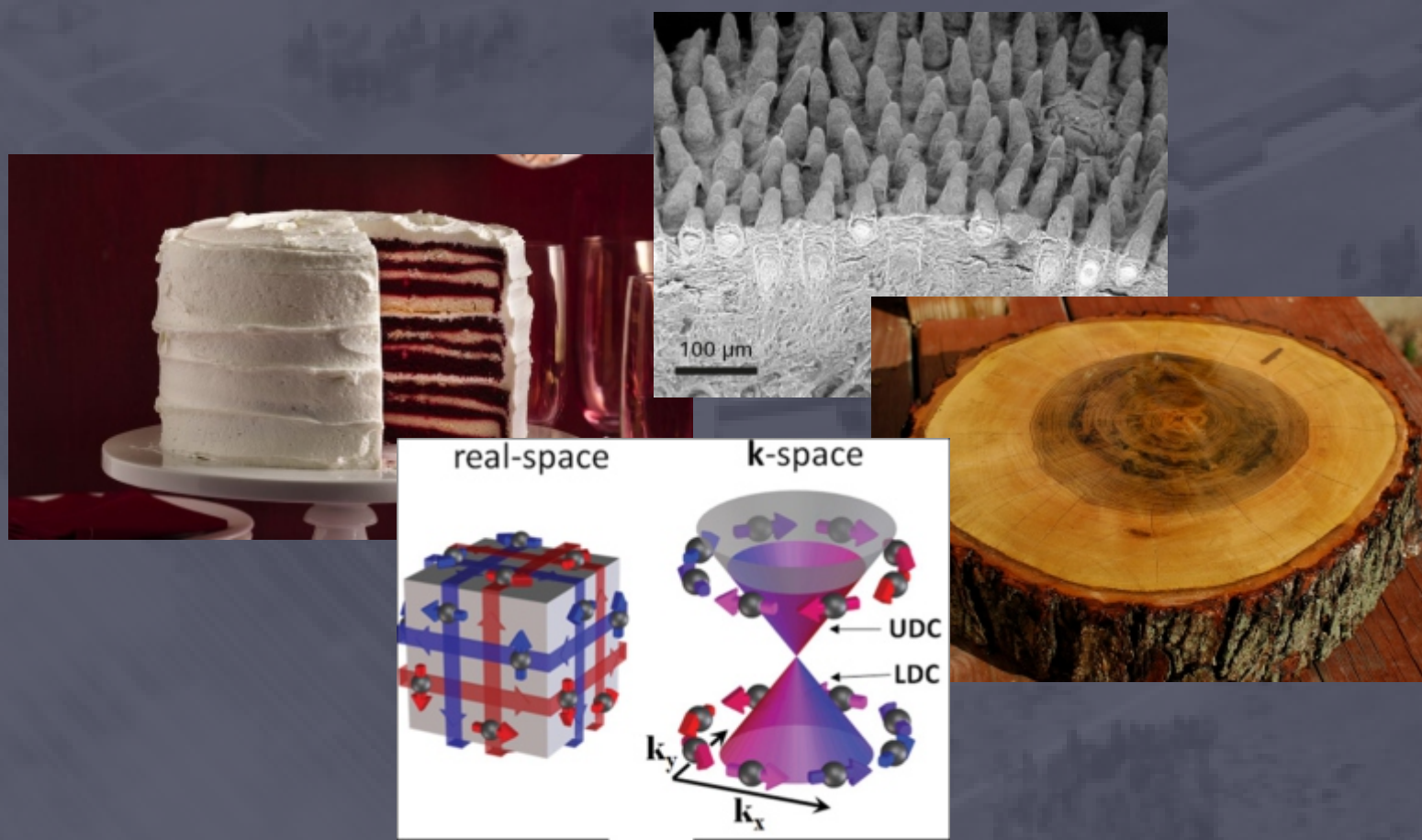


- Neutron mass yields that such wave-length equals an energy of 0.1 - 100 meV ('chicken-egg')
- This energy-scale fits perfectly to many atomic/molecular/spin excitations: phonons, molecular dynamics, ion diffusion, magnetic spinwaves/magnons



Why is NS Optimal for Probing Materials (II) ?

- Point-interaction with nuclei (not only e^-) →
- Possible to investigate also light elements, e.g. **Hydrogen**, which is more or less impossible with x-rays.
- Point-interaction → Q-independent form-factor (c.f. x-rays!)
- Neutral particle that penetrates → probe bulk (intrinsic material) properties as well as buried structures. [**surface vs. bulk!!!**]



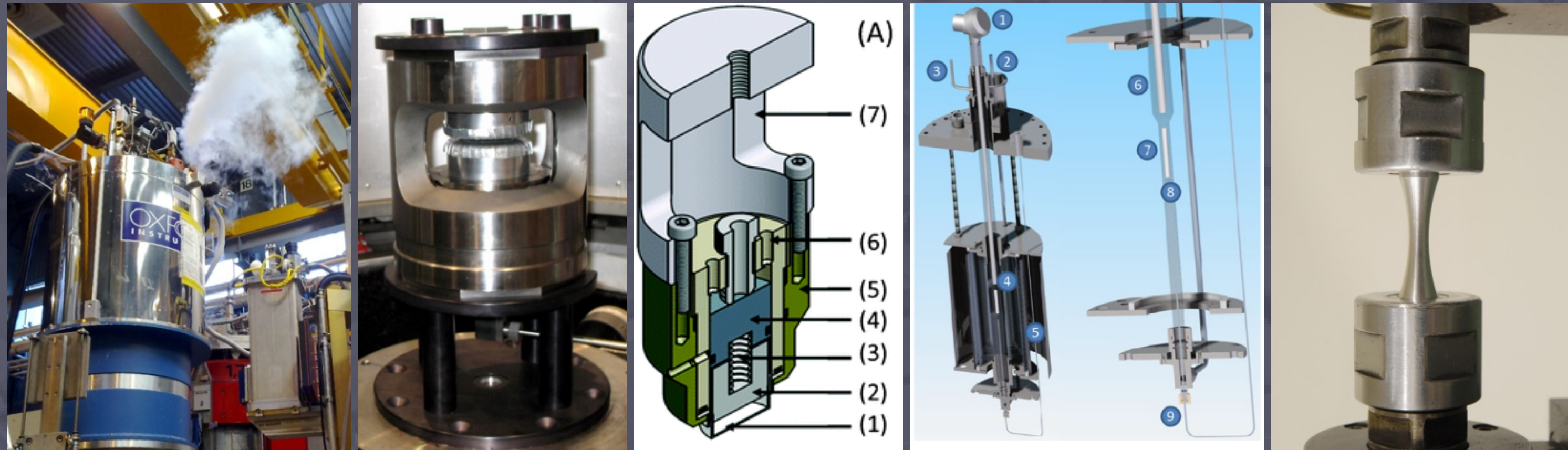
<u>X-rays</u>		<u>Neutrons</u>	
○	H/D	⊖	⊕
○	C	○	○
○	O	○	○
○	Ti	●	●
○	Fe	○	○
○	Ni	○	●

Scattering Strengths

- Some materials (e.g. Aluminium) are 'transparent' for neutrons → easy to make sample holders, containers for the experiment **and also...**

Why is NS Optimal for Probing Materials (III) ?

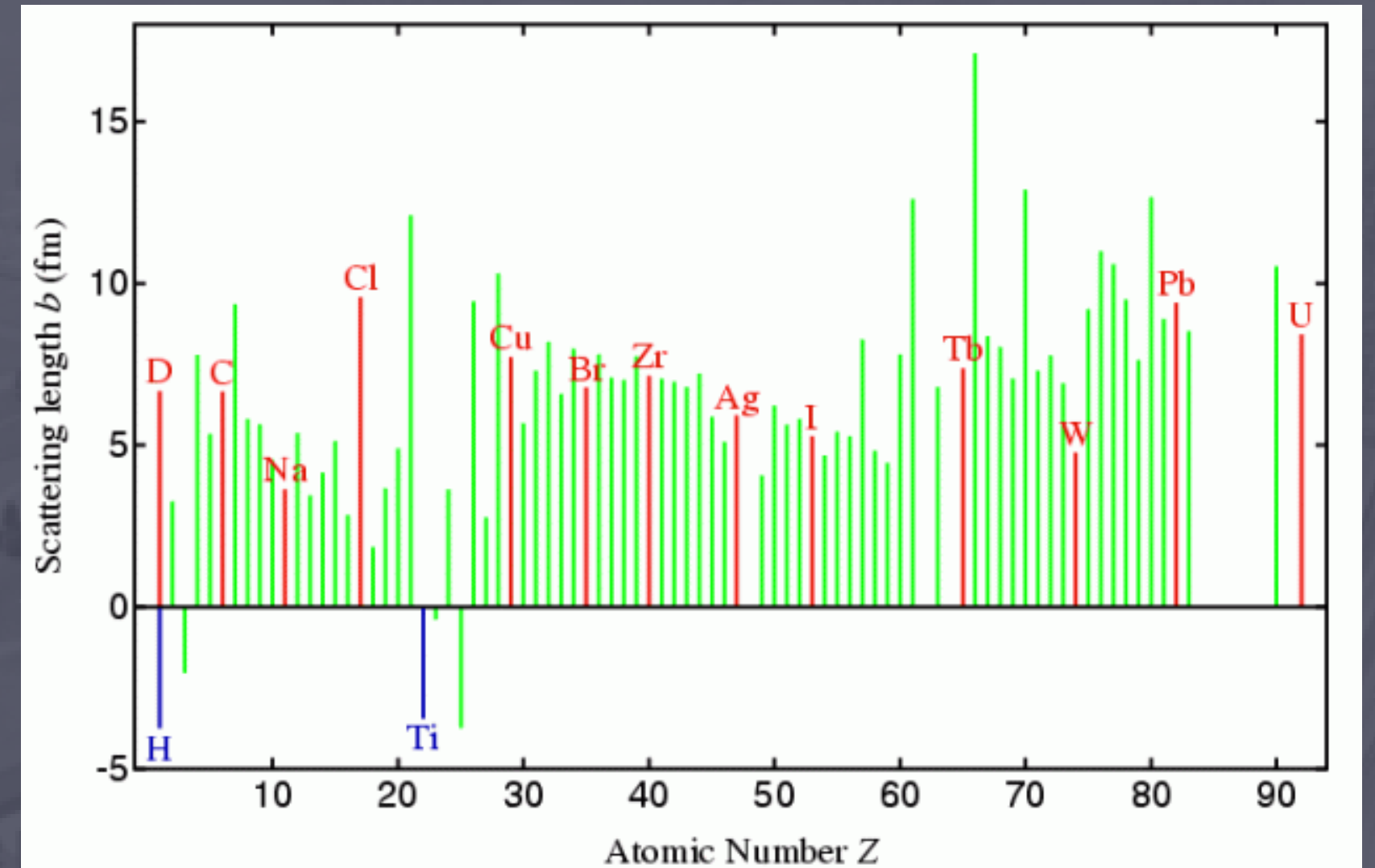
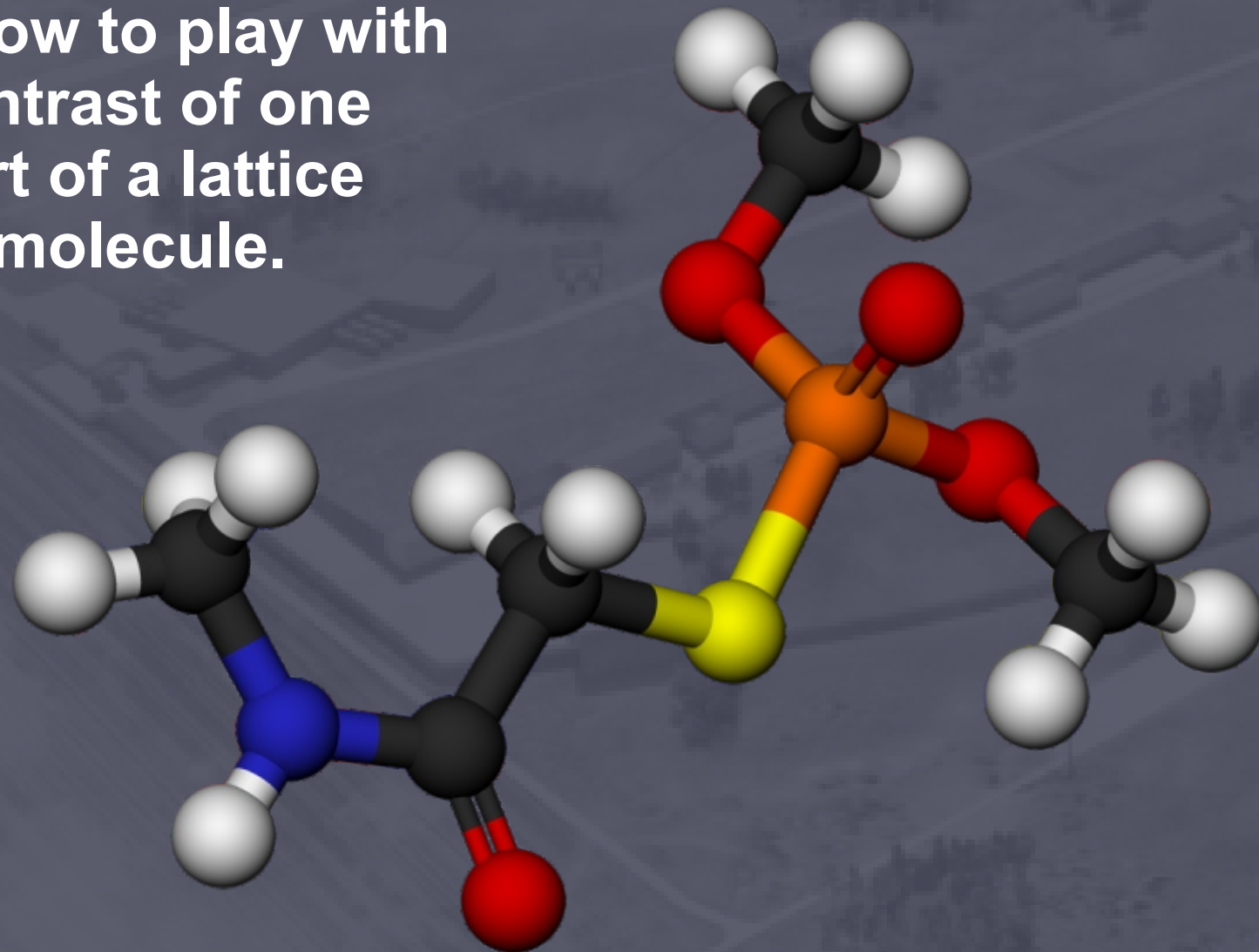
- Some materials (e.g. Aluminium) are ‘transparent’ for neutrons →
- Good materials for building sample environments (cryostats, magnets, pressure cells...).



- Measurements under extreme conditions: low ($T = 10 \text{ mK}$) & high (1500 K) temperatures, high pressures ($P = 500 \text{ kbar}$) & magnetic fields ($H = 27 \text{ T}$).
- Also opens the door to make in situ / in operando measurements of e.g. real batteries, flow cells, catalysis, engineering materials fatigue tests...

Isotope Sensitivity

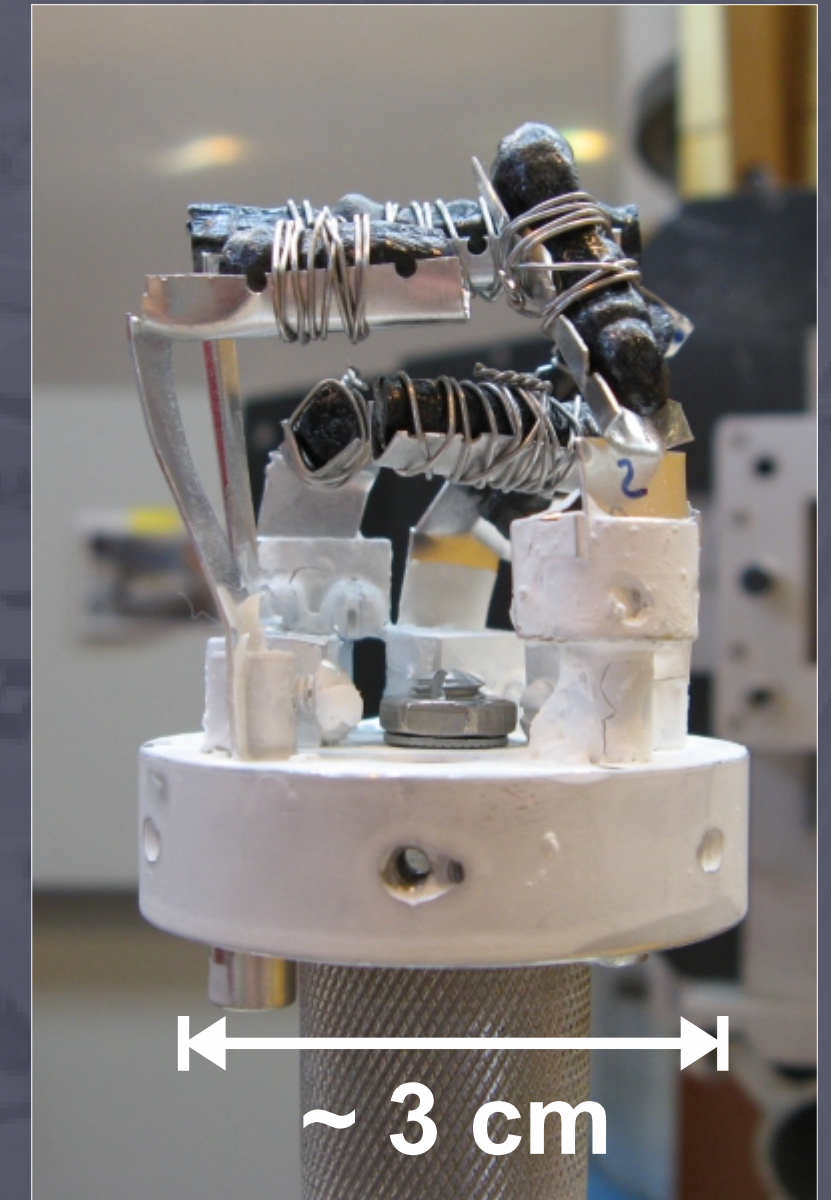
- Isotopes of the same element have different scattering lengths (and absorption).
- Some of them even have different signs (phases) e.g. H/D or ${}^6Li/{}^7Li$
- Allow to play with contrast of one part of a lattice or molecule.



- Isotopic labeling of a part of an organic/bio molecule by using deuterated reaction chemicals.
- Discern e.g. details regarding specific molecular dynamics.
- Can also play with contrast matching to remove background from a sample in solution (H_2O / D_2O)

Drawbacks of Neutron Scattering

- **Slow method**, new high-brilliance neutron sources are needed (ESS) e.g. for INS/QENS studies or spectroscopic/time-resolved measurements.
- **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 (better with new sources).
- Some elements **strongly absorbs** neutrons (Eu, Cd).
- Neutral particle → technically **hard to manipulate** particle beam (focus, bend, accelerate and detect).



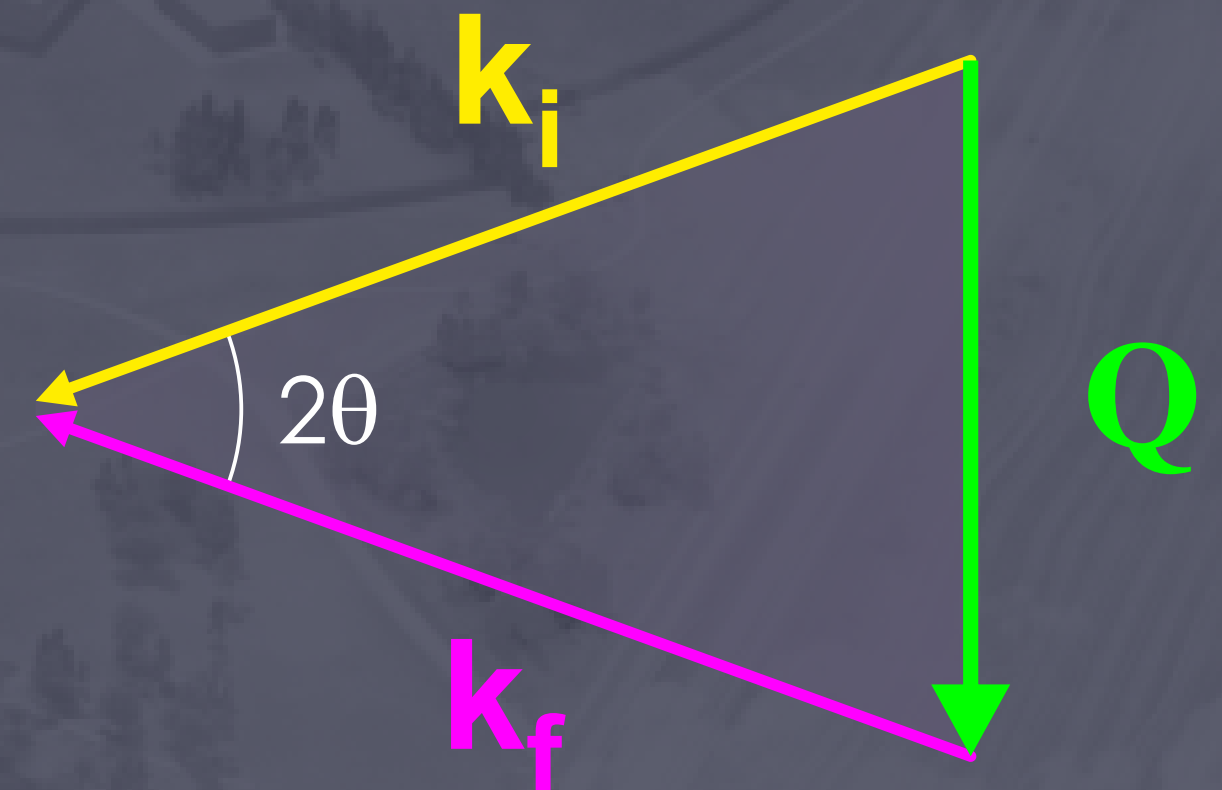
- **Kinematic restrictions** on Q for large energy transfers → Difficult to study excitations at higher (eV) energies (...RIXS !!!)
- Some **samples** gets highly **activated** in the neutron beam, which is hazardous and sometimes not 'practical'.

