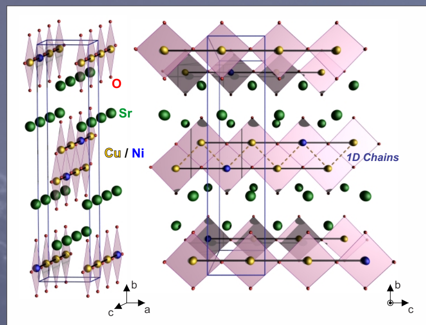
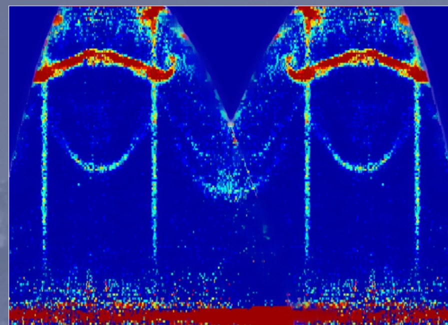
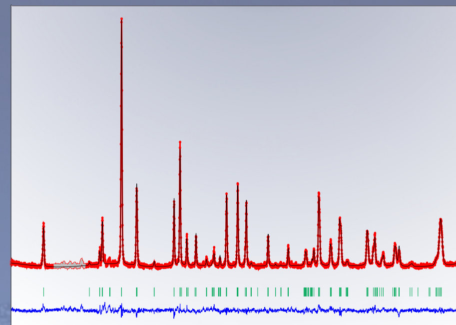
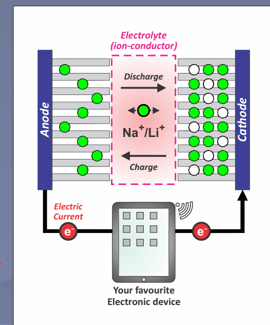
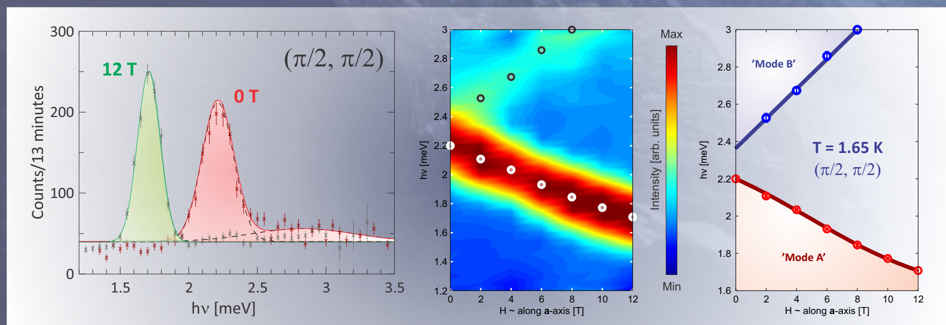
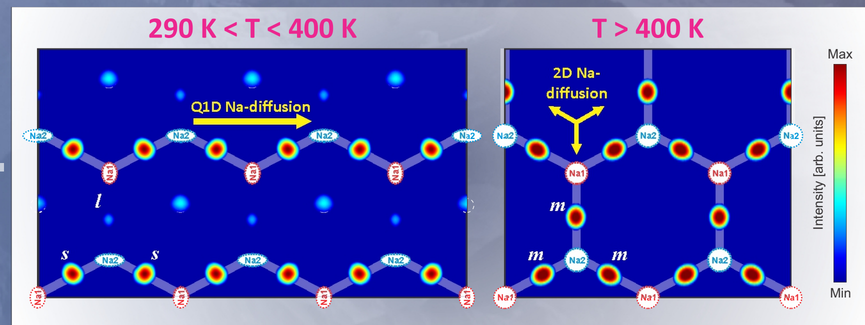
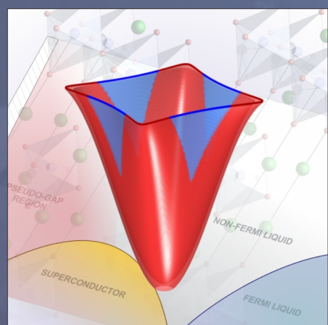
Overview of the Intro Course in Neutron Scattering

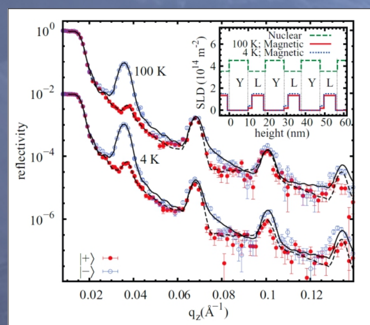


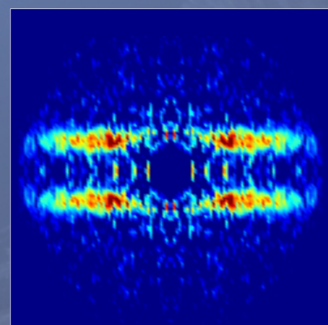
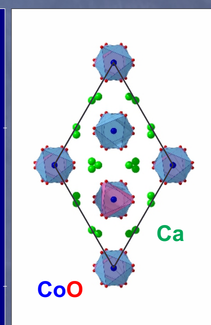












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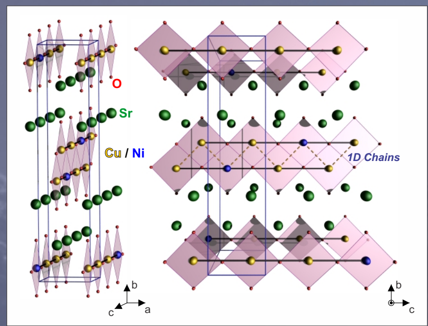
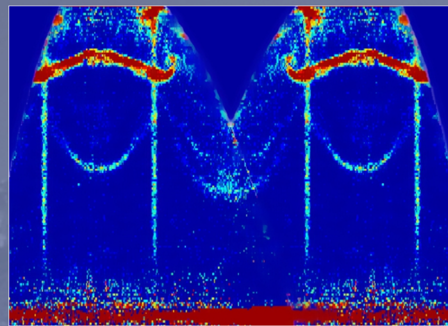
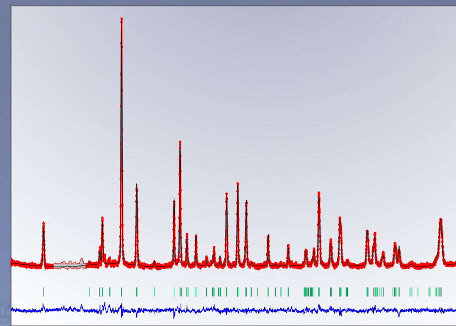
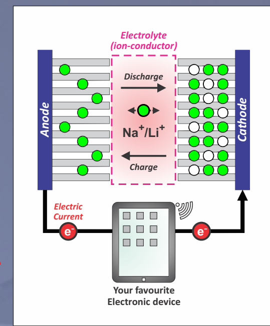
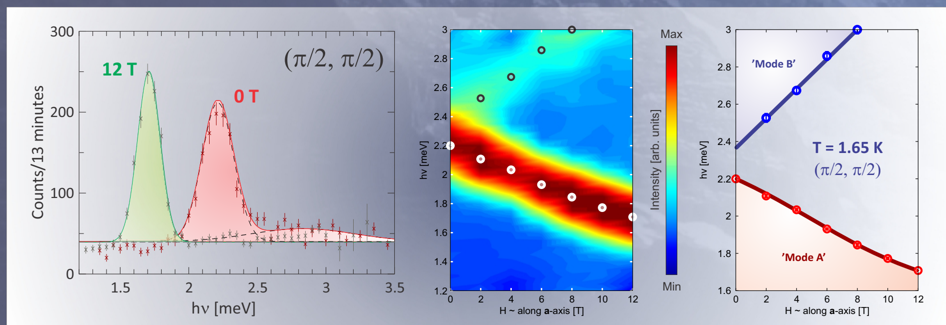
A.K.A
Crash Course in Neutron Scattering

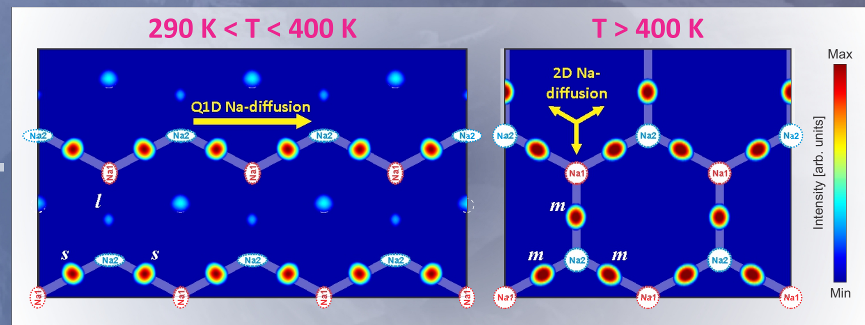


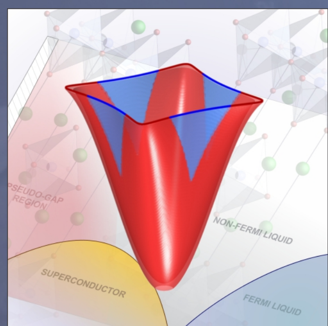


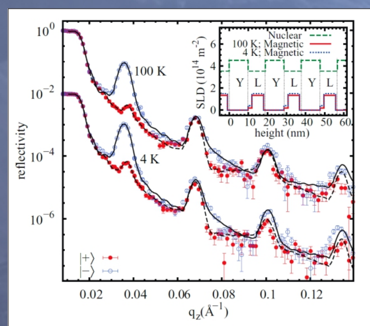


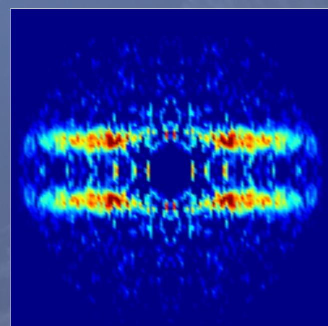


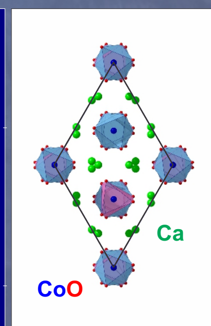












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Stockholm, Sweden

About Me

- As. Prof. in Neutron Scattering at KTH (since 2015)

KTH · PAUL SCHERRER INSTITUT PSI · TOYOTA CENTRAL R&D LABS., INC. · ETH zürich · EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE · KTH

- Neutron instrument responsible for 4 years (Swiss Spallation Neutron Source)
- Board member Swedish Neutron Scattering Society - SNSS (since 2014)
- Director of Studies, Swedish graduate school in neutron scattering (SwedNess)
- Member of the Scientific Advisory Committee (SAC) for ESS
- Member of the VR reference group for a Swedish ESS Strategy
- Project leader for an ESS related VR neutron grant: BIFROST @ ESS

Σ = "I like neutrons"

+ *X-rays*
+ *muons*

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

- From 2022 there will be excellent possibilities for young scientists / industry to perform world-leading science & developments.

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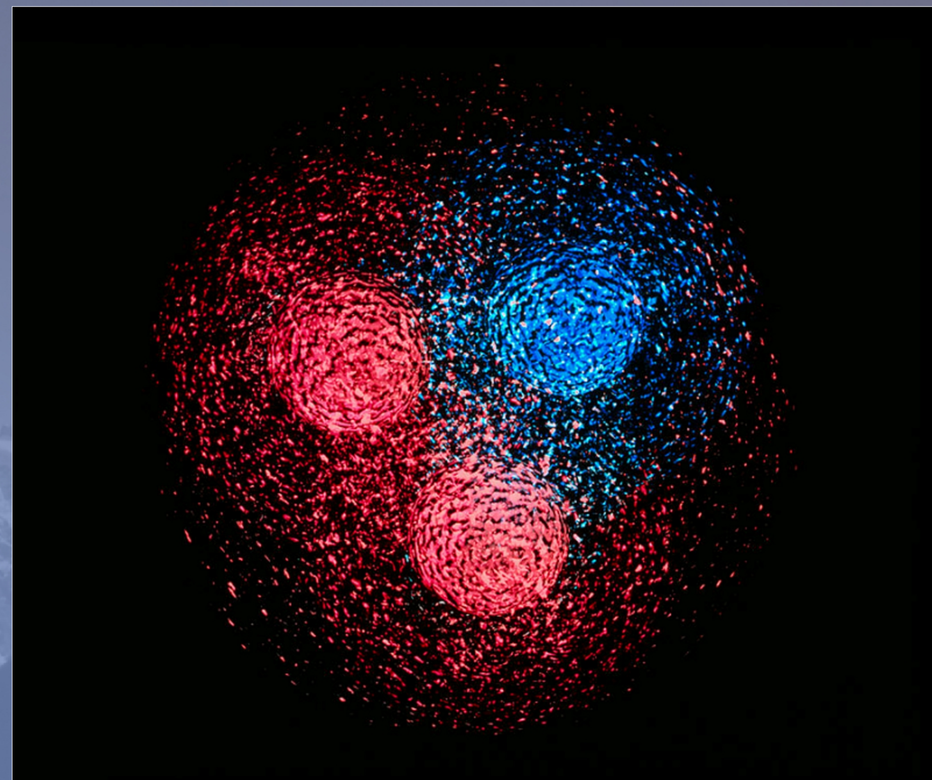
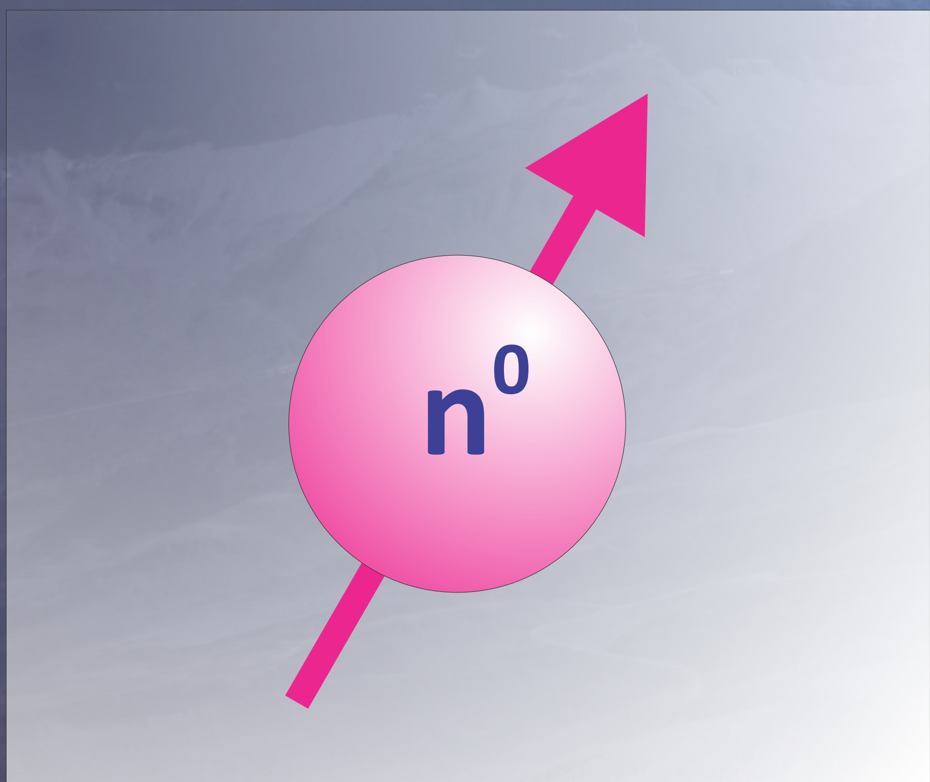
What is a Neutron (n^0)?

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 / macroscopic materials / device properties.
- "Can show where atoms are and what they do" + magnetism

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Neutron Properties

NEUTRAL

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

HAS A SPIN

S = ½ → Initial state can be polarized & polariz. of 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 τ = 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: $E = \hbar \mathbf{k}^2 / 2m \rightarrow \ldots$

$\lambda = 5$ Å → 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 i.e. condensed matter physics !!!

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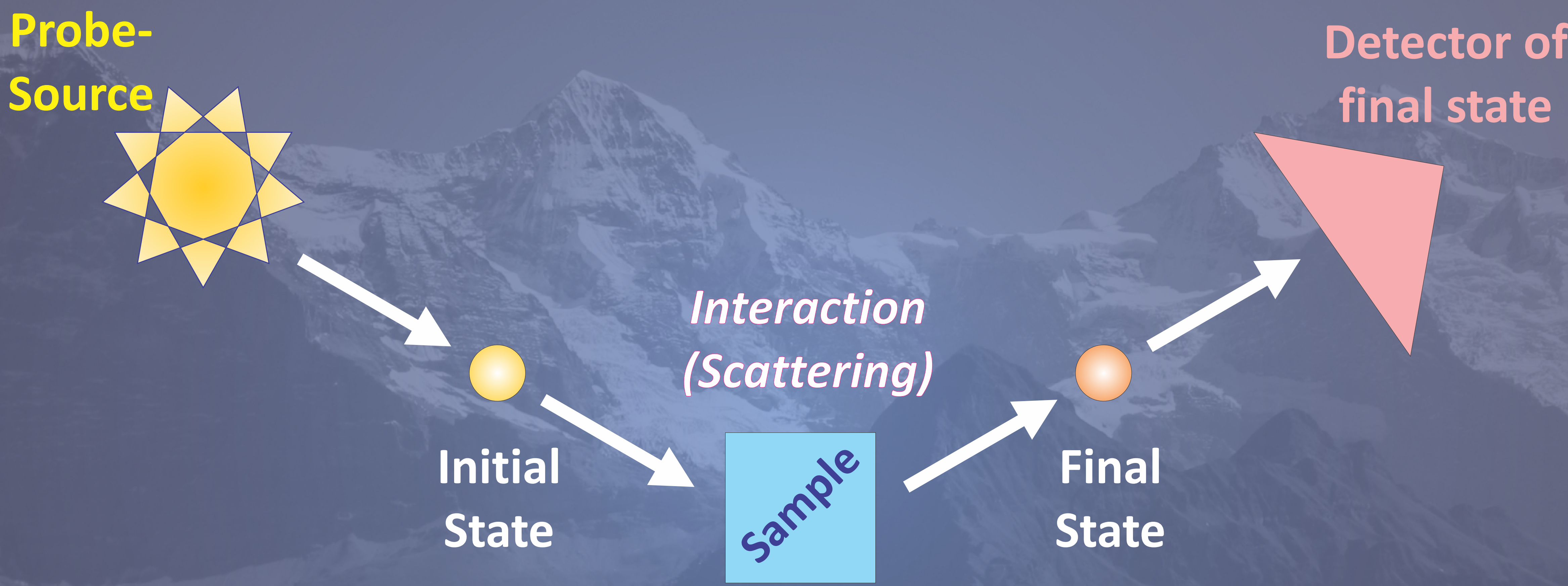
A Scattering Experiment



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

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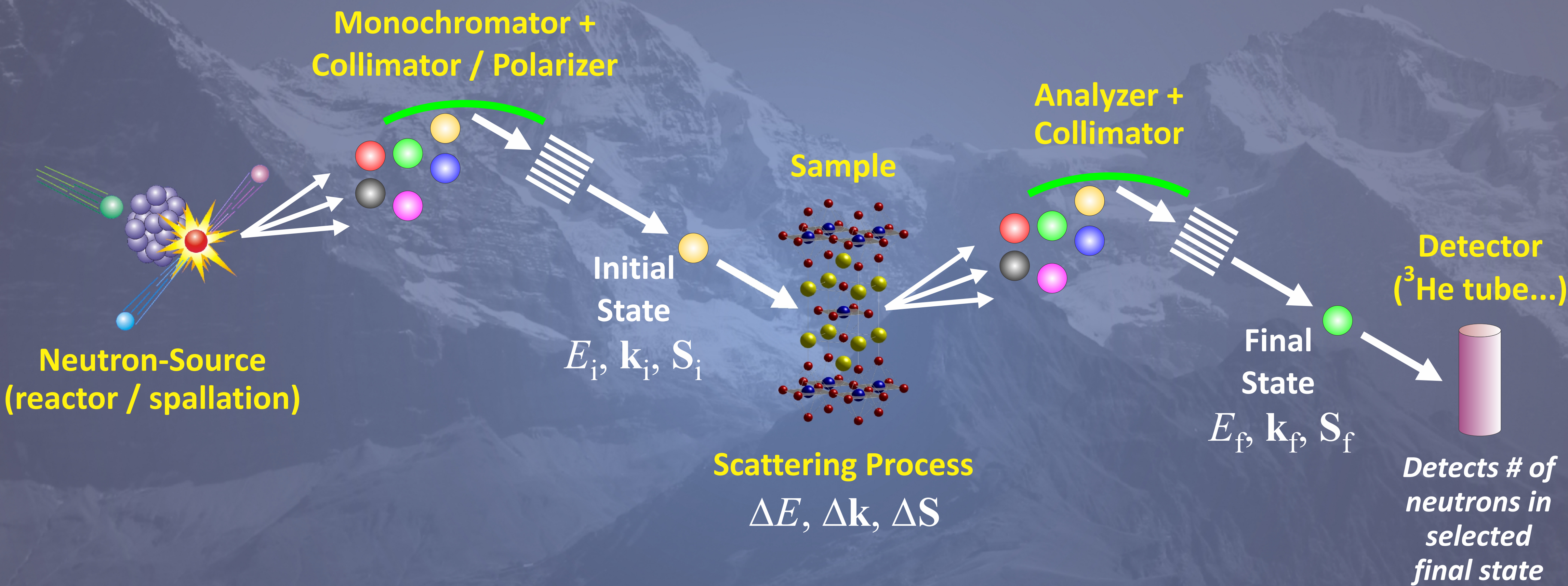
A Neutron Scattering Experiment

- **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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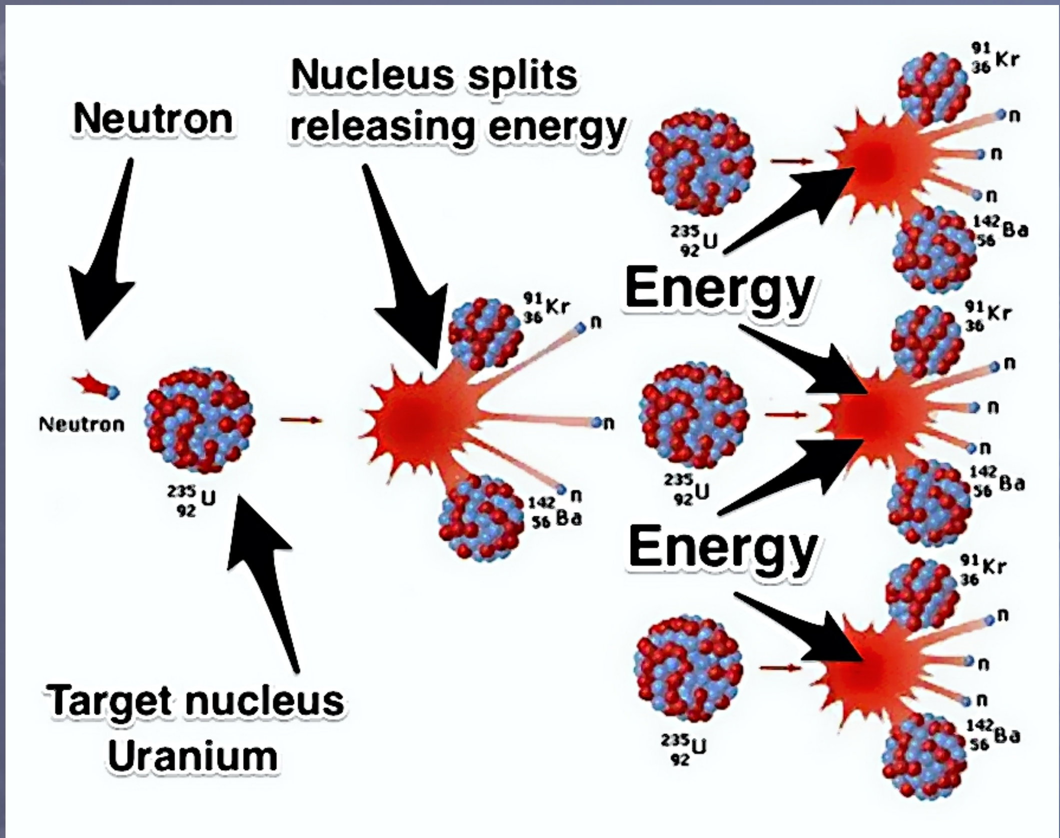
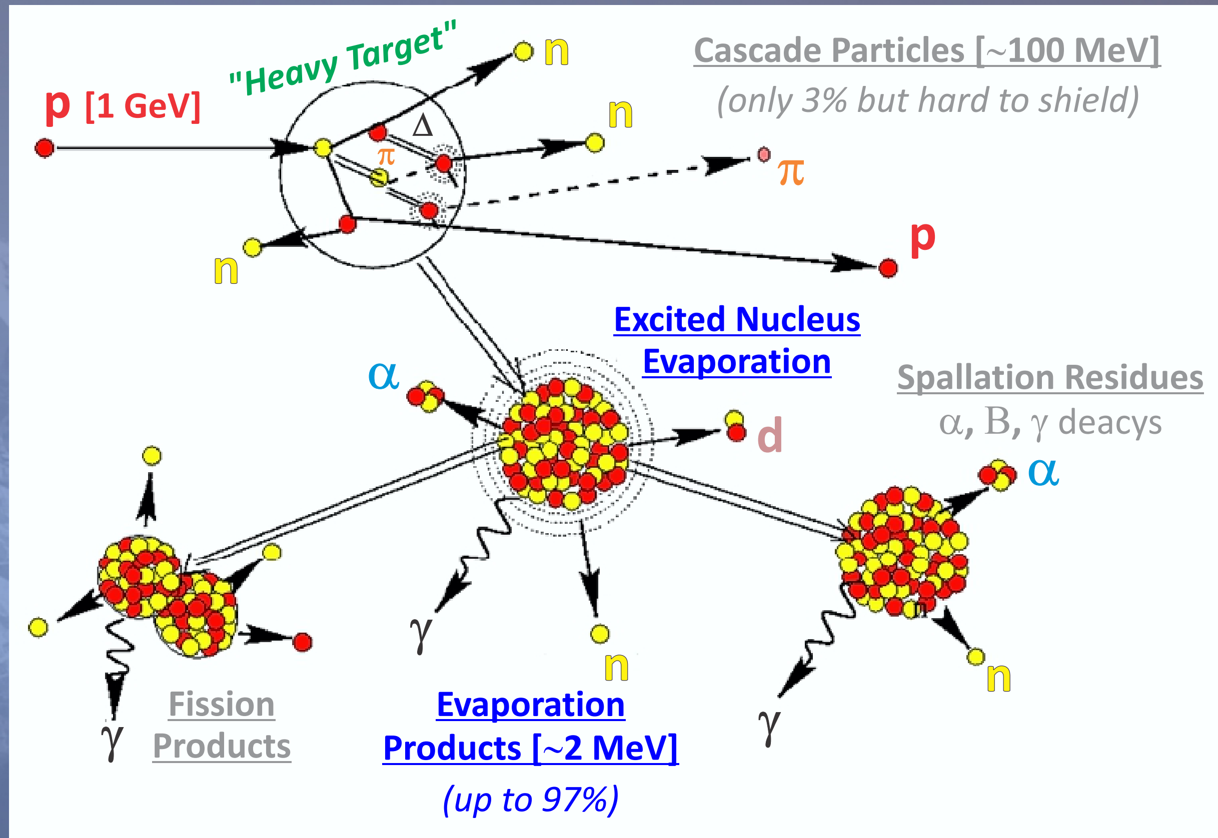
Neutron Production / Sources

Soon to be the past
Reactors (fission)