Elastic Neutron Scattering

- The aim of a NS experiment is to determine the probability that an initial neutron of wavevector \mathbf{k}_i is scattered into a final state \mathbf{k}_f .
- Intensity of the scattered neutrons is measured as a function of momentum transfer (\mathbf{Q}) and energy transfer (E):
- These two equations describe the momentum and energy conservation of the neutron scattering process !!!
- If the scattering occurs without any loss/gain of neutron energy ($E = 0$ i.e. $|\mathbf{k}_i| = |\mathbf{k}_f|$) this is called Elastic Neutron Scattering:

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

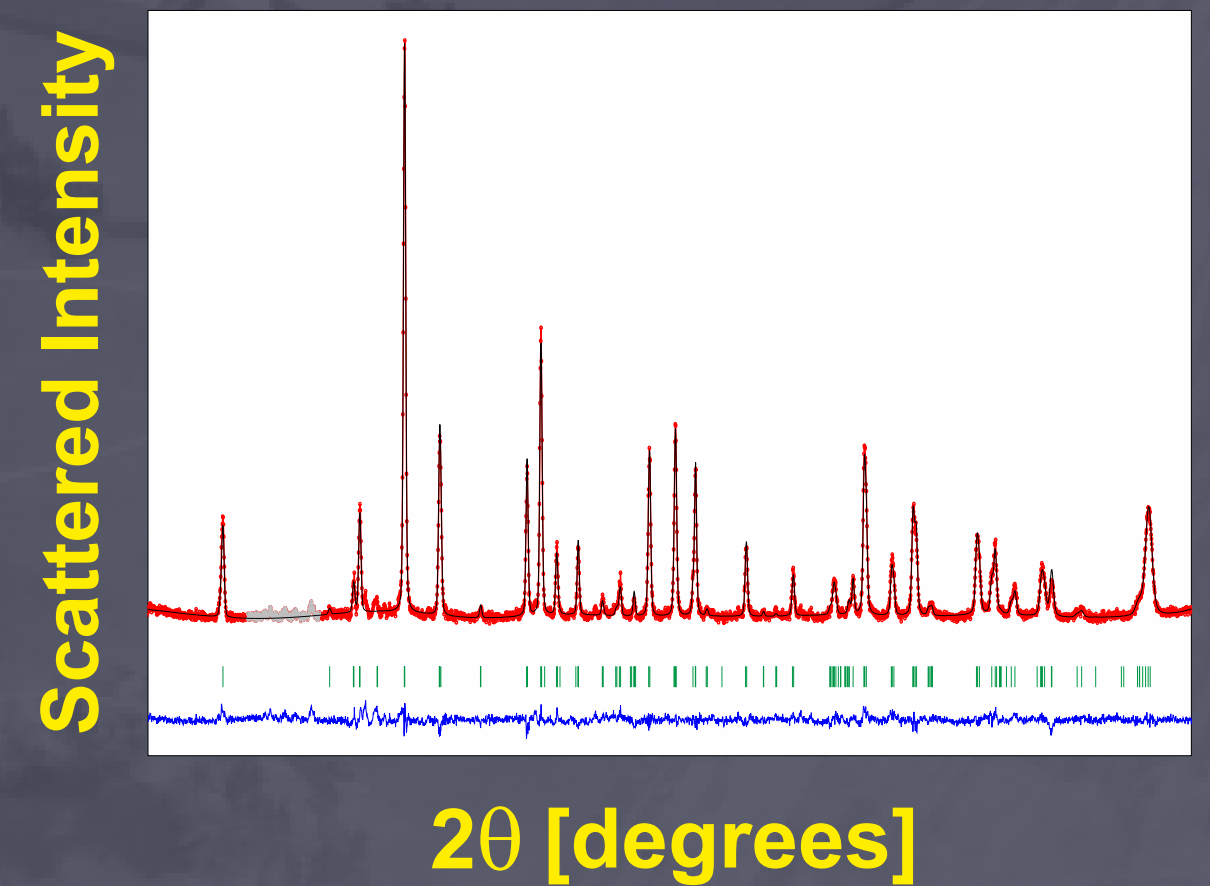
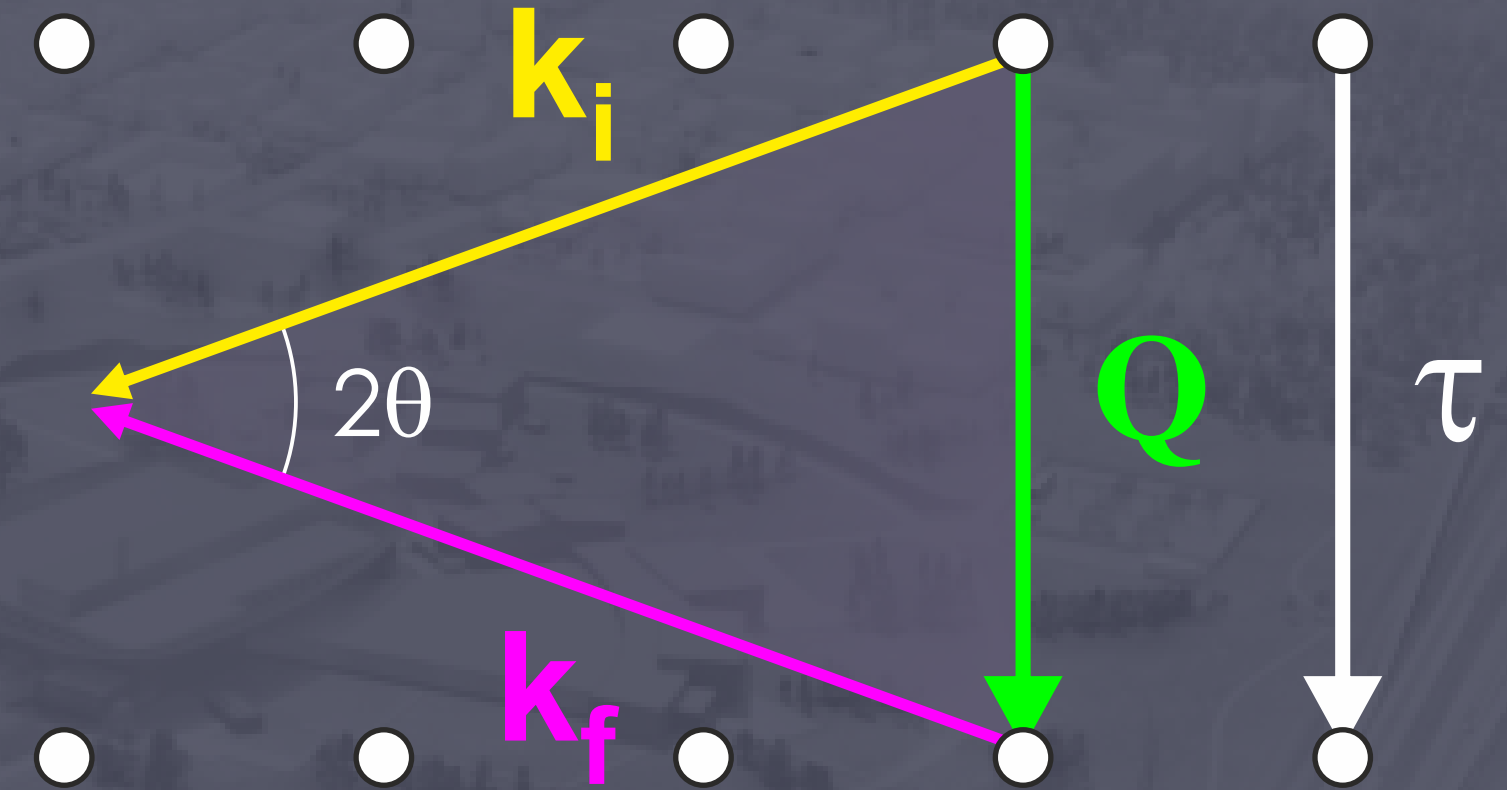
$$E = \hbar\omega = \hbar^2(\mathbf{k}_i^2 - \mathbf{k}_f^2) / 2m$$



Tells us about where atoms are and how spins align

Neutron Diffraction

- If the scattering vector $Q = \tau$ 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 $\theta / 2\theta$ 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 $Q = \tau$, 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)].
Modern sources → mg and minutes !!!

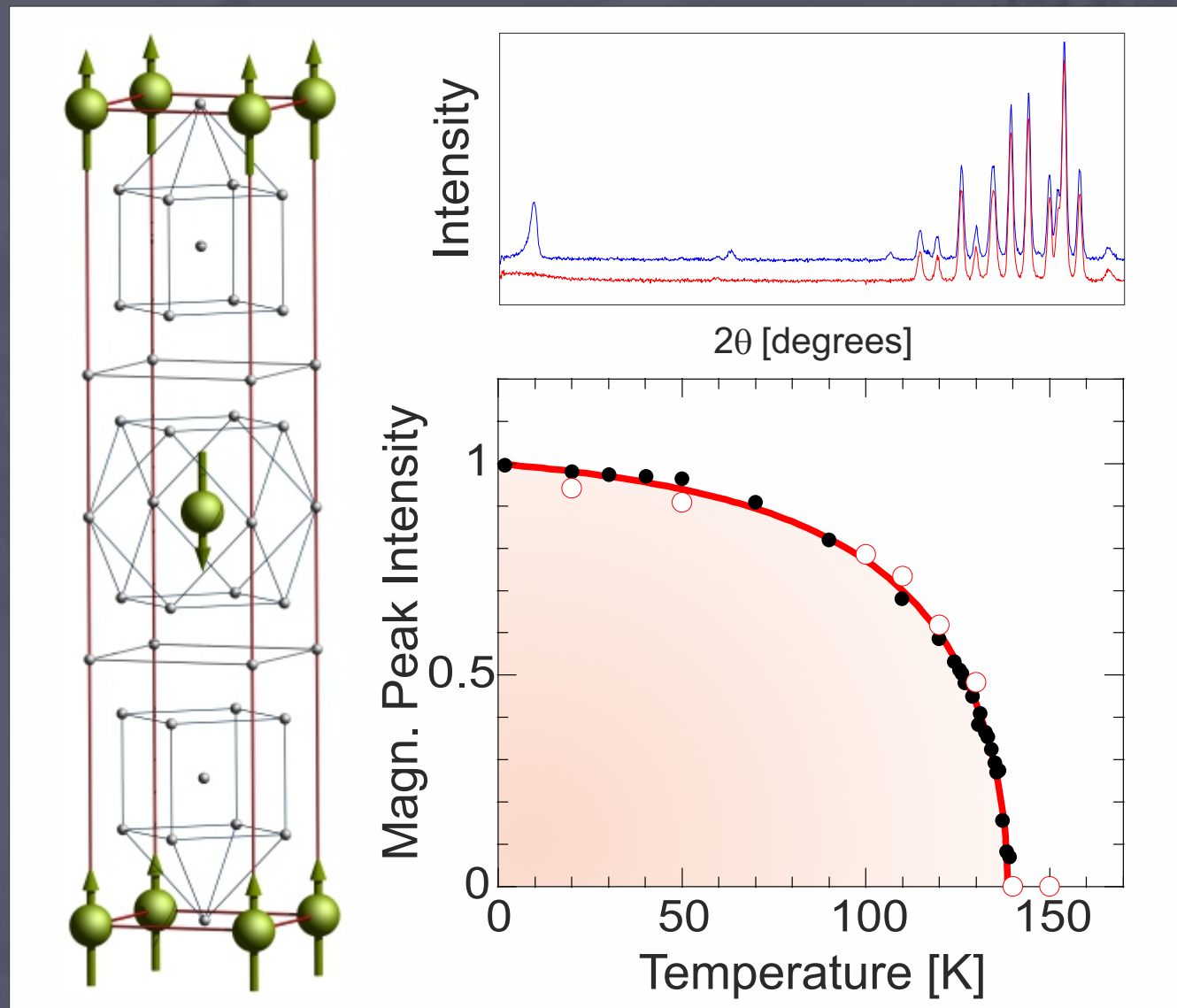
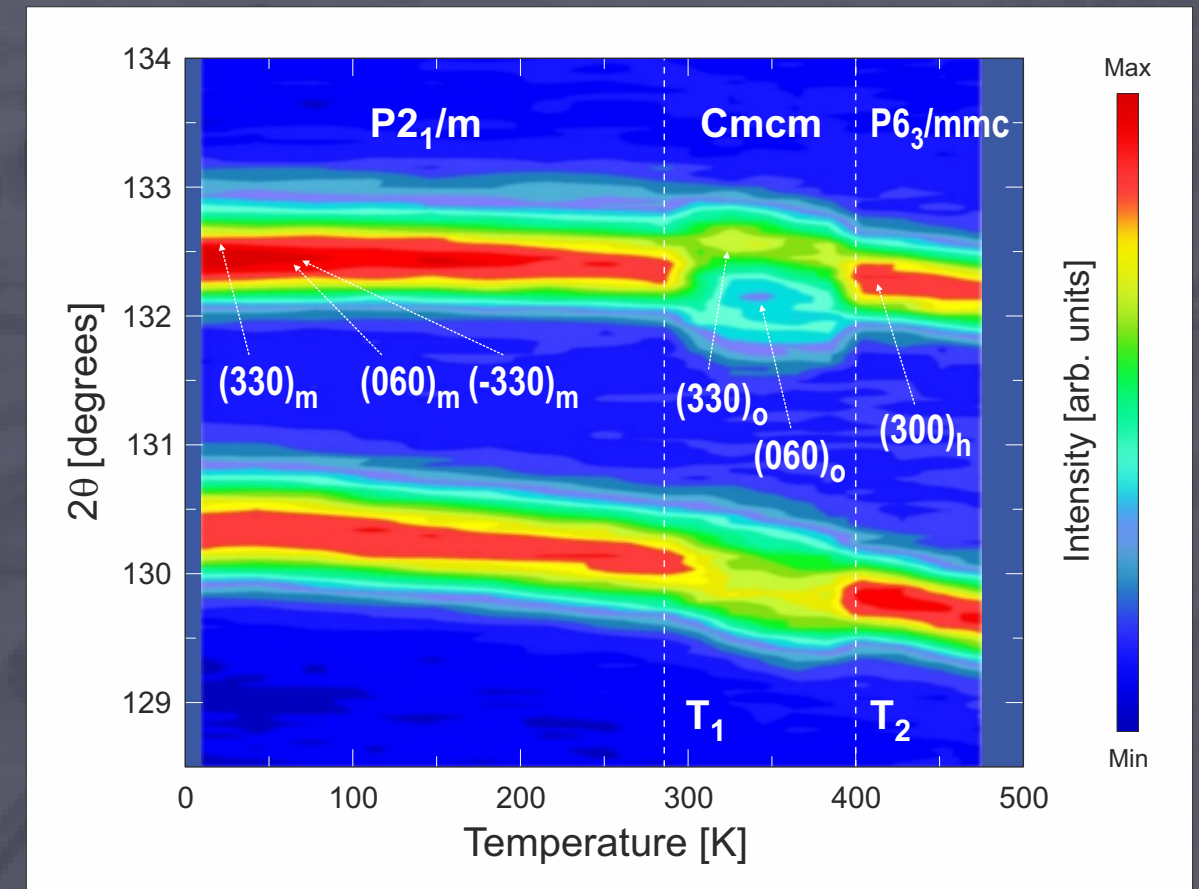


Neutron Diffraction Examples

Nuclear Diffraction

- Determination of & 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 (also H !)

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



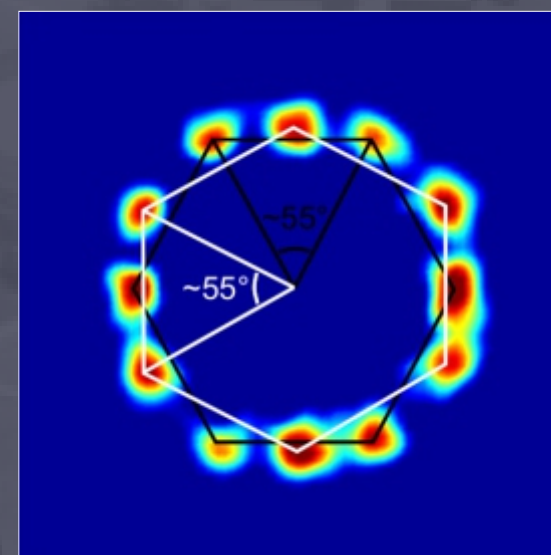
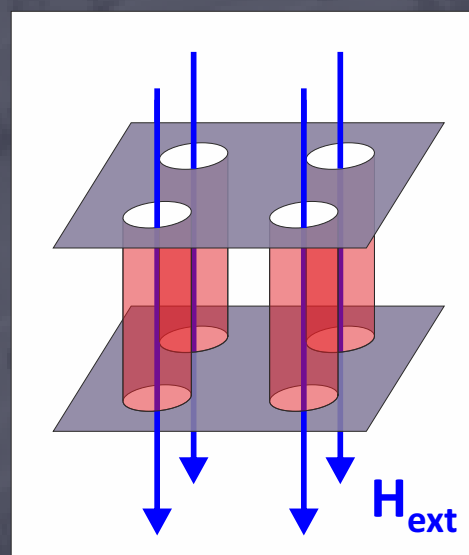
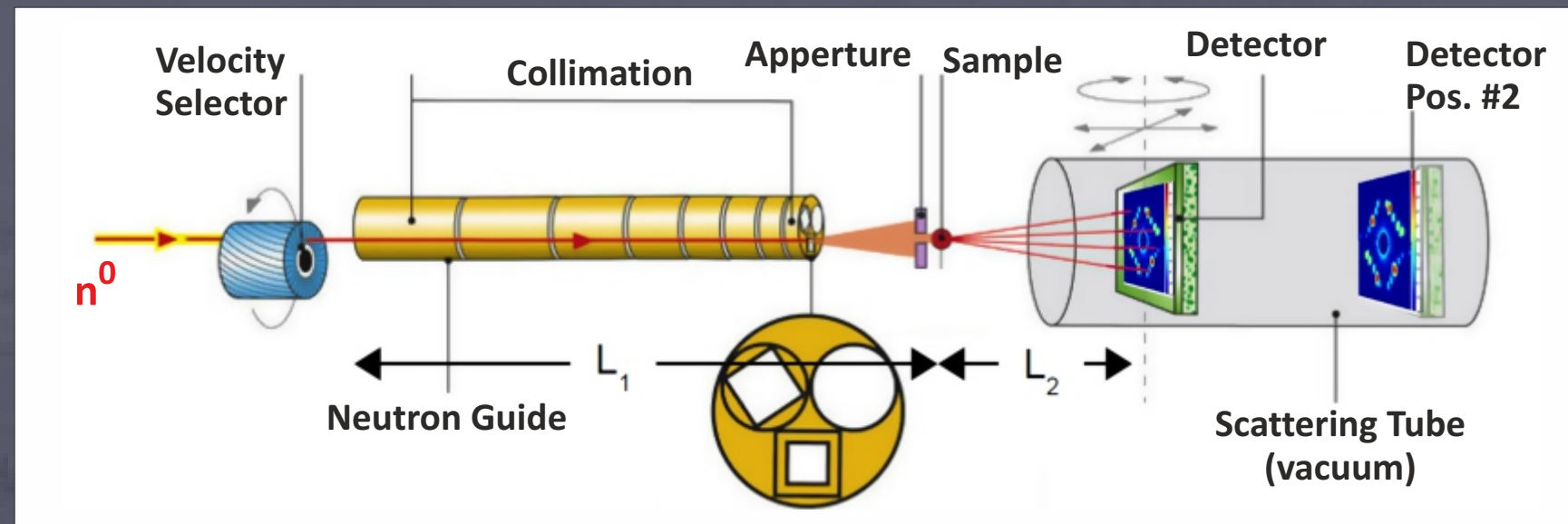
Magnetic Diffraction

- Only available tool (!!!) to directly 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

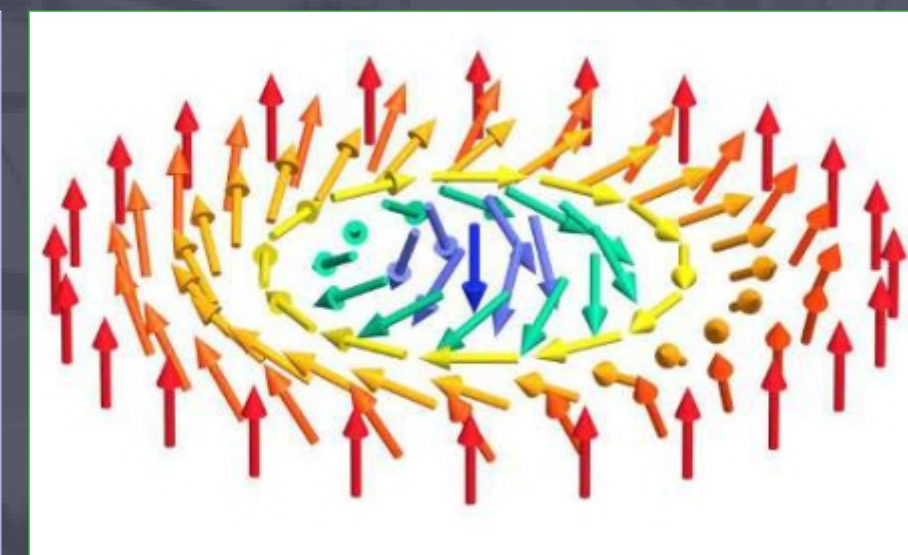
Other Elastic NS Techinques

Small-Angle Neutron Scattering (SANS)

- Order/distribution of **nm- μ m** sized objects
 - ◆ *Micelles in liquids, creep cavities in steel, ...*
 - ◆ Magnetic nano-particles
 - ◆ Flux-line (vortex) lattice in superconductors
 - ◆ Magnetic Skyrmions



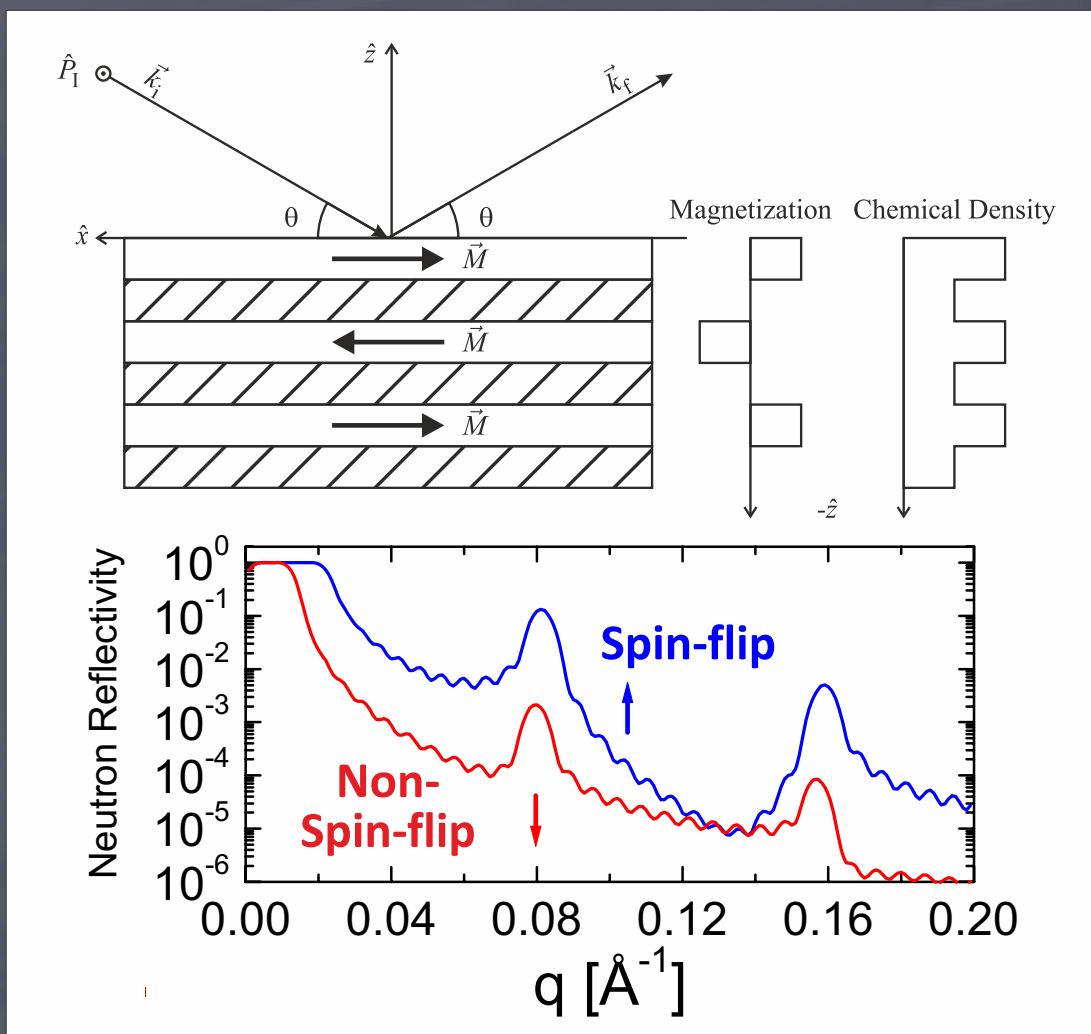
H. Kawano-Furukawa, Phys. Rev. B 84, 024507 (2011)



S. Mühlbauer, et al., Science 323, 915 (2009)

Neutron Reflectometry

- Determine **film/layer** thickness, roughness & structural interfaces
 - ◆ *Solid-liquid interfaces, spin coated polymer films, ...*
 - ◆ 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 (INS)

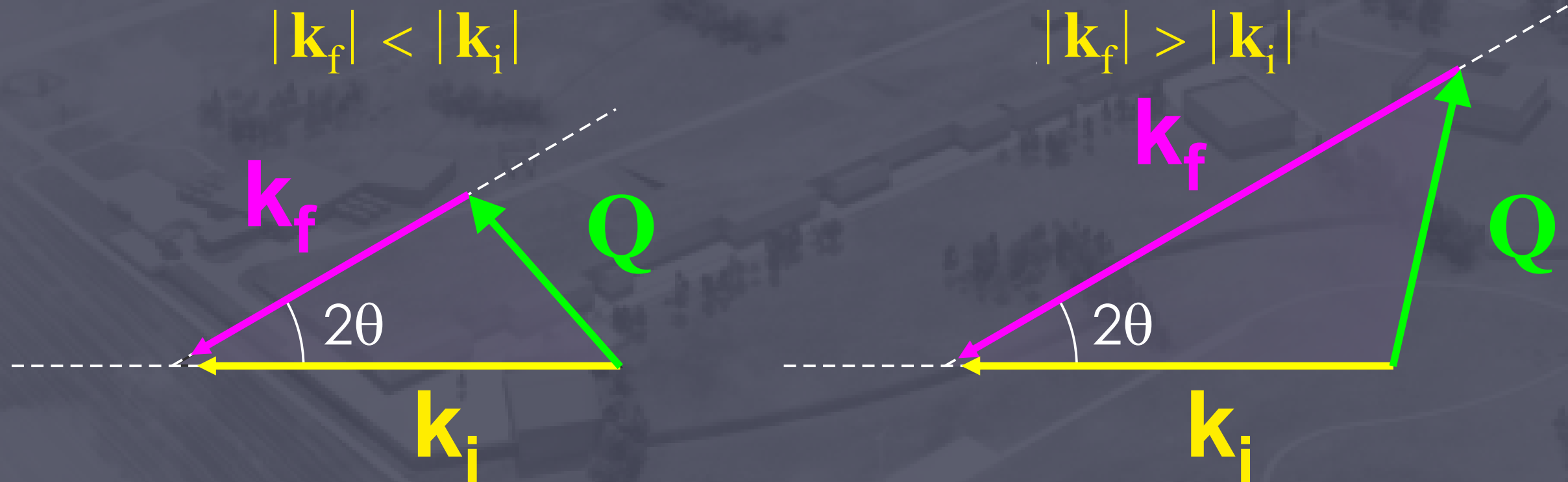
- Intensity of the scattered neutrons is measured as a function of momentum transfer (\mathbf{Q}) and energy transfer (E):
- If the neutrons lose or gain energy in the scattering process ($E \neq 0$ i.e. $|\mathbf{k}_i| \neq |\mathbf{k}_f|$) this is called Inelastic Neutron Scattering (INS):

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

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

Neutron Loses Energy

Neutron Gains Energy

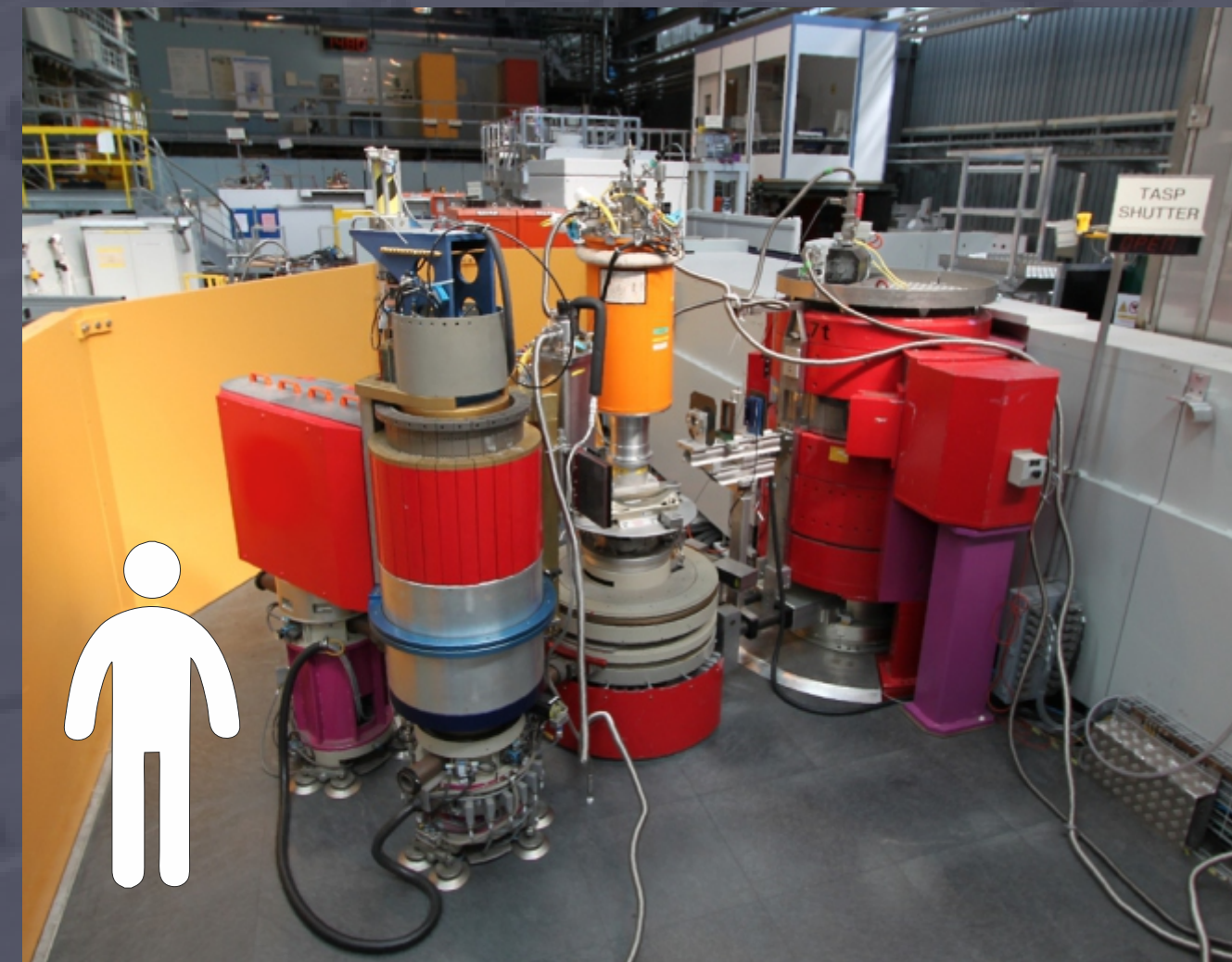
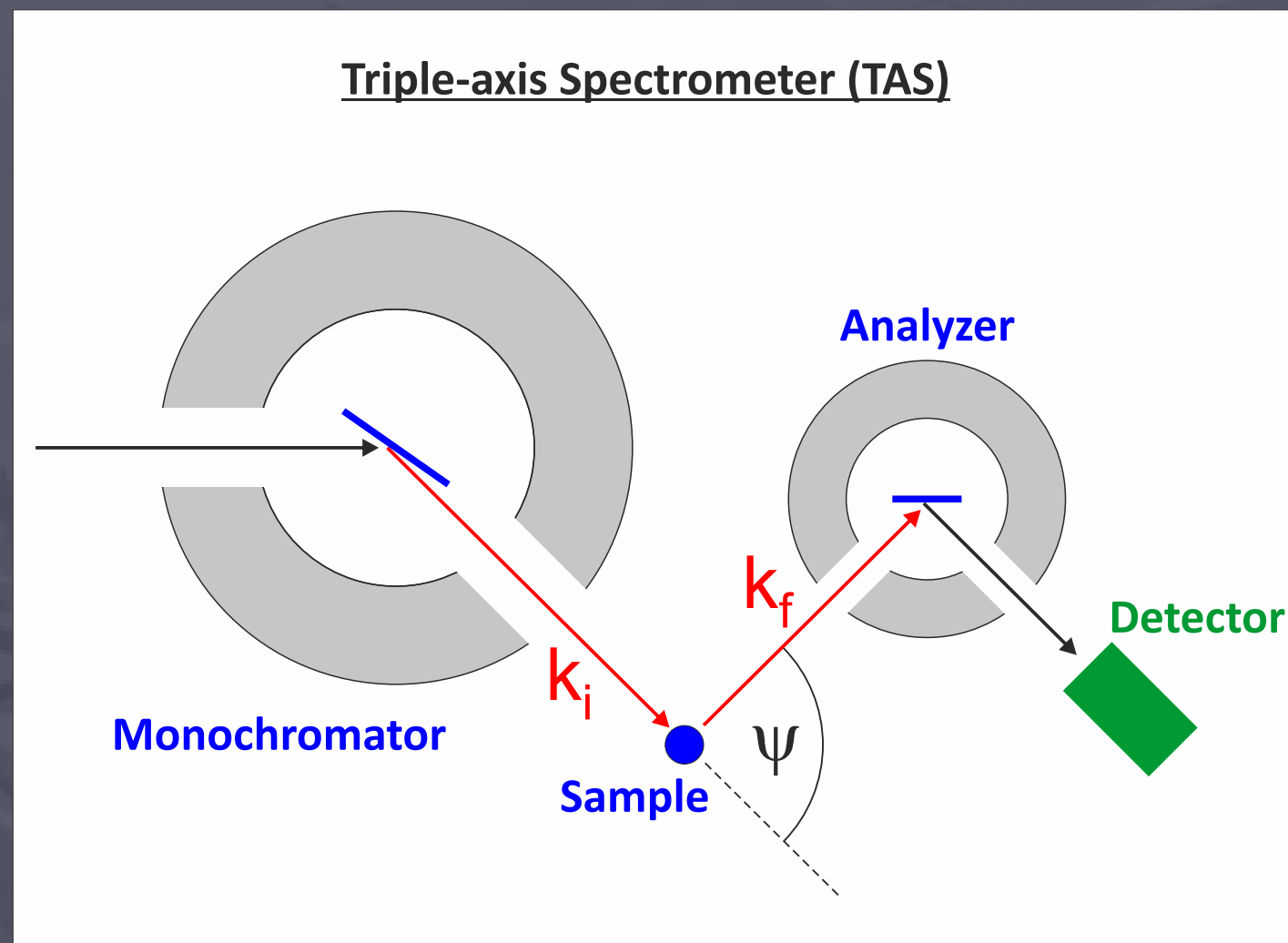


Tells us what the atoms & electron spins 'do'

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

Classic Triple-Axis Spectroscopy (TAS)

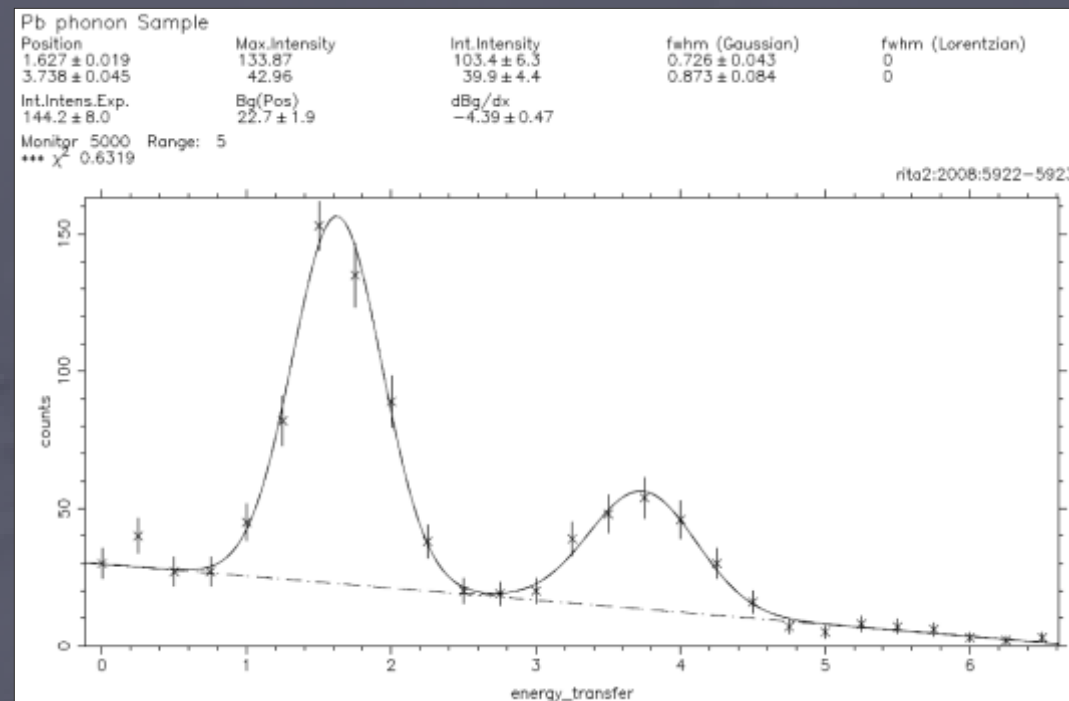
- Measure a single Q,E point at a time by using monochromators and "filters" to define initial state and to detect a specific final state.



- This is a very inefficient and slow method where most neutrons are wasted (twice) and it can take several minutes for one single data point.

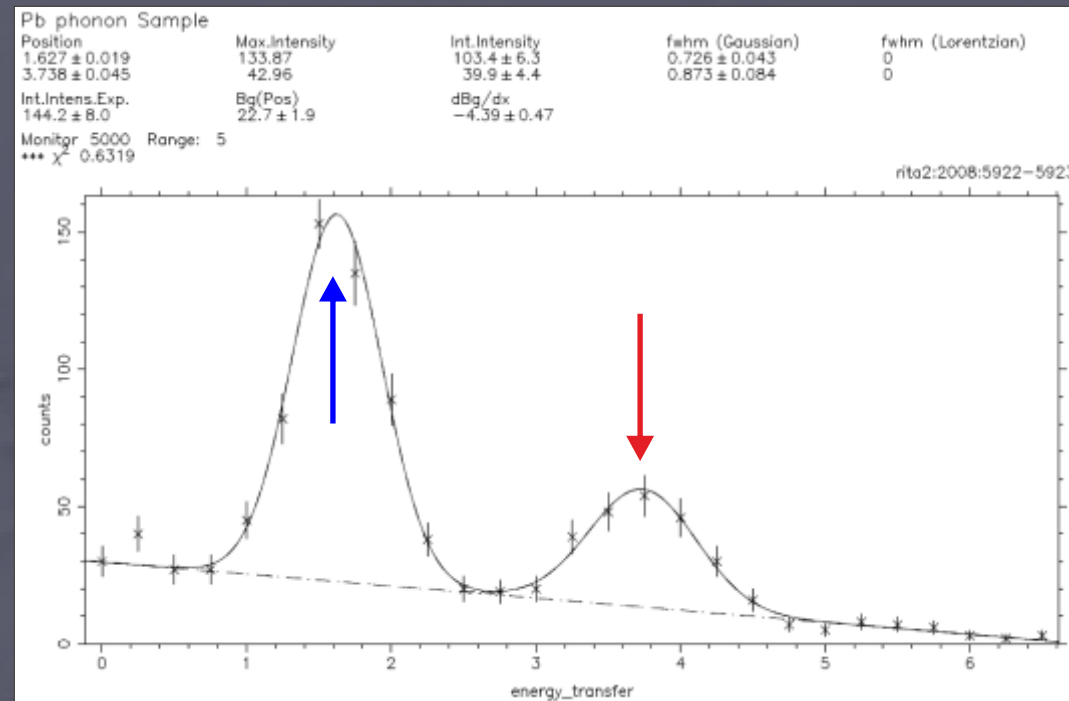
Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.

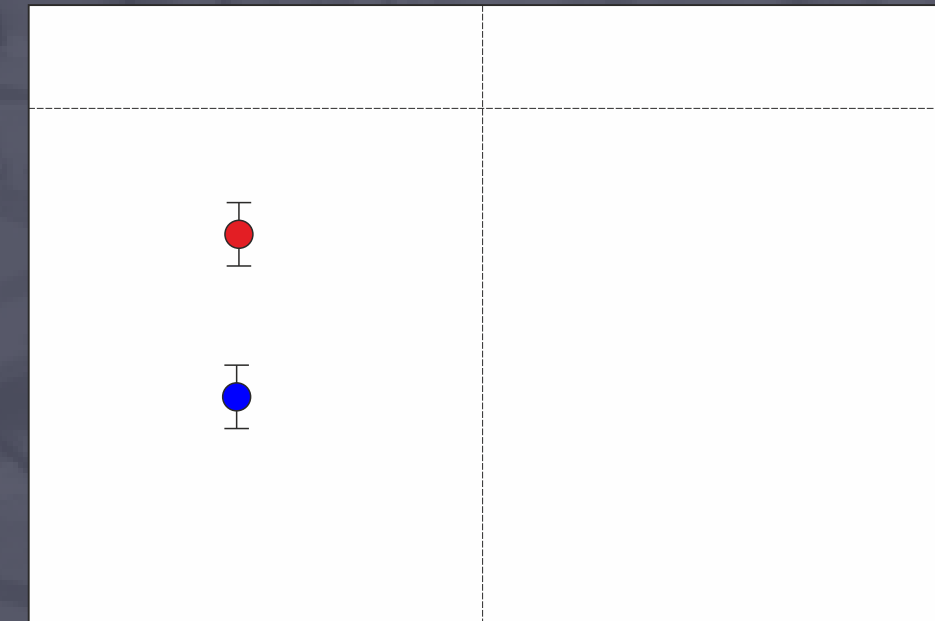


Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.



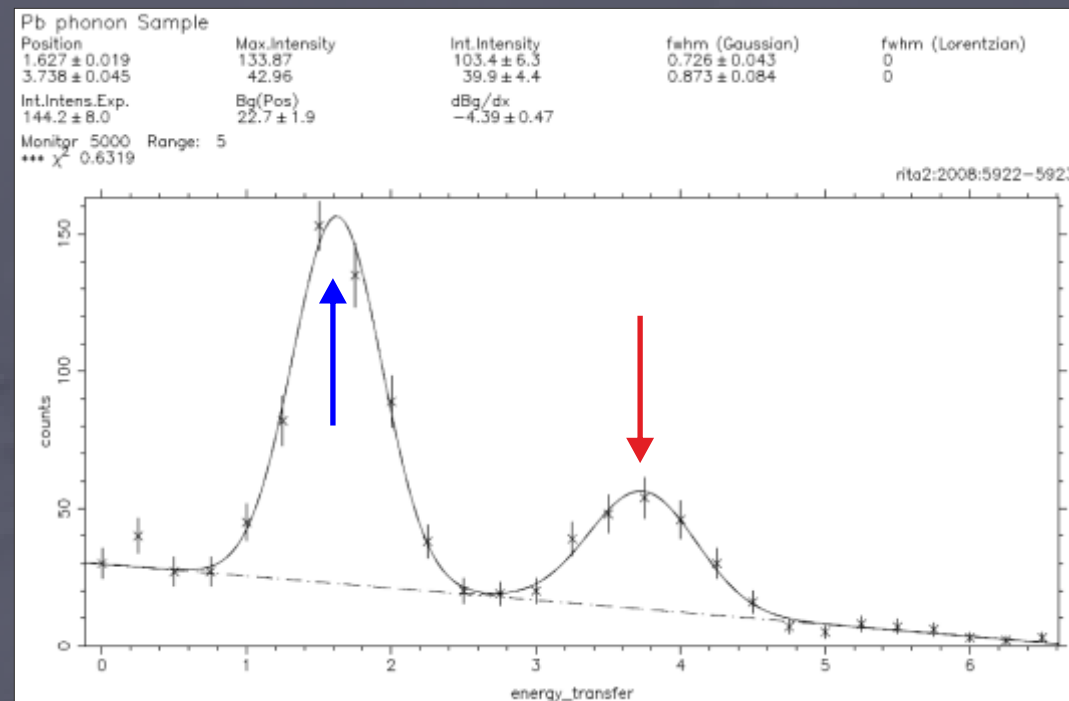
Energy-transfer, E [meV]



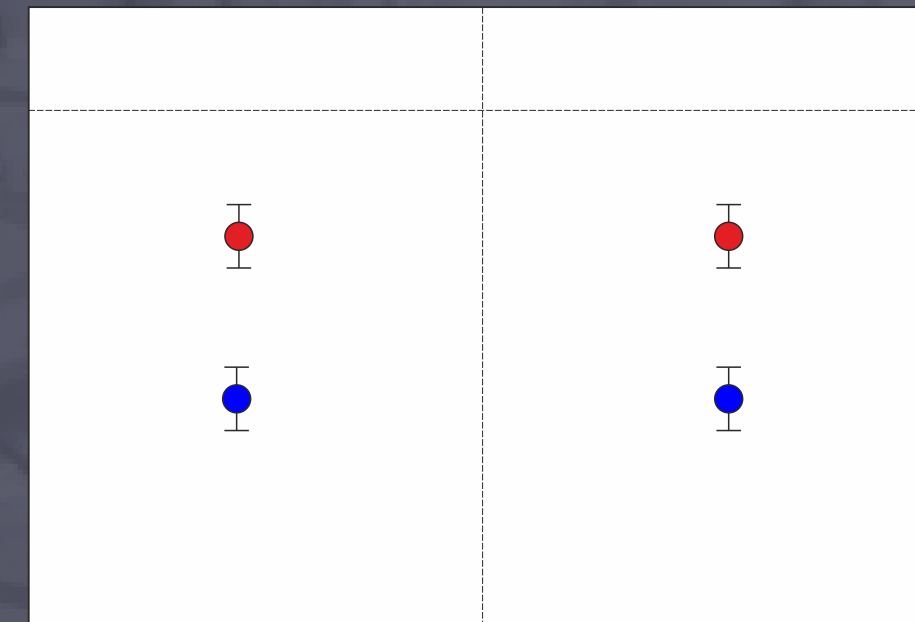
Momentum-transfer, q [r.l.u.]

Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.