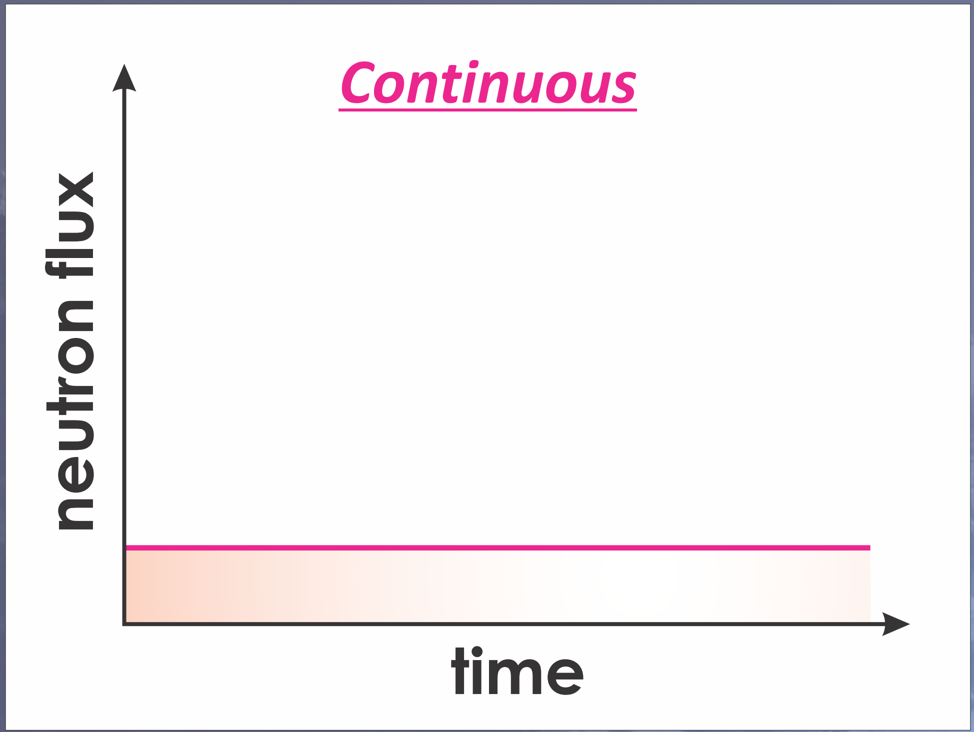
- Energy per neutron ~180 MeV
- High and continuous flux
- Waste a lot of neutrons in ToF
- Rare beam down, but if...
- Safety / Politics complicated

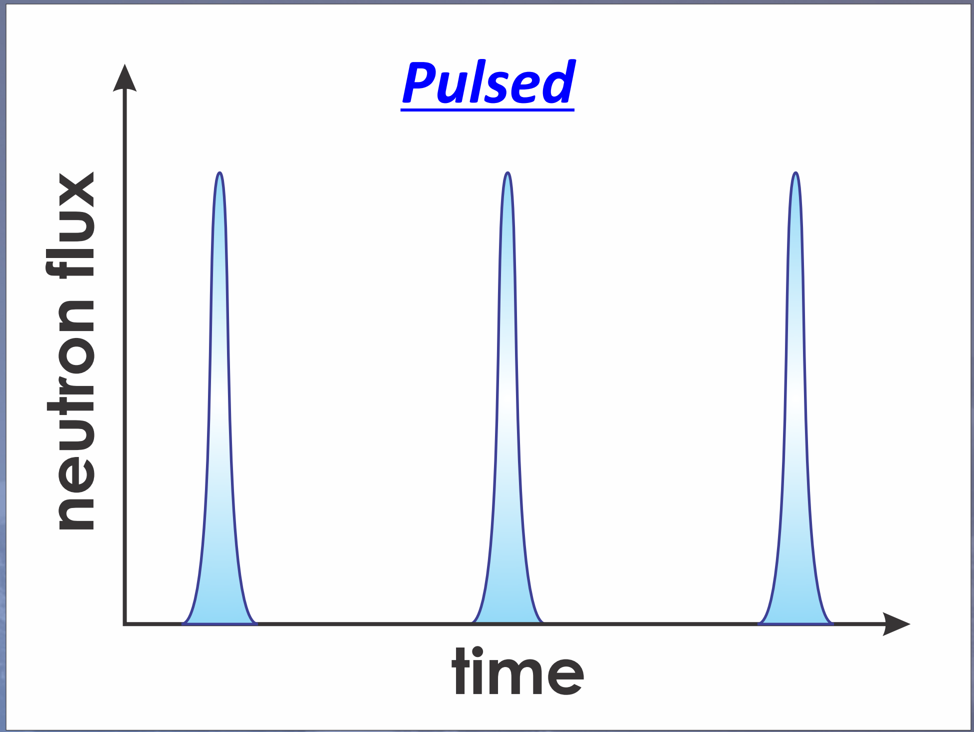
Future already here
Spallation Sources



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

Continuous vs. Pulsed Sources



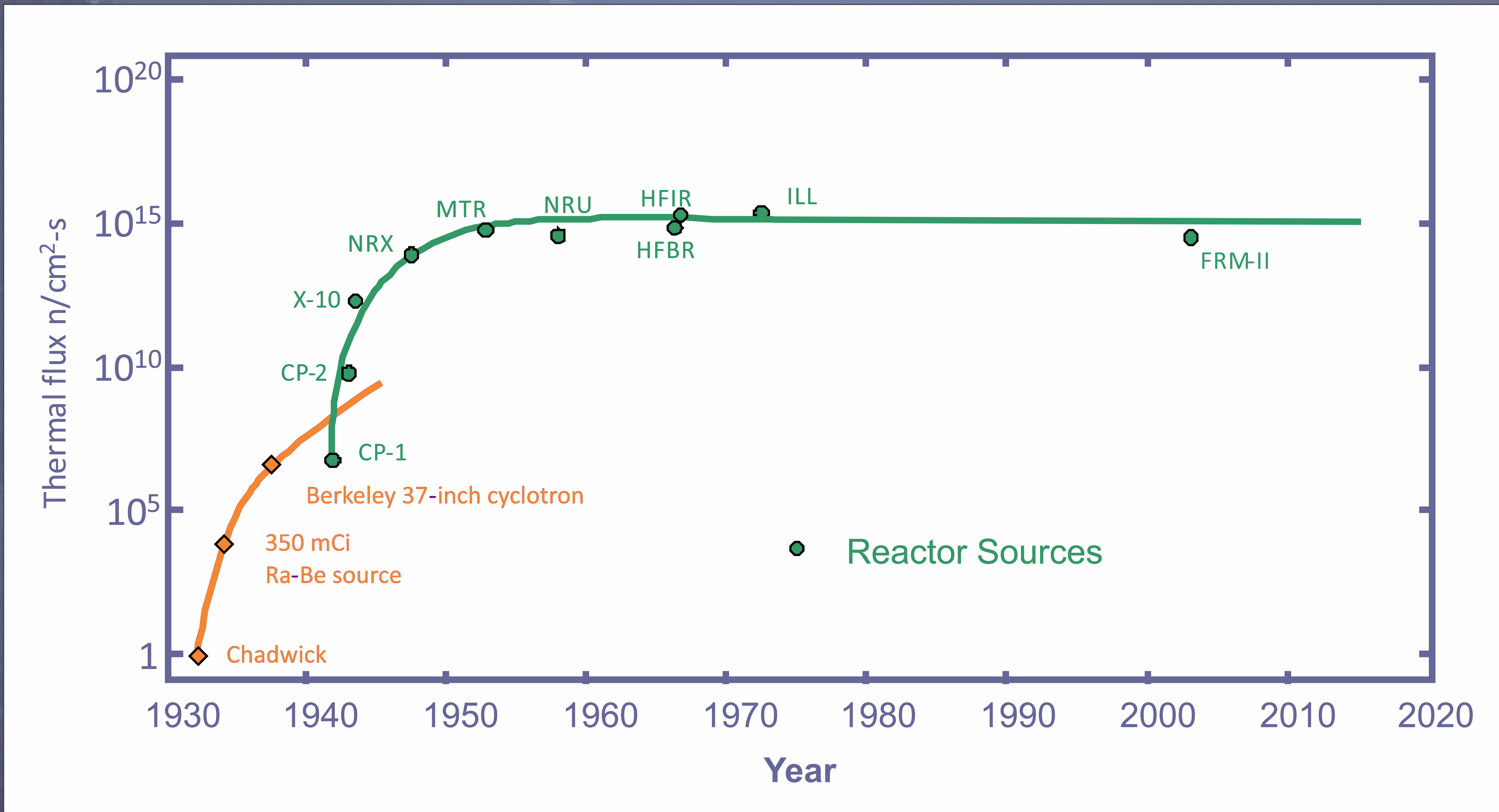


- Optimized for average flux
- Good enough for most applications
- Fission neutrons easier to shield
- Easy to build compact and simple instruments
- Simple electronics / data
- Tried and tested ('Old School')

- 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

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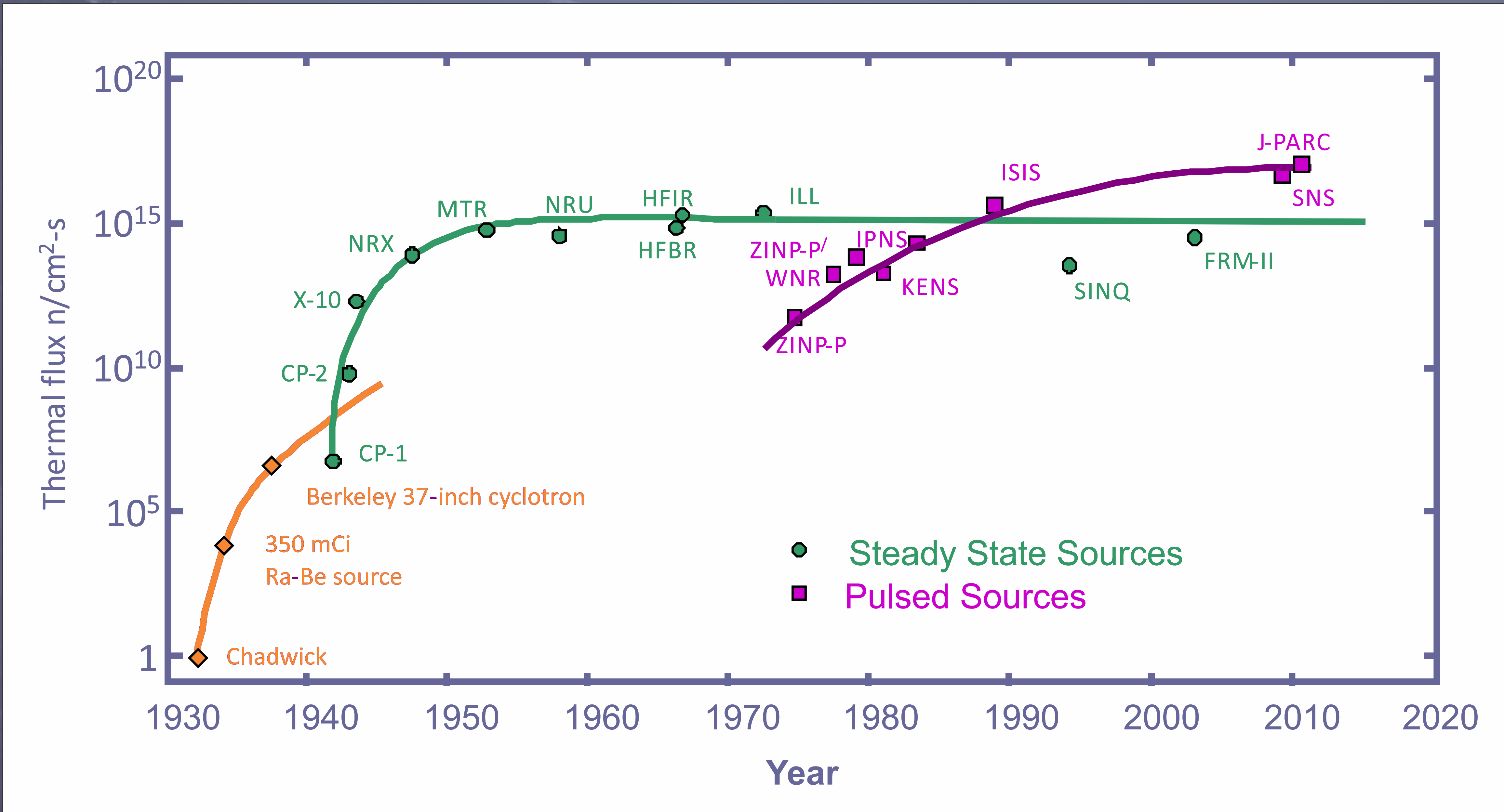
- Also pulsed spallation sources have had the same development



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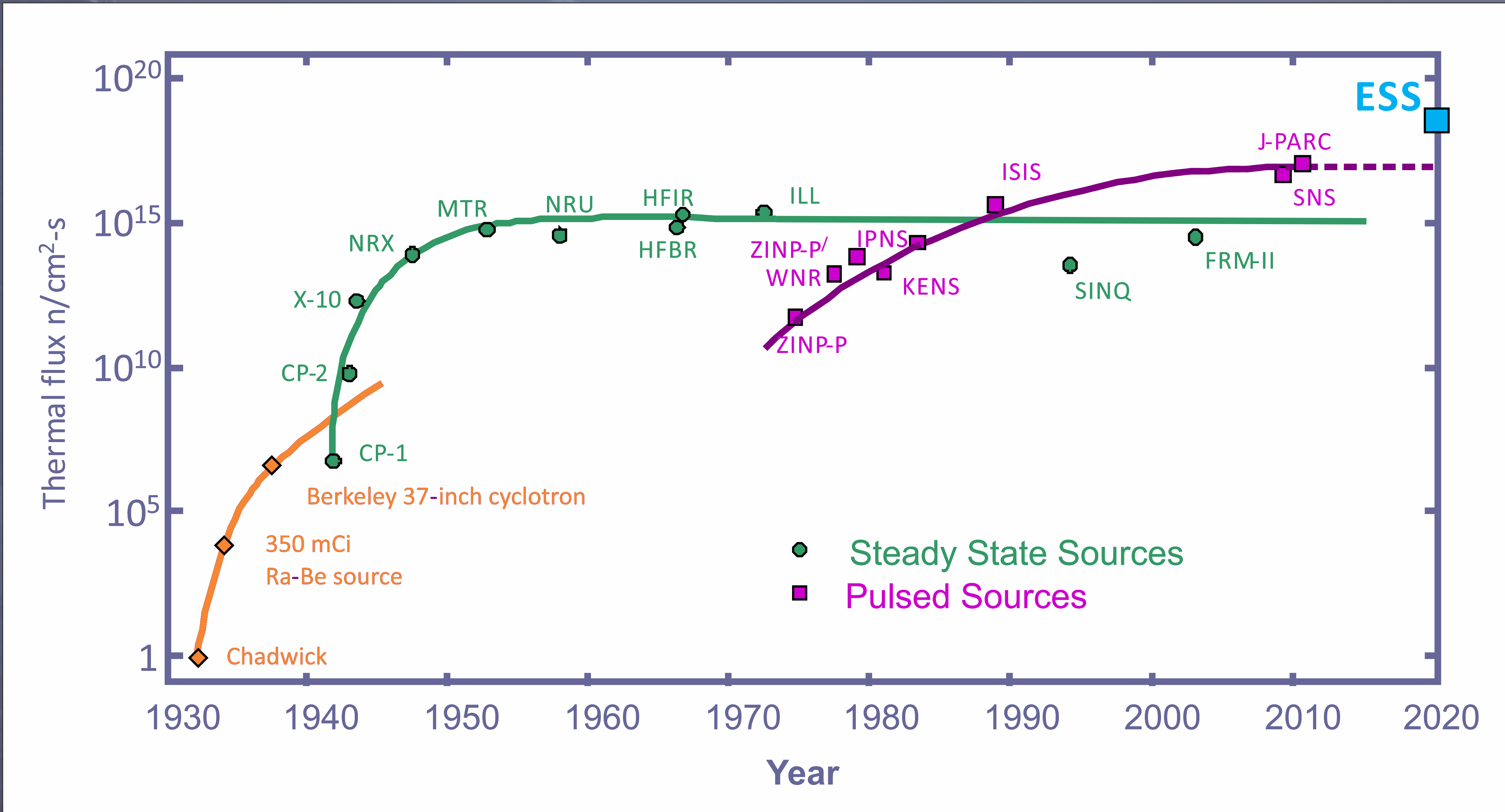

- Hope surpass such trend with new technological developments at ESS !!!

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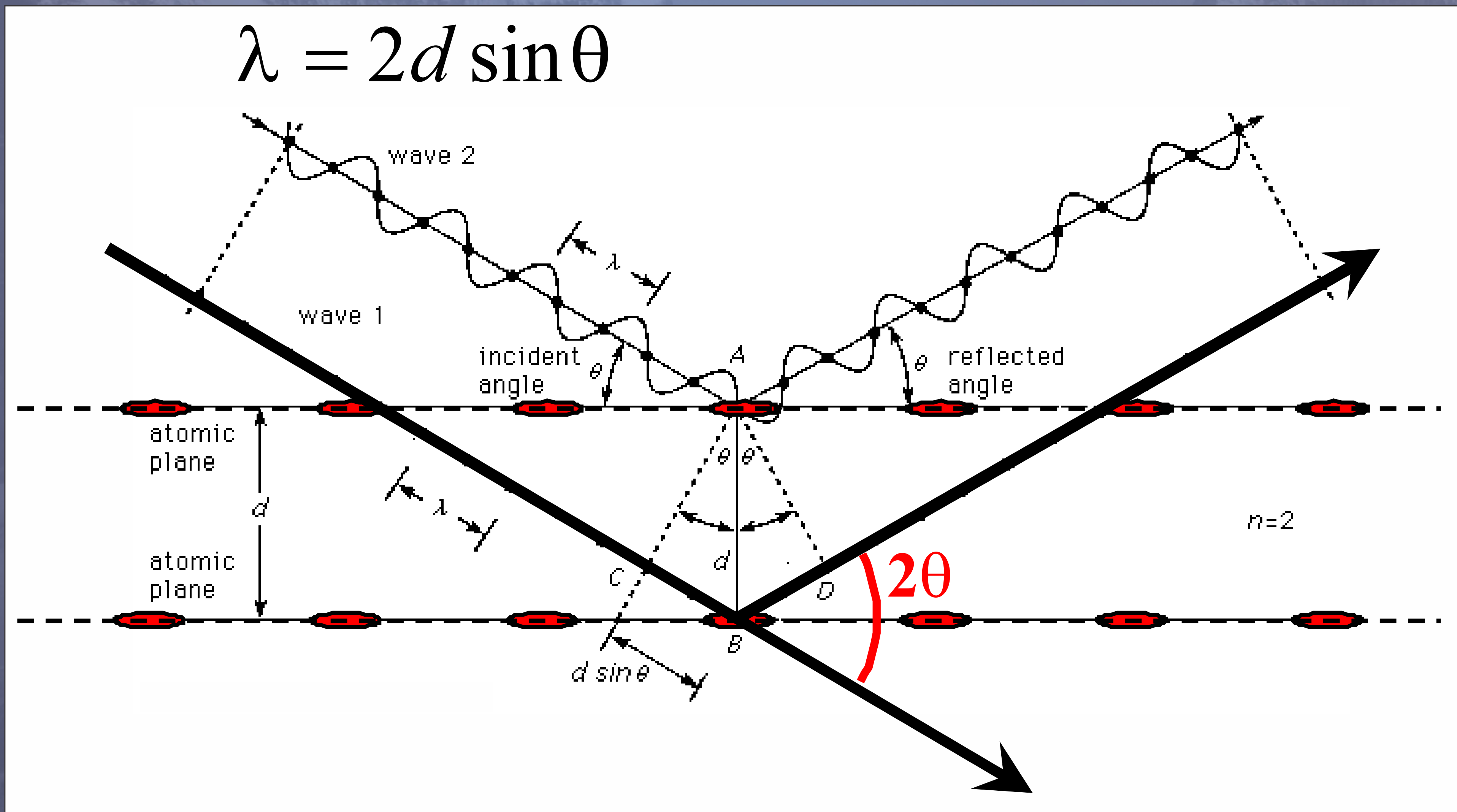
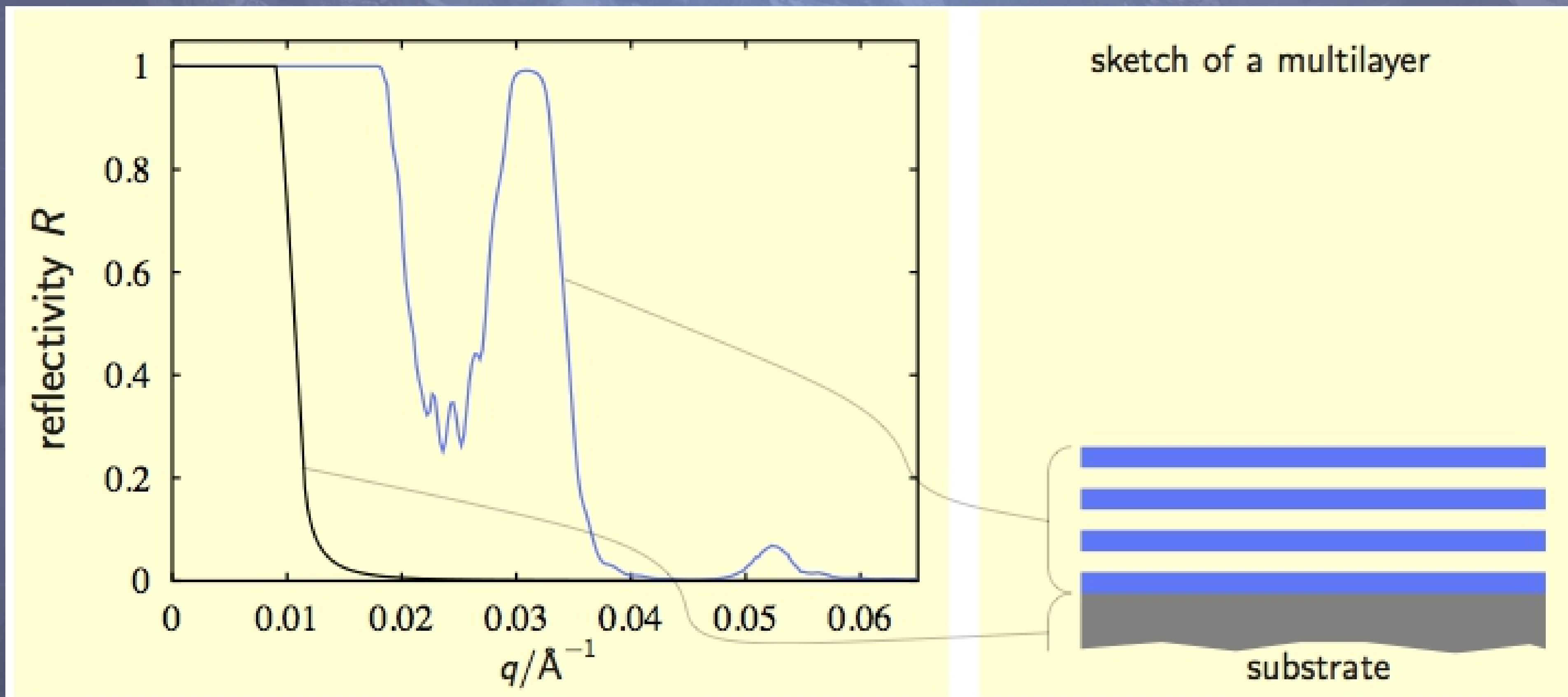
Neutron Guides

- 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.



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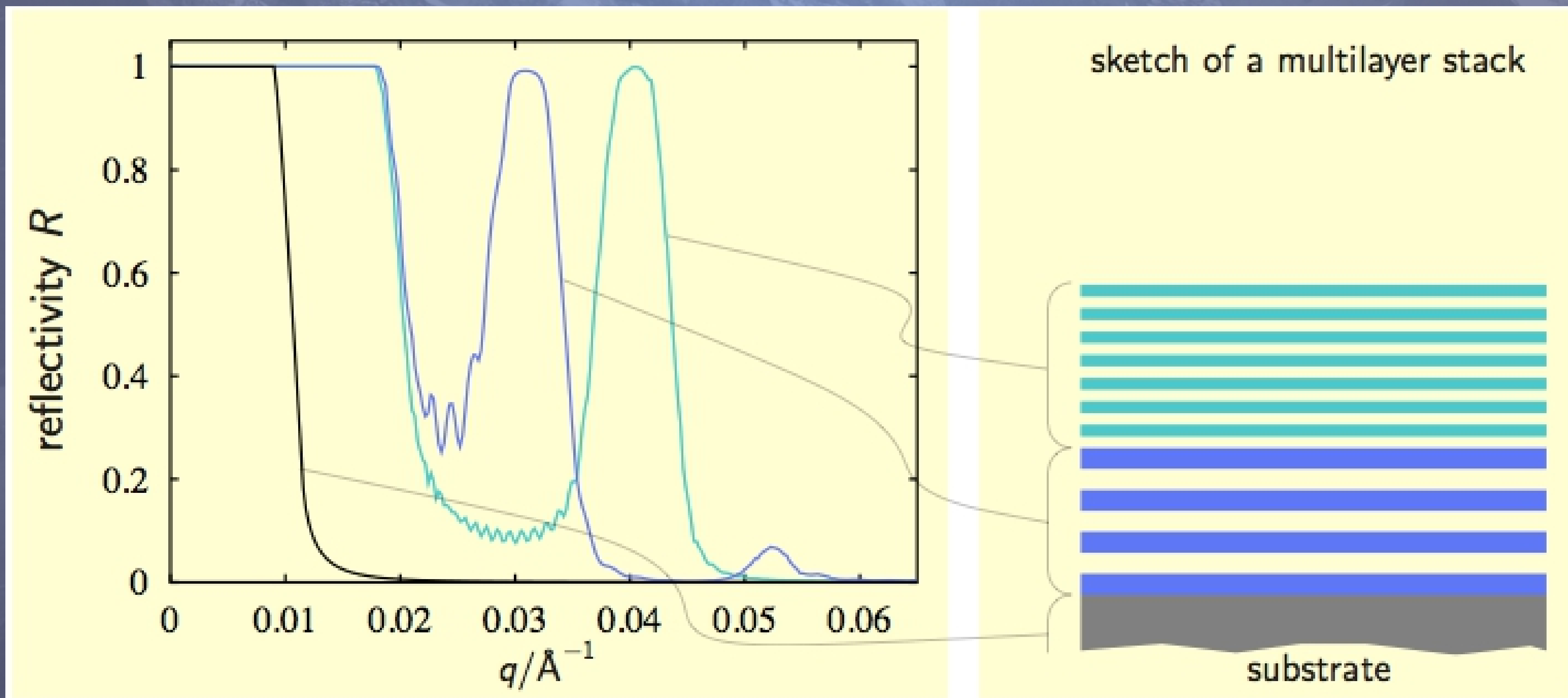

- So we grow several different multi-layers on top of each other in order to guide a broader band-width of neutrons.

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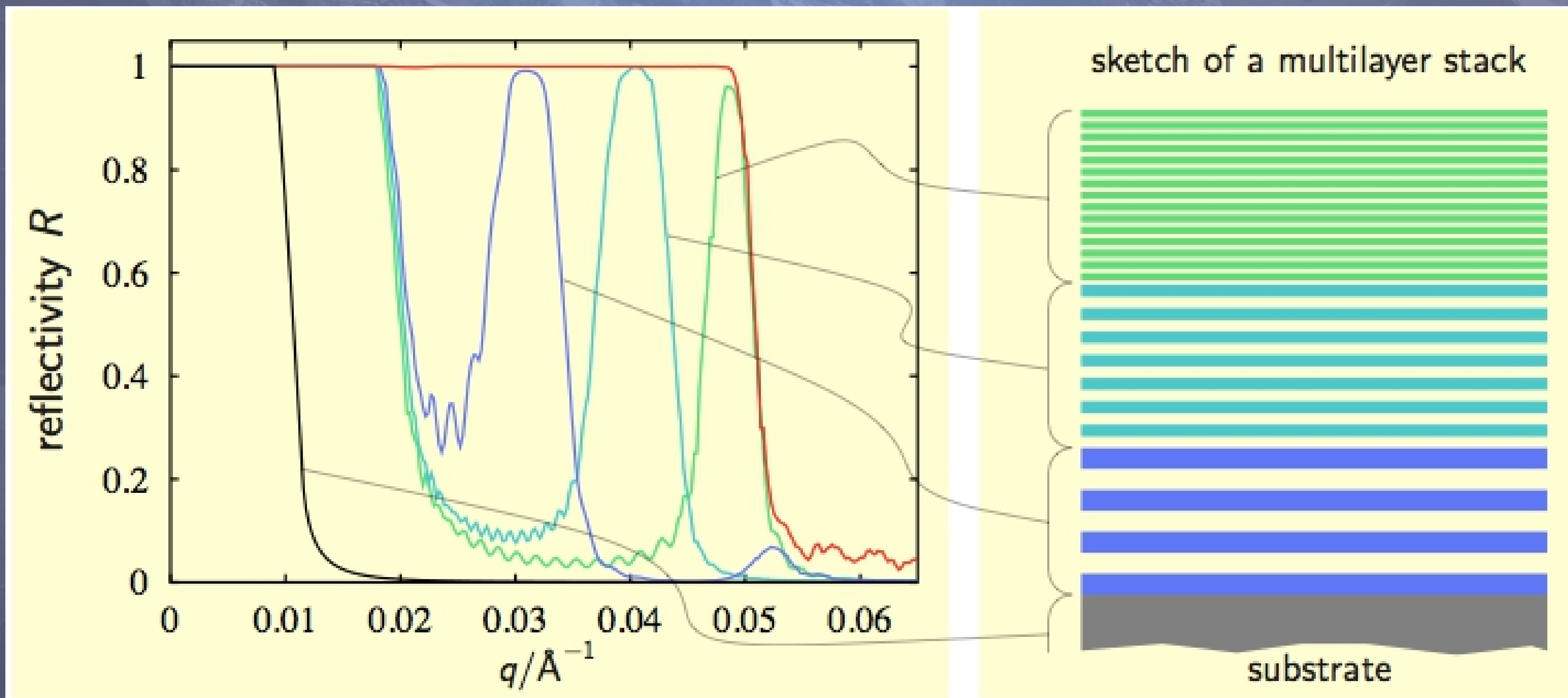

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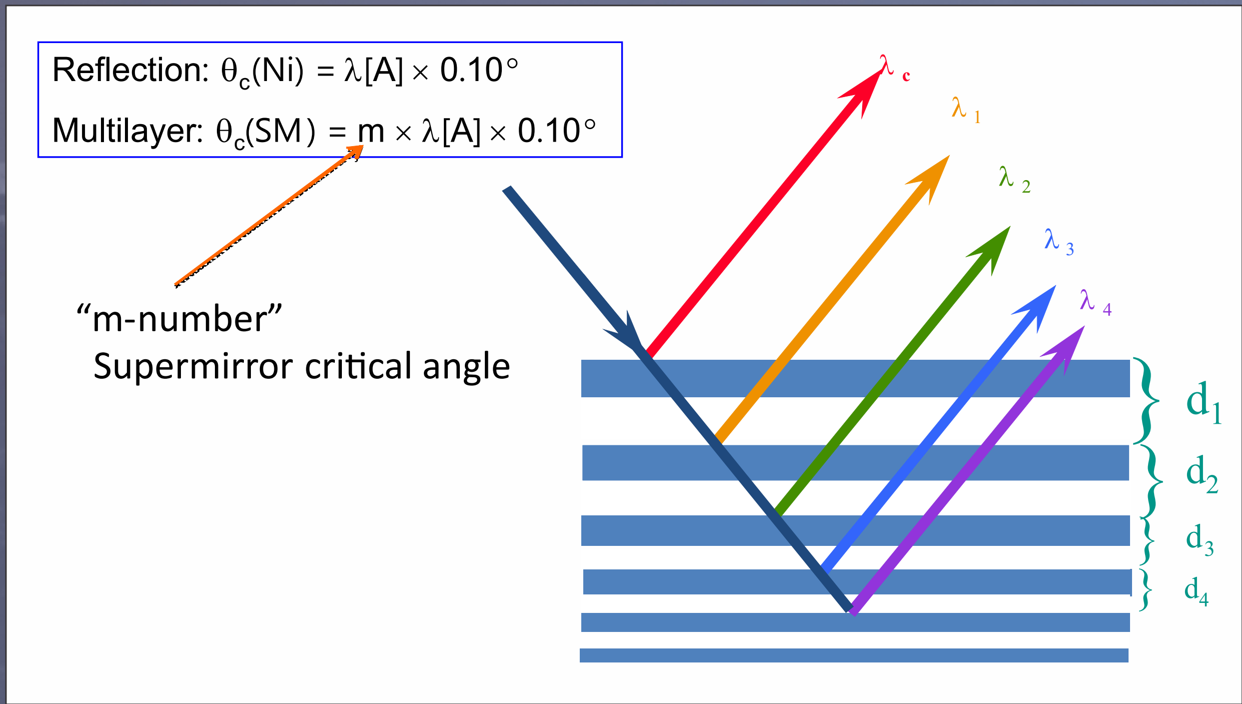
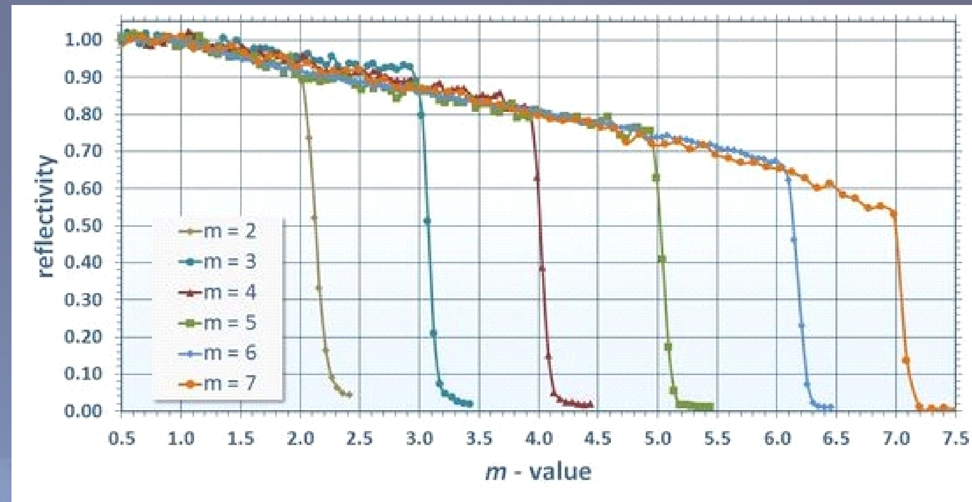
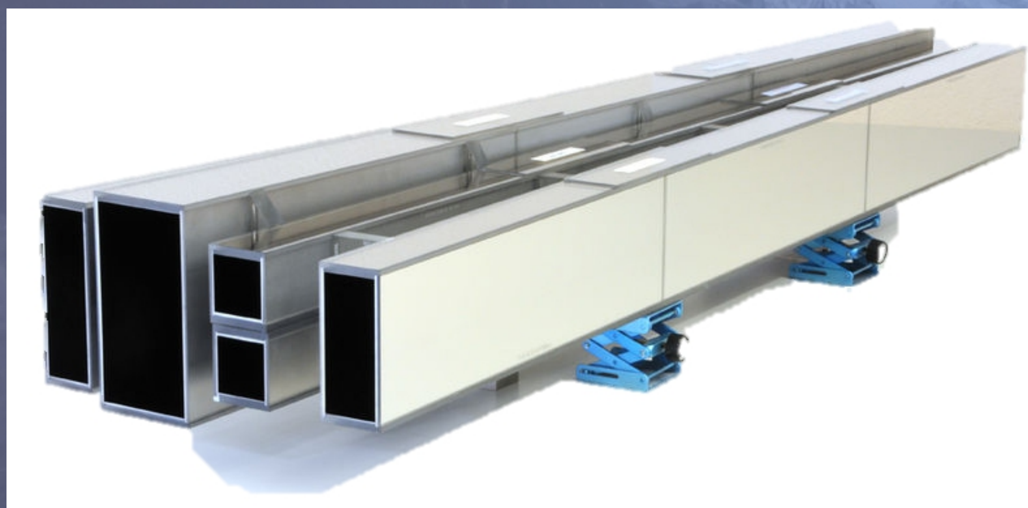
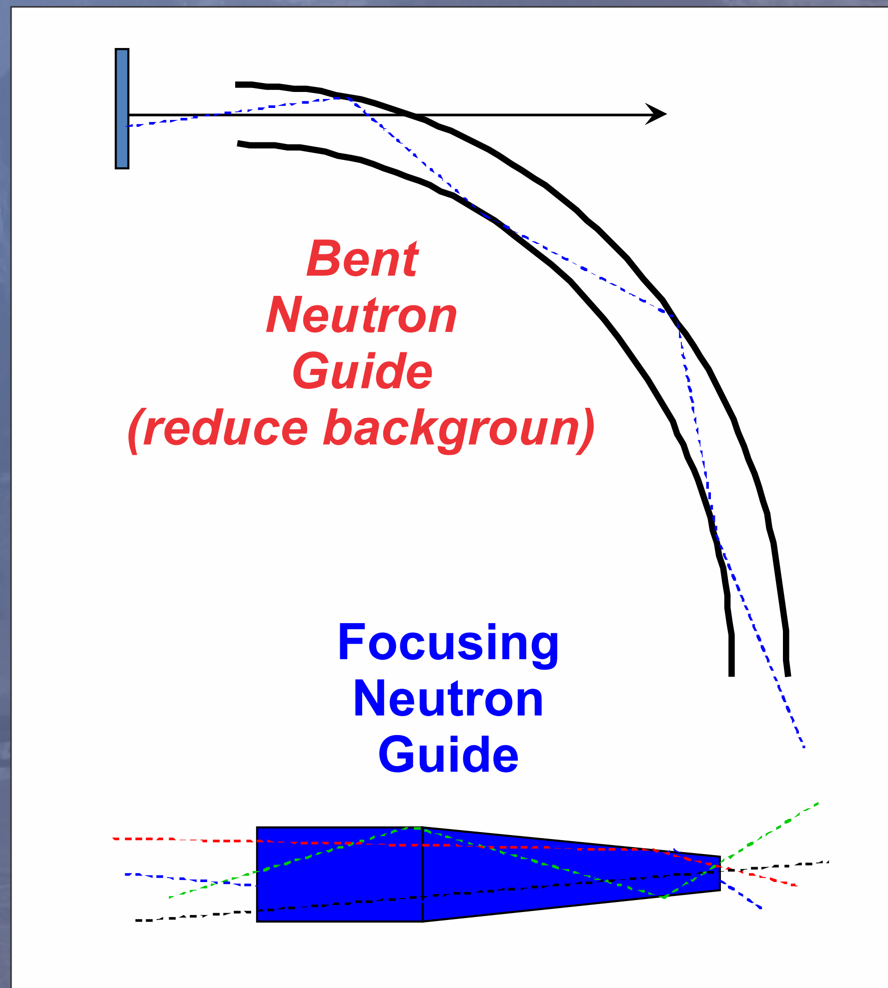
Neutron Super Mirrors





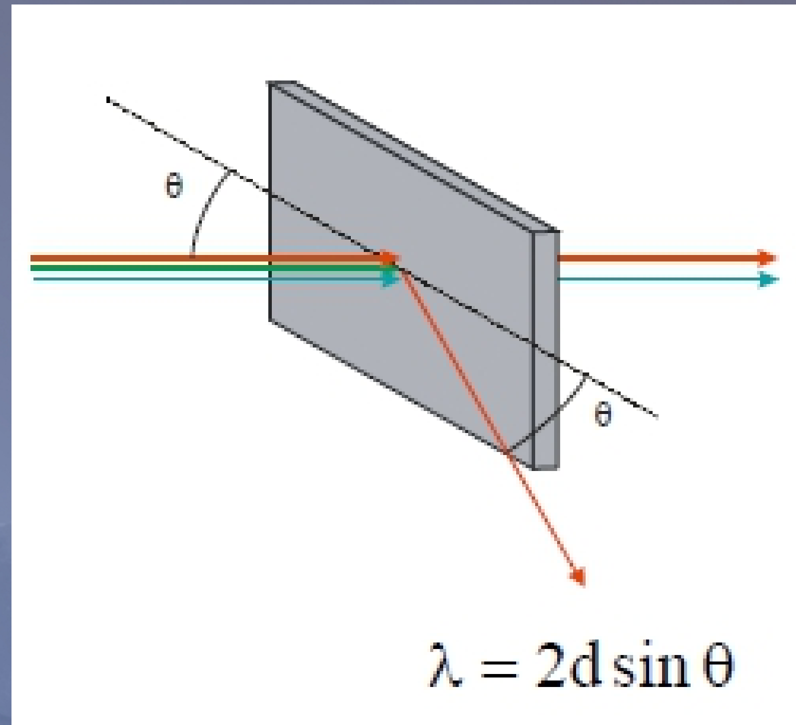




- **Neutron guides can also be focusing, "bending" (to reduce background) or even polarizing!**

Defining E: Crystal Monochromators

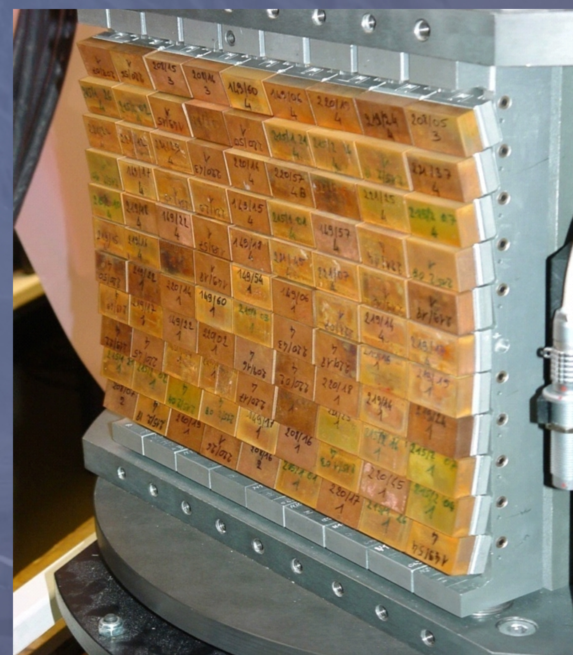
- **Same idea as supermirrors but use single crystals of pure materials.**
- **Several very carefull co-aligned crystals are put together into a monochromator.**
- **Angle and crystal type selects the out-going neutron energy**
- **Can be made to also focus the beam.**



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]

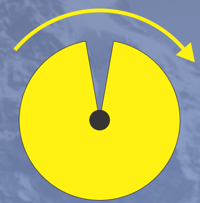


- **Mainly used in the "old type" of reactor/continuous neutron sources.**

Defining E/t: Neutron Choppers

- **Another way to select neutron energy is to use so-called choppers.**

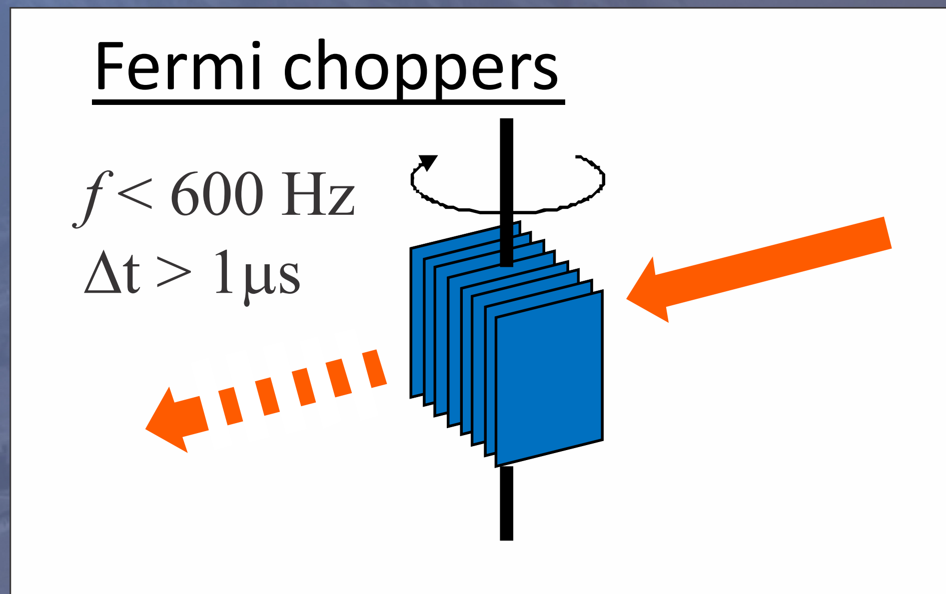
- **Simplest form is a spinning disc made out of a neutron absorbing material with a gap that works as a velocity selector.**

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.**

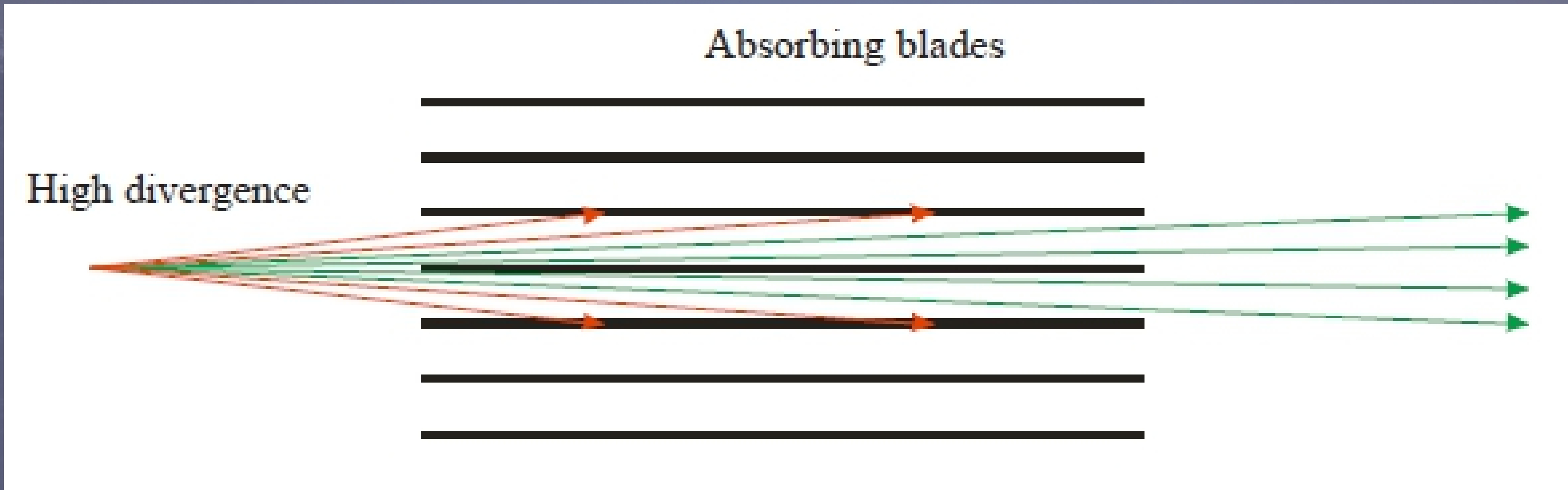
- **Can be used at any type of source but of course much more efficient for pulsed sources where "time = energy is used"**



- **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...)**

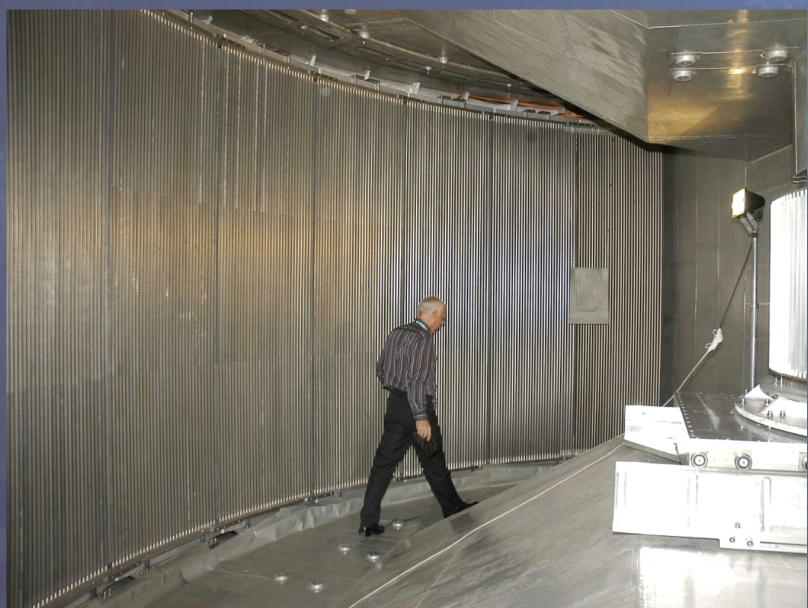
Detecting the Neutrons

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

^{3}He Tubes

$n + {}^3He \rightarrow {}^1P\ [570\ keV] + {}^3H\ [200\ keV]$

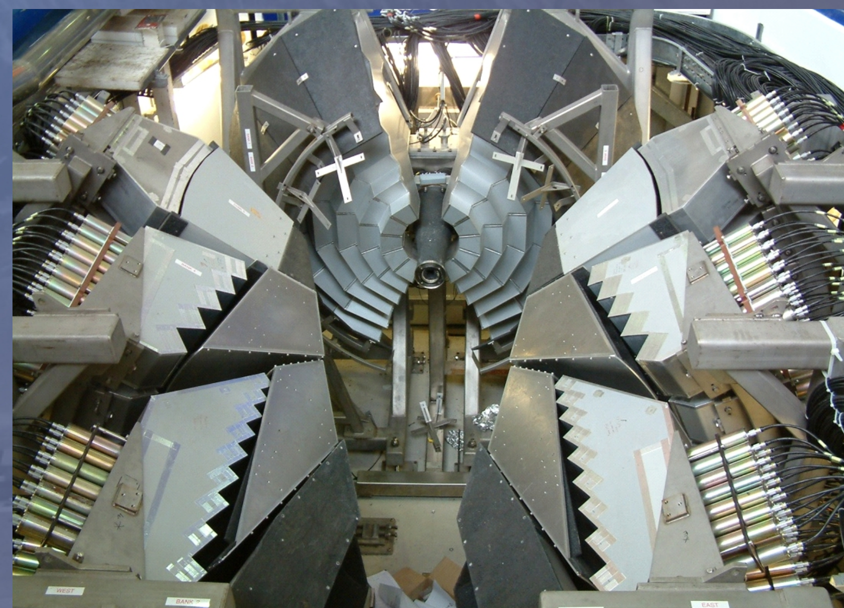
> 1mm resolution
High Efficiency
Low gamma sensitivity
Supply/cost problem!!!



Scintillators

$n + {}^6Li \rightarrow {}^4He + {}^3H + 4.79\ MeV$

< 1mm resolution
Medium Efficiency
Some gamma sensitivity
Magnetic Field Sensitive!



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

Detecting the Neutrons

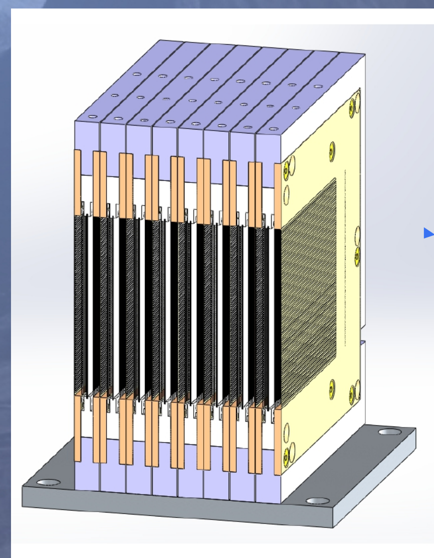
- New technology under development based on ^{10}B:

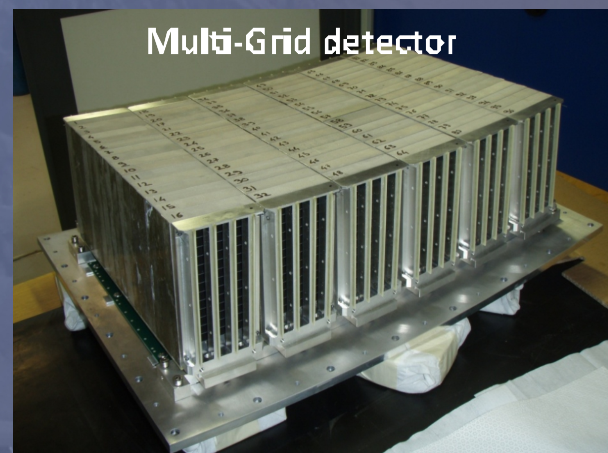
<u>^{10}B Detectors</u>

$n + {}^{10}B \rightarrow {}^{4}He$ [1.5 meV] + ^{7}Li [830 keV] + γ

<<< 1mm resolution
70% Efficiency of ^{3}He
10B is abundant (20% of natural B)
<u>New Technology under development!!!</u>

- $\sim$1 μm thin solid ^{10}B-containing layer (α and 7Li need to exit) $\Rightarrow$ only 5% efficiency $\Rightarrow$ multi-layers and multisegment / blades





- Use $^{10}B_4C$ since it is mechanically, chemically & thermally very stable

- Big development program and production at LiU for ESS

Linköping University

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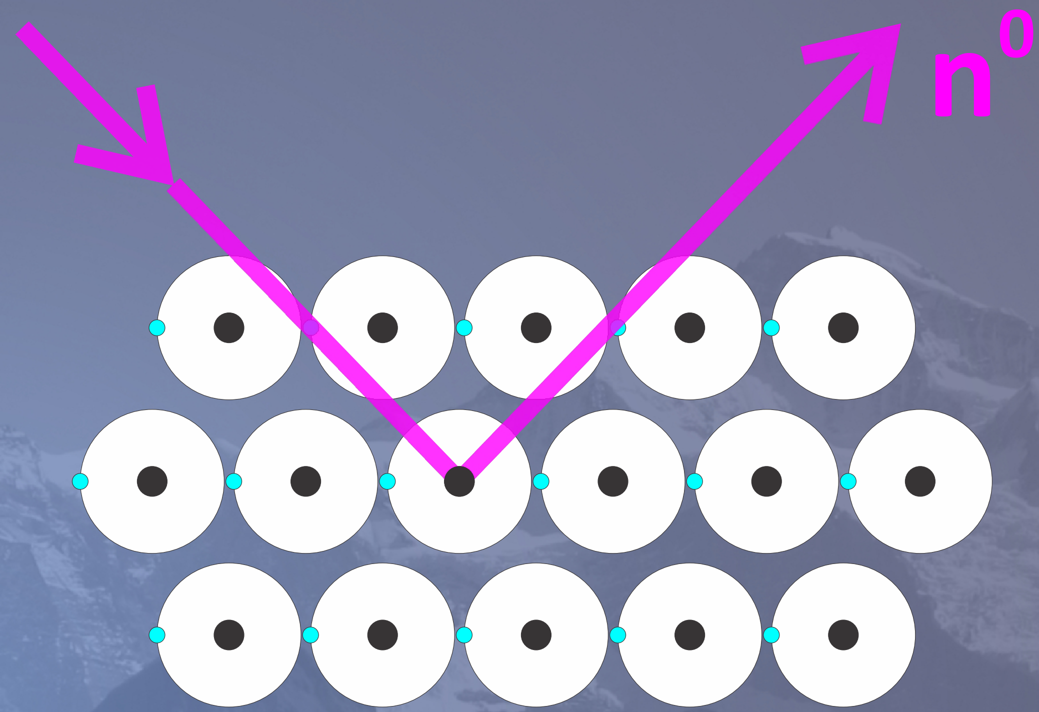
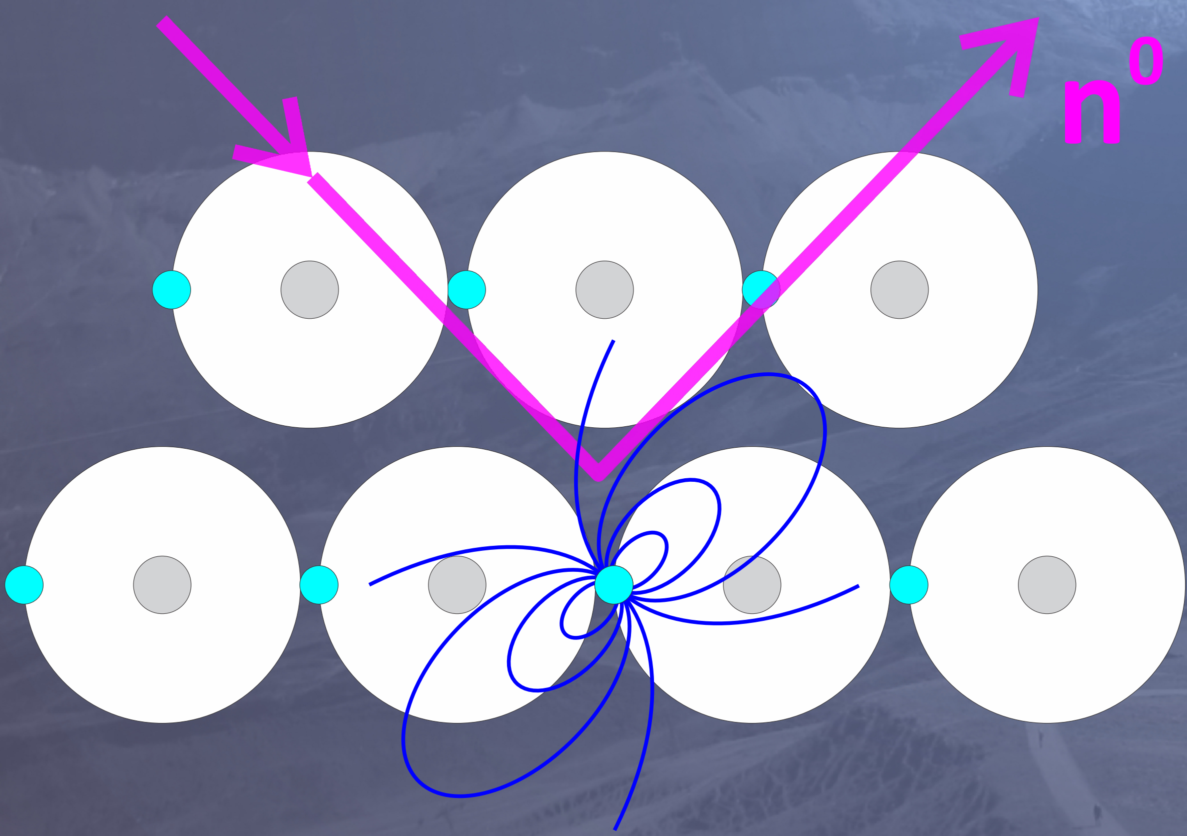
Neutron Interaction with Matter