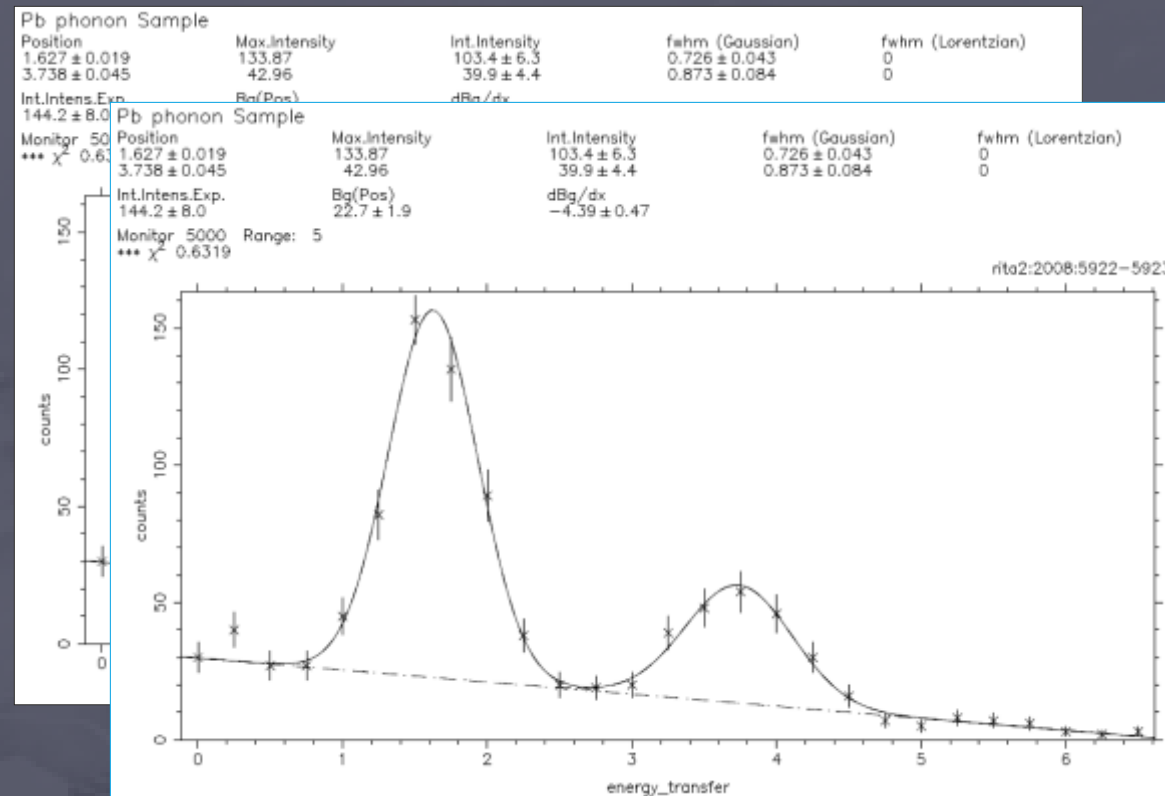
Energy-transfer, E [meV]



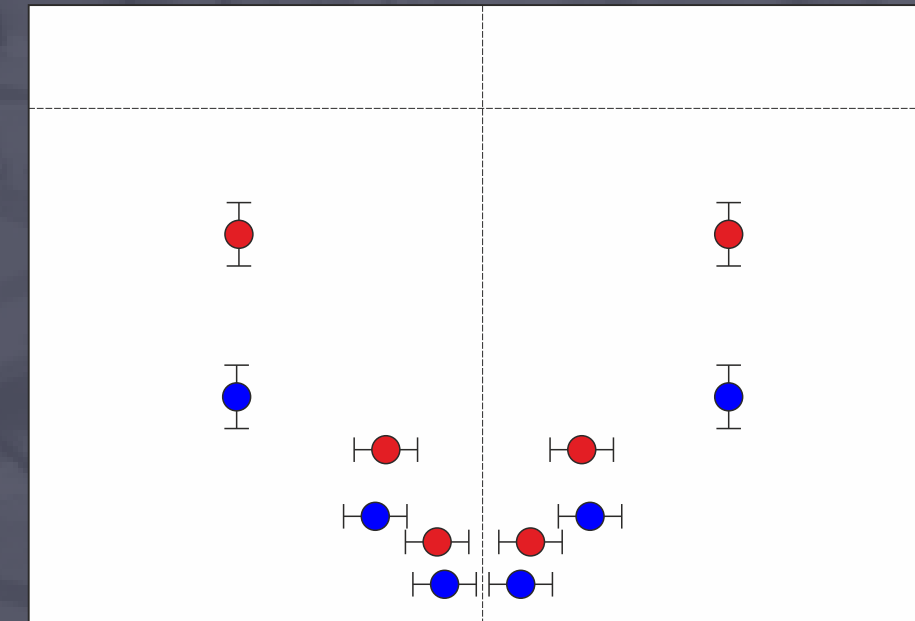
Momentum-transfer, q [r.l.u.]

Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.



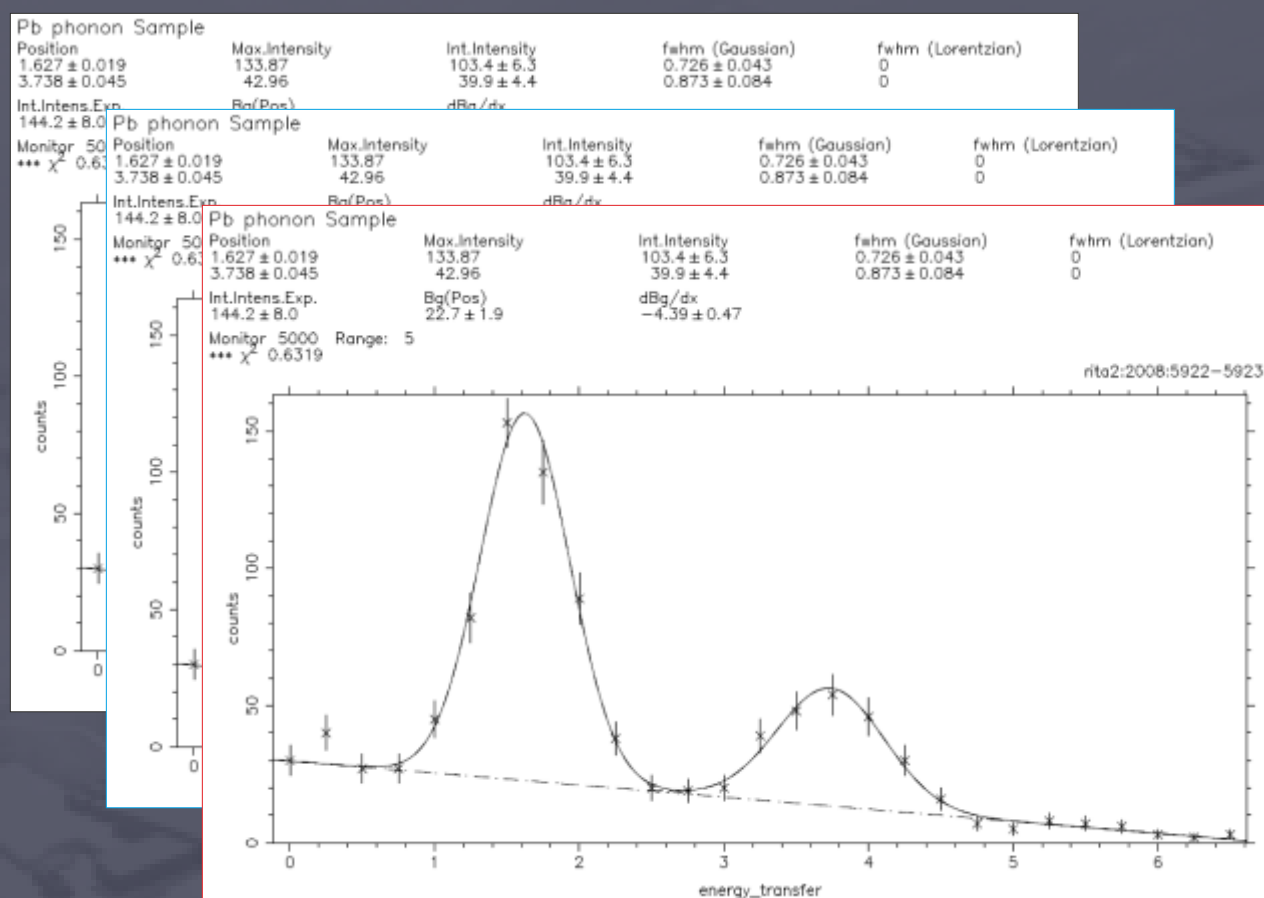
Energy-transfer, E [meV]



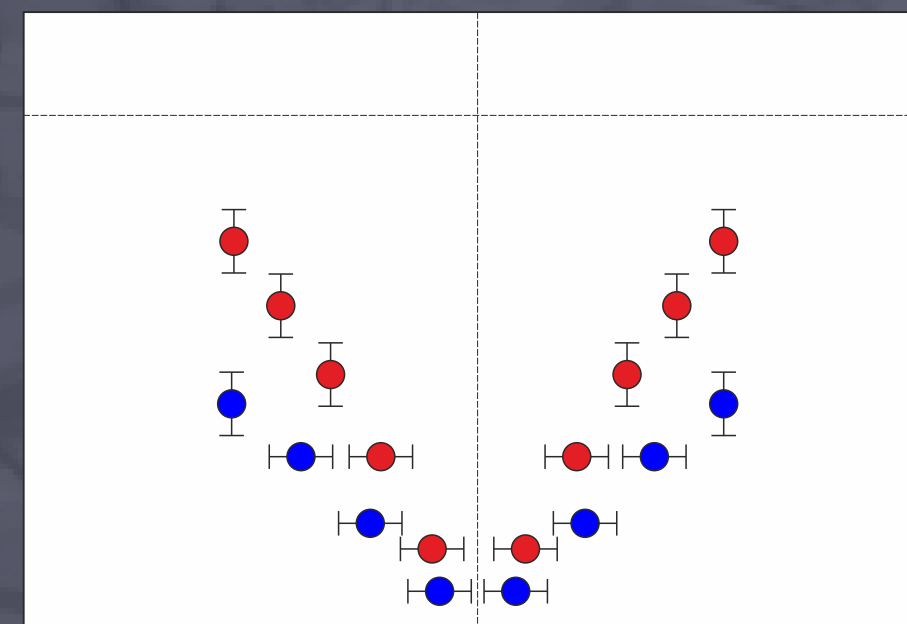
Momentum-transfer, q [r.l.u.]

Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.



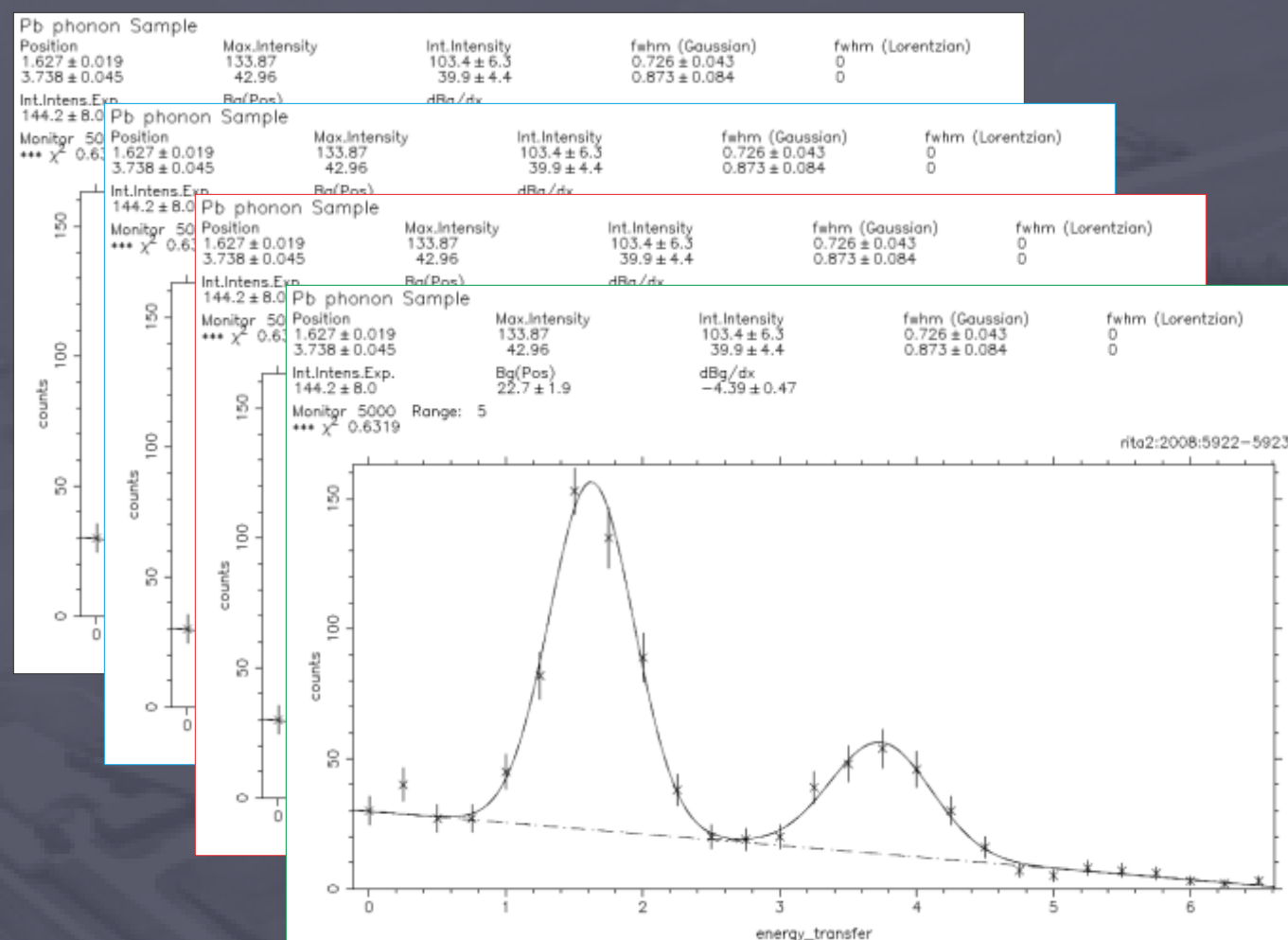
Energy-transfer, E [meV]



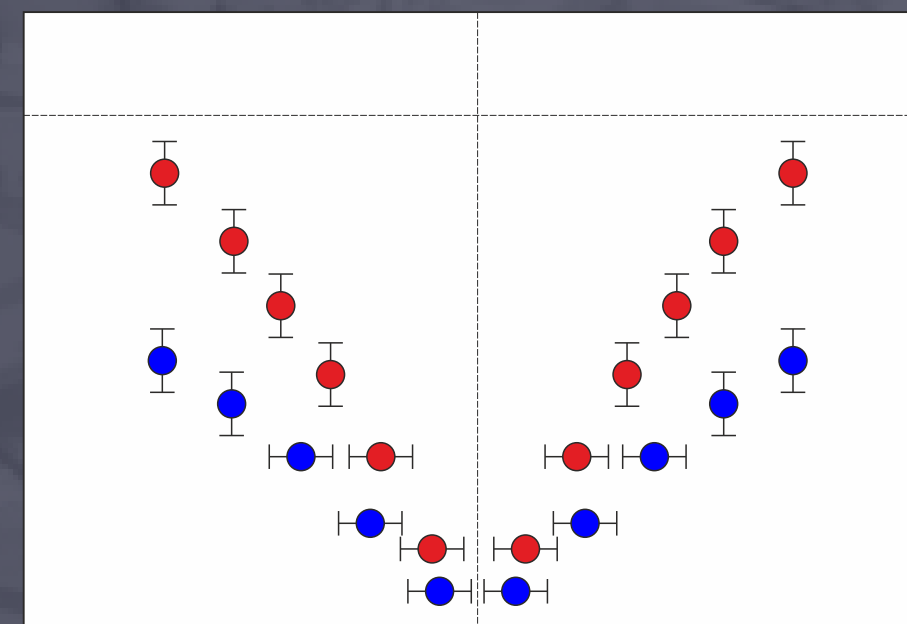
Momentum-transfer, q [r.l.u.]

Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.



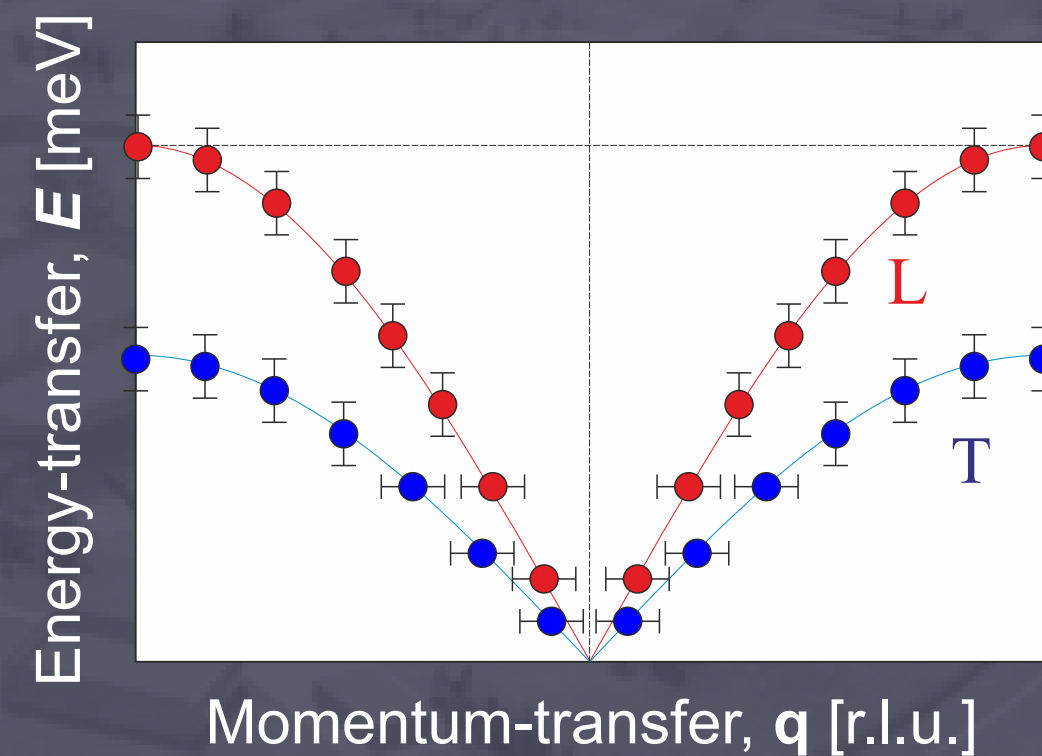
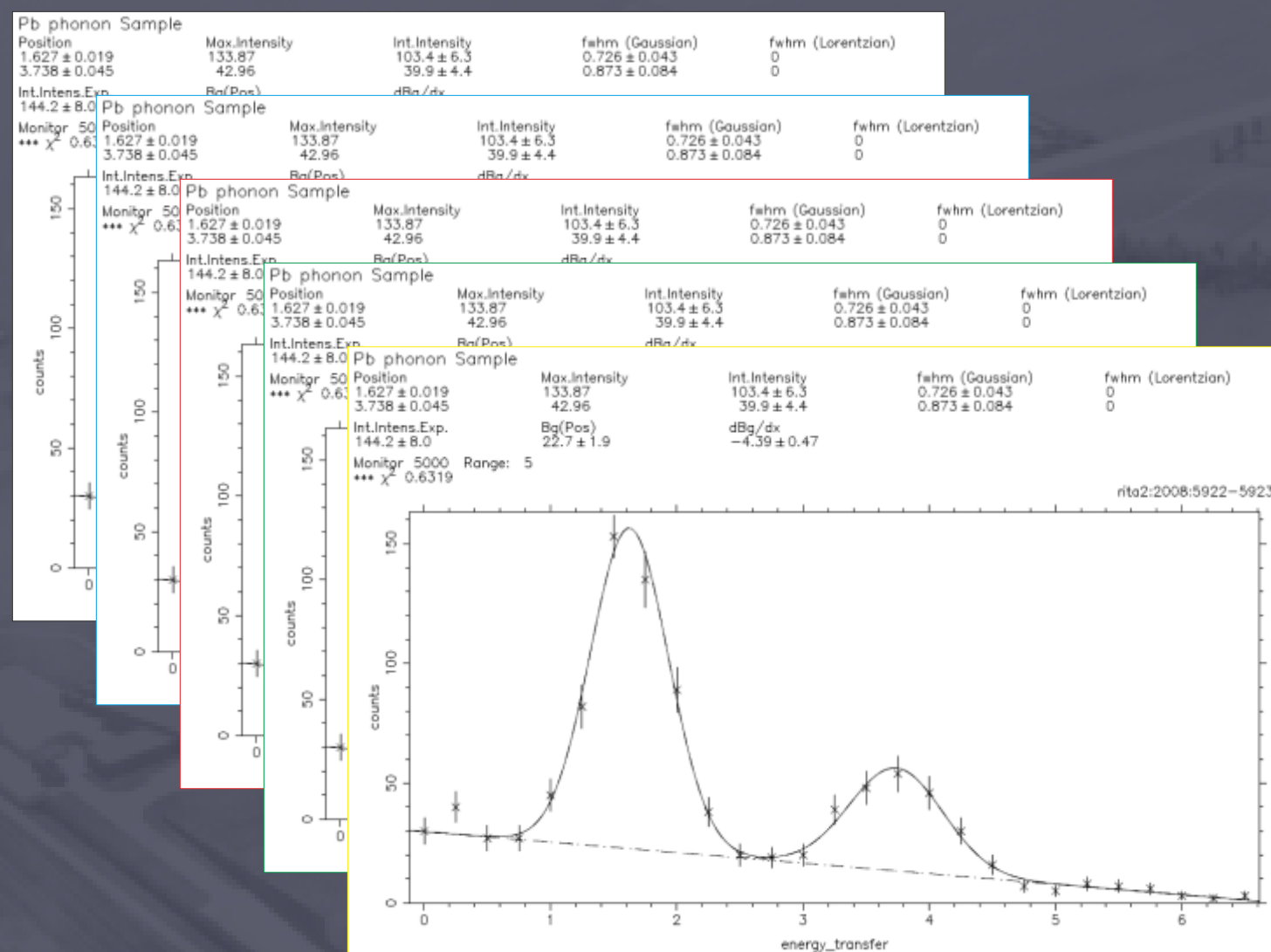
Energy-transfer, E [meV]



Momentum-transfer, q [r.l.u.]

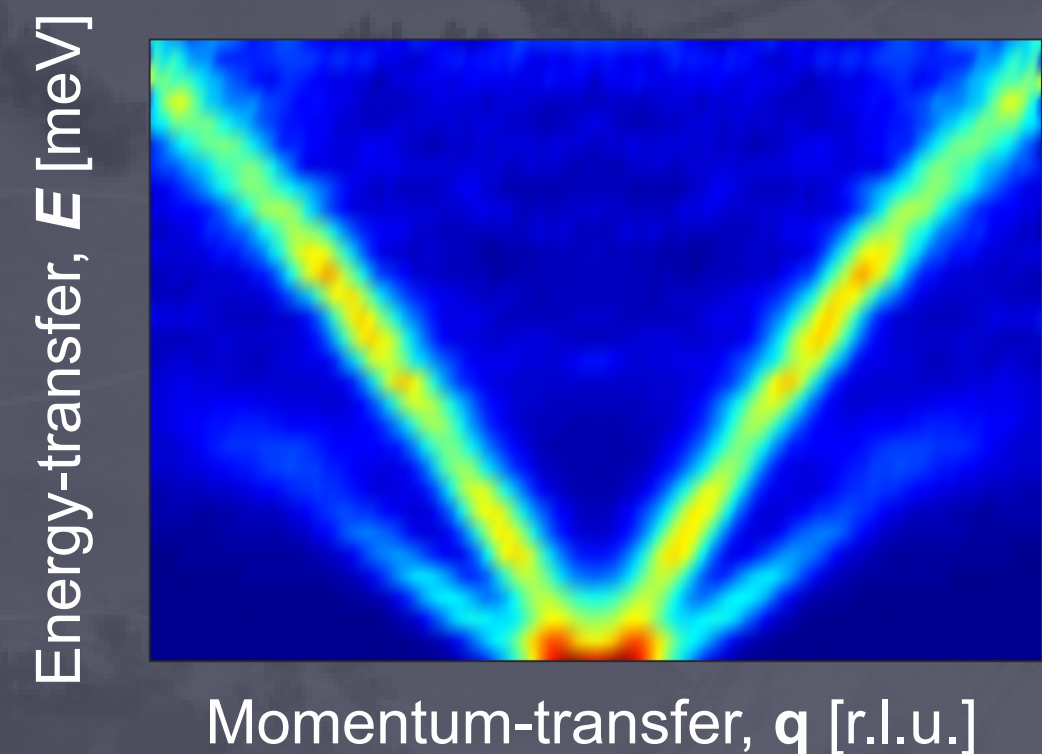
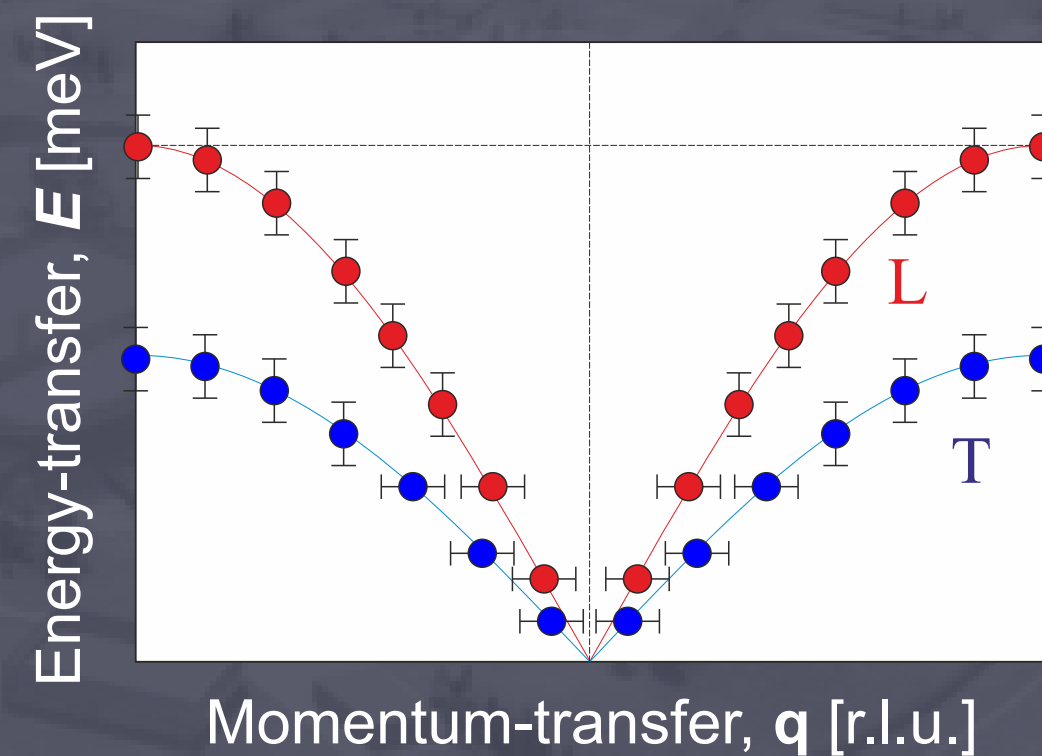
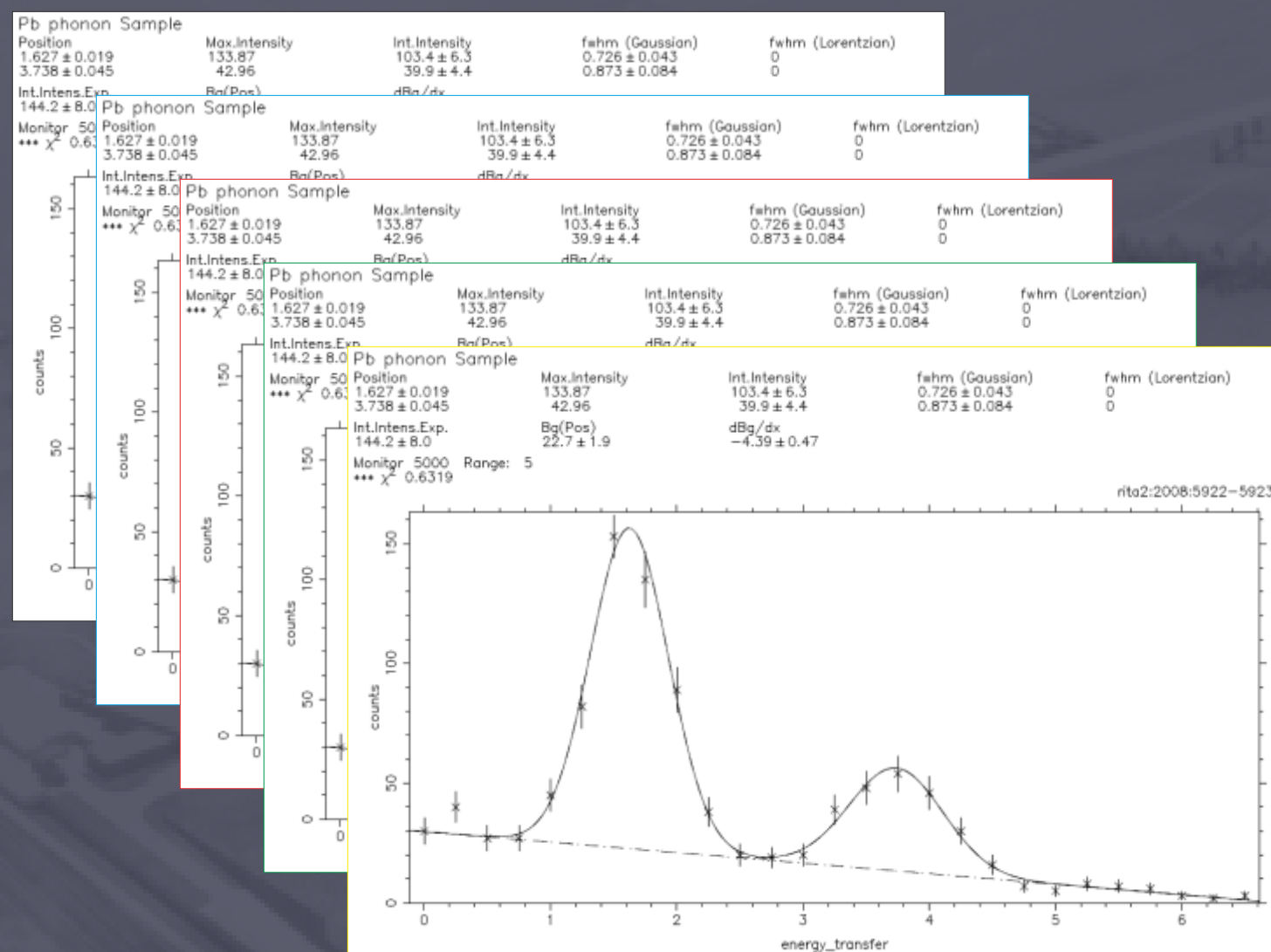
Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.



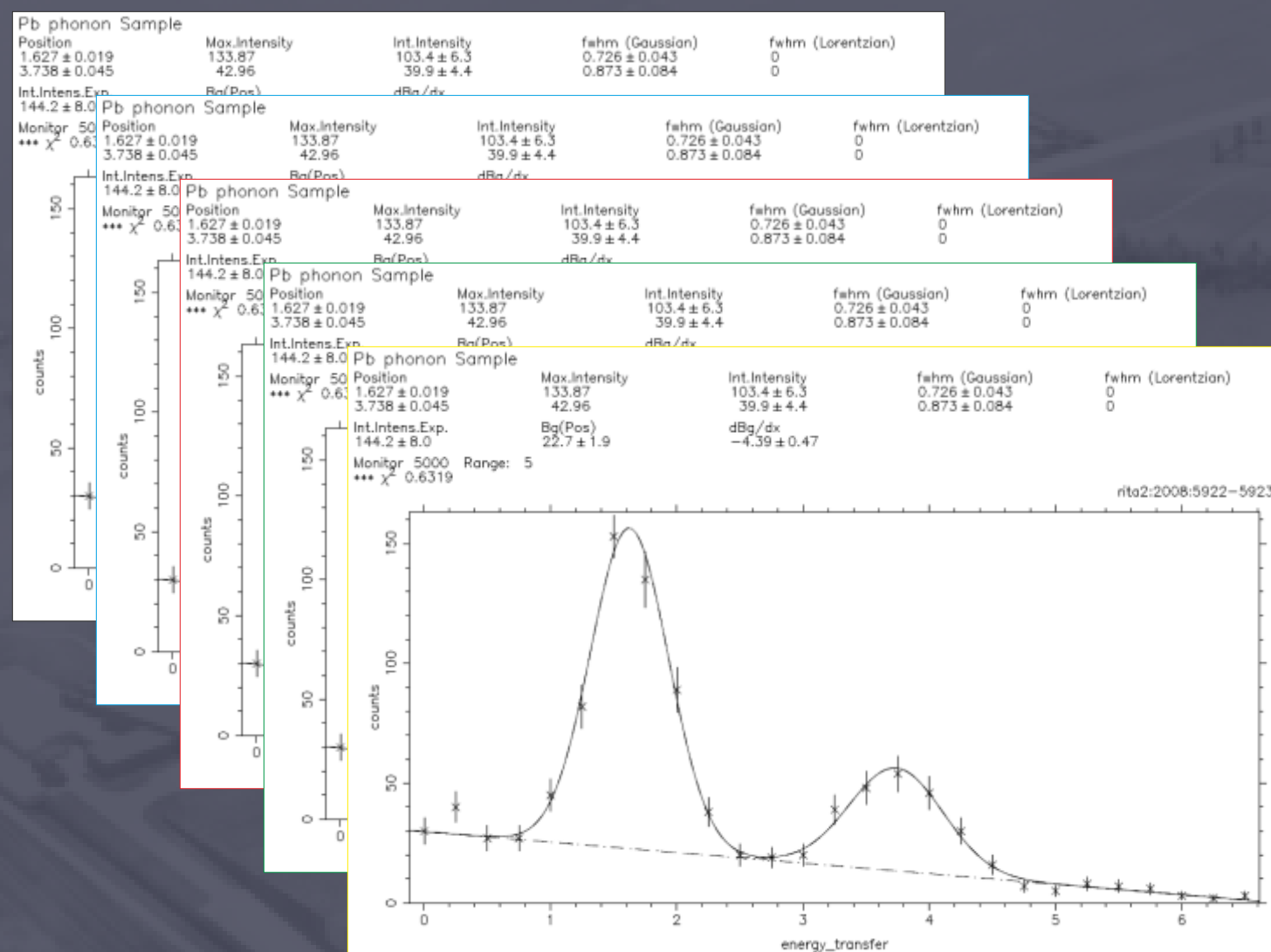
Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.

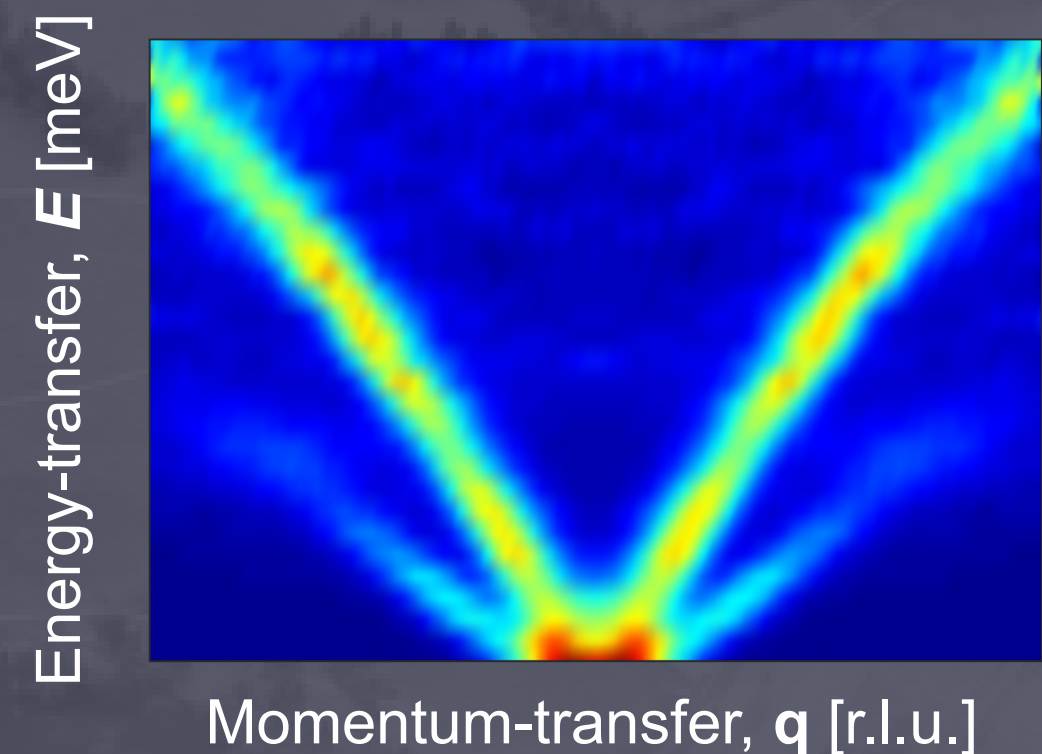
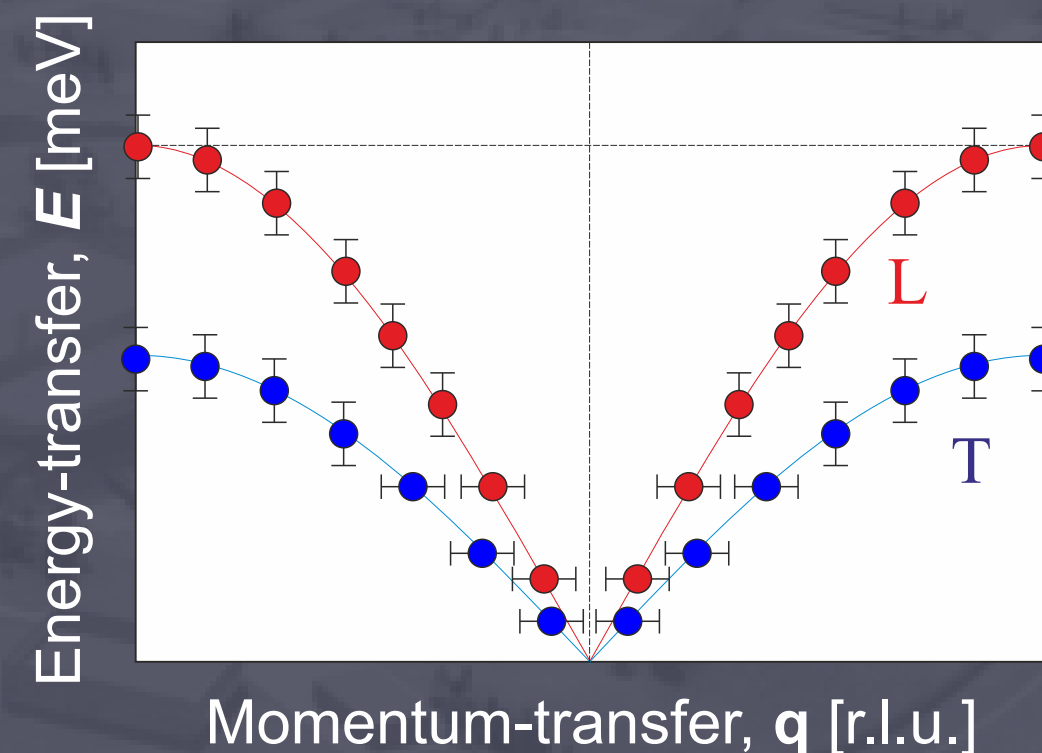


Classic TAS: Data Acquisition & Analysis

- Build up an excitation dispersion curve (E vs. Q) by acquiring 1D cuts (1 spectra) and fitting the peaks to give 1 or several points of the dispersion.

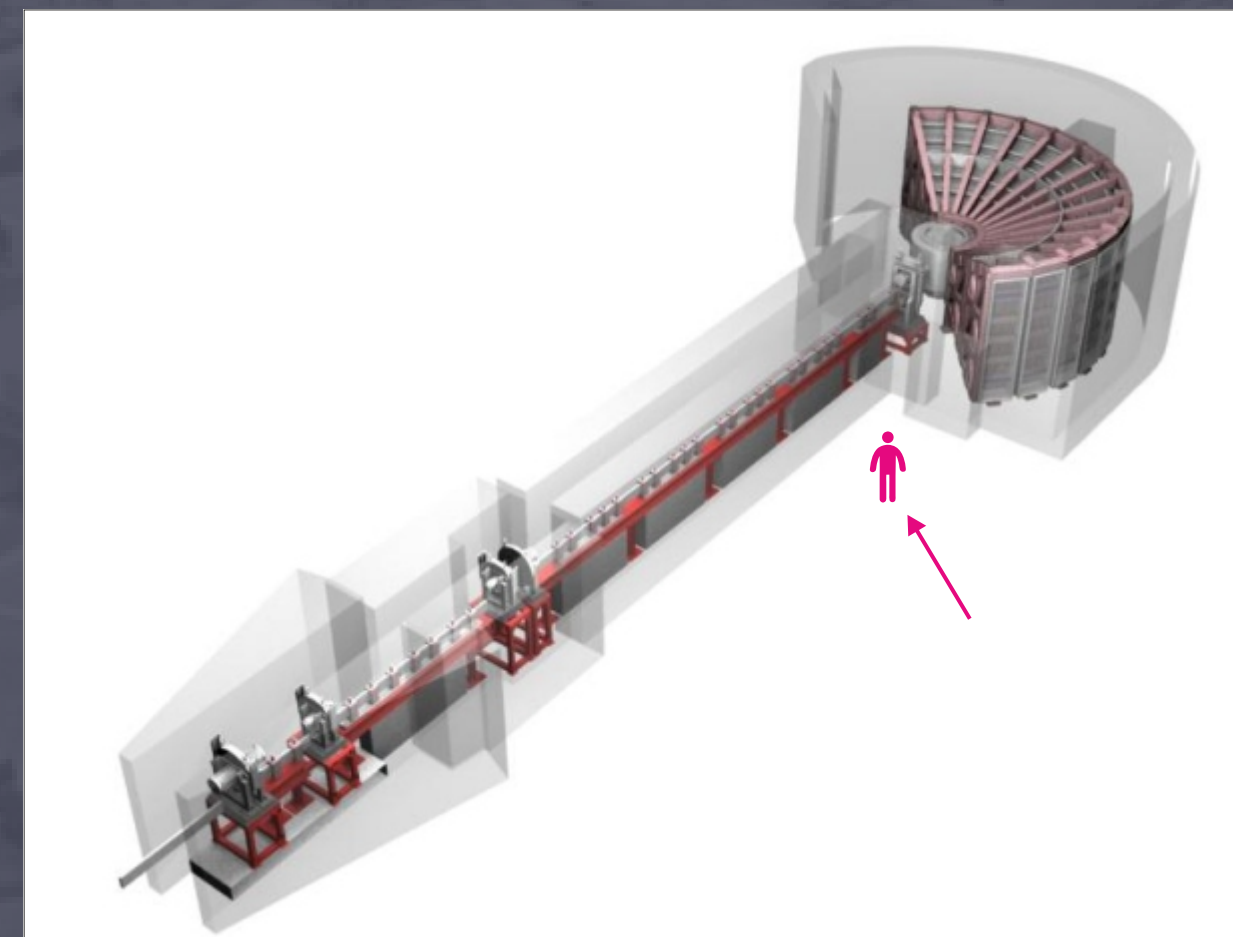
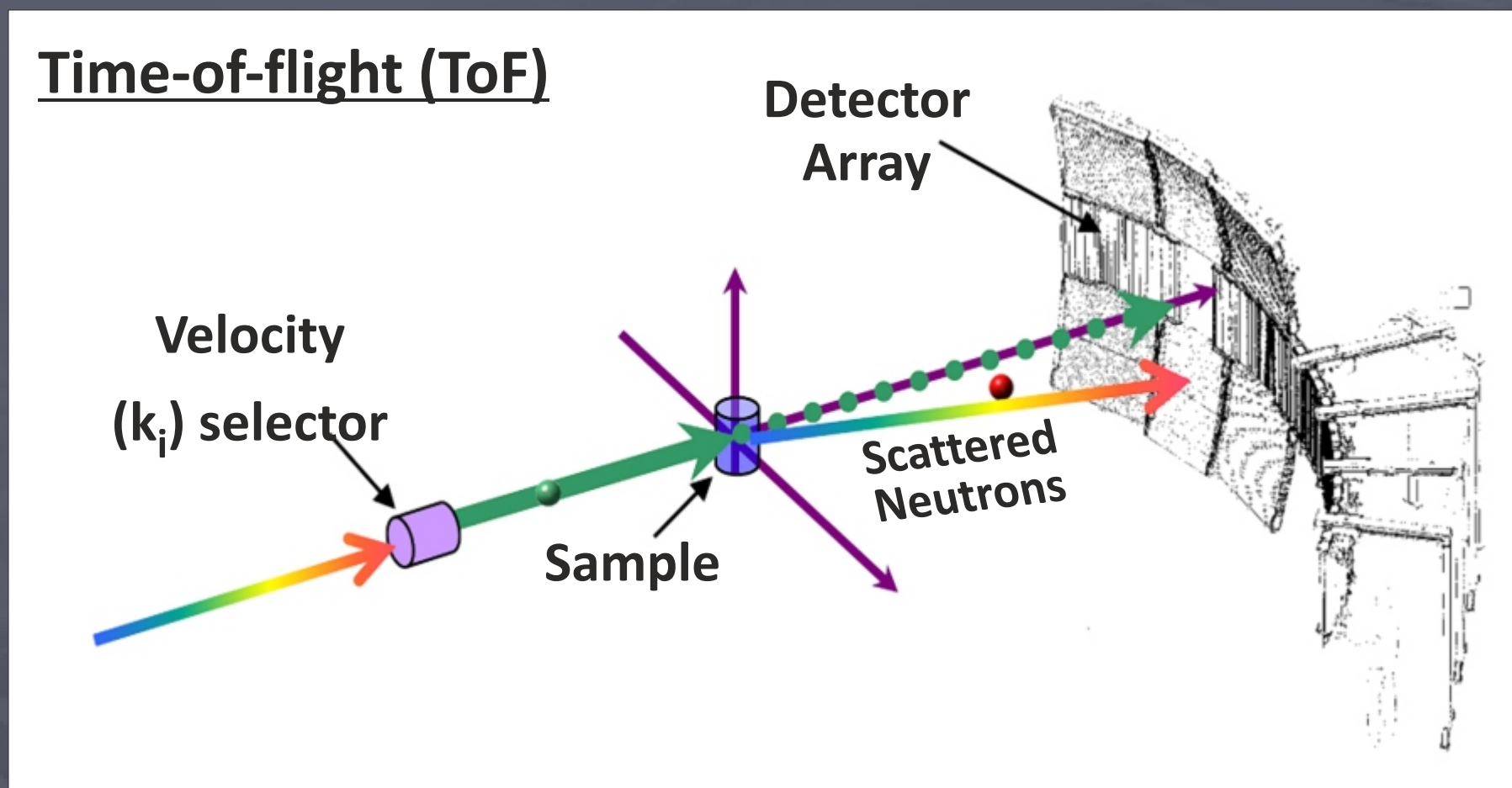


- Online data analysis is made in 1 minute while scanning next point. Full analysis is done in 1 hour/spectra. Total data volume 100 kbyte acquired in 5 days (magnetic).