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

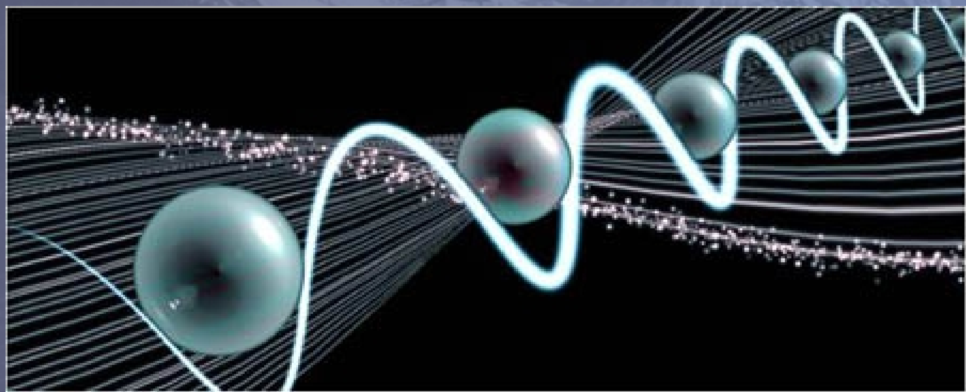


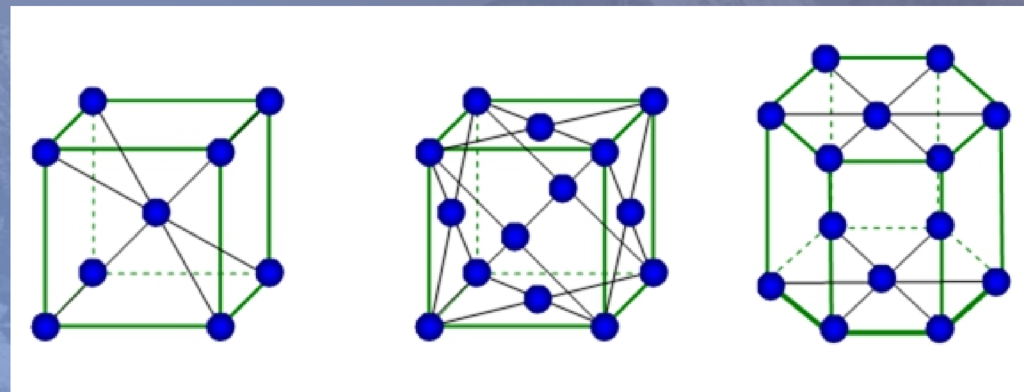


- **Neutrons also interact with un-paired electrons via a weaker magnetic dipole interaction.**
- **Neutrons see magnetic struc-tures, spin waves and other magnetic excitations.**
- ***"Show how spins align and what they do"***

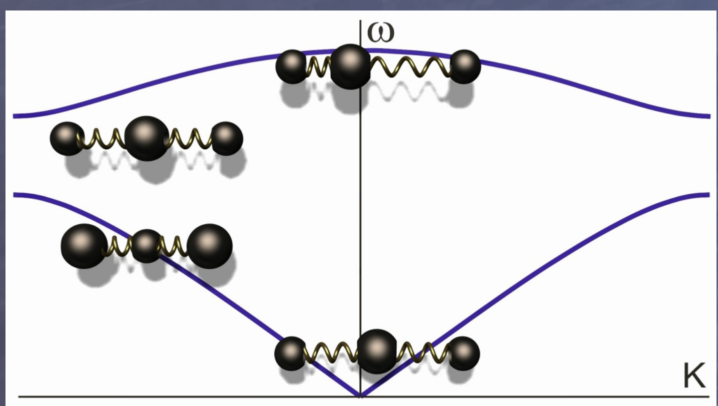
Why is NS Optimal for Probing Materials?

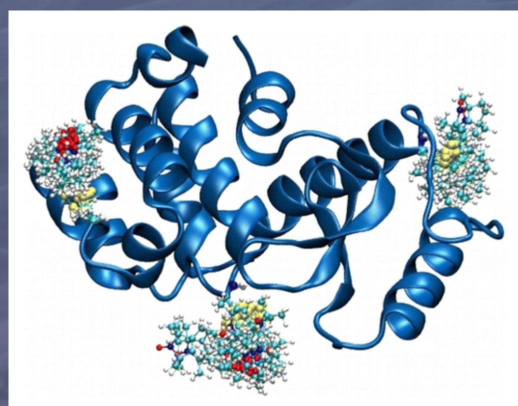
- Strong nuclear scattering <u>AND</u> magnetic scattering
- Neutron wave-length is approximately ”a few Ångström” (~1-30 Å)
- This is the same length-scale as interatomic distances i.e. ideal probe and characterize atomic lattices, molecules and spin-order!

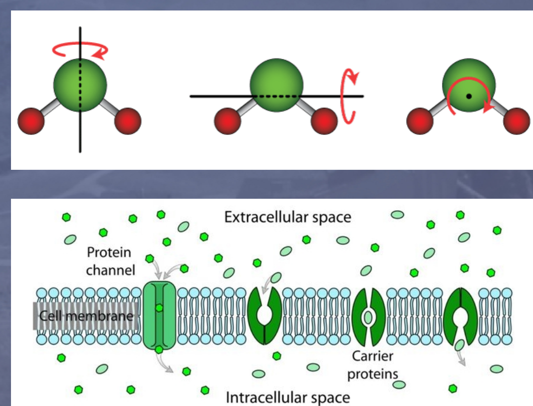


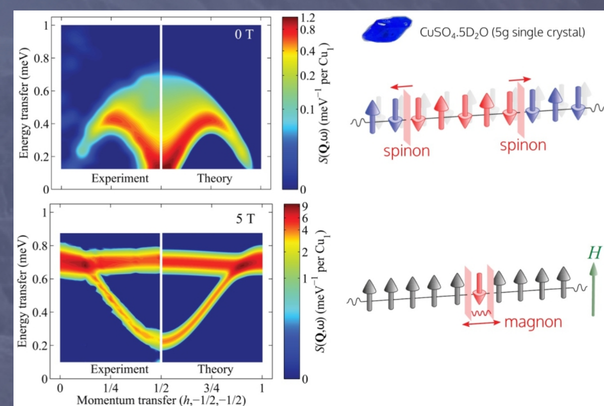


- Neutron mass gives that such wave-length equals an energy that is of the order 0.1 - 100 meV (energy gives wave-length, *chicken-egg*).
- This energy-scale fits perfectly to many atomic/molecular/spin excitations: phonons, molecular dynamics, ion diffusion, magnetic spinwaves/magnons









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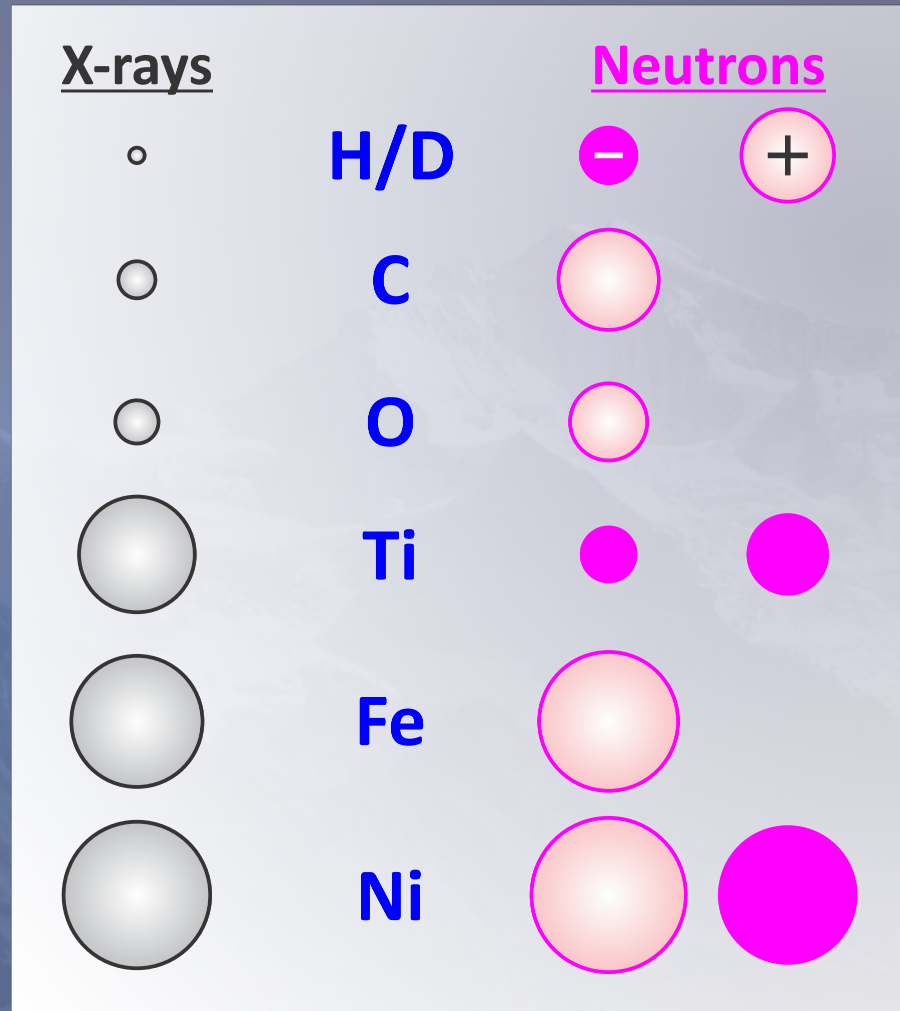
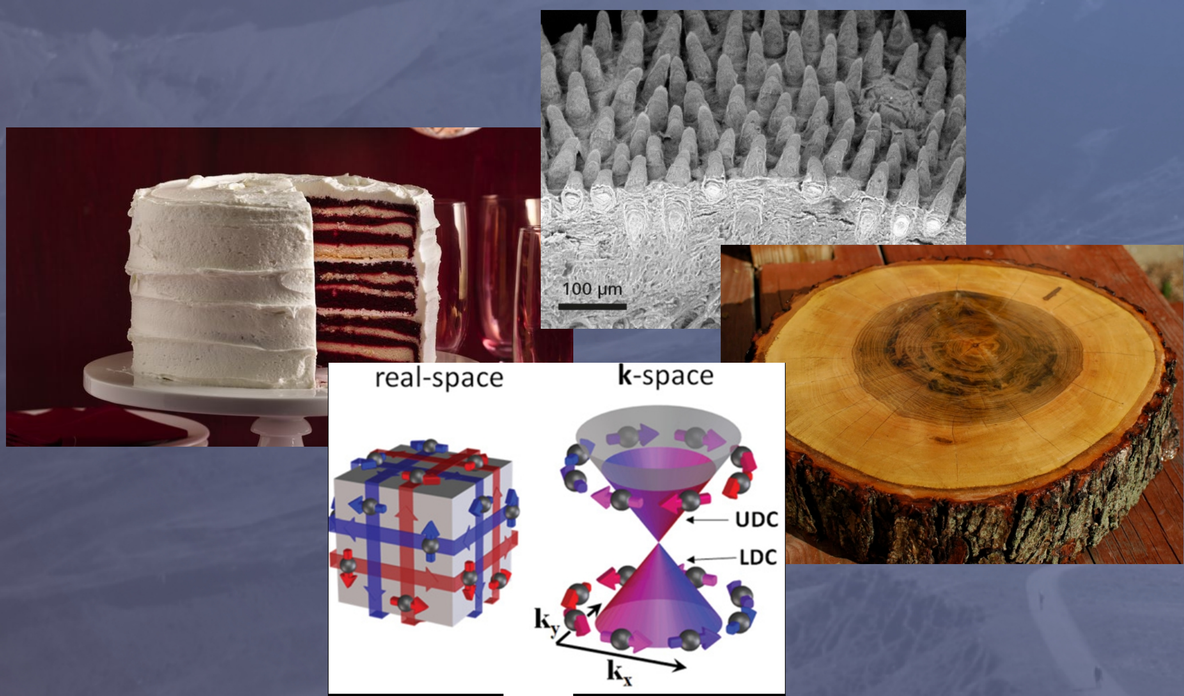
Why is NS Optimal for Probing Materials?

- 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!!!]



Scattering Strengths

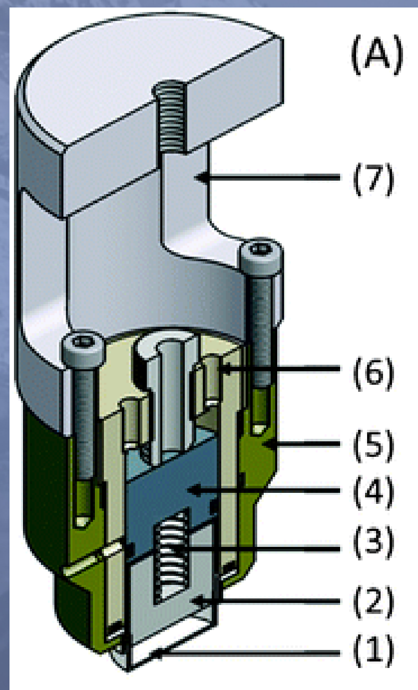


- Some materials (*e.g.* Aluminium) are 'transparent' for neutrons → easy to make sample holders, containers for the experiment and also...

Why is NS Optimal for Probing Materials?

- Some materials (*e.g.* Aluminium) are 'transparent' for neutrons →

- Good materials for building sample environments (cryostats, magnets, pressure cells...).

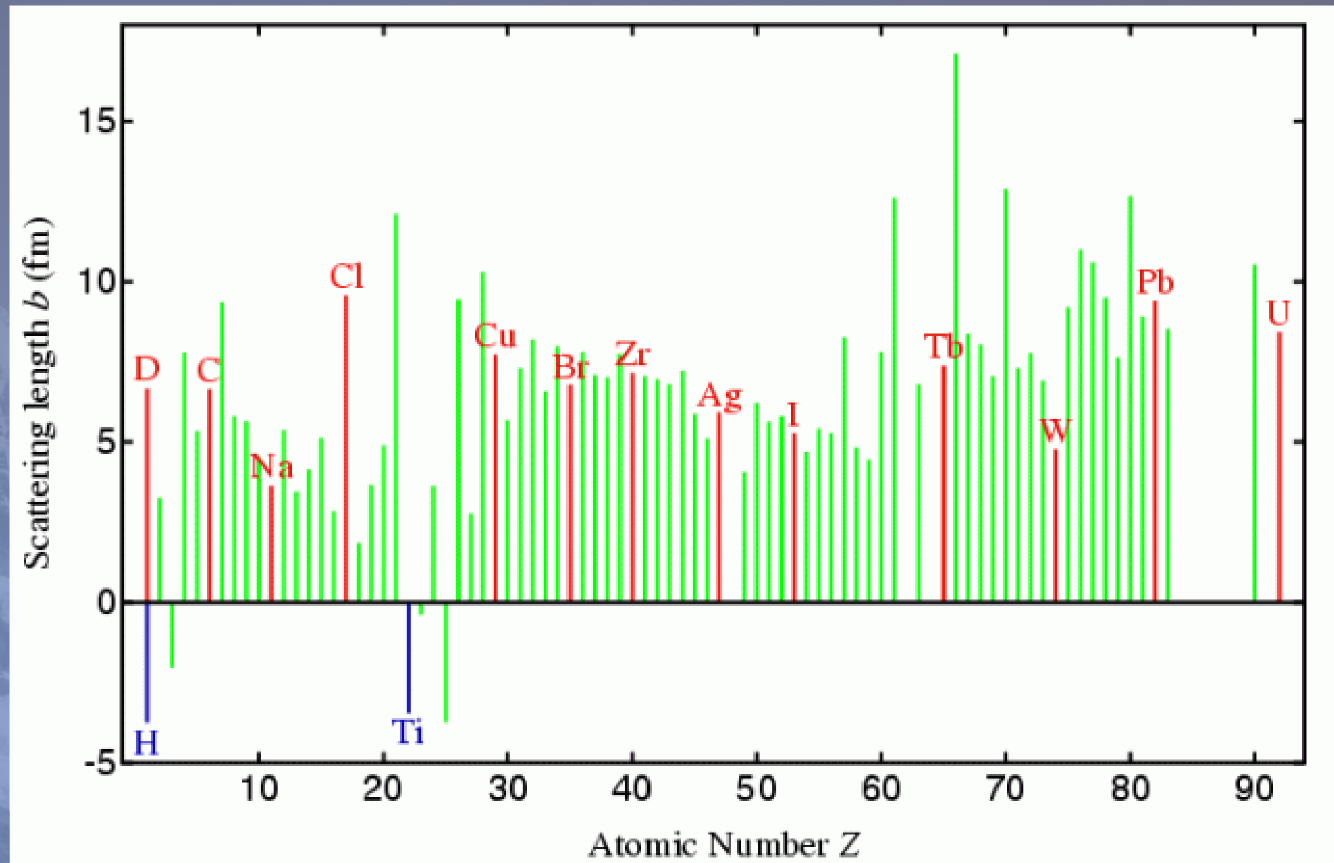


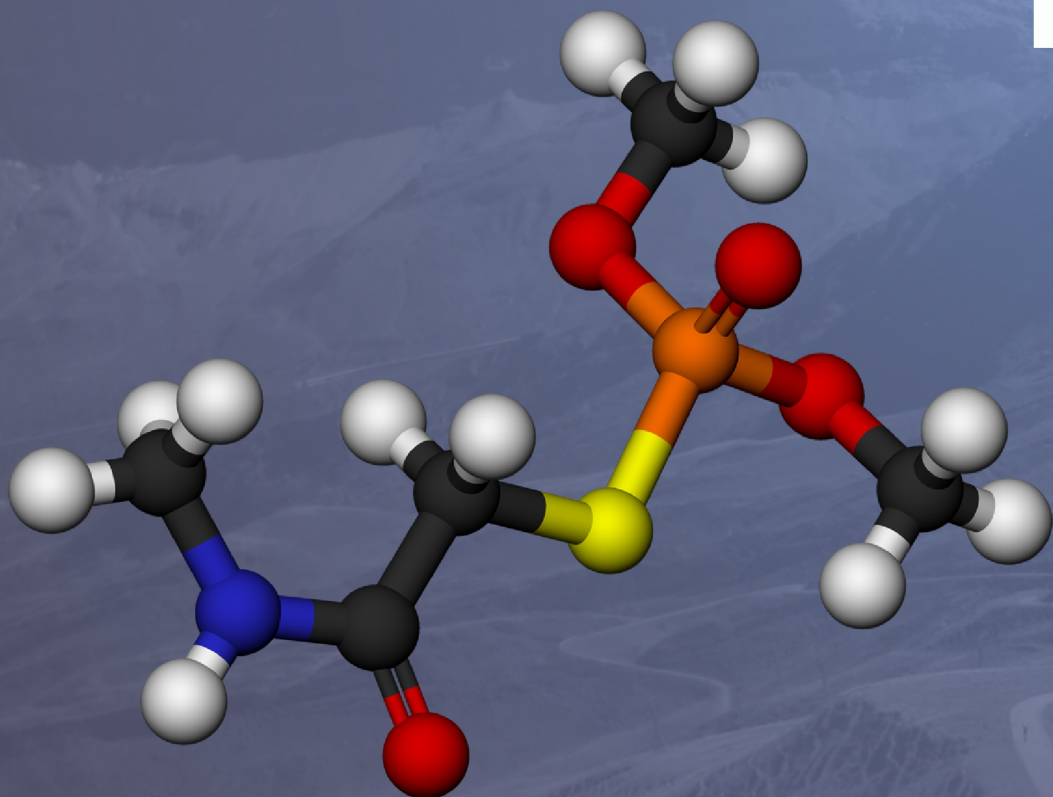
- Measurements under extreme conditions: low (*T* = 10 mK) & high (1500 K) temperatures, high pressures (*P* = 500 kbar) & magnetic fields (*H* = 27 T).

- 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 ^{6}Li / ^{7}L.





- 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.

Deuterated Cellulose

- It is possible to grow deuterated (bacterial) cellulose without causing any structural changes!

Production of Bacterial Cellulose with Controlled Deuterium–Hydrogen Substitution for Neutron Scattering Studies ☆

Hugh O'Neill*[,1], Riddhi Shah*[,†], Barbara R. Evans[‡], Junhong He*, Sai Venkatesh Pingali*, Shishir P.S. Chundawat[§], A. Daniel Jones[¶,||], Paul Langan*, Brian H. Davison[#], Volker Urban*

Methods in Enzymology, Volume 565
ISSN 0076-6879
http://dx.doi.org/10.1016/bs.mie.2015.08.031

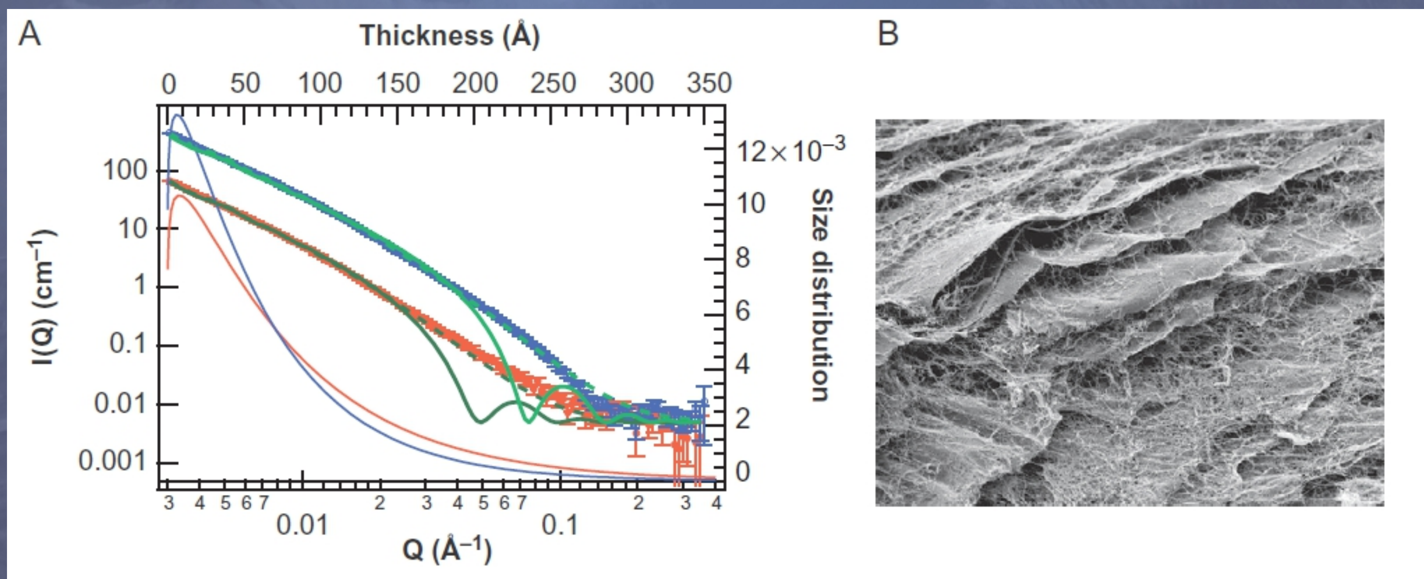
Cellulose (2014) 21:927–936
DOI 10.1007/s10570-013-0067-4

ORIGINAL PAPER

Controlled incorporation of deuterium into bacterial cellulose

Junhong He · Sai Venkatesh Pingali · Shishir P. S. Chundawat · Angela Pack · A. Daniel Jones · Paul Langan · Brian H. Davison · Volker Urban · Barbara Evans · Hugh O'Neill

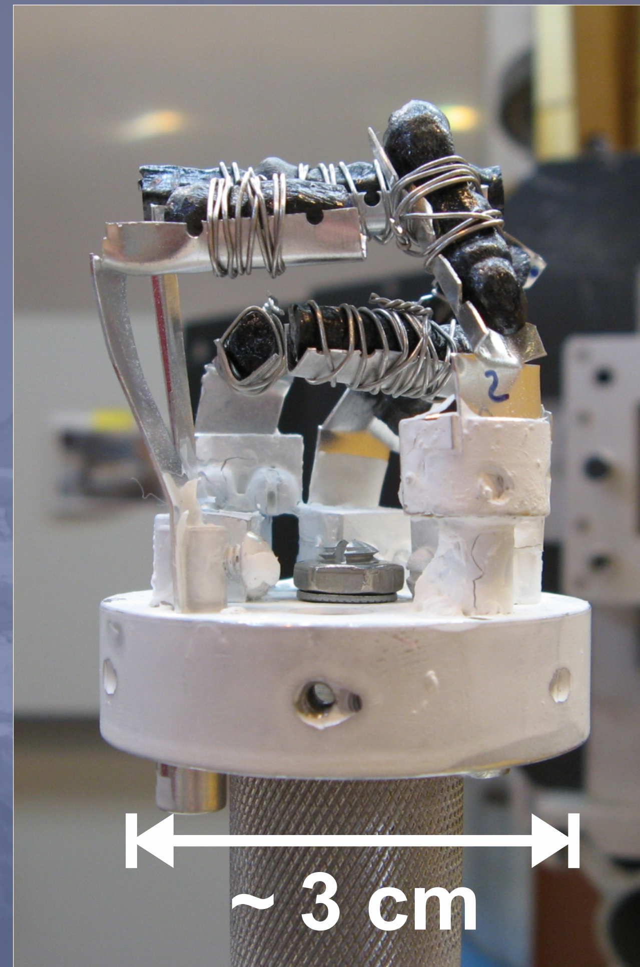
- This allow you to play with contrast between cellulose and water in neutron experiments (e.g. SANS).