Modern INS: Time-of-Flight (ToF)

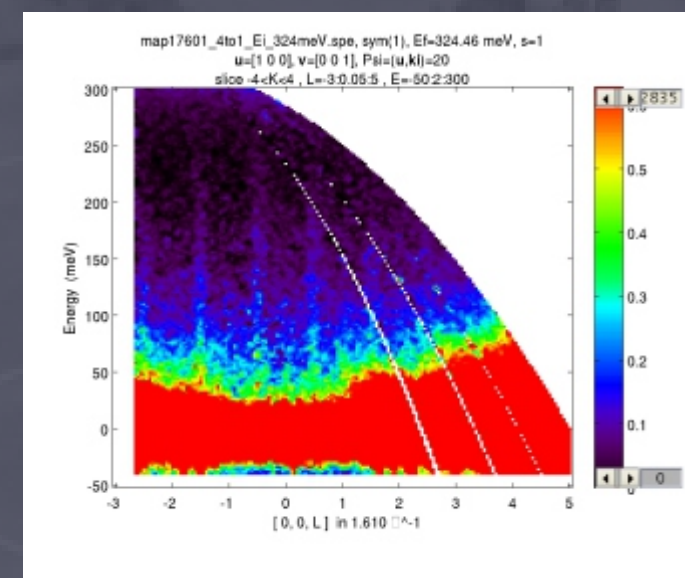
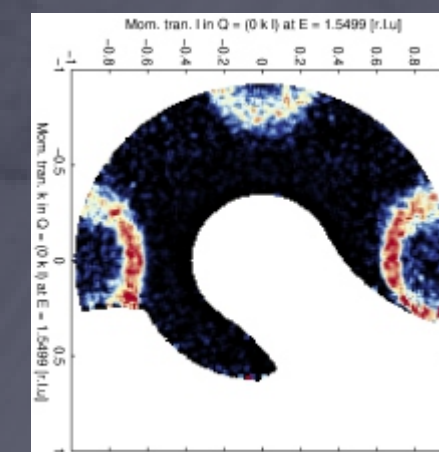
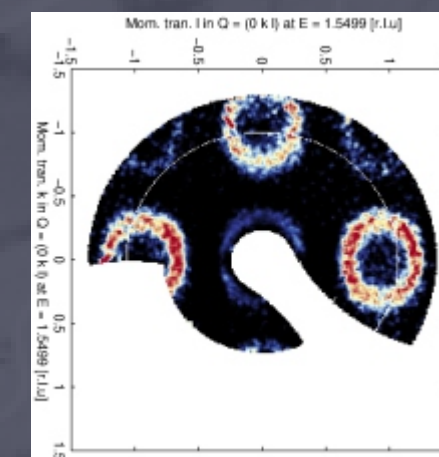
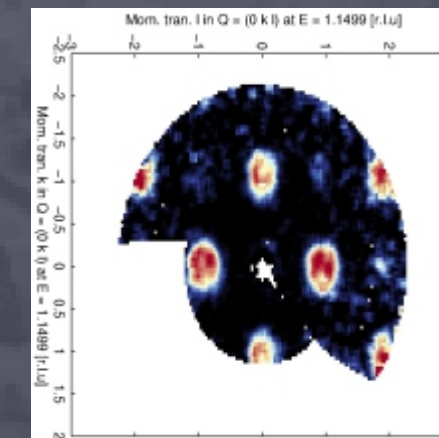
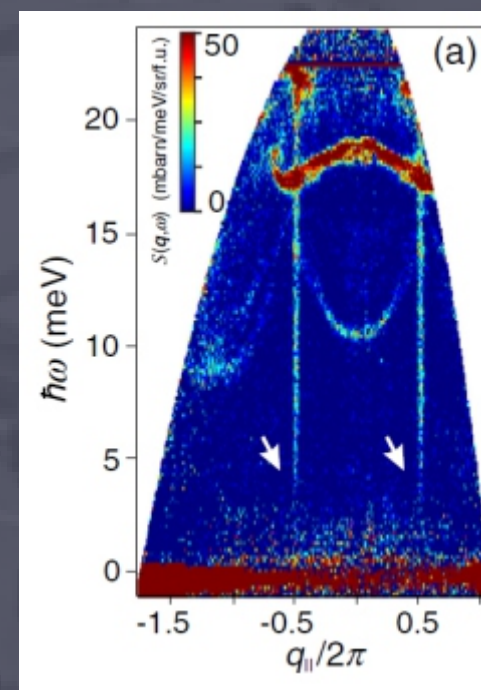
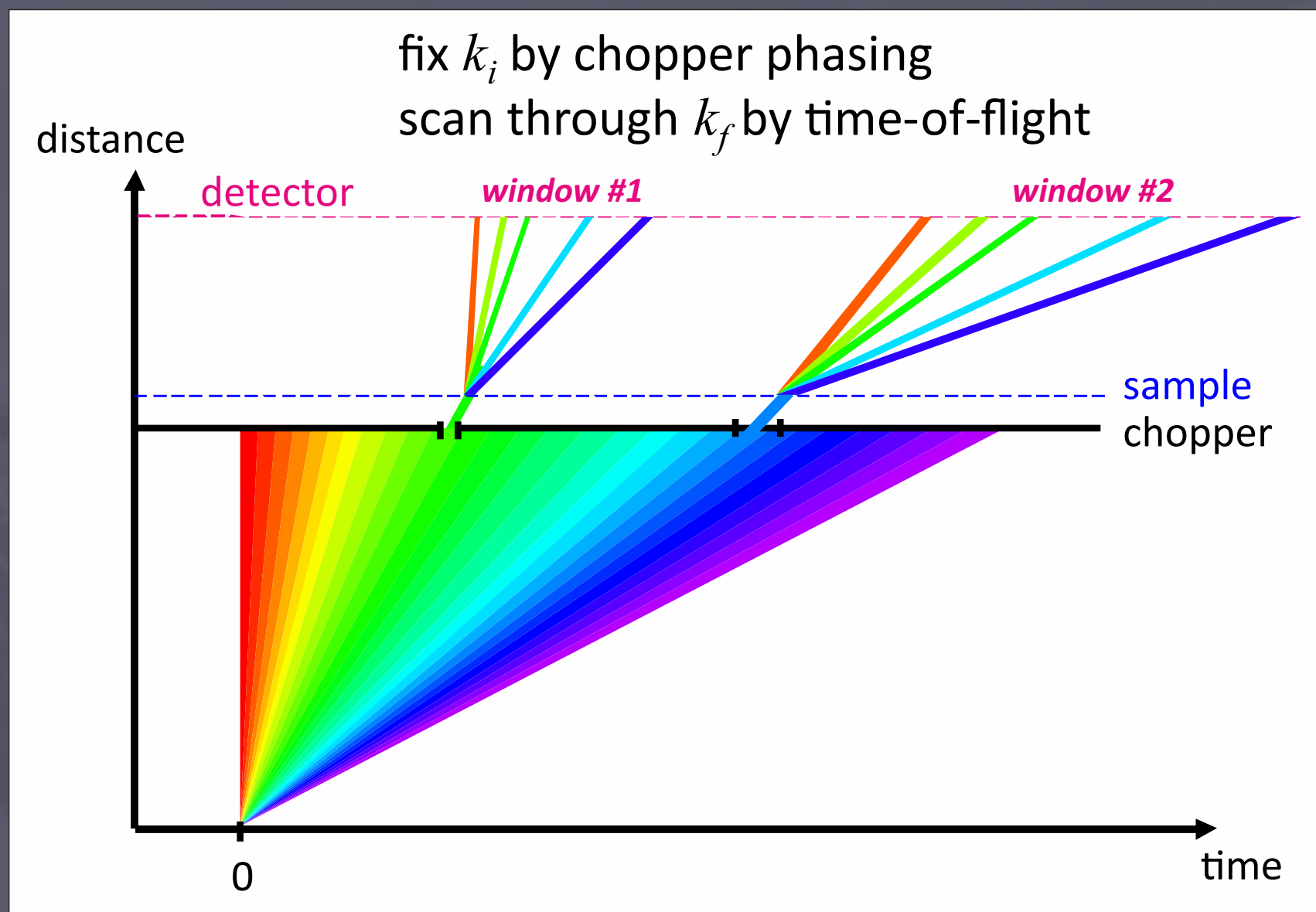
- Modern time-of-flight instruments (on modern pulsed sources) have huge detector banks.



- Data come out as a 3D/4D matrix with a huge number of measured Q-points (q_x , q_y , q_z). Each point is also resolved in energy-transfer... and H, T, E, P !!!
- Raw data files are 100 GB or even several TB
- Data collection can be a few days, while data analysis months or even years (first perform the experiment and then the PhD project).

Multiple Time/Energy Windows

- By clever tuning of several chopper speeds and phases it is possible to gain several neutron energies in one single frame i.e 2 or 3 complete data sets simultaneously (high-resolution zoom + lower-resolution overview).



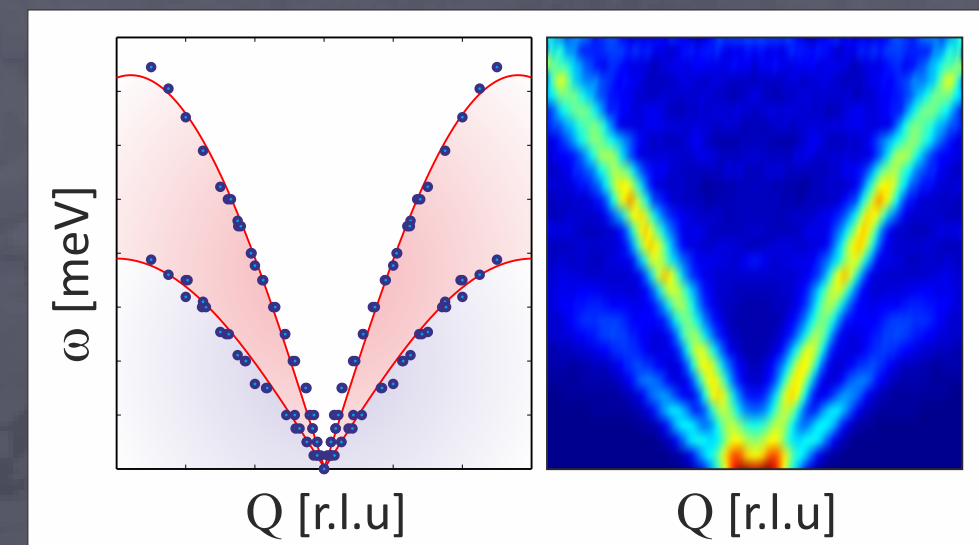
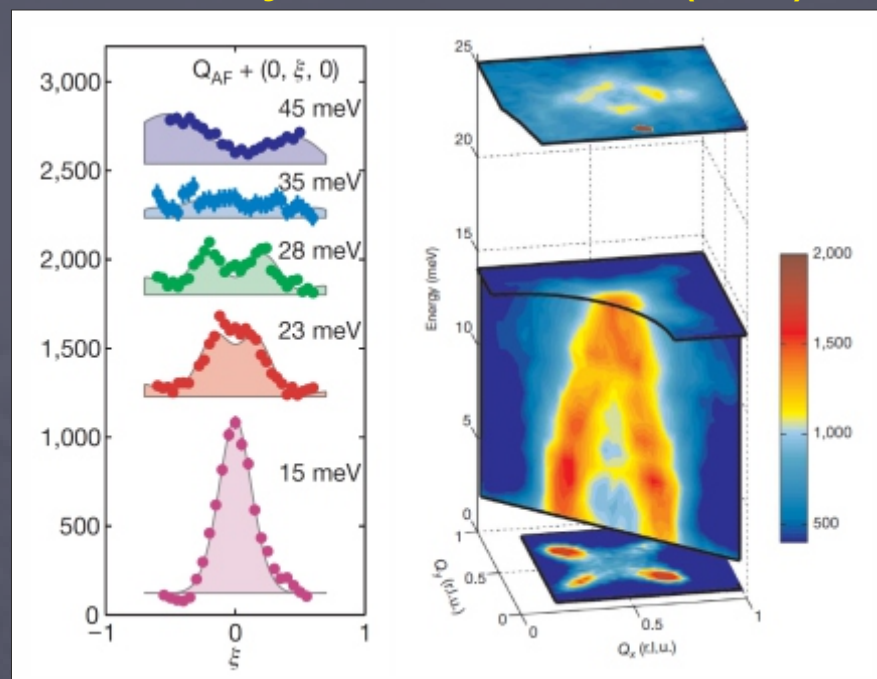
- Very efficient use of produced neutrons (much larger fraction of scattered neutrons are collected/counted (i.e. data)).

INS: Examples

NUCLEAR EXCITATIONS

- Lattice vibrations i.e. **phonons** have traditionally been extensively investigated (e.g. cooper-pair formation in conventional superconductors)

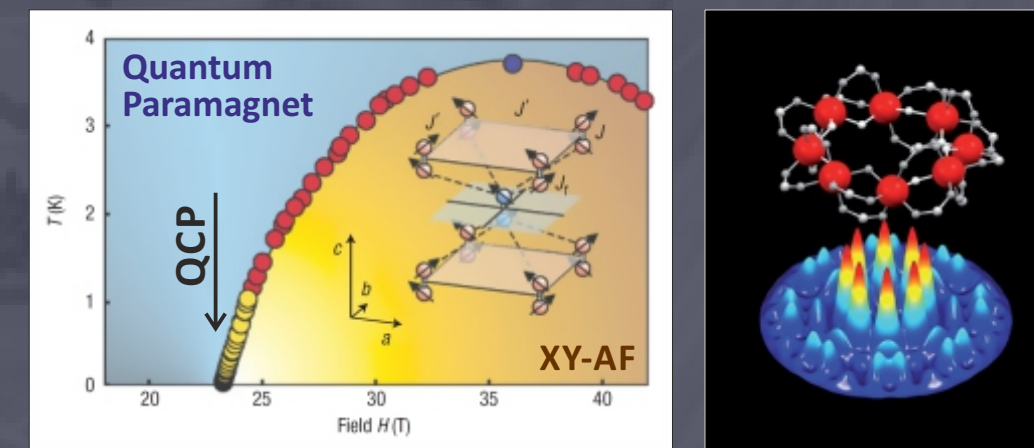
Boothroyd, Nature 471, 341 (2011)



HIGH-TEMPERATURE SUPERCONDUCTIVITY

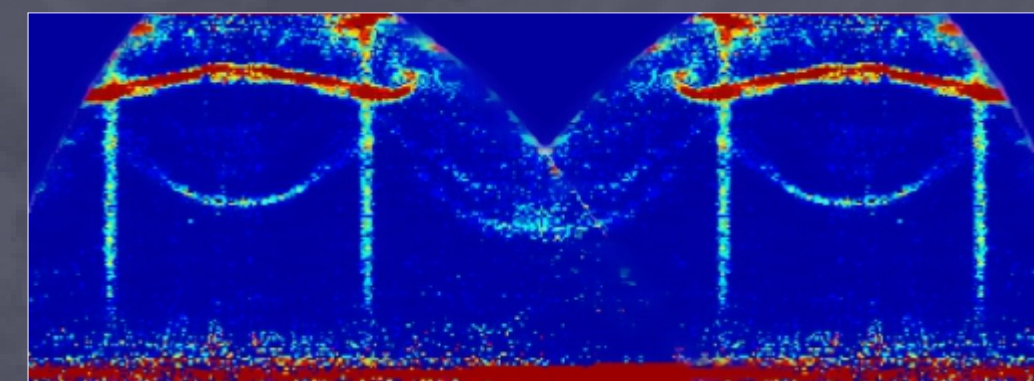
- HTSC emerges from AF parent compounds. INS has shown that **spin excitations** remain even in the SC phase.

GIAMARCHI, Nature Physics 4, 198 (2008)



MAGNETISM

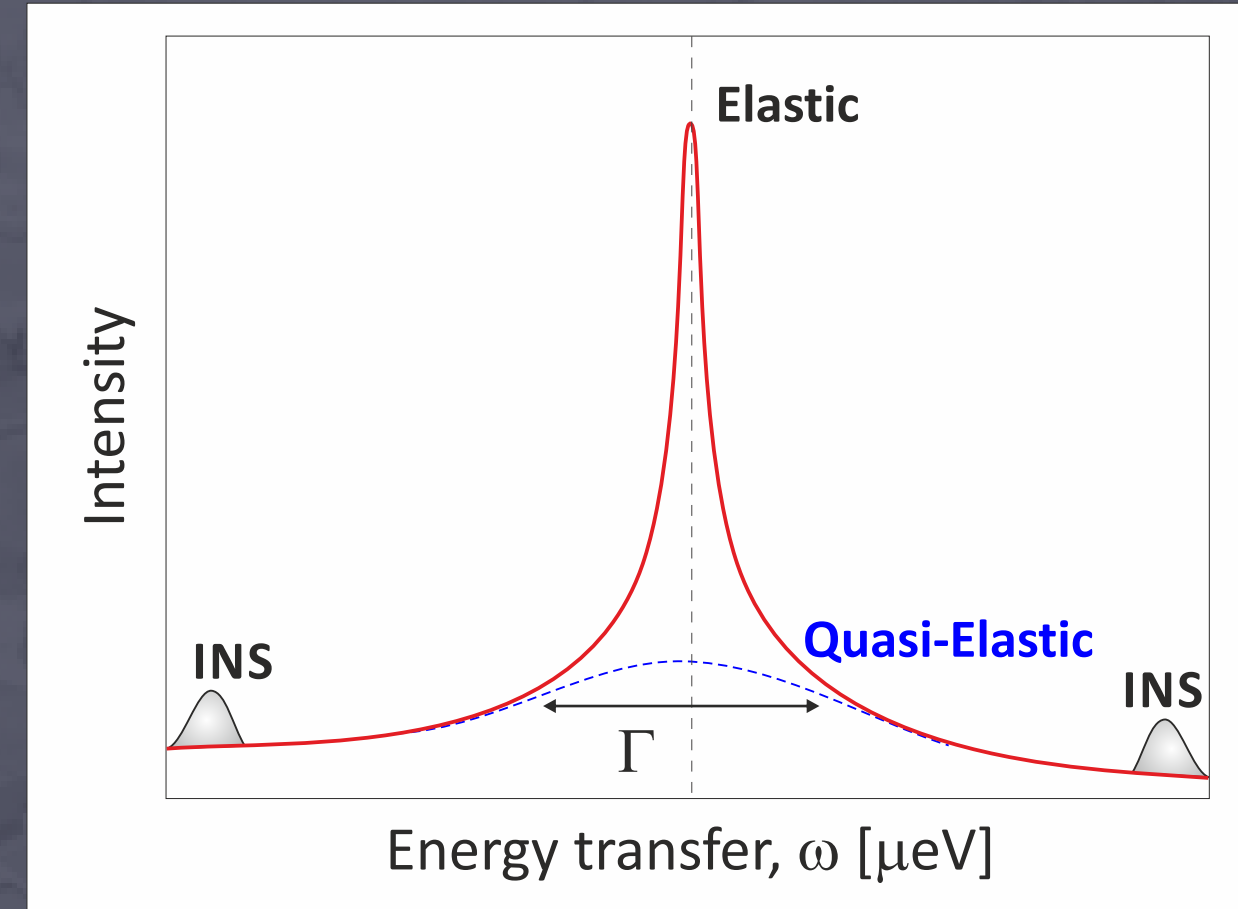
- Spin-wave/magnon** mapping in exotic magnets (triangular frustration, square lattice AF etc.)
- Induce magnetic order by pressure, external field (**Bose Einstein Condensation and QCP** in quantum/molecular magnets).



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

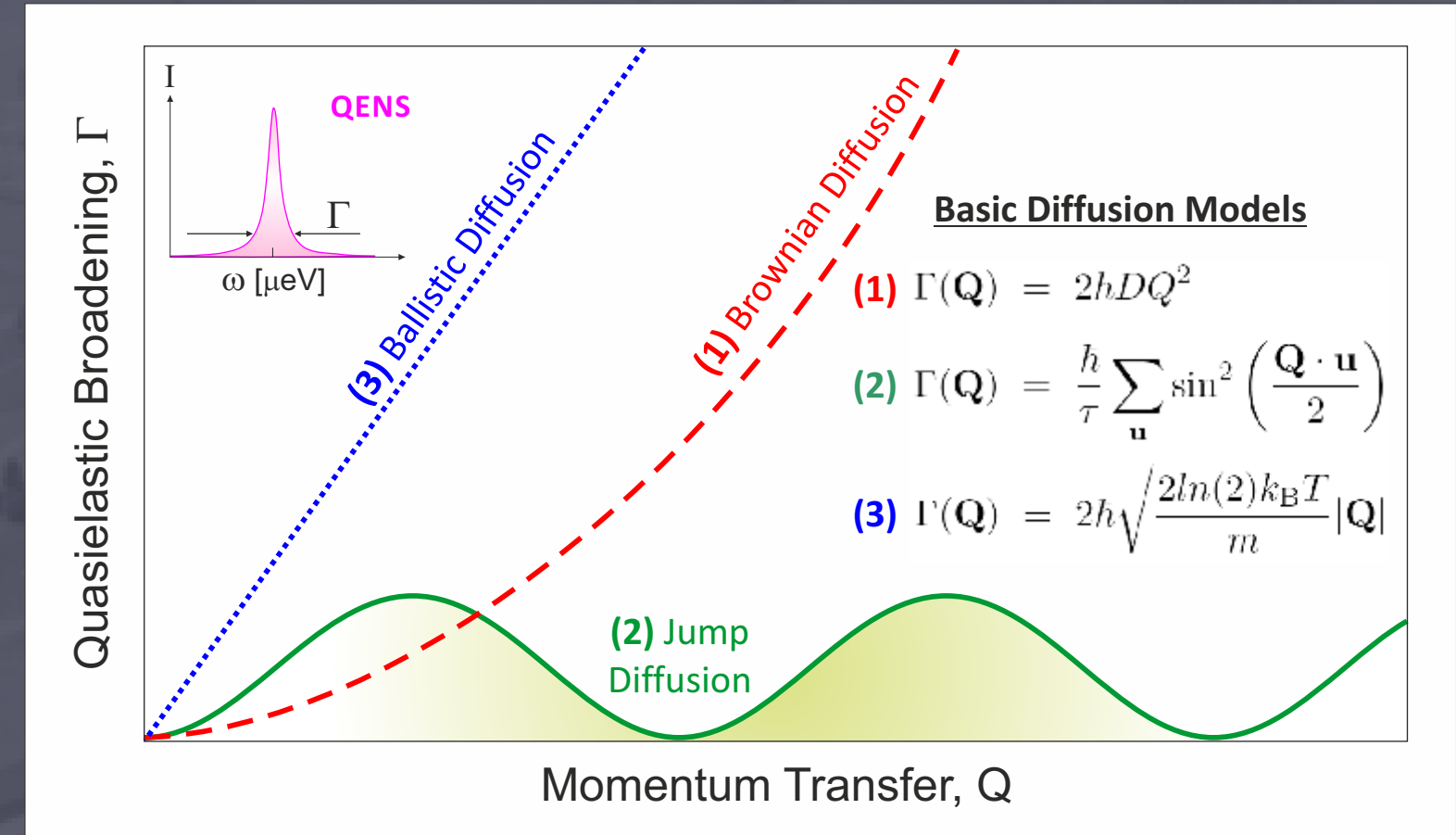
Quasi-Elastic Neutron Scattering (QENS)

- QENS is a 'sub-genre' of INS dealing with $\omega_{\max} \approx \pm 2 \text{ meV}$ using high-resolution [μeV]
- QENS signal/line-width (Γ) supply info on particle/ion/molecular diffusion and/or dynamics on a 0.1–100 nm & ps–ns scale. Temperature dependence give activation energy (E_a) and Q-dependence information on geometry of the diffusion process (continuous, jump, rotation...).



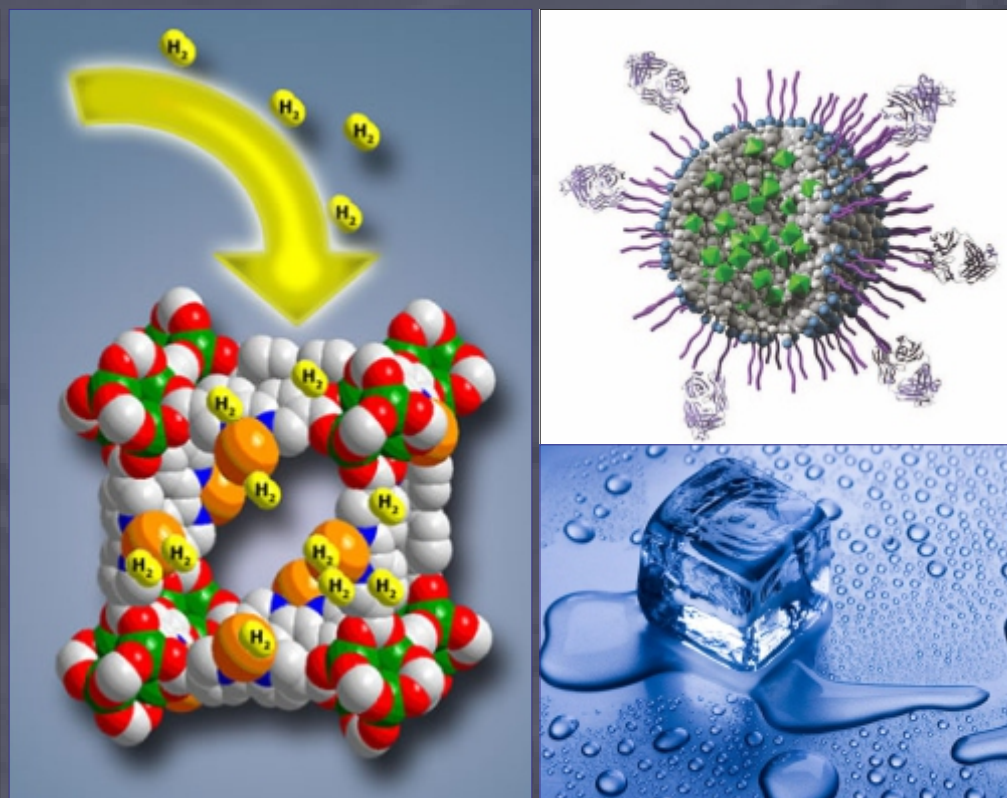
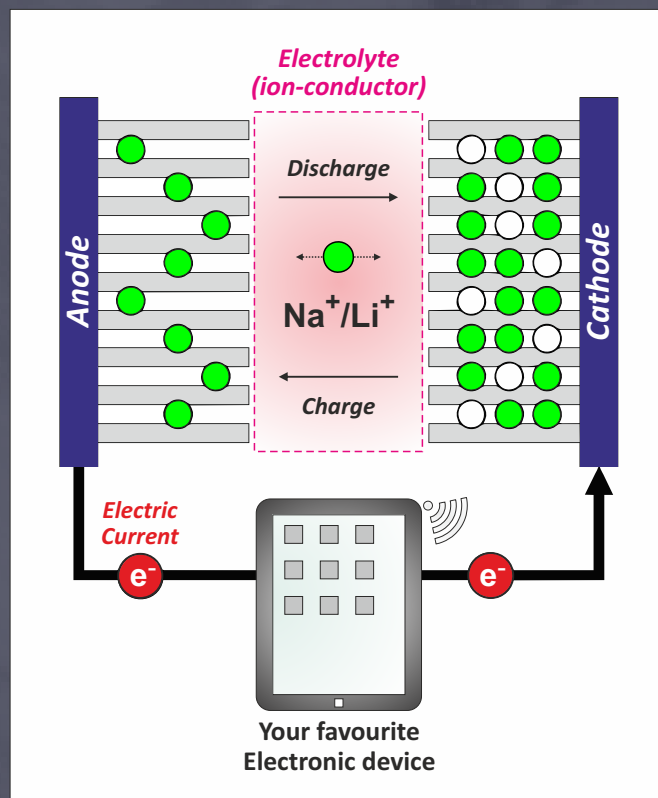
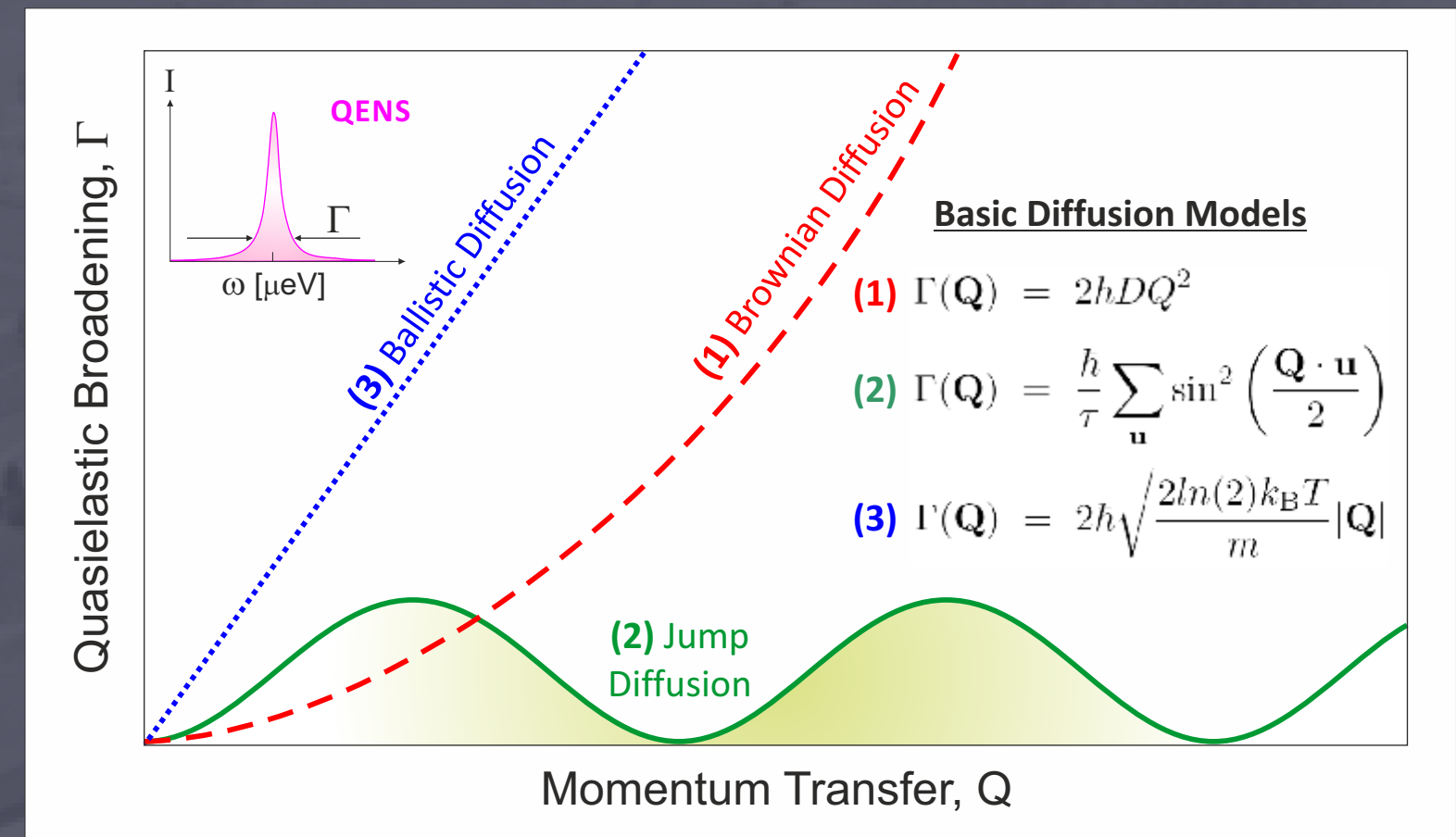
Quasi-Elastic Neutron Scattering (QENS)

- QENS is a ‘sub-genre’ of INS dealing with $\omega_{\max} \approx \pm 2 \text{ meV}$ using high-resolution [μeV]
- QENS signal/line-width (Γ) supply info on particle/ion/molecular diffusion and/or dynamics on a 0.1–100 nm & ps–ns scale. Temperature dependence give activation energy (E_a) and Q-dependence information on geometry of the diffusion process (continuous, jump, rotation...).



Quasi-Elastic Neutron Scattering (QENS)

- QENS is a ‘sub-genre’ of INS dealing with $\omega_{\max} \approx \pm 2 \text{ meV}$ using high-resolution [μeV]
- QENS signal/line-width (Γ) supply info on particle/ion/molecular diffusion and/or dynamics on a 0.1–100 nm & ps–ns scale. Temperature dependence give activation energy (E_a) and Q-dependence information on geometry of the diffusion process (continuous, jump, rotation...).

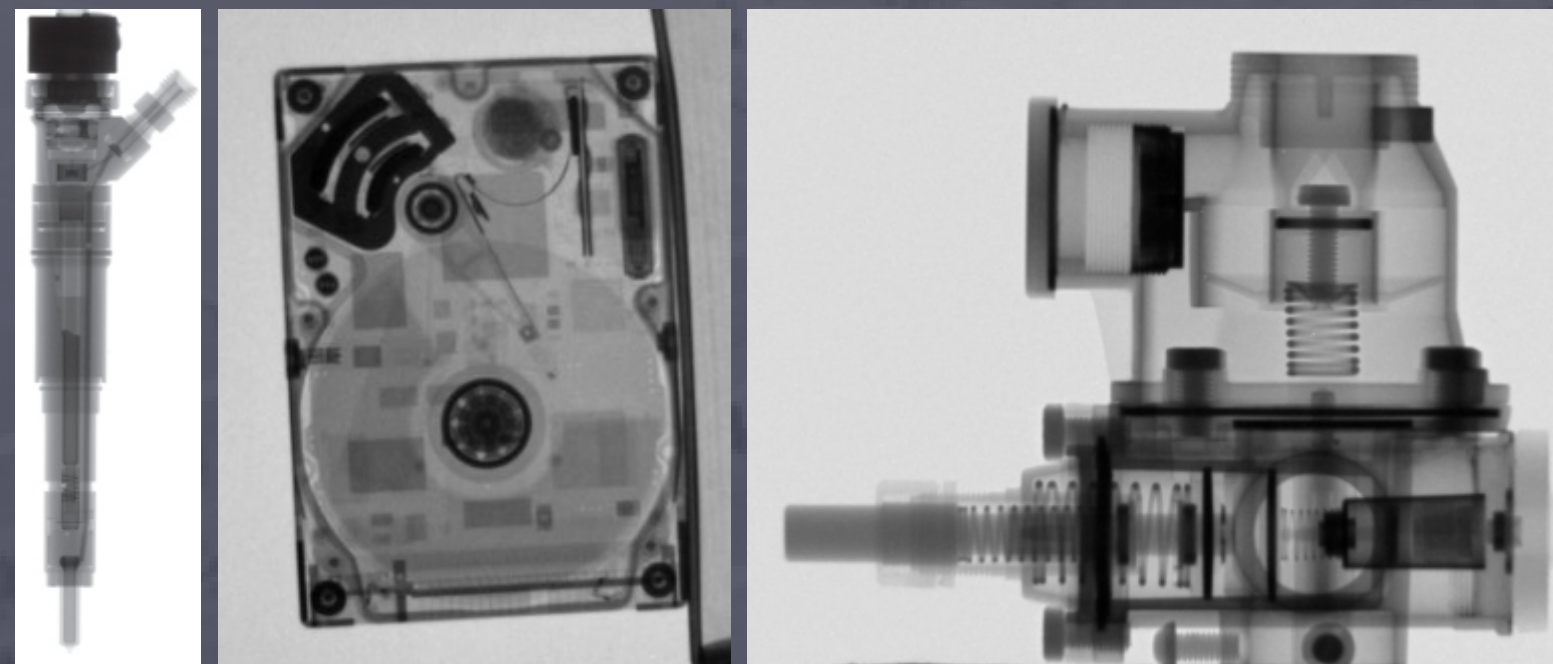


- Molecular dynamics (bond rotations...) and dynamics in bio / life-science
- Fluid dynamics including e.g. confined liquids and melting processes
- Energy materials including e.g. battery, hydrogen storage and fuel cells.

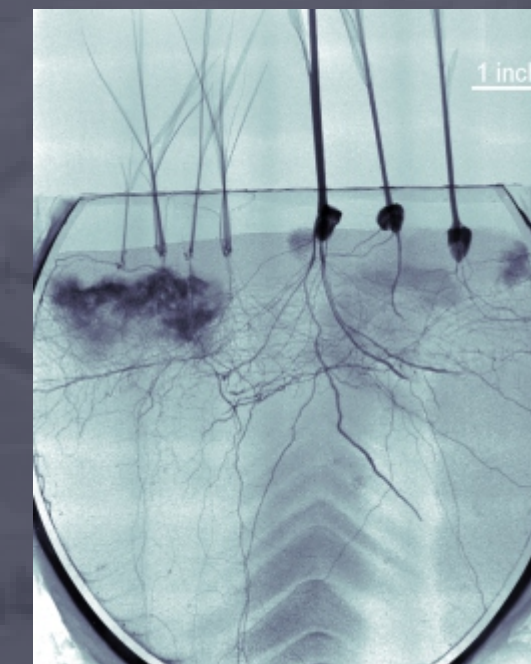
Neutron Imaging

- Similar to an X-ray radiography but technically not a scattering technique
- Resulting image is based on the neutron attenuation properties of the different parts of the imaged object.
- Due to the different interaction mechanism of neutrons and X-rays with matter, neutrons delivers complementary information.
- Spatial resolution is on the order of micro-meter, but this is continuously being improved.

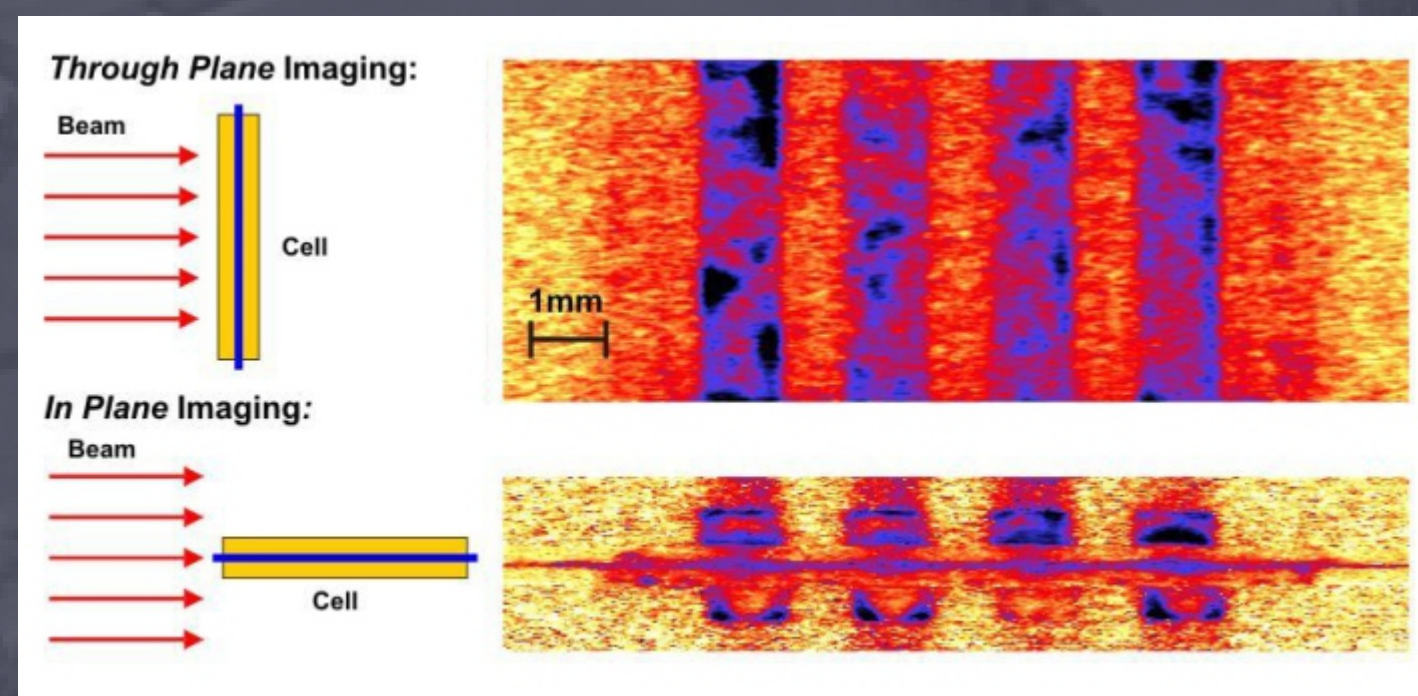
Non-destructive testing of mechanical components