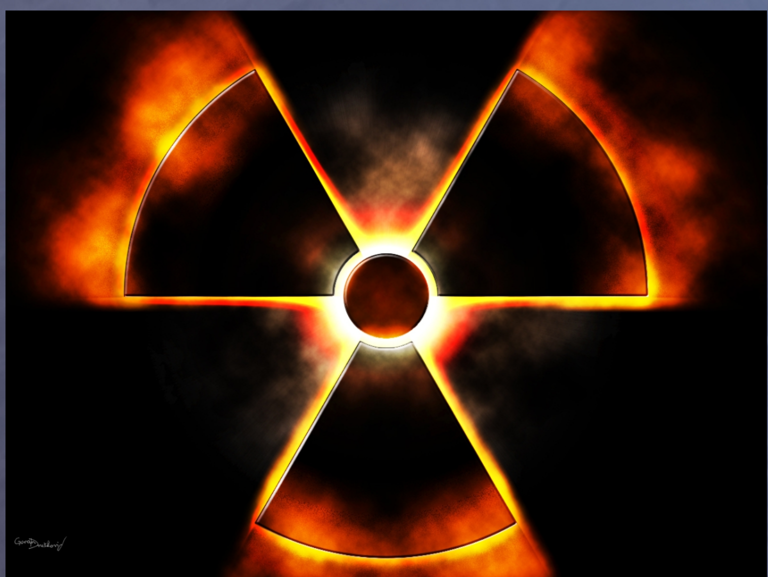


- Also helps to separate interactions with other biomolecules and polymers for development of composite materials.

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'.

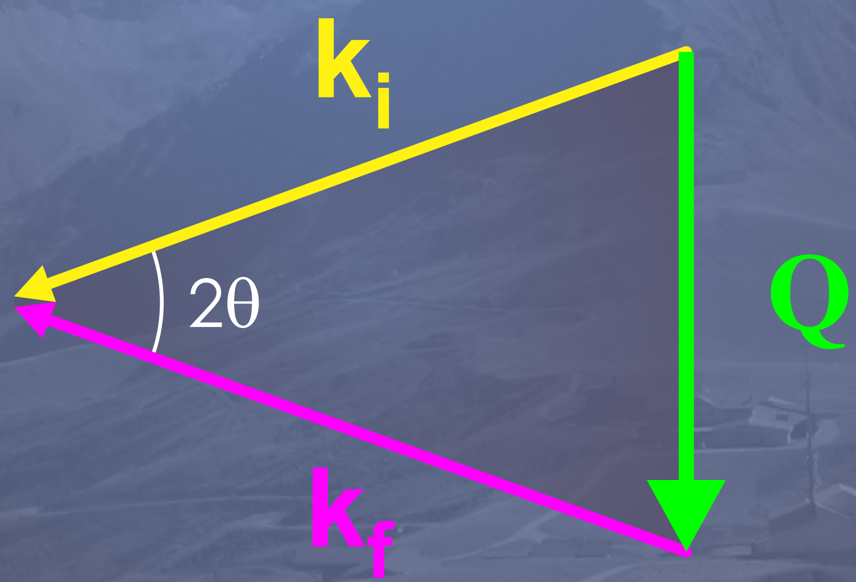
Elastic Neutron Scattering

- 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

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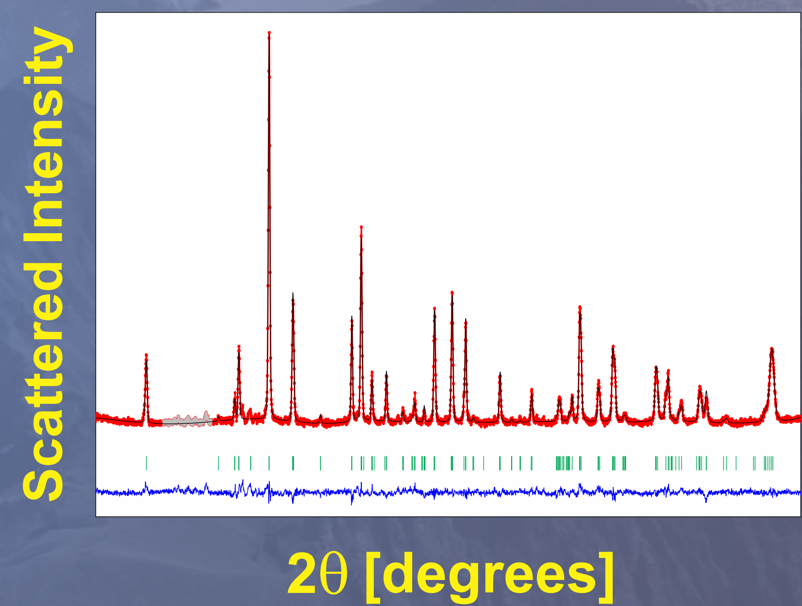
Neutron Diffraction

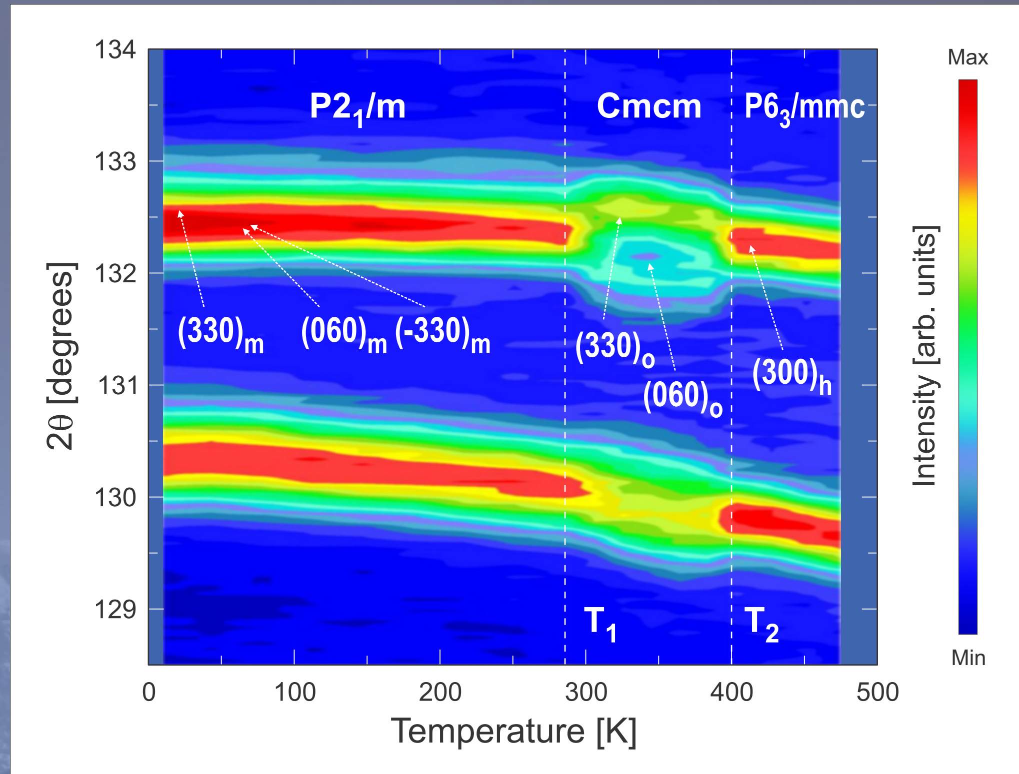
- If the scattering vector $\mathbf{Q} = \tau$ where τ is a reciprocal lattice vector for a nuclear and/or magnetic lattice we obtain coherent elastic scattering.
- As for a normal XRD experiment this is done by performing θ / 2θ scans (2-axis instrument) using fixed & monochromatic incident neutron 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)]. Modern sources → mg and minutes !!!

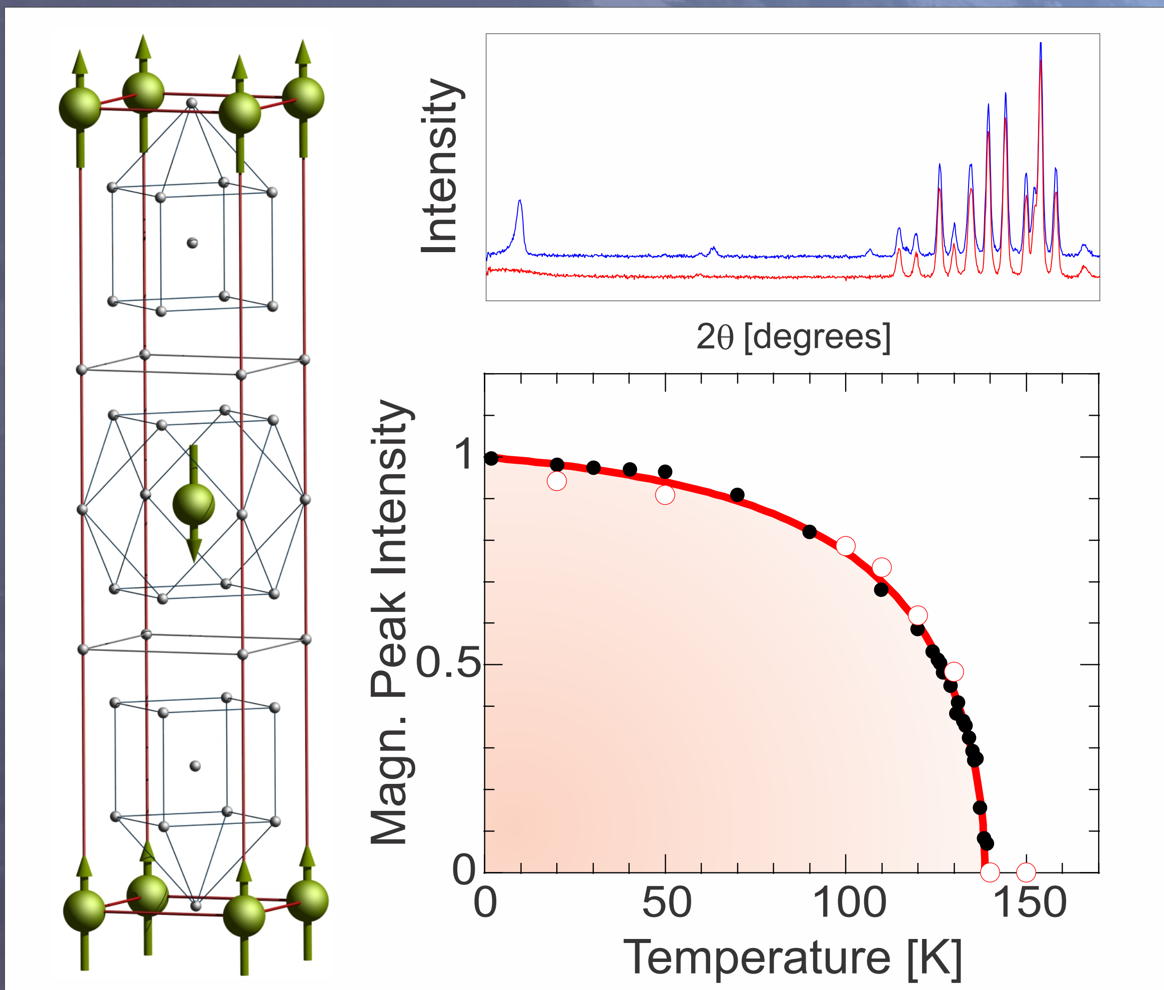
Neutron Diffraction - Examples

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 (also H !)

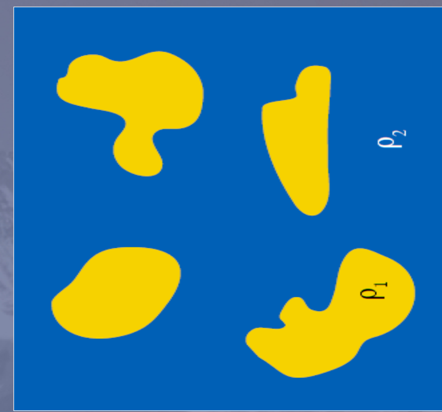


Magnetic Diffraction

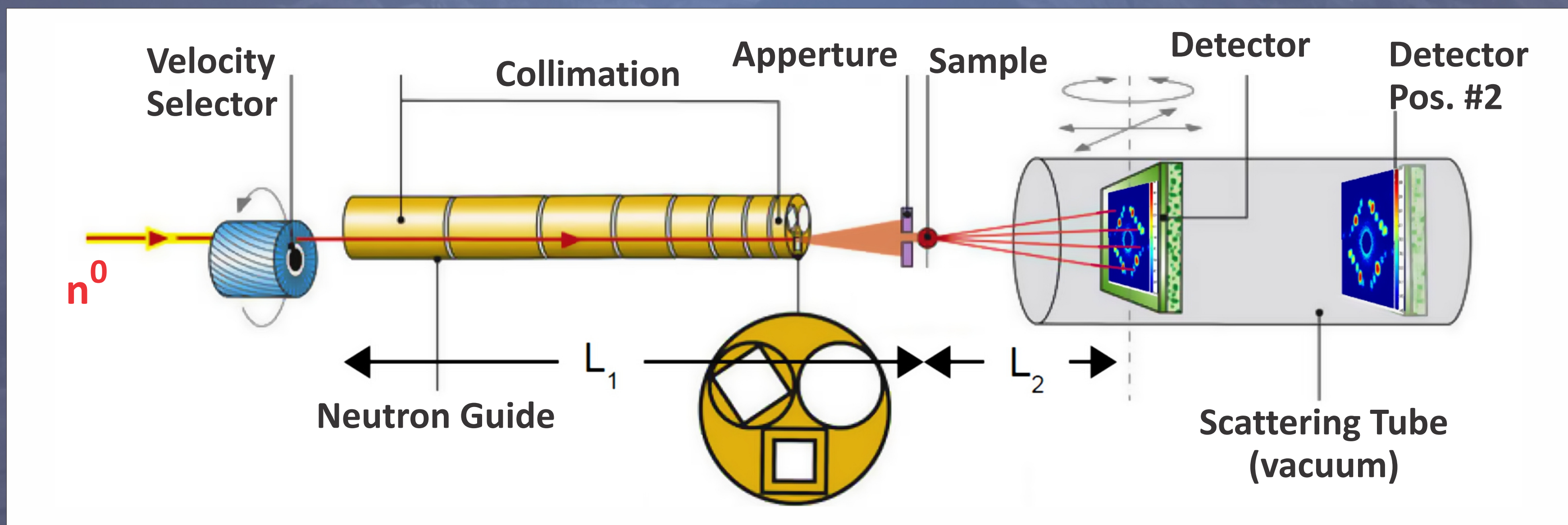
- Only available tool (!!!) to directly study magnetic order:
  - Determine complex spin-structures and size + direction of magnetic moment for spintronics, storage, novel materials...
  - Magnetic order parameters as a function of T/H to understand formation of spin order *e.g.* frustrated/quantum magnets.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

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.

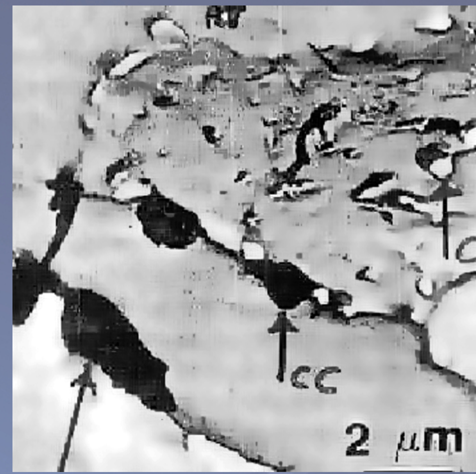


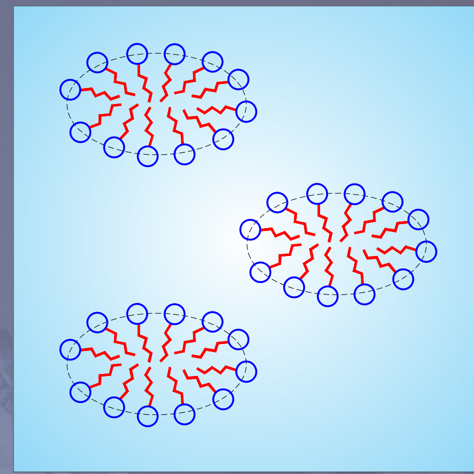
- Good resolution for small scattering angles → good collimation + large spectrometers (L = 10-50 m, H = 2-5 m) with adjustable detector distance.

SANS - Examples

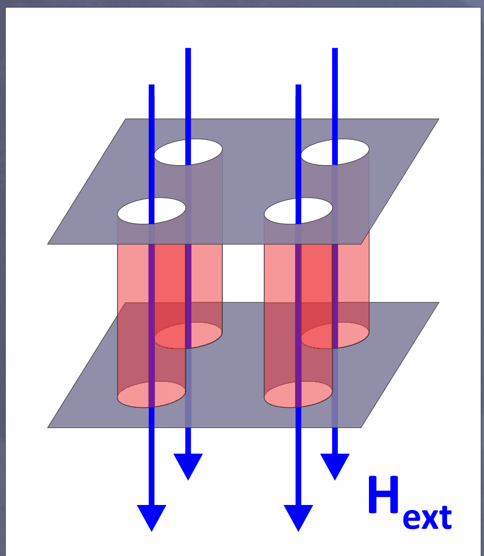
'LARGE' STRUCTURES

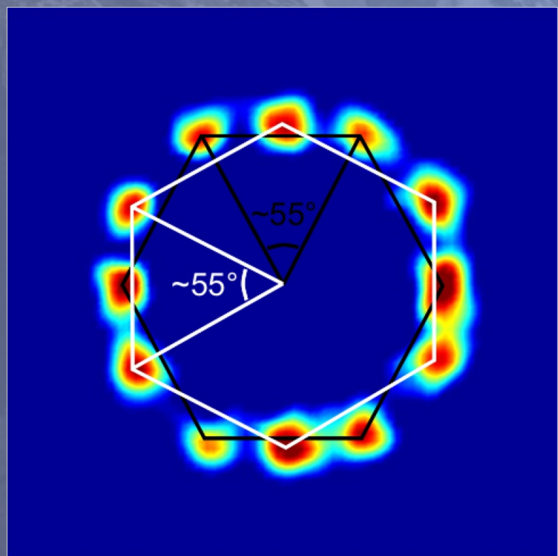
- **Metallurgy: creep cavitation damage in steel at high T where volume fraction and size distribution of cavities is obtained.**
- **'Soft' matter: size, shape and interaction of particles *e.g.* proteins/micelles in solution or nano-phases in polymers. [H vs. D!]**





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





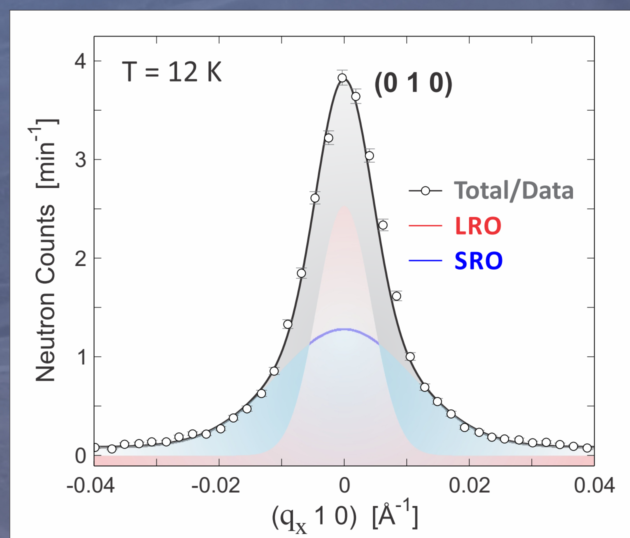
HIGH-TEMPERATURE SUPERCONDUCTIVITY

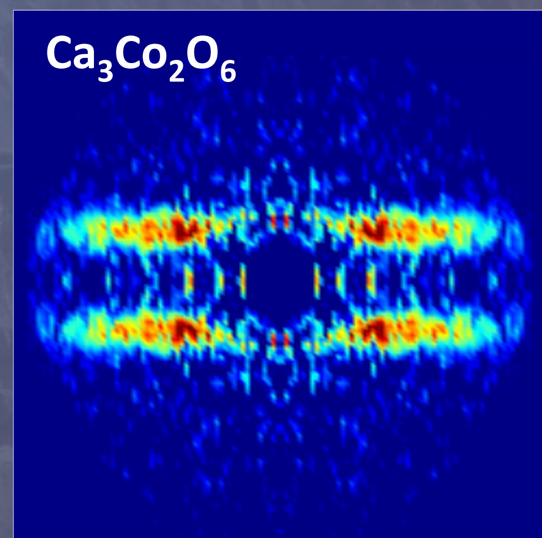
- **Vortex lattices in TYPE-II superconductors created by externally applied magn. field.**
- **The size, distribution and elasticity tells a lot about the underlying physics, FS/OP symmetry and transport properties.**

Prsa, arXiv:1404.7398

MAGNETISM

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





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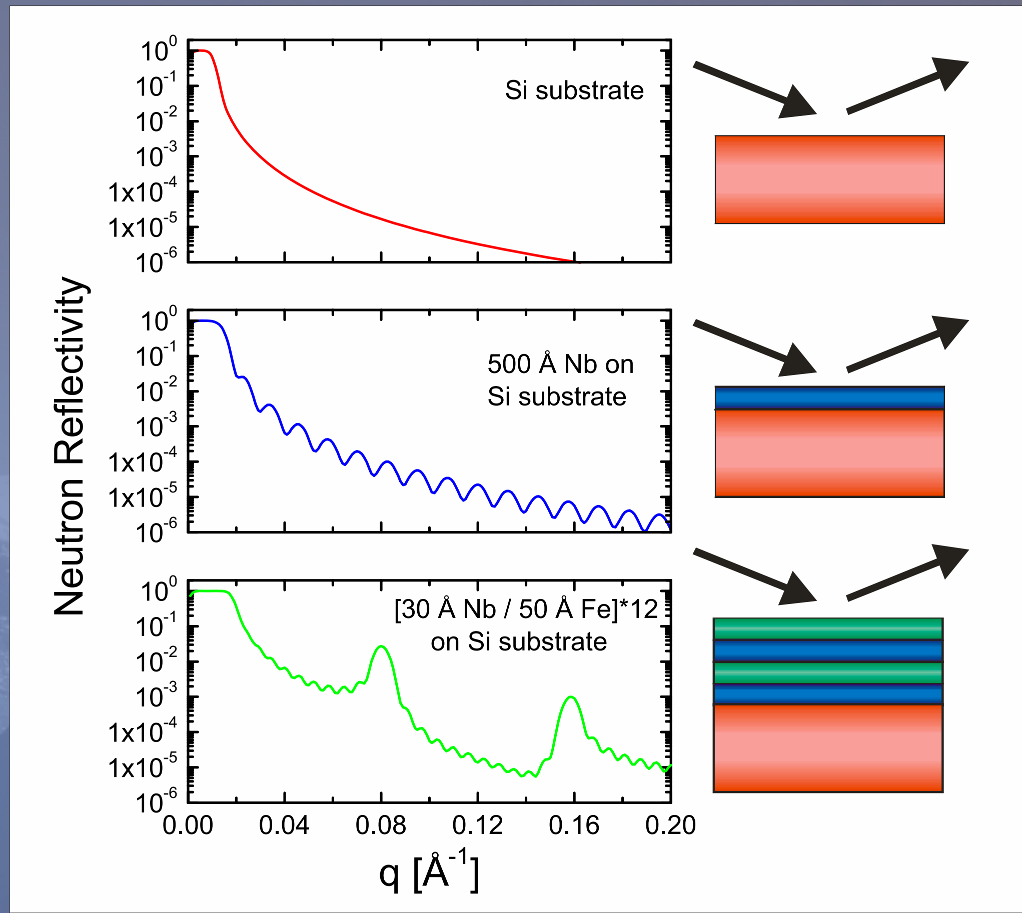
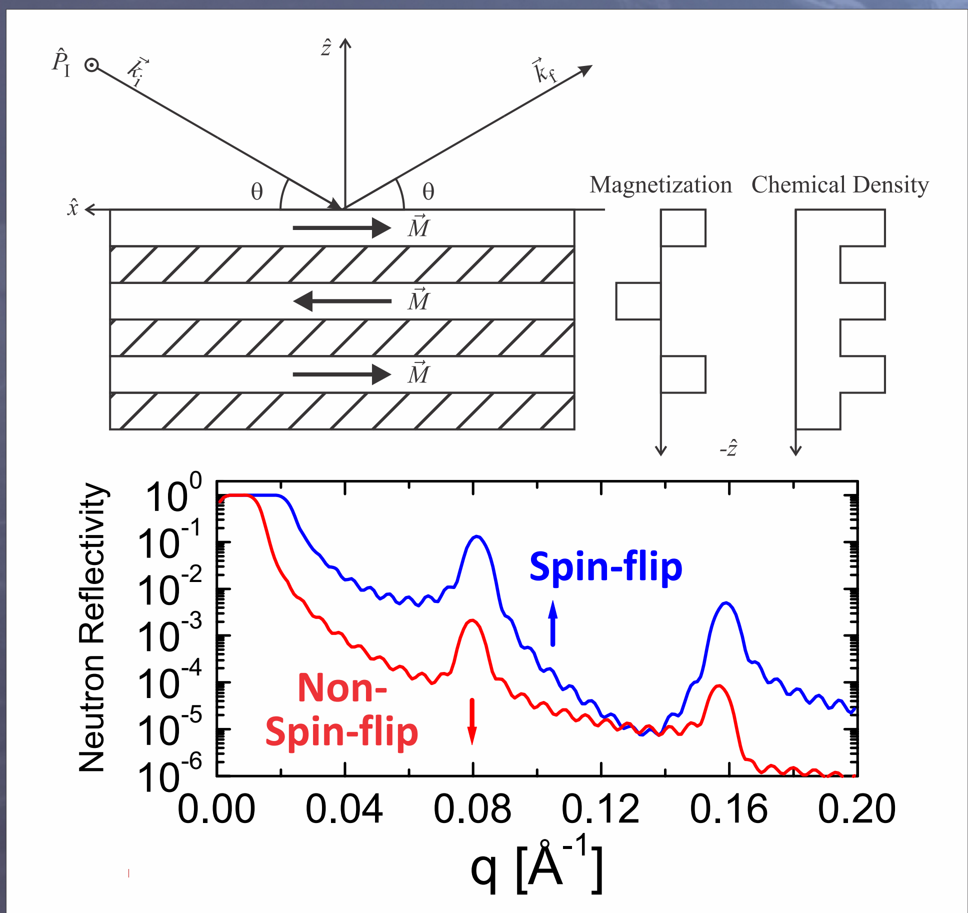
Neutron Reflectometry

- 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...