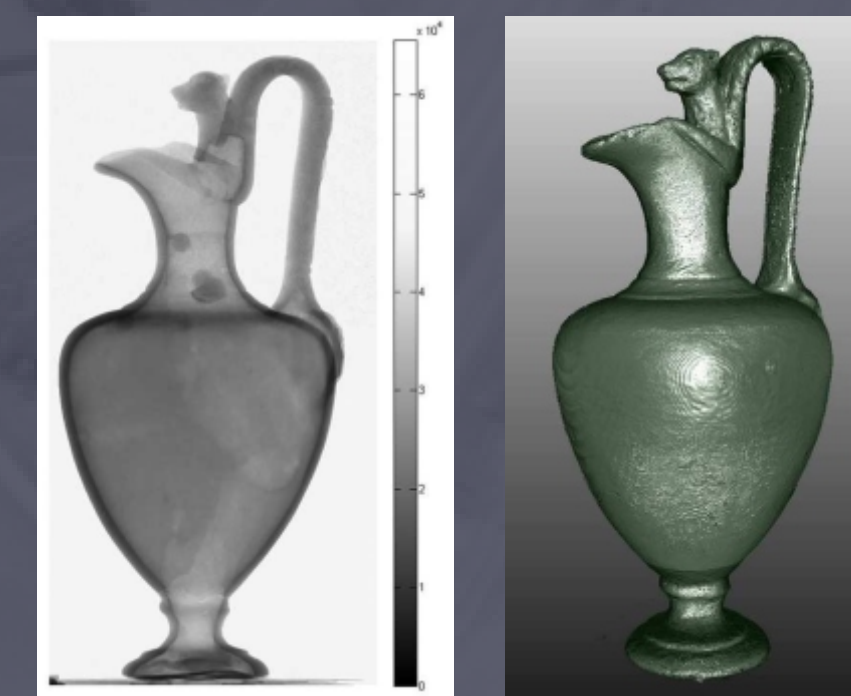
Root-system of plants



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

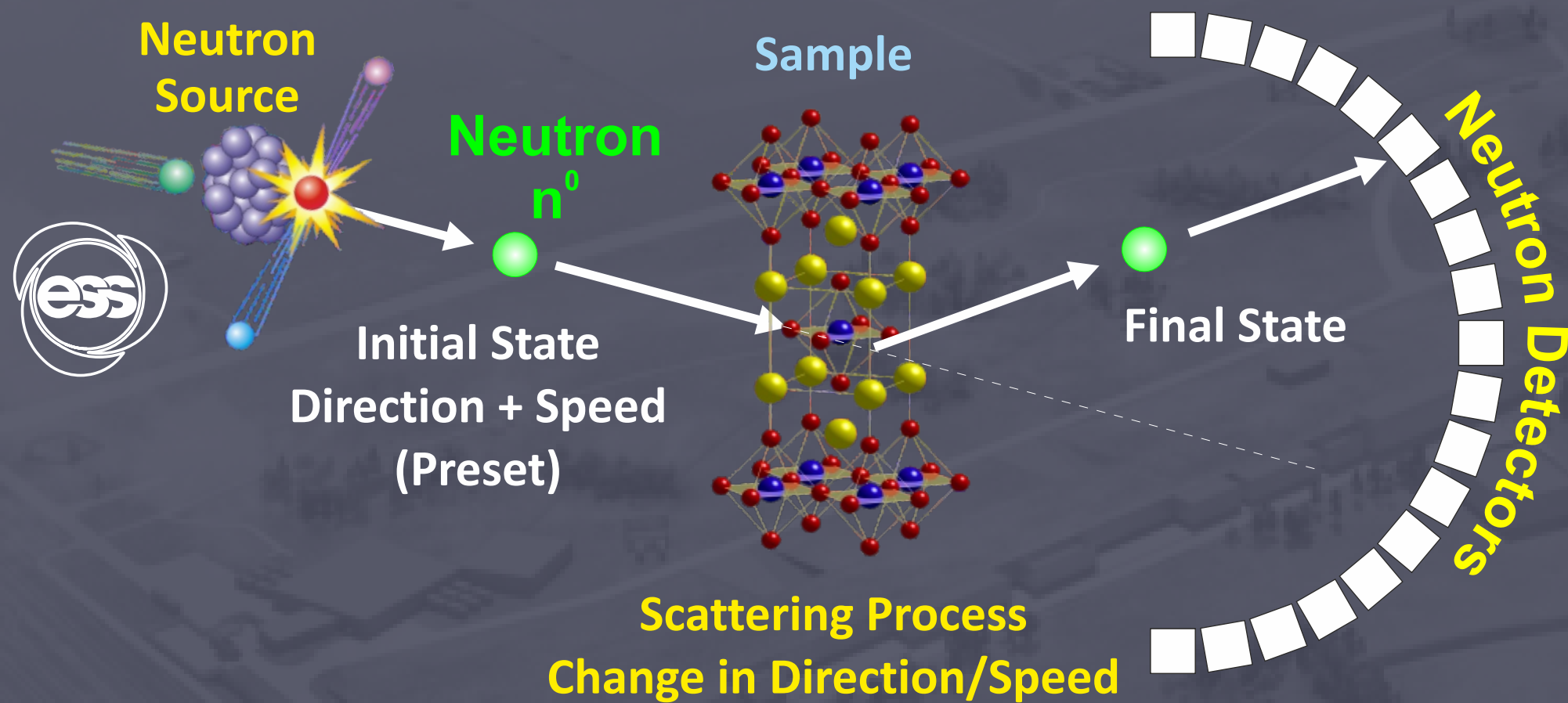


Radiography / Tomography of archeological artefacts

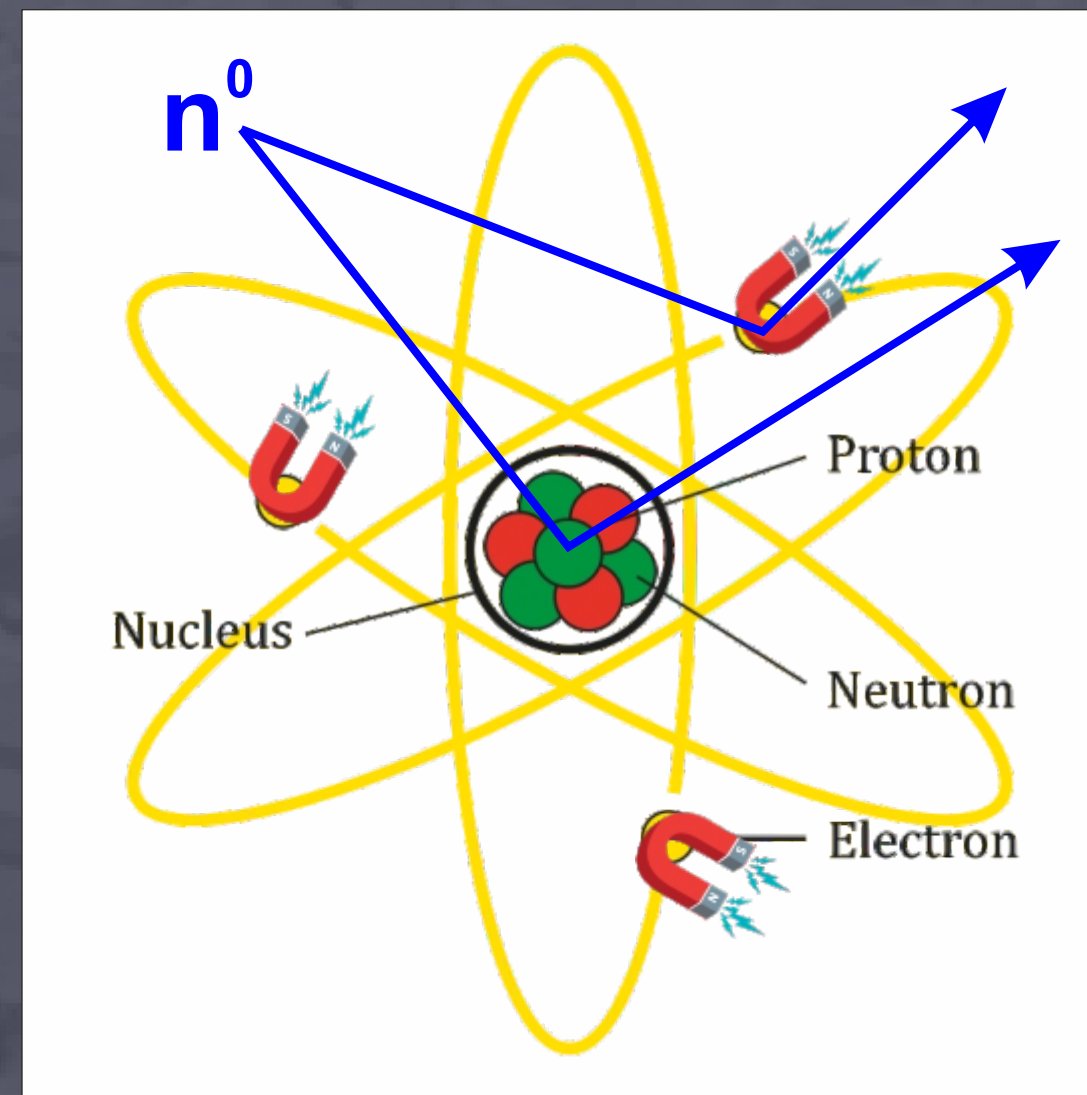


Neutron Scattering 101

- Neutron is a subatomic (very small) particle without charge (i.e. neutral) but with a magnetic moment (spin = 1/2).



Neutrons interact with both atomic nucleus and electron spins (magnetism) of the atoms



Scattering Process

“Elastic Neutron Scattering”

Only detect change in direction/angle

Tells us about where atoms are and how spins align

“Inelastic Neutron Scattering”

Detect change in direction/angle + speed/energy

Tells us what the atoms and electron spins ‘do’

Atomic Structure & Dynamics + Magnetism

Neutron Sources of the World



EUROPE

ILL, Grenoble, France

ISIS/RAL, UK

SINQ, PSI, Switzerland

FRM-II, Germany

BER II, HZB, Berlin, Germany (closed !!!)

LLB, Saclay, France (closed !!!)

IFE, Kjeller, Norway (closed !!!)

OTHER EXAMPLES

HFIR/SNS, Oak Ridge, USA

J-PARC, Japan

ANSTO, Bragg Institute, Australia

UNDER CONSTRUCTION

Lund, Sweden



Dongguan, China



<http://www.neutrons.se/>

<http://www.neutronsources.org/>

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

European Spallation Source (ESS)

- European flagship project constructed in Lund with 15 member countries & Sweden as host
- Construction cost: 1843 M€ with Sweden contributing 37.5% (+ operations costs)



European Spallation Source (ESS)

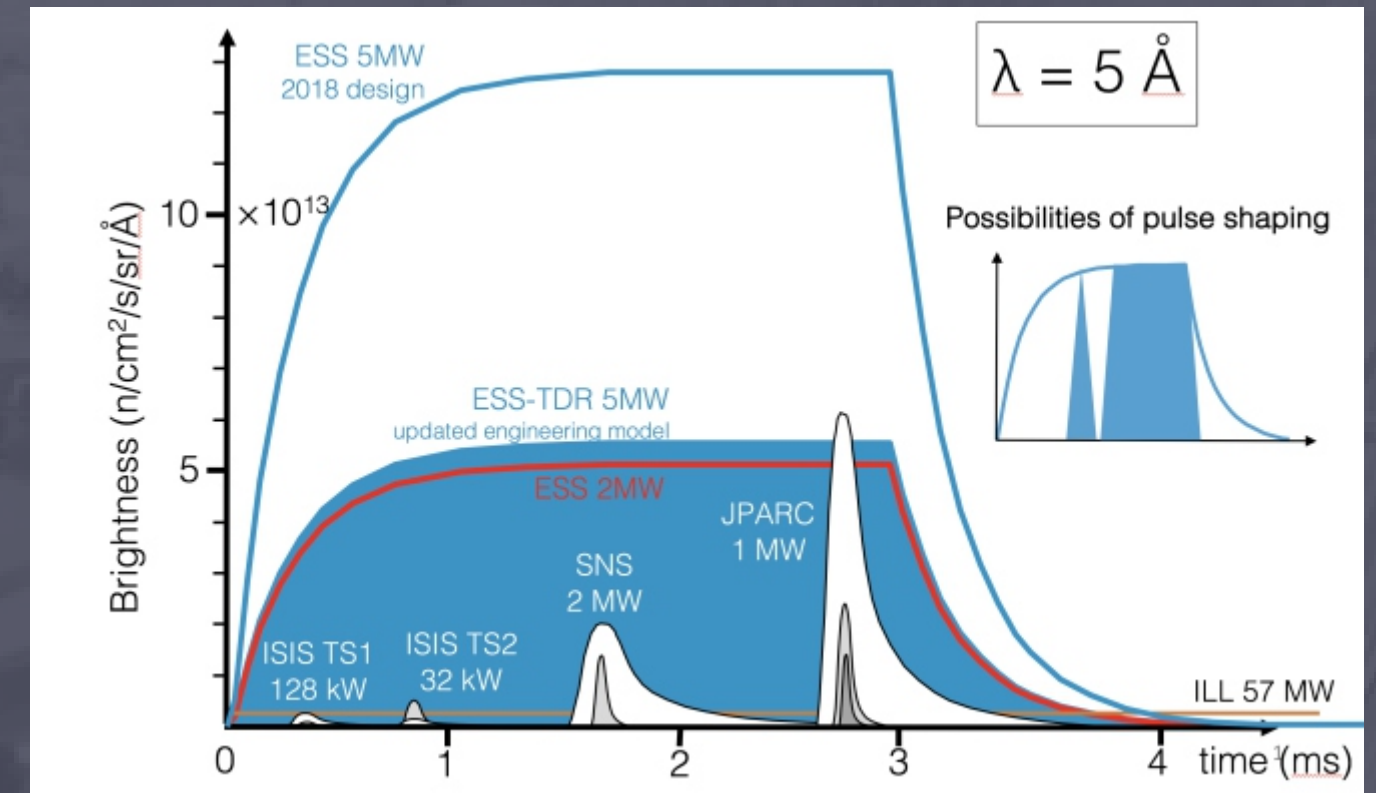
- European flagship project constructed in Lund with 15 member countries & Sweden as host
- Construction cost: 1843 M€ with Sweden contributing 37.5% (+ operations costs)



- Neutrons and then user operation expected ~2025...

ESS: A world-leading Neutron Facility

- ESS will clearly be the world's most intense neutron source
- But all technical aspects are “better”: moderators, detectors wave-guides = also more efficient use of produced neutrons
- First 15 instruments are on average $\times 20$ better (at 2 MW) than best existing instruments. But some ultimately $\times 250$!!!
- Now: measure for 20 or 250 days \rightarrow ESS: measure 1 day !!!
- The result is that we can measure faster and/or study much smaller samples.
- “**Game changer**” for many many fields e.g. protein crystallography, quantum materials, energy, ...
- **In situ/operando** studies will strongly benefit with better time-resolution and lower background
- **Extreme conditions** much easier, where we can push the limit + use multiple conditions!
- Measurements of dynamics (inelastic + QENS = **spectroscopy**) will have a new world to explore
- Completely new way of conducting neutron scattering (J-PARC/SNS show a teaser...)



"The instrument suite of the European Spallation Source" – Nuclear Inst. and Methods in Physics Research, A 957, 163402 (2020)

ESS Construction Phase



ESS Construction Phase



ESS Construction Phase



April 2015

ESS Construction Phase



ESS Construction Phase



November 2015

ESS Construction Phase



ESS Construction Phase



October 2016

ESS Construction Phase



ESS Construction Phase



ESS Construction Phase



ESS Construction Phase



ESS Construction Phase

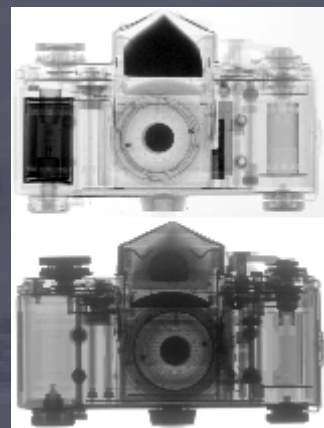
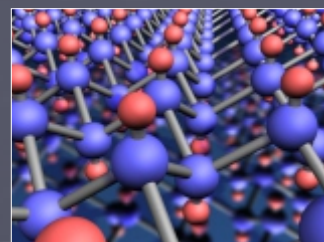
January 2021 (~80% Complete)



EUROPEAN
SPALLATION
SOURCE

Neutrons & X-rays

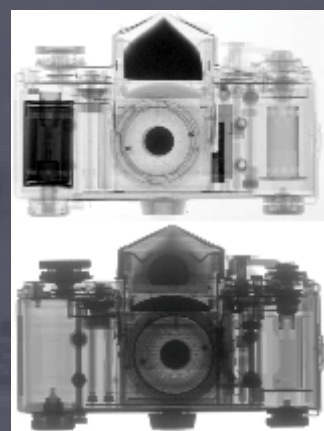
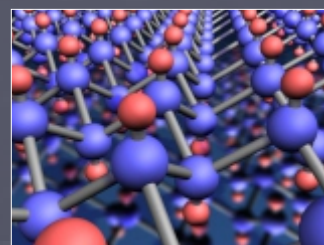
- Neutron and X-ray scattering techniques are complementary to each other.
- Together they create a very powerful experimental tool-box for a wide range of research fields.



- 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.

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.



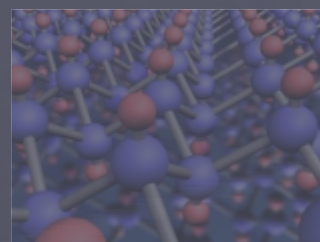
- Deduce complex crystallographic structures that contains atoms visible/unvisible by X-rays and neutrons, respectively.
- Connection between changes in magnetic spin structure and very subtle structural transitions.
- Contrast variation in imaging/tomography techniques.
- Covering different inelastic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



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.

Swedish Beamline @ PETRA III



- Deduce atomic structures that contains neutrons, respectively.
- Connect and verify magnetic spin structure
- Contrast microscopy techniques.
- Covering a wide range of excitation



Neutrons vs. X-rays

NEUTRONS

Low Intensity

Slow Measurement

Bulk properties

Extreme Conditions /In operando

No beam damage

Access to light elements
Isotope Sensitive / Labelling

Better energy resolution

Direct access to magnetism

Difficult to manipulate beams

X-RAYS

High Intensity

Fast Measurement

Not always bulk properties

"Difficult"

Potential beam damage (bio/organic)

No access to light elements or
Isotope labelling (especially H/D)

Worse energy resolution

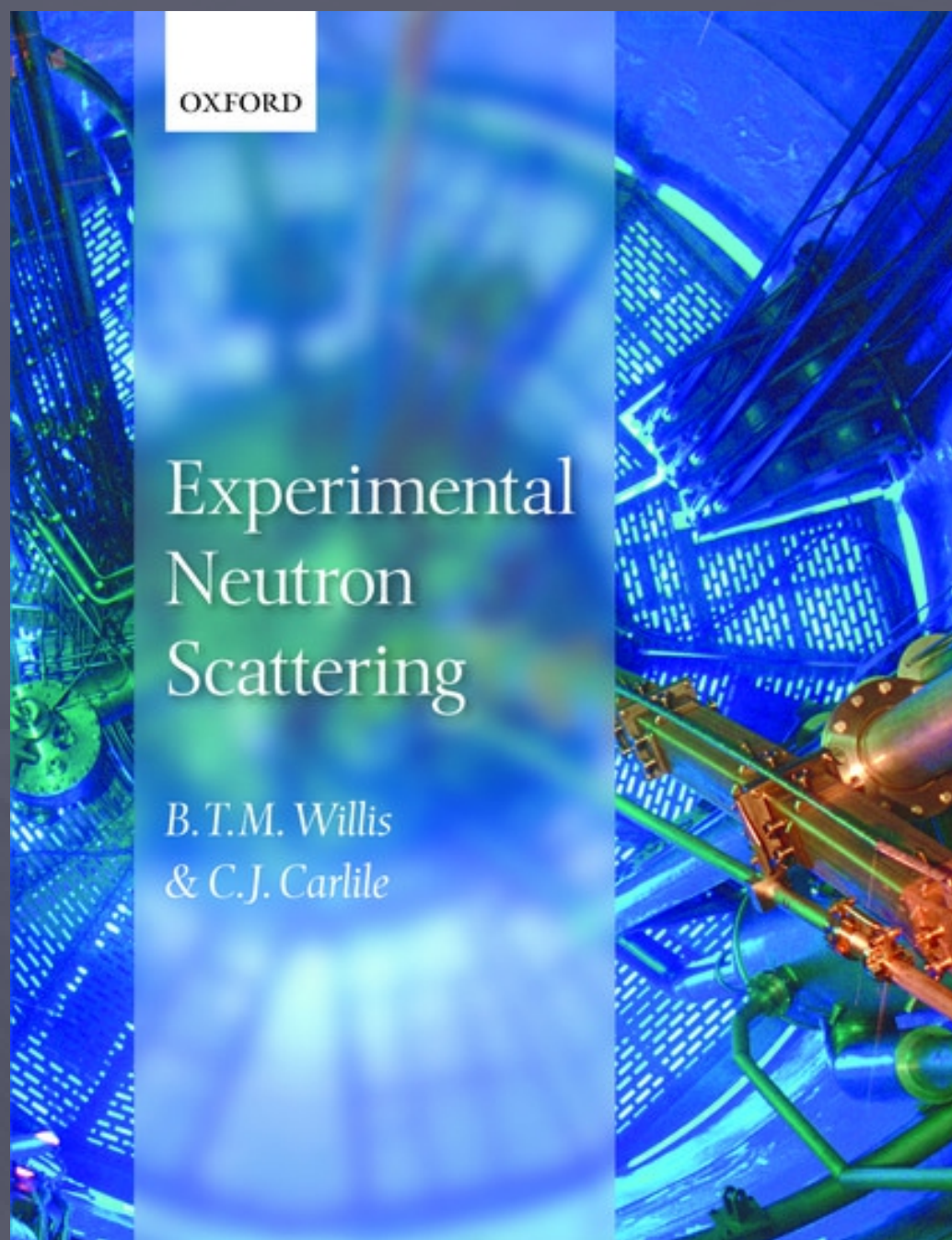
No direct access to magnetism

Easy to manipulate beams

How to Practically do Neutron (X-ray) 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 (>1 week 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 References



Experimental Neutron Scattering
 B. T. M. Willis and C. J. Carlile
 Oxford University Press (2013)
 ISBN-13: 978-0199673773

SwedNess/NNSP Neutron School 2019 in Tartu, Estonia

Material for the Introductory Days

- Mathematical background
- Wave physics
- Fourier transforms

General Reference Material for the Entire Course

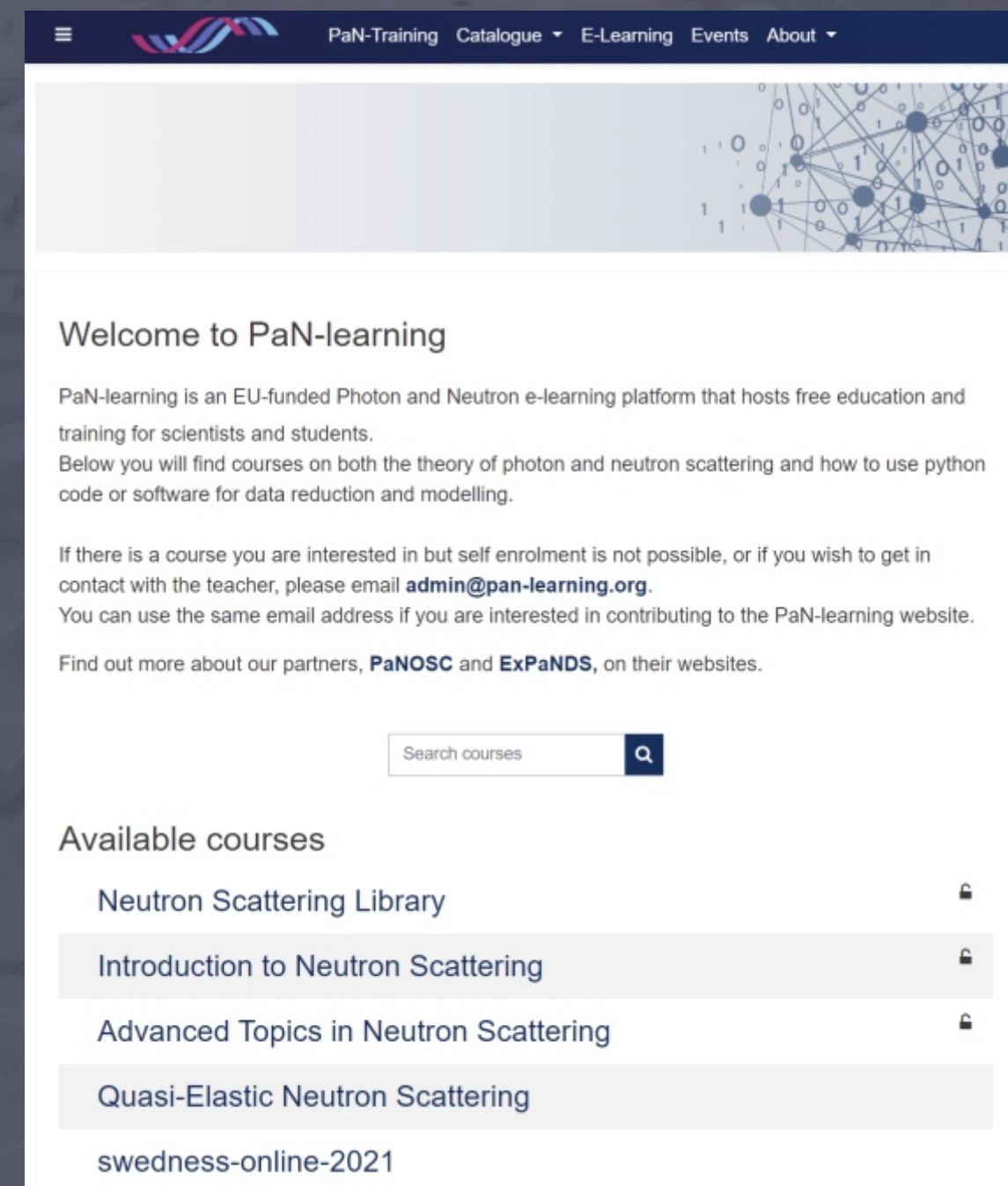
- Scattering Physics Compendium
- Neutron Scattering Notes
- Lecture Notes Imaging (M. Strobl)
- Program

Slides from the Lectures

- 01 - Welcome & Practical Information
- 02 - Overview Lecture (Martin Mansson, KTH)
- 05 - Crystallography (Nami Matsubara, KTH)
- 06 - Diffraction I (Nami Matsubara, KTH)
 - Working Fullprof-files
- 07 - Diffraction II (Nami Matsubara, KTH)
- 08 - Neutron Reflection, Intro and Practical (Adrian Rennie, UU)

<http://www.neutrons.se/Tartu2019/>

<http://www.SwedNess.se>



PaN-Training Catalogue E-Learning Events About

Welcome to PaN-learning

PaN-learning is an EU-funded Photon and Neutron e-learning platform that hosts free education and training for scientists and students. Below you will find courses on both the theory of photon and neutron scattering and how to use python code or software for data reduction and modelling.

If there is a course you are interested in but self enrolment is not possible, or if you wish to get in contact with the teacher, please email admin@pan-learning.org. You can use the same email address if you are interested in contributing to the PaN-learning website.

Find out more about our partners, **PaNOSC** and **ExPaNDS**, on their websites.

Search courses

Available courses

- Neutron Scattering Library
- Introduction to Neutron Scattering
- Advanced Topics in Neutron Scattering
- Quasi-Elastic Neutron Scattering
- swedness-online-2021

<https://pan-learning.org/>

Conclusions

- Neutron scattering is the most versatile & powerful experimental technique for studying intrinsic material properties.
- Tell us where atoms are and how spins align (elastic)
- Tell us how atoms and spins move / excitations (inelastic)
- The world's most intense neutron source, **ESS**, is currently being built in Sweden (Lund), user operation starts **~2025**.
- Governments & funding agencies now put a lot of funding for strengthening the neutron scattering community.
- **ESS + MAX IV + PETRA III = Great Opportunities !!!**

Acquiring experience and expertise in neutron scattering will be favorable for science/industry and a career in the North !!!



Thank You for Your Attention !!!



Prof. Martin Mansson
condmat@kth.se