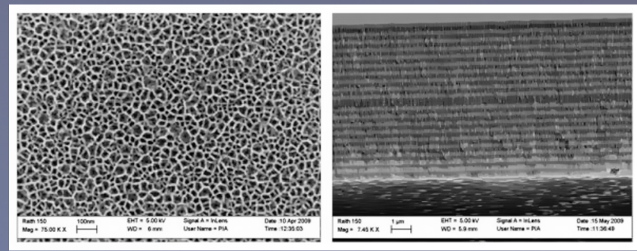


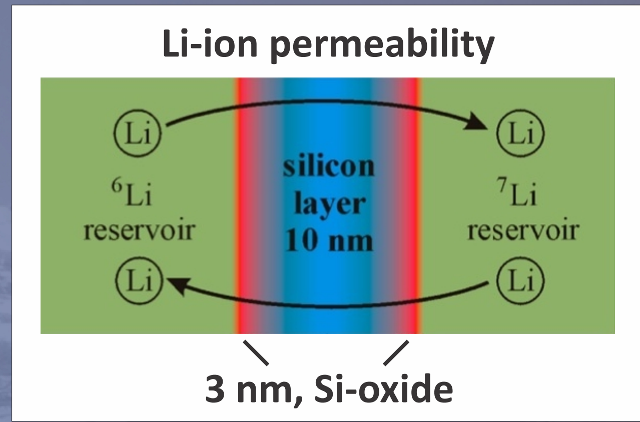
- ...the exact shape of the reflectivity profile can provide very detailed info about the structure of the surface, including the thickness, density, and roughness of any thin films layered on the substrate.
- If the measurement is done polarized (PNR) it is possible to deduce also the magnetic spin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

Reflectometry - Examples

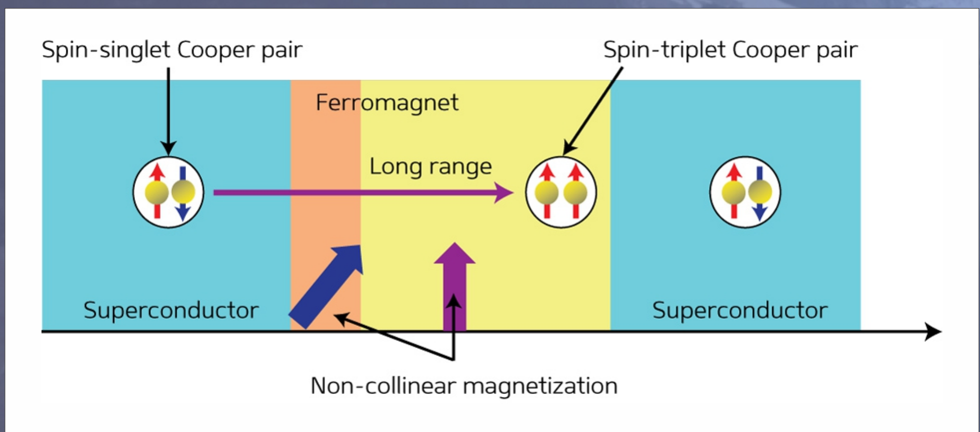
Non-polarized / Structural

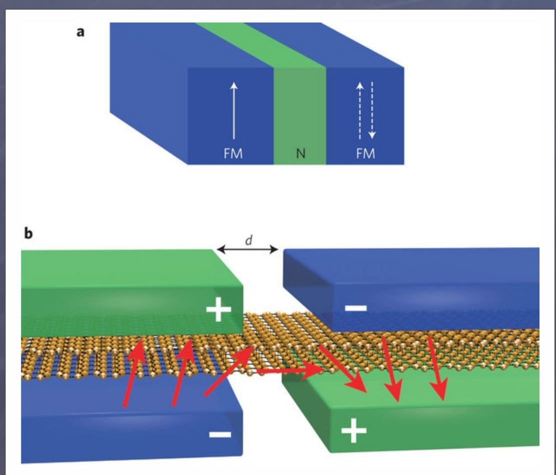
- Determination of film thickness, depth-resolved density profile, roughness and interface properties of multilayers:
  - Spin-coated polymer films (e.g. insulation in electrical motors, solar cells...) and other surface coatings
  - Semiconductor multilayers
  - Liquid adhesion and chemical aggregation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

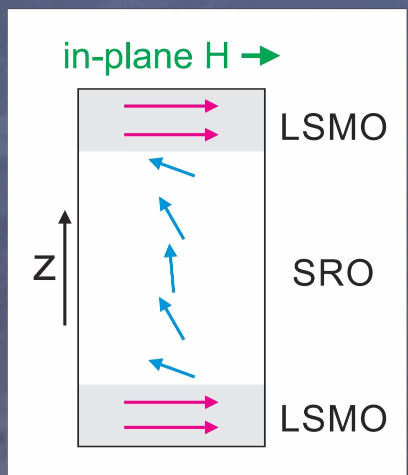




Hüger, Nano Letters 13, 1237 (2013)







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*):

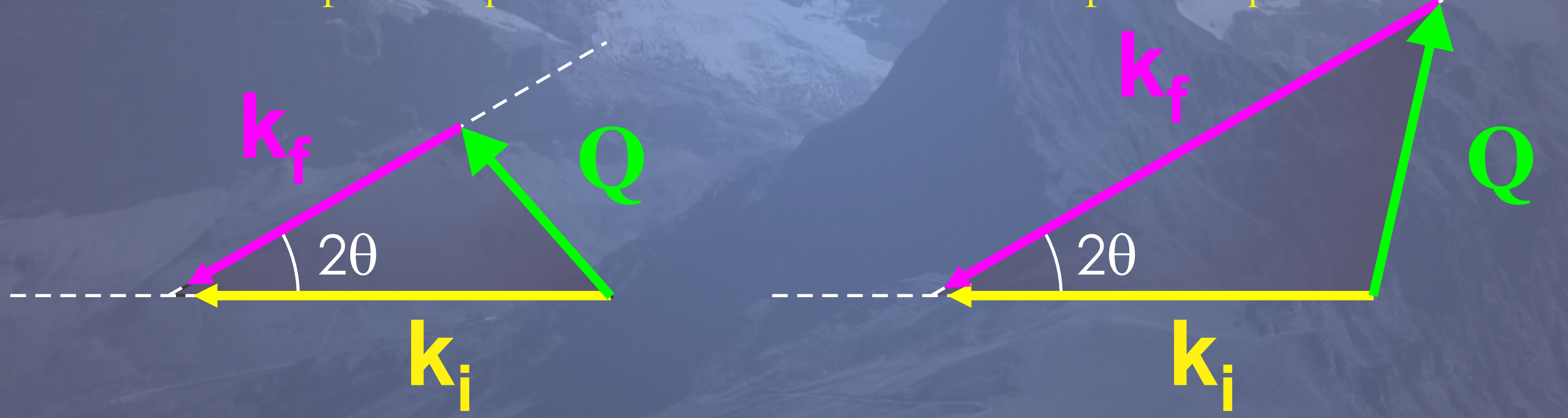
$$\mathbf{Q} = (\mathbf{k}_i - \mathbf{k}_f)$$

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

- 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 <u>Inelastic Neutron Scattering (INS)</u>:

<u>Neutron Loses Energy</u> $|\mathbf{k}_f| < |\mathbf{k}_i|$

<u>Neutron Gains Energy</u> $|\mathbf{k}_f| > |\mathbf{k}_i|$



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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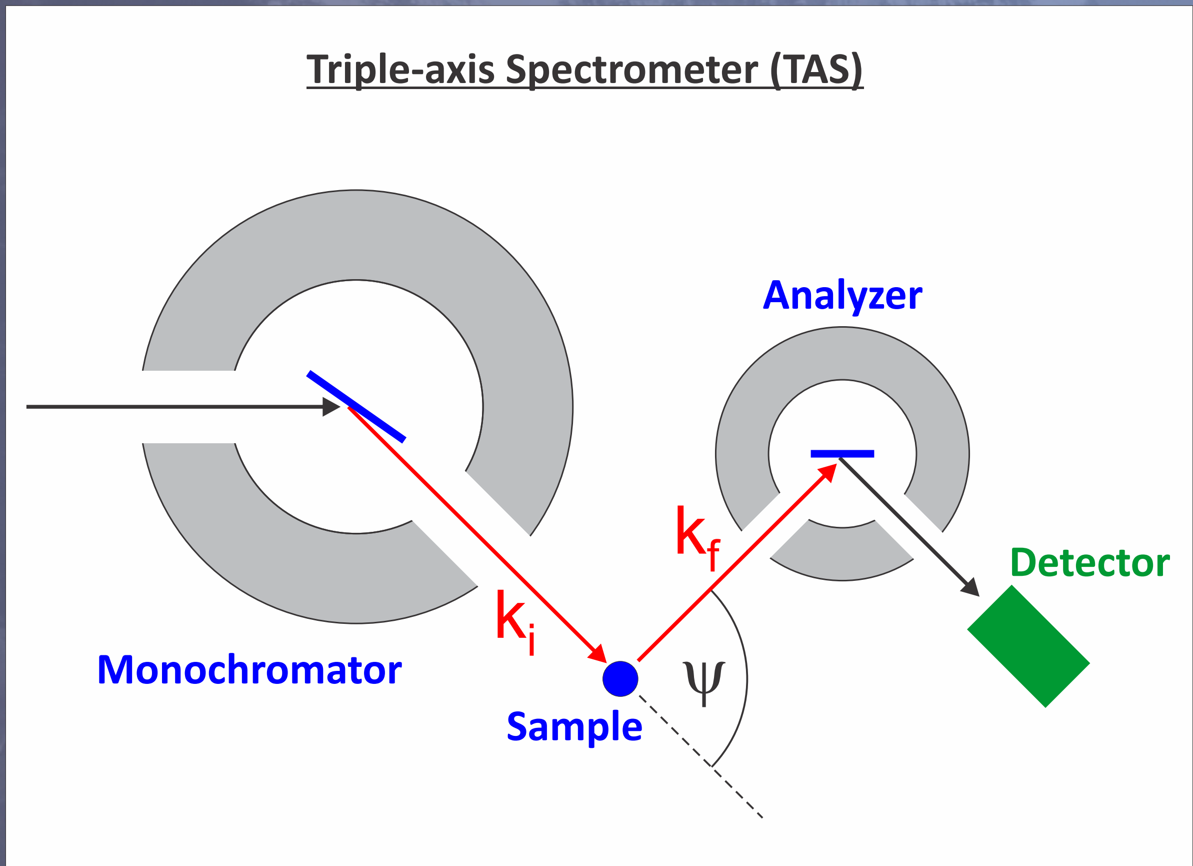
Classic Triple-axis Spectrometer (TAS)

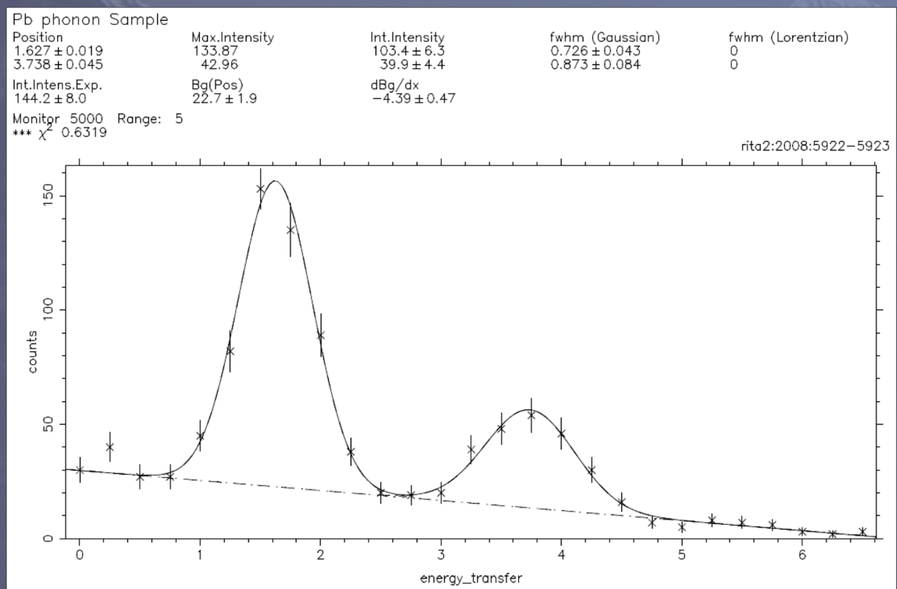
- Measure a single Q,E point at a time by using monochromators and "filters" to define initial state and to detect a specific final state.



- 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.**



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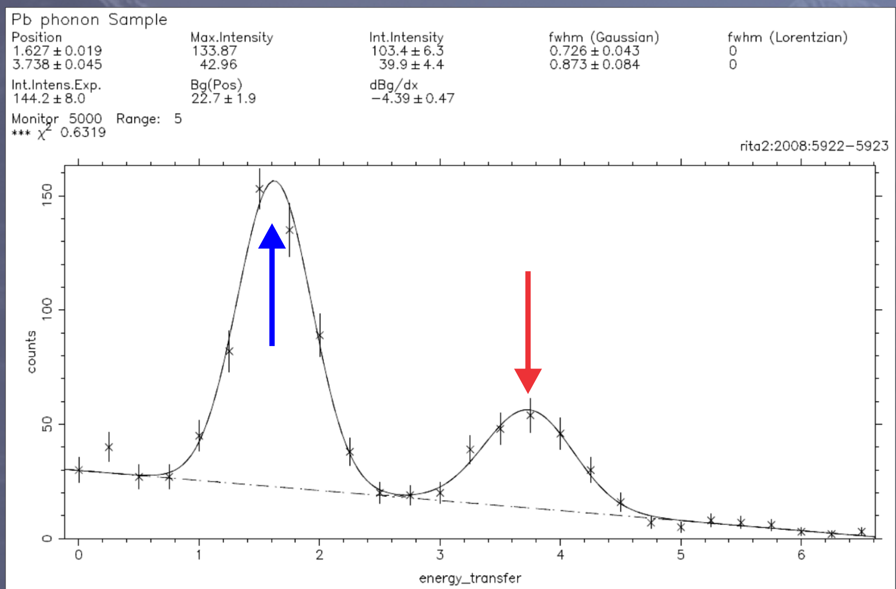

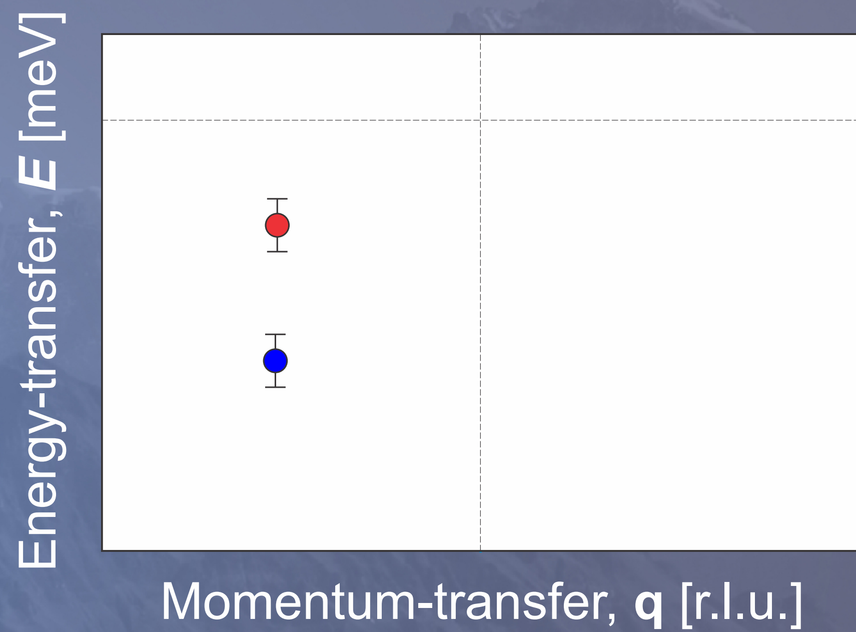

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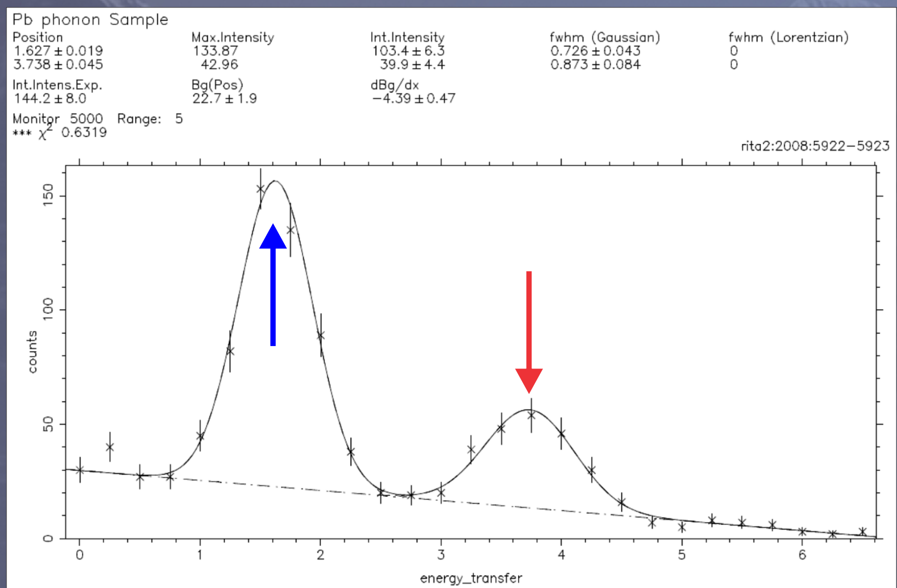

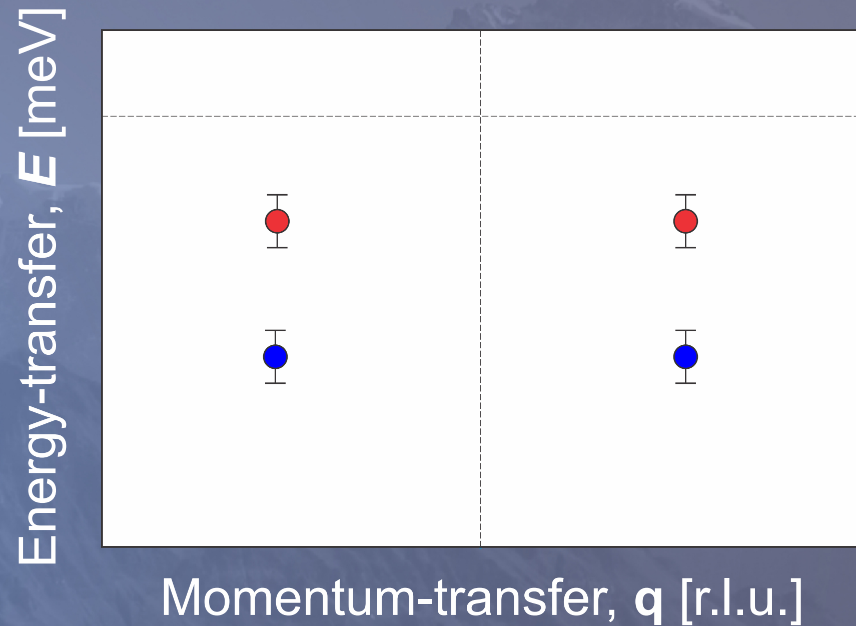

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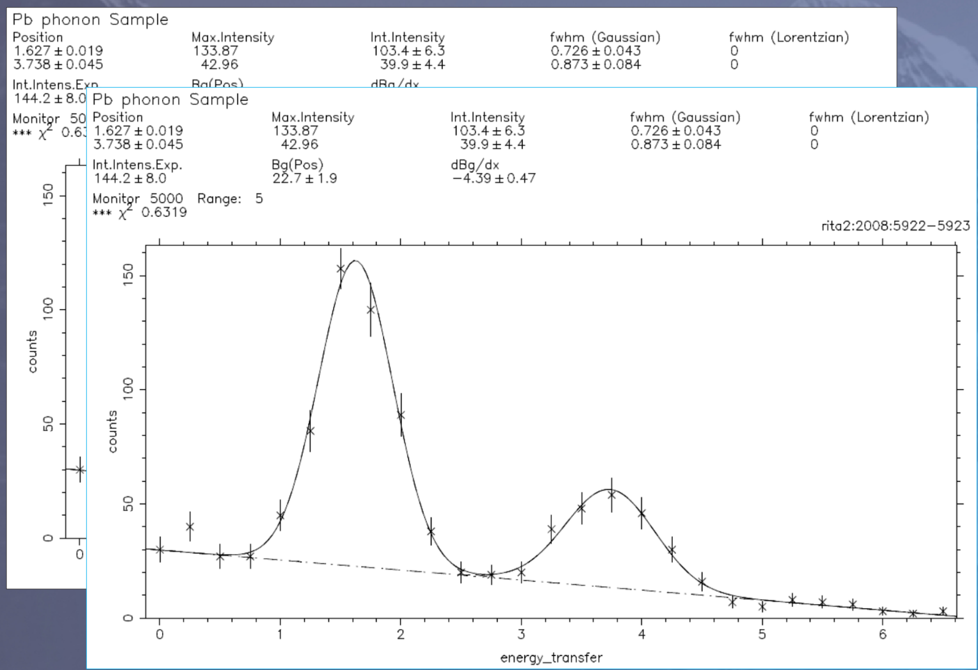

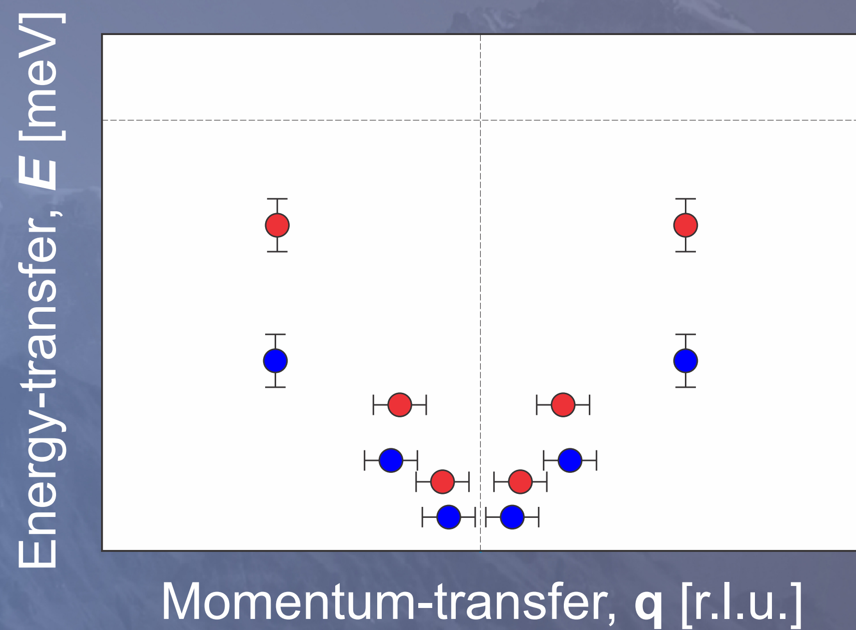

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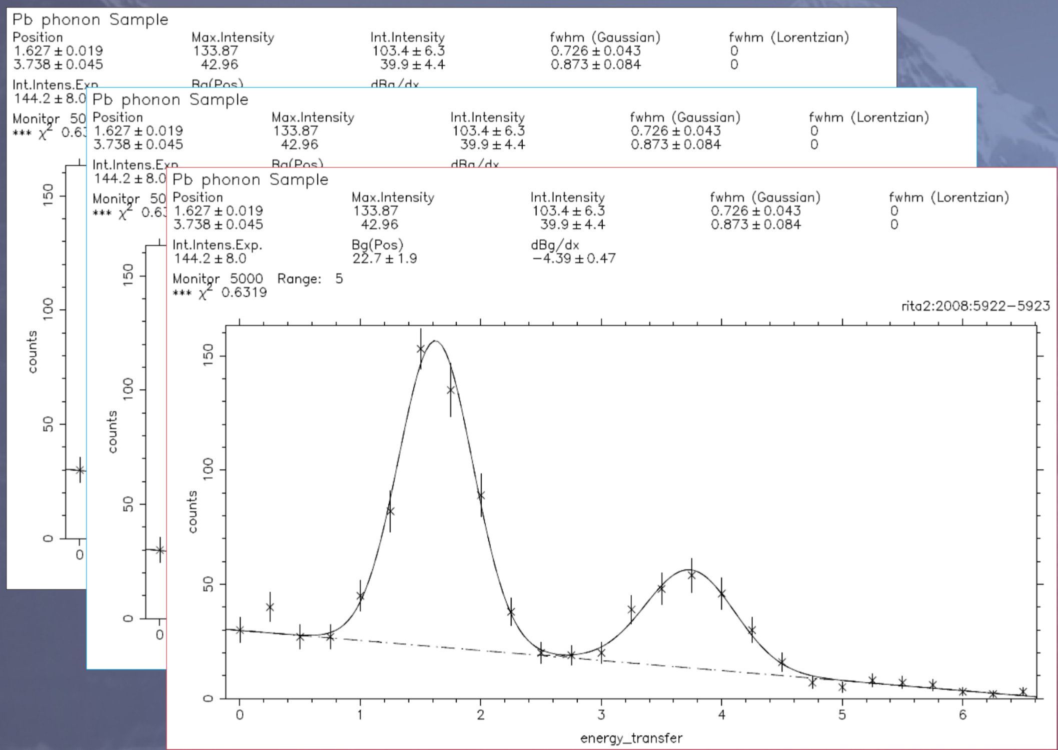

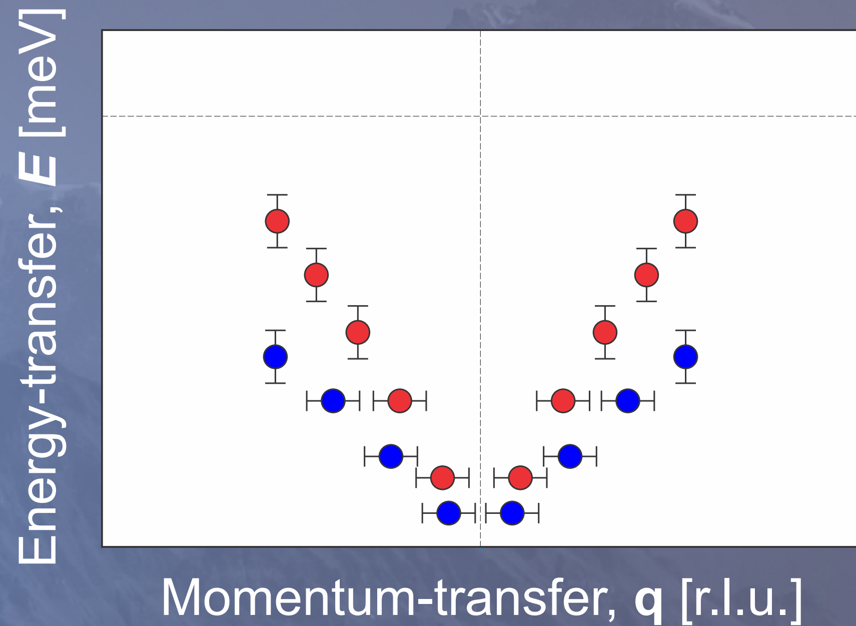

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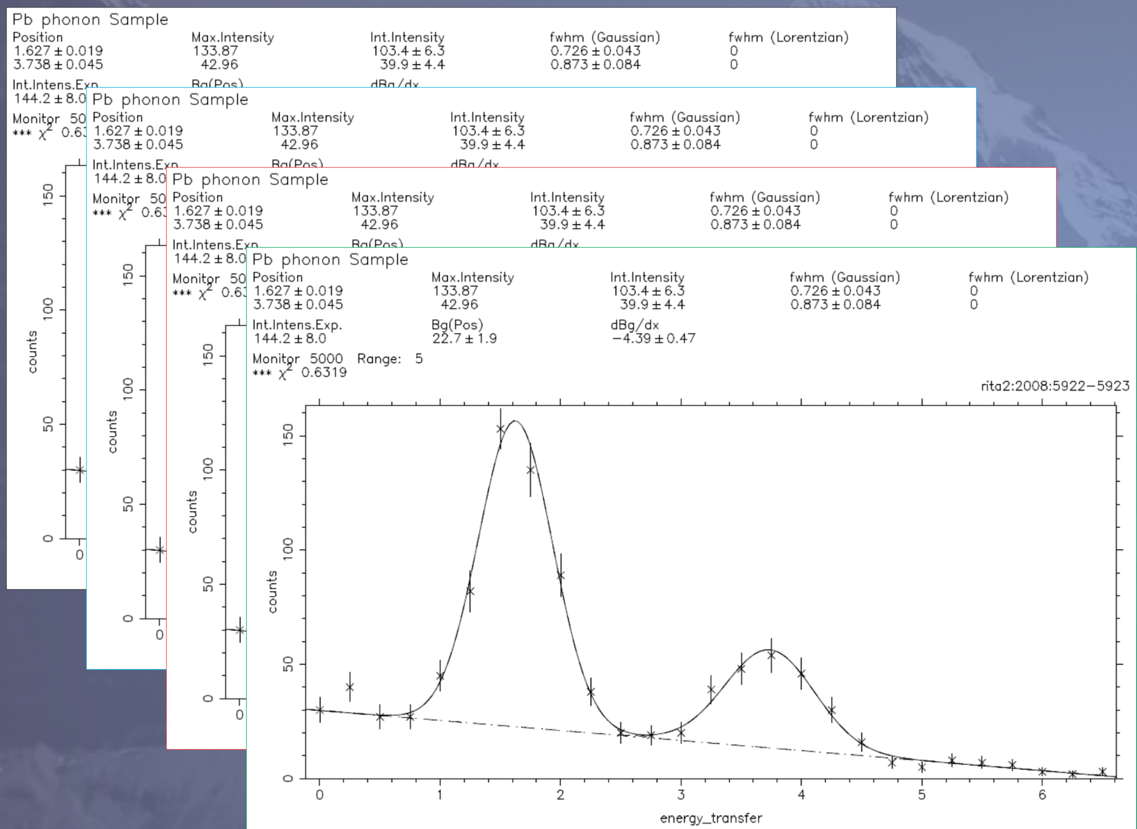

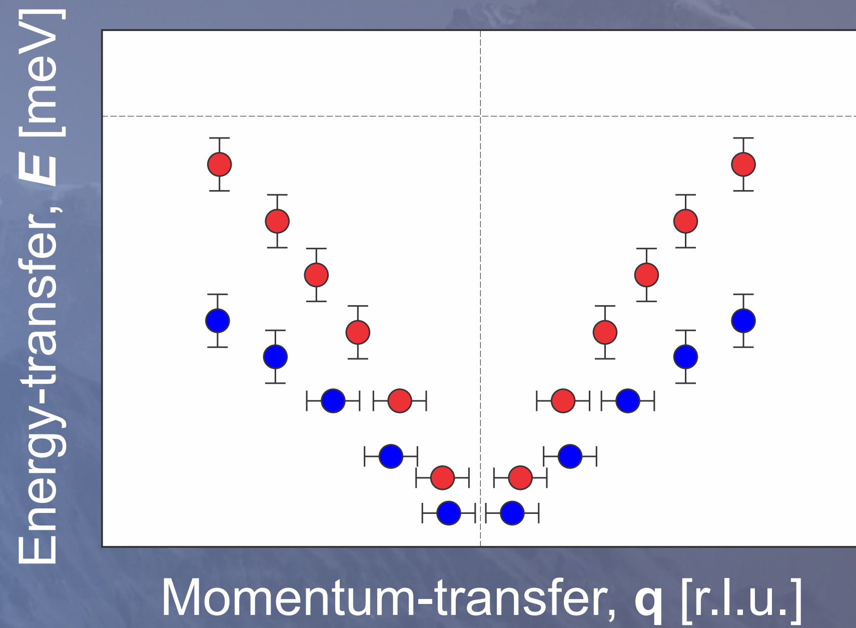

Classic TAS: Data Acquisition/Analysis

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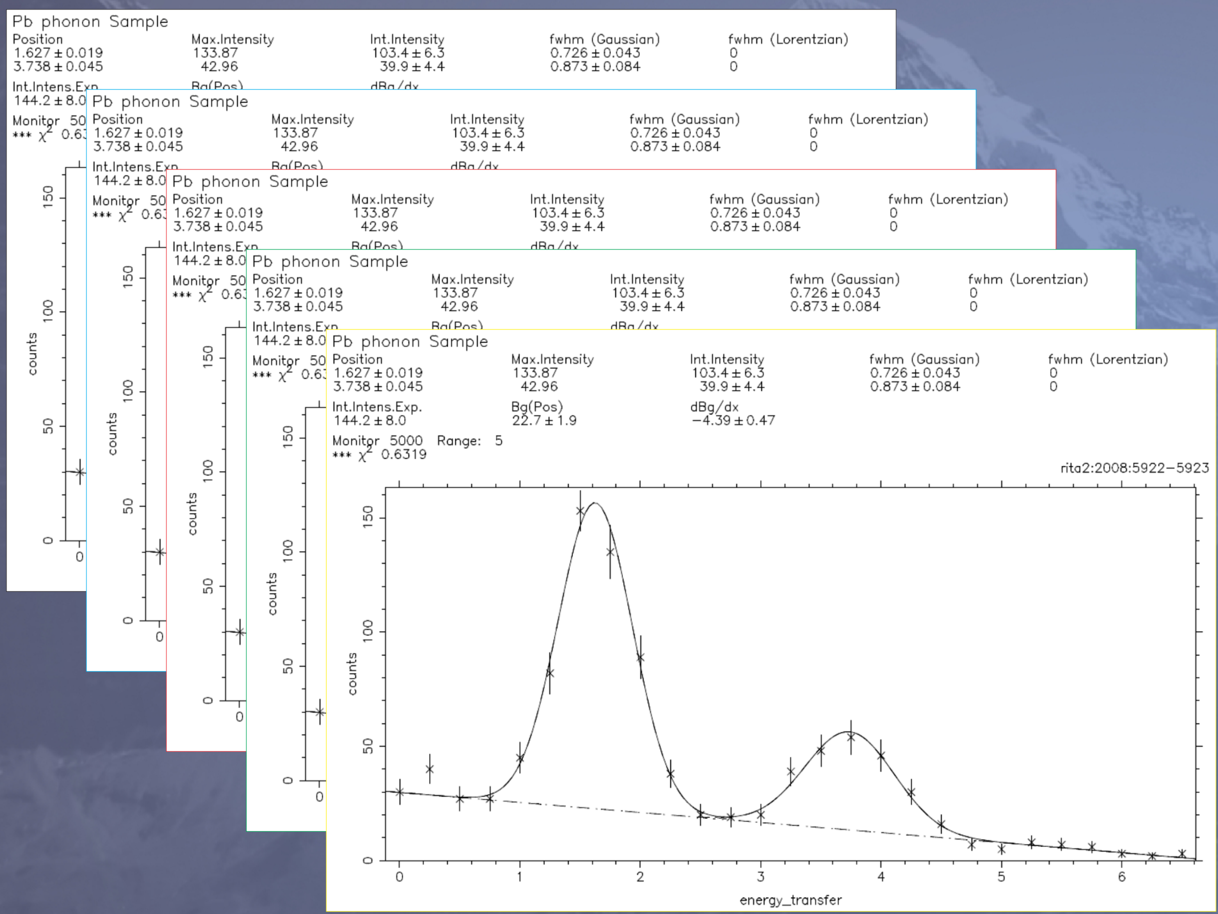

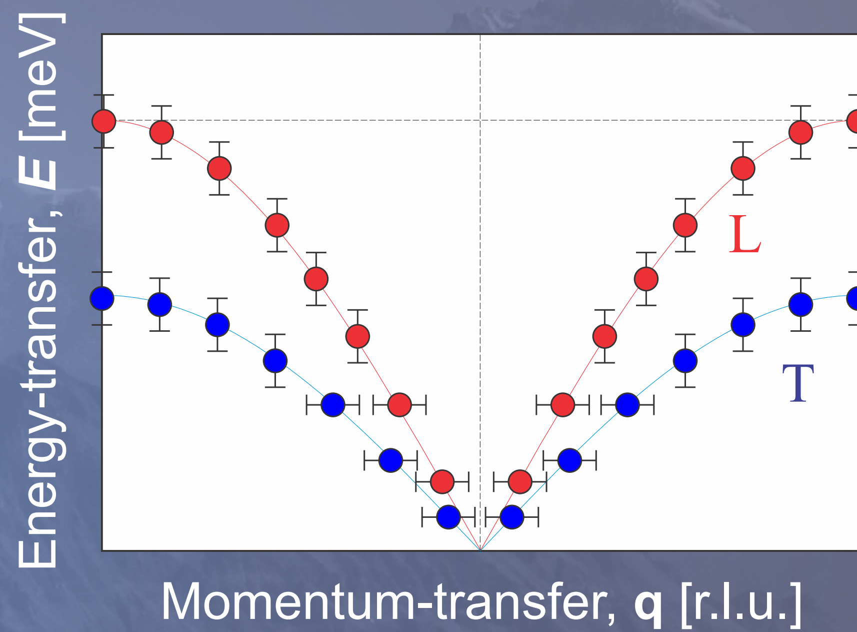

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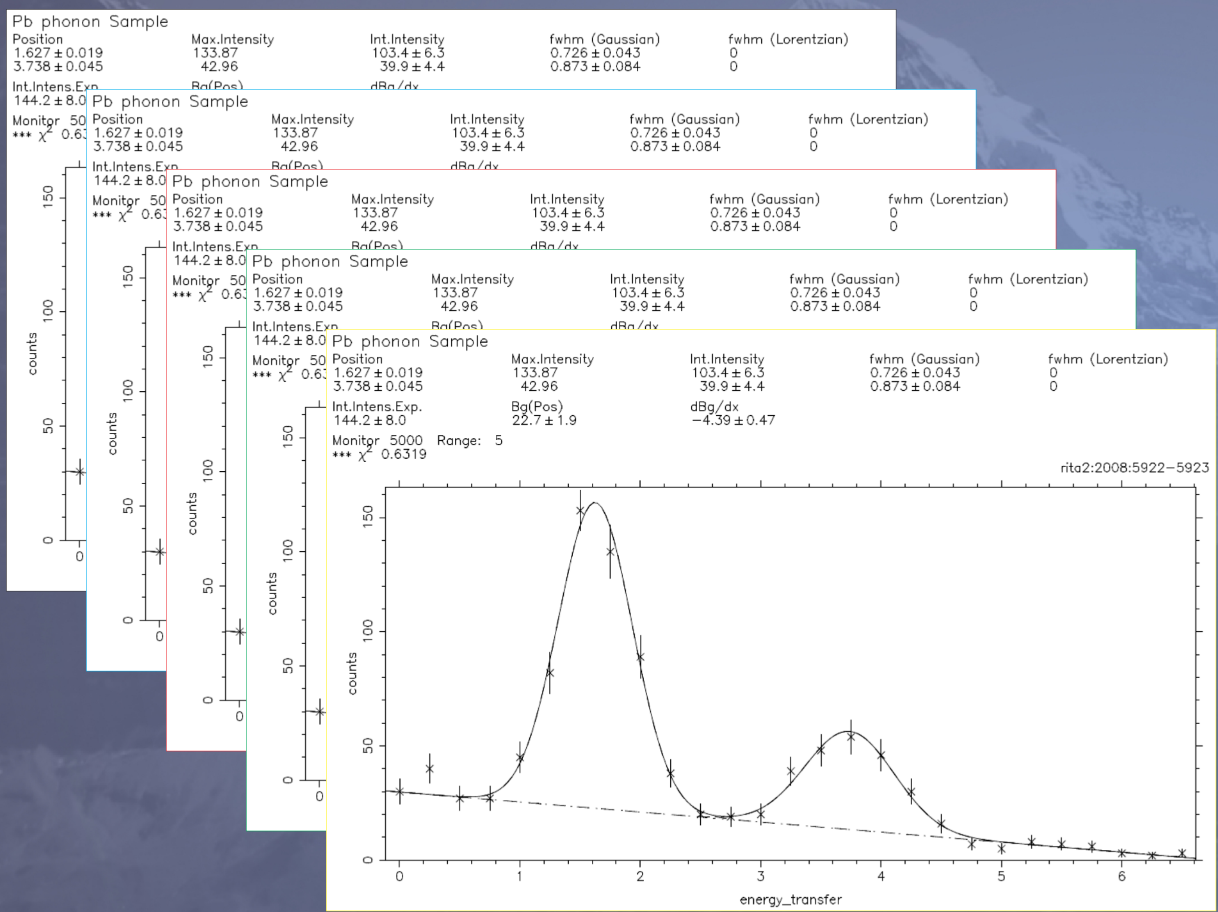

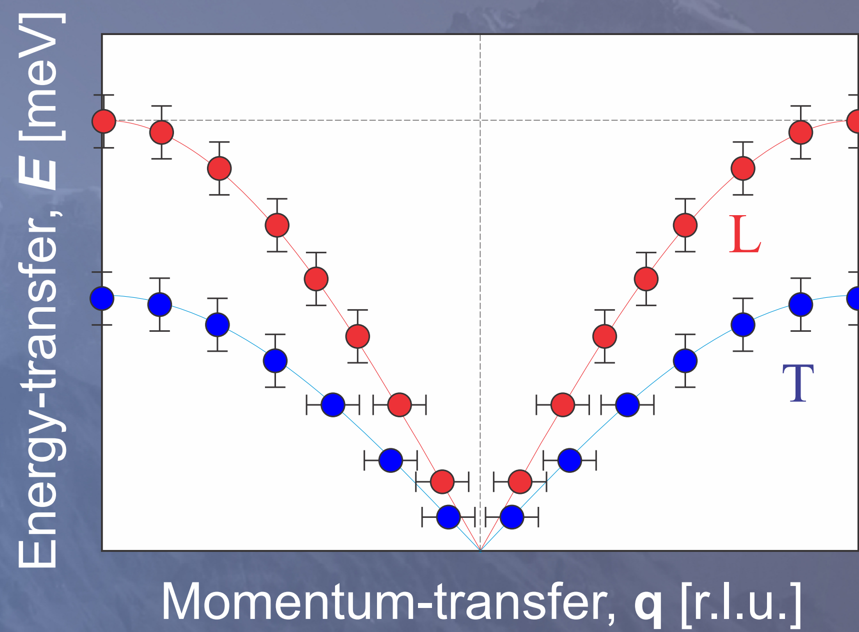

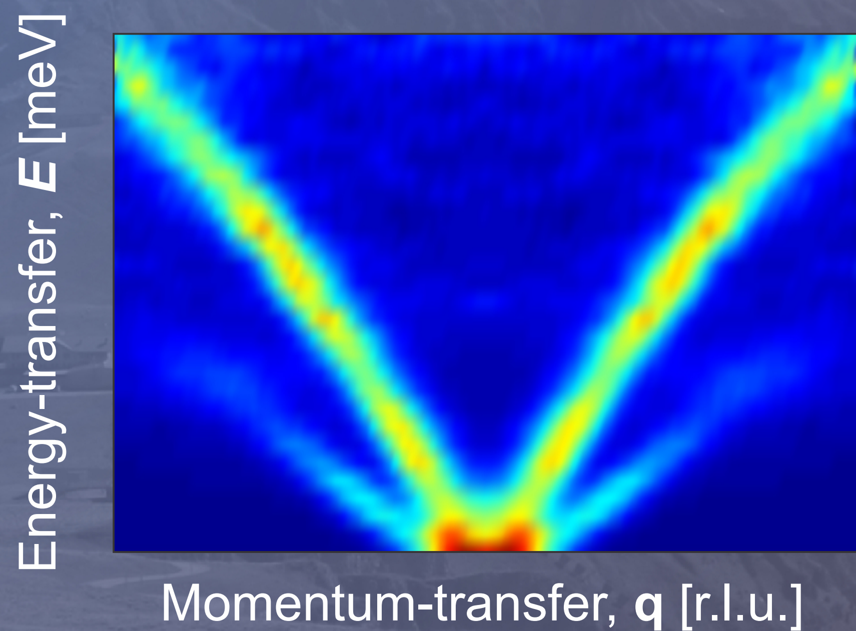

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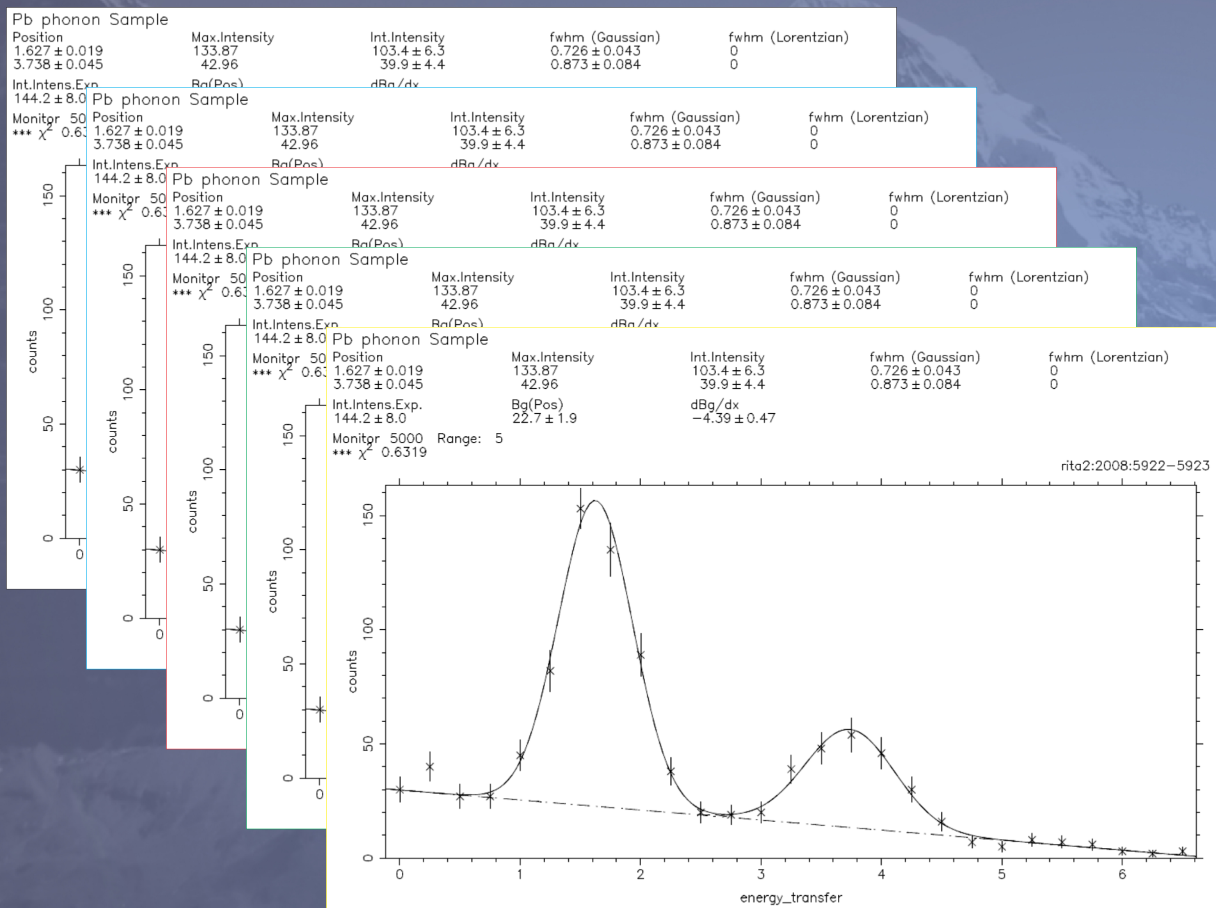

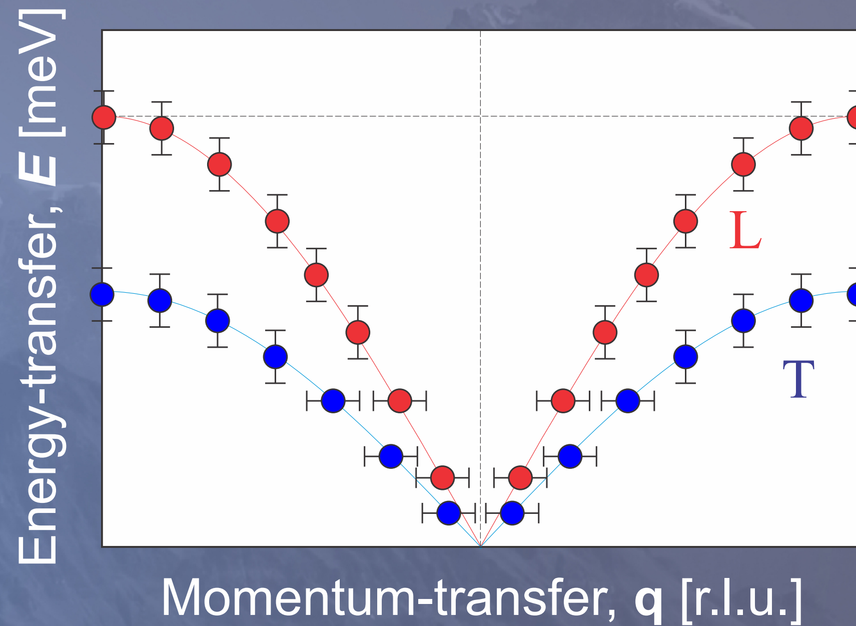

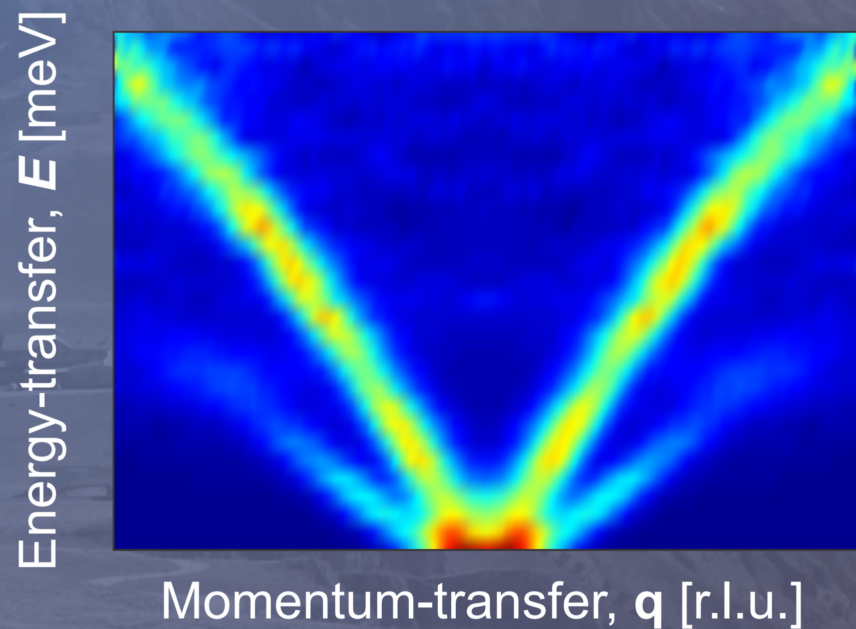

- **Online data analysis is made in 1 minute while scanning next point. Full analysis is done in 1 hour/spectra. Total data volume 100 kbyte acquired in 5 days (magnetic).**

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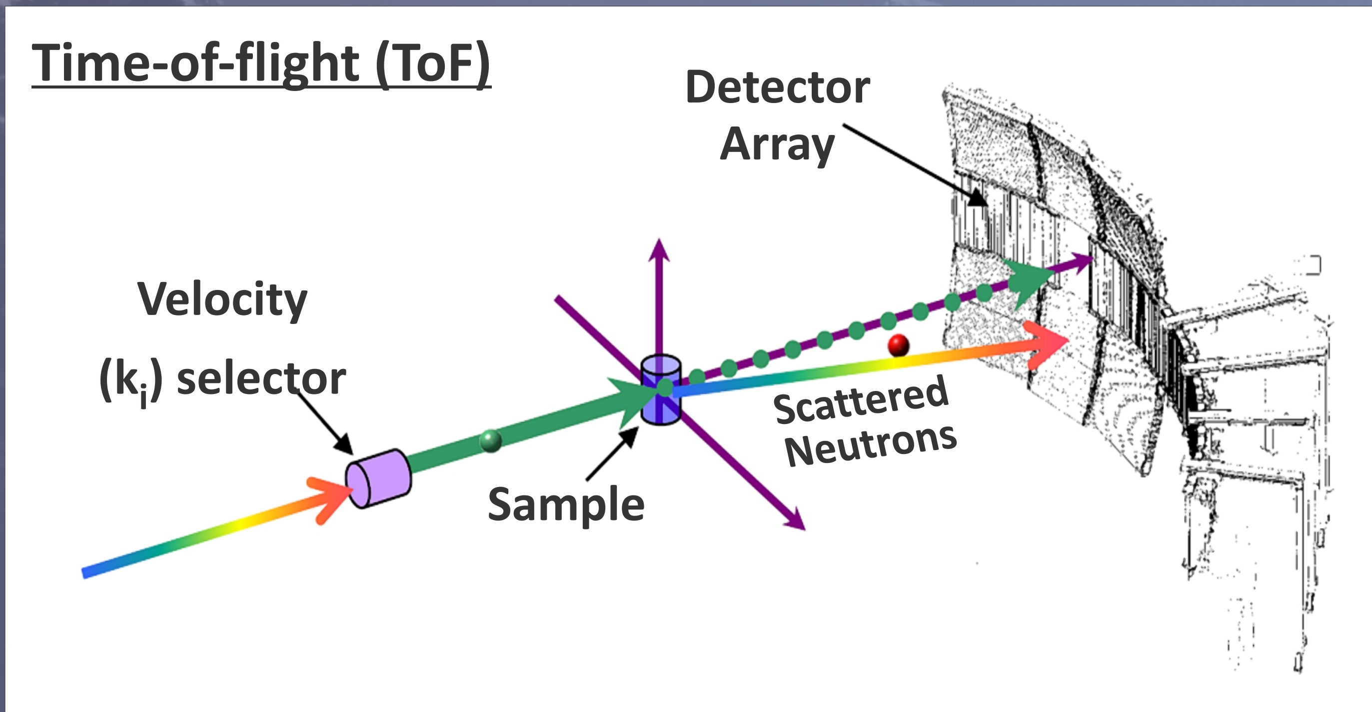
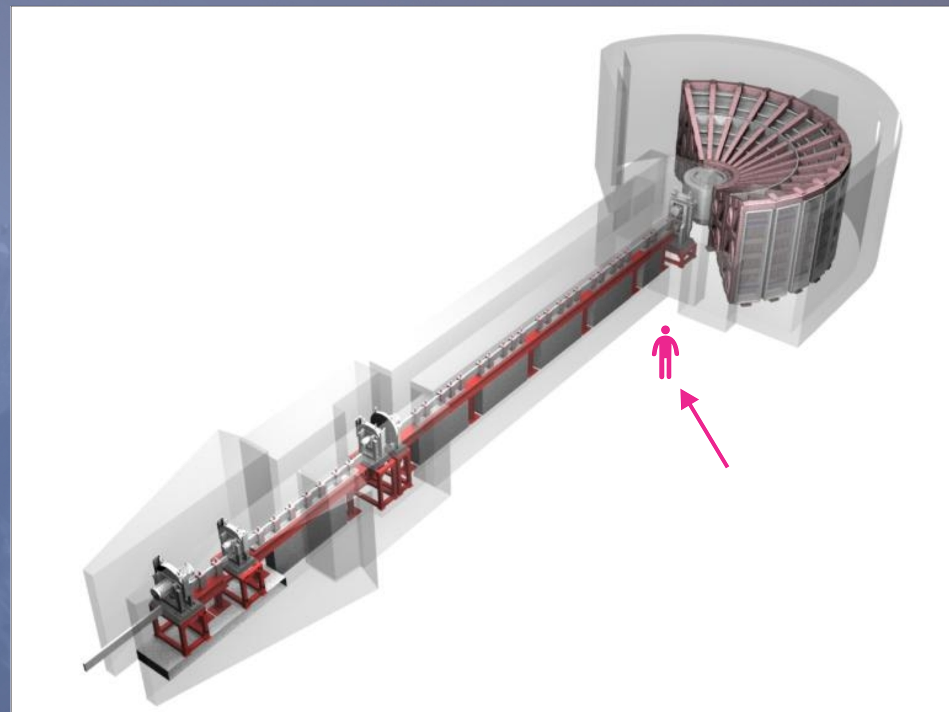
Modern INS: Time-of-Flight (ToF)

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





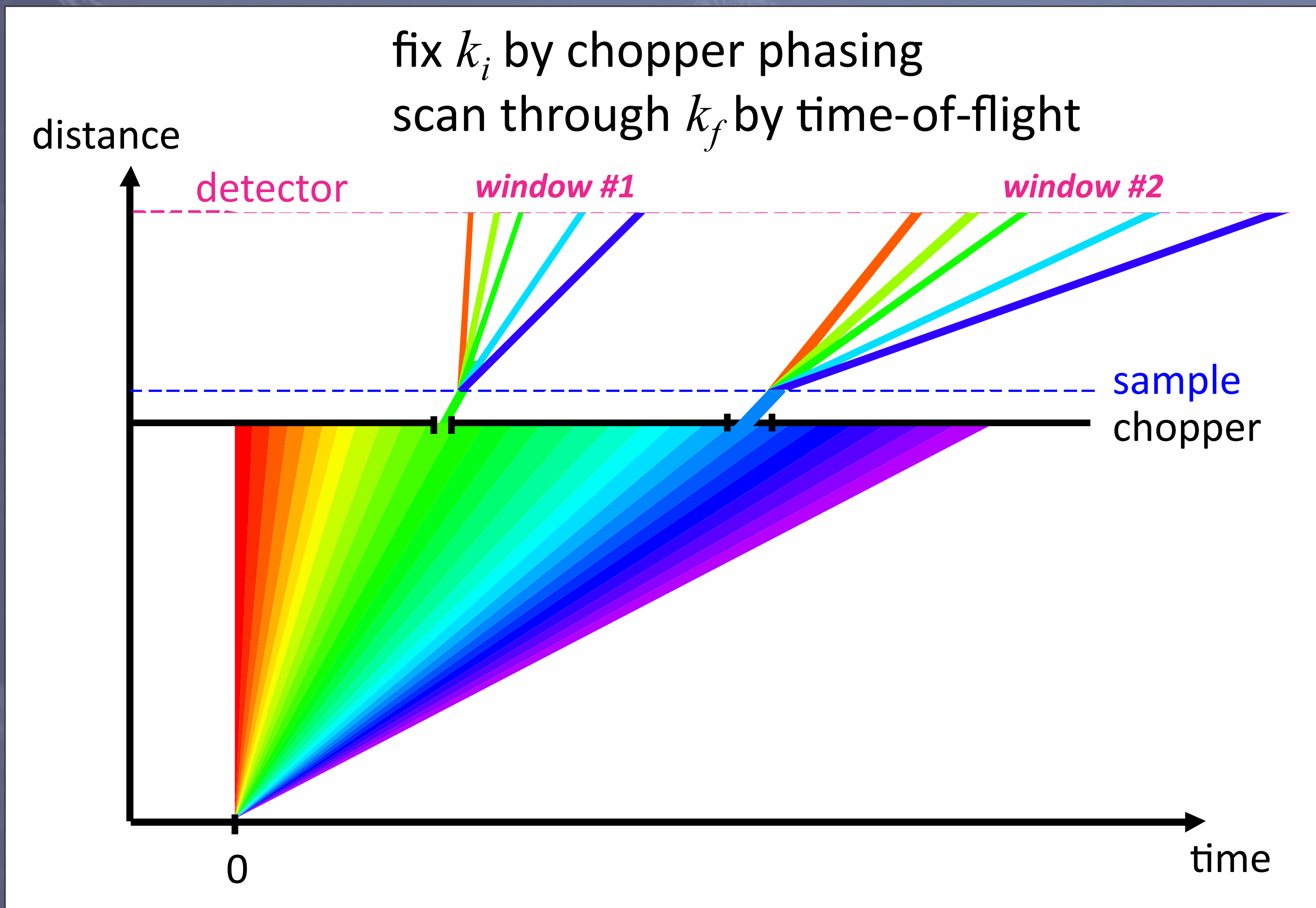
- Data come out as a 3D/4D matrix with a huge number of measured Q-points (qx, qy, qy). Each point is also resolved in energy-transfer... and H, T, E, P !!!

- Raw data files are 100 GB or even several TB

- Data collection can be a few days,while data analysis months or even years (do the experiment then the PhD project).

Modern INS: Time-of-Flight (ToF)

- 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).



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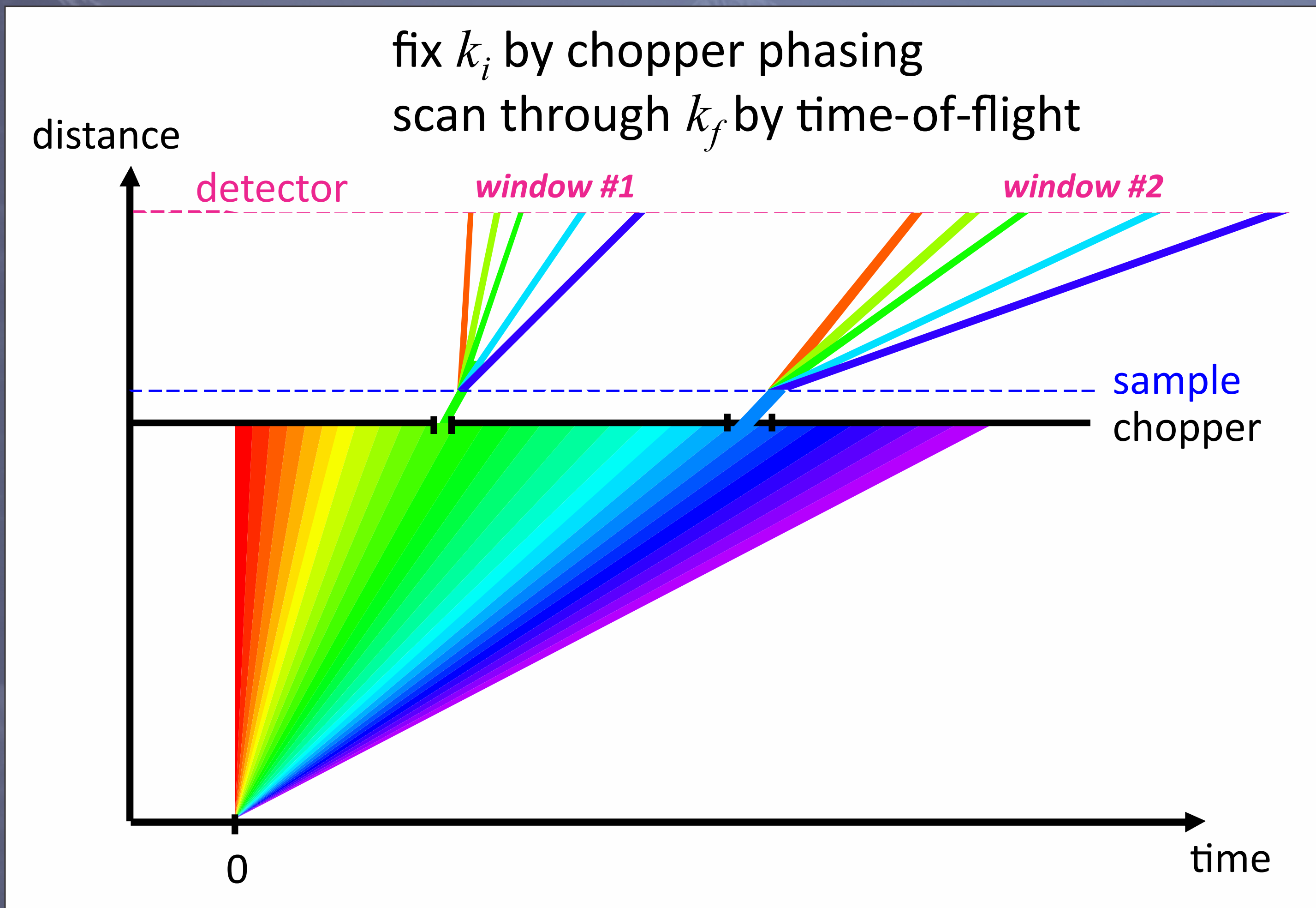

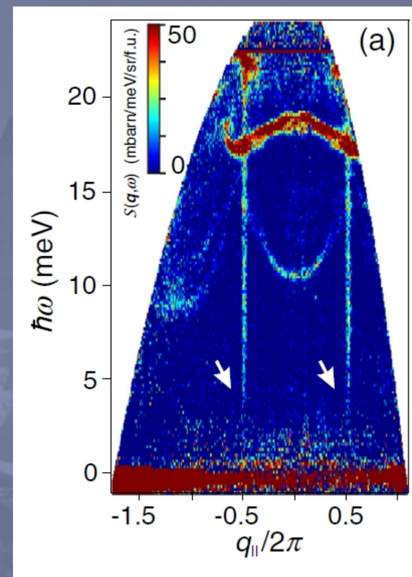

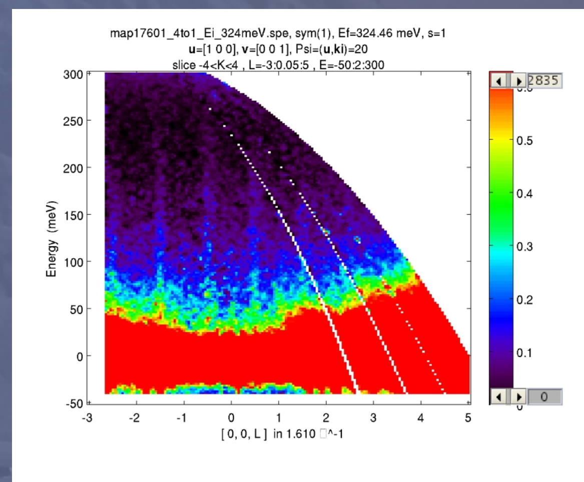

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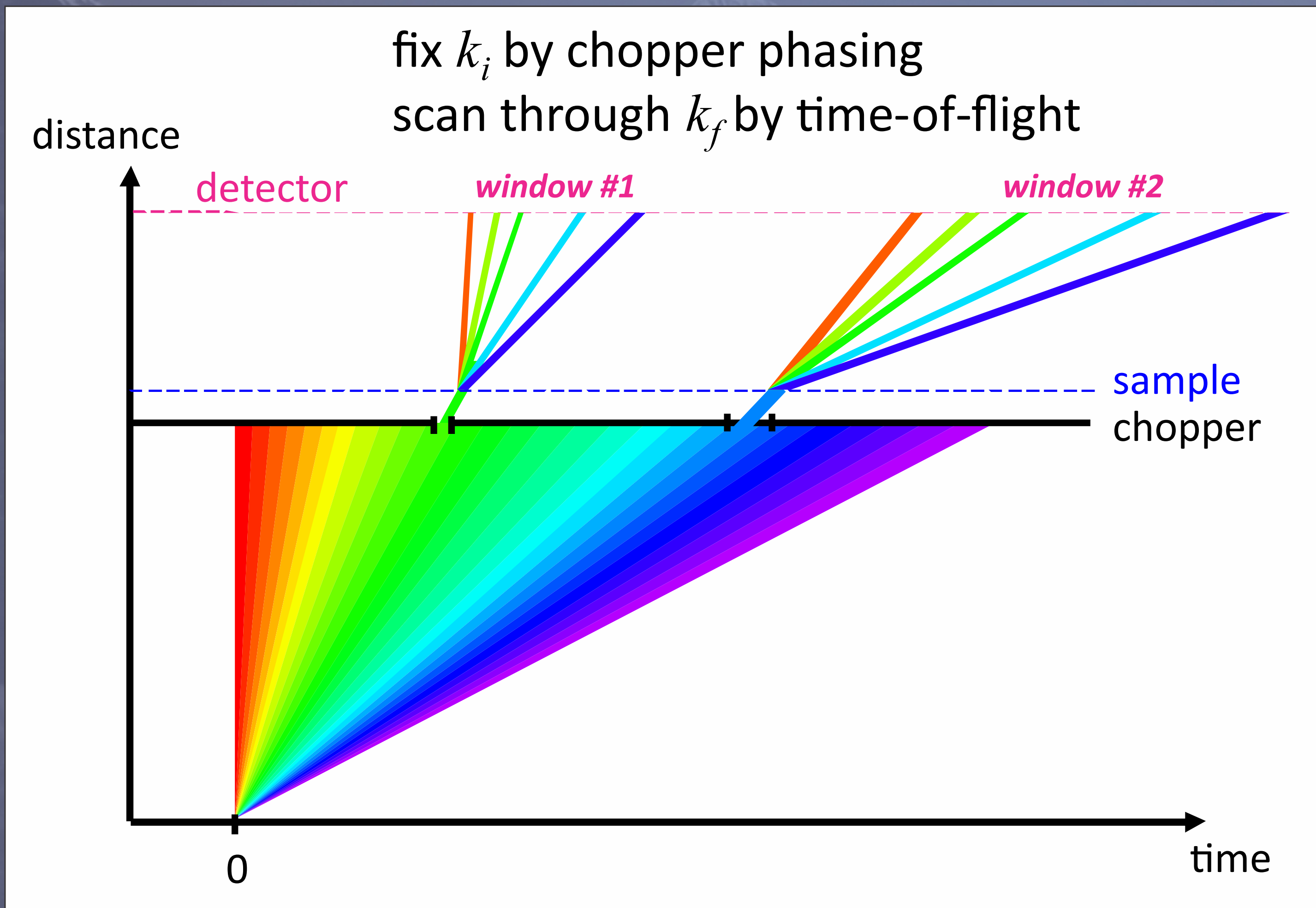

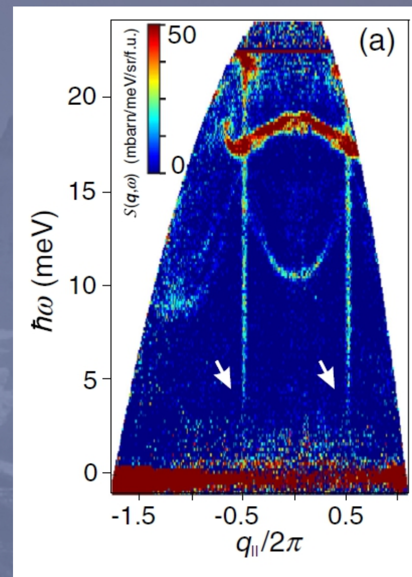

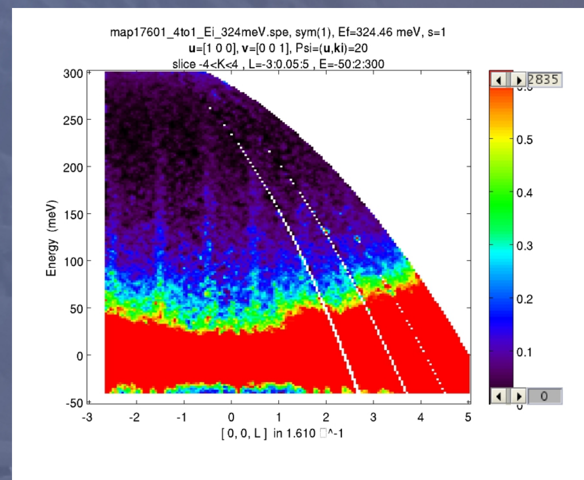

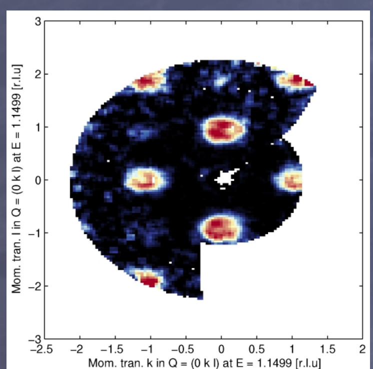

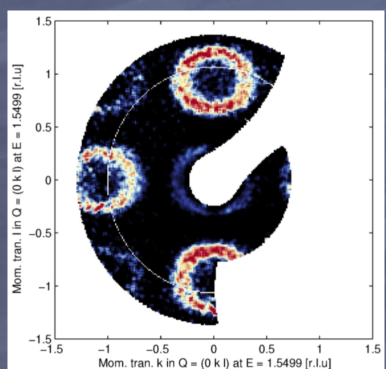

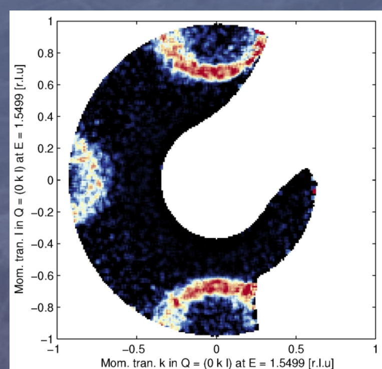

- **Very efficient use of produced neutrons (much larger fraction of scattered neutrons are collected/counted (i.e. data).**

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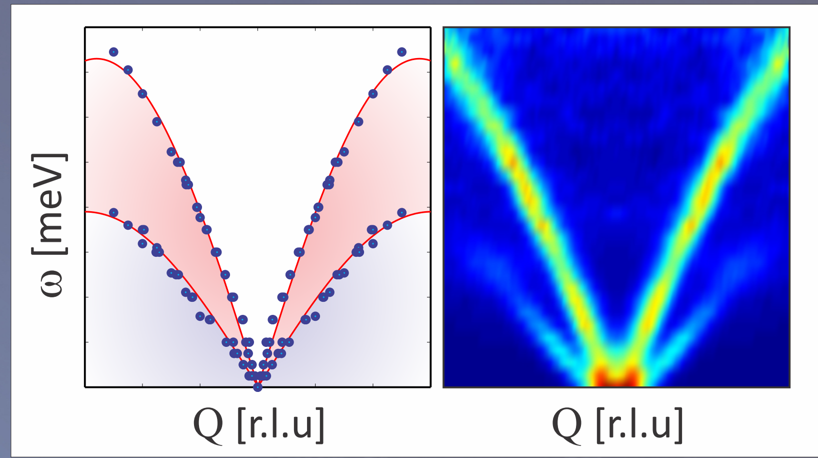
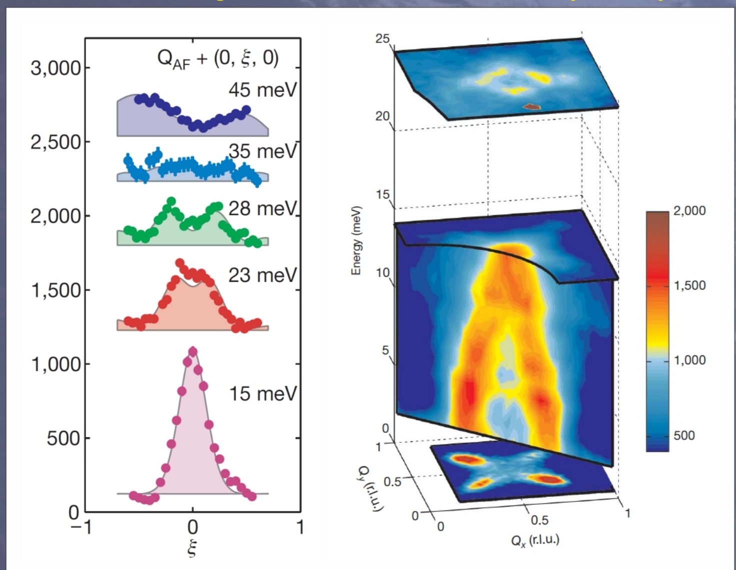
INS - Examples

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)



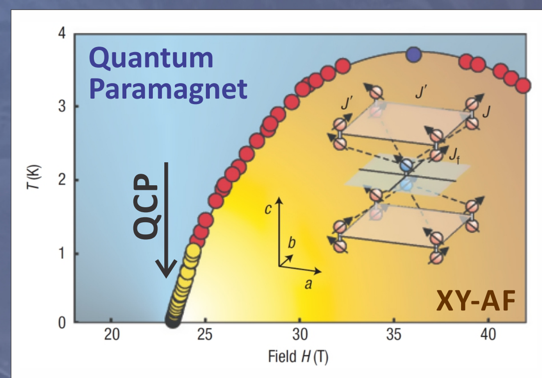
Boothroyd, Nature 471, 341 (2011)

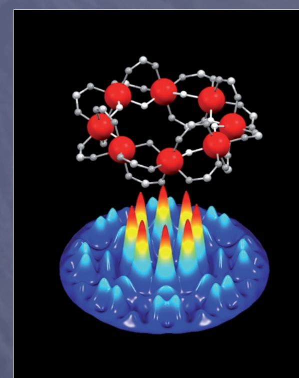


HIGH-TEMPERATURE SUPERCONDUCTIVITY

- 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)

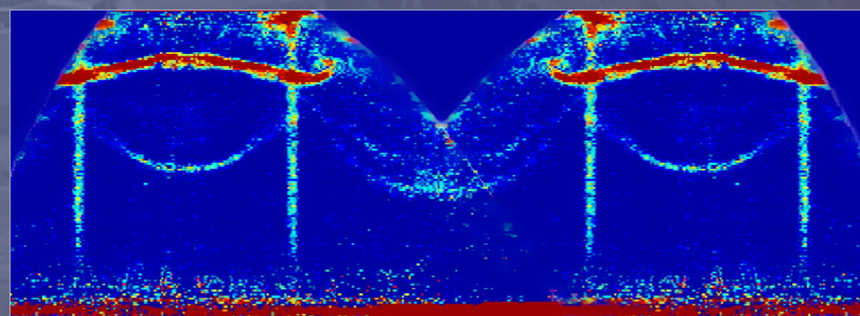
GIAMARCHI, Nature Physics 4, 198 (2008)





MAGNETISM

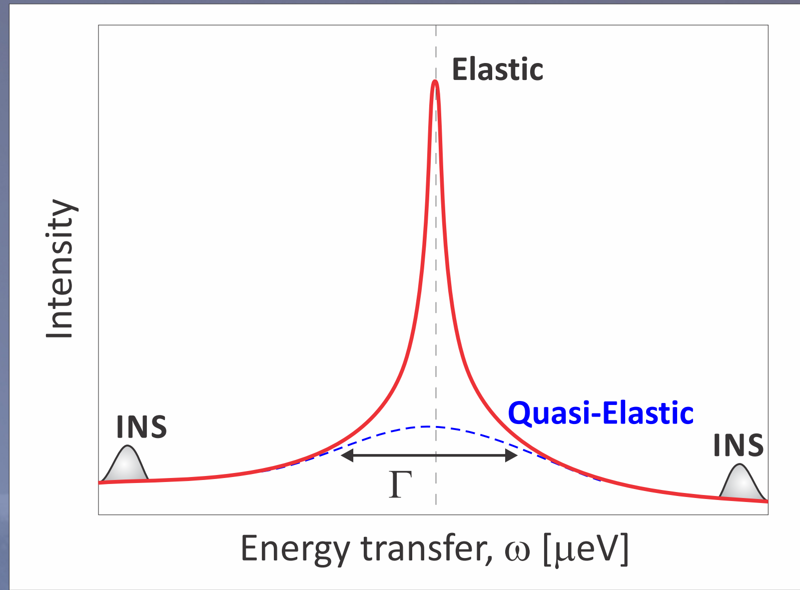
- **Spin-wave/magnon** mapping in exotic magnets (triangular frustration, square lattice AF etc.)
- Induce magnetic order by pressure, external field (**Bose Einstein Condensation and QCP** in quantum/molecular magnets).
- Destroy magnetism by *e.g.* creating **disorder** (defects,doping) → opening of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



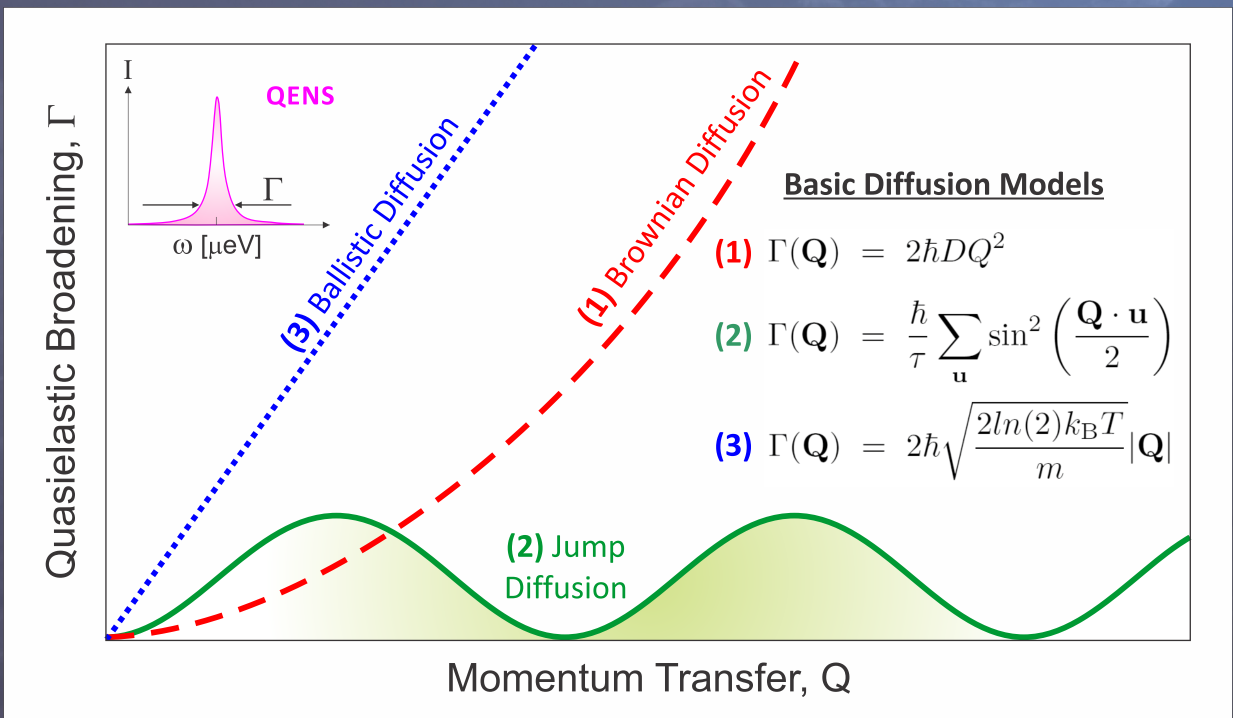
Simutis, Phys. Rev. Lett. 111, 067204 (2013)

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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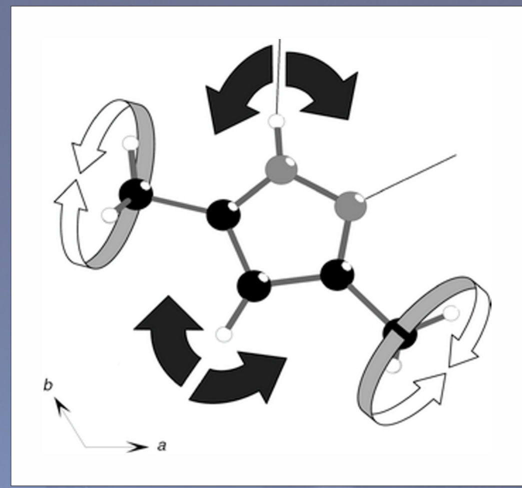
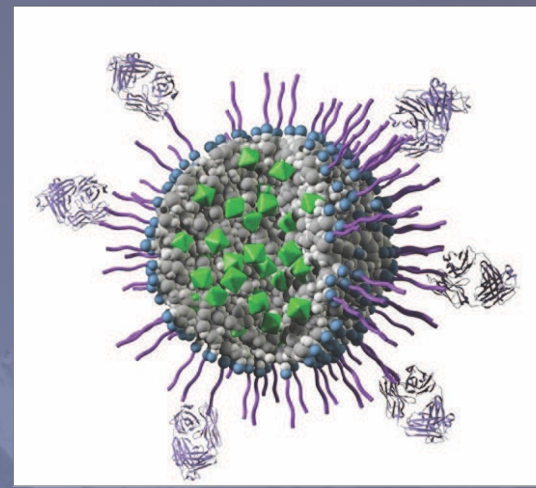
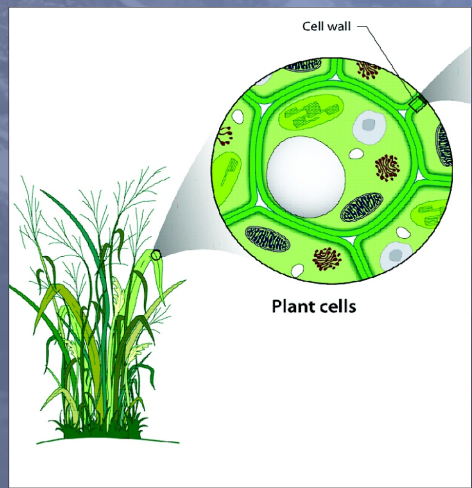
QENS - Examples

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

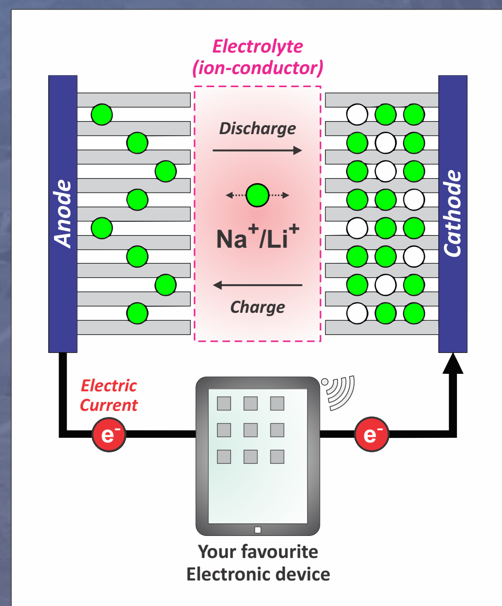


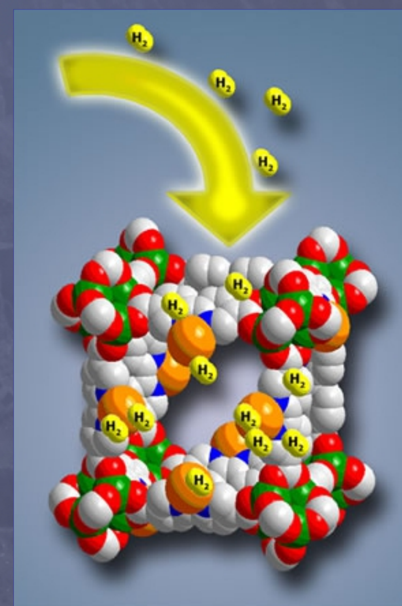




- **Fluid dynamics:**
  - Confined liquid *e.g.* water in wood/plants
  - Complex liquids and clays
  - Melting processes (*e.g* ice/water)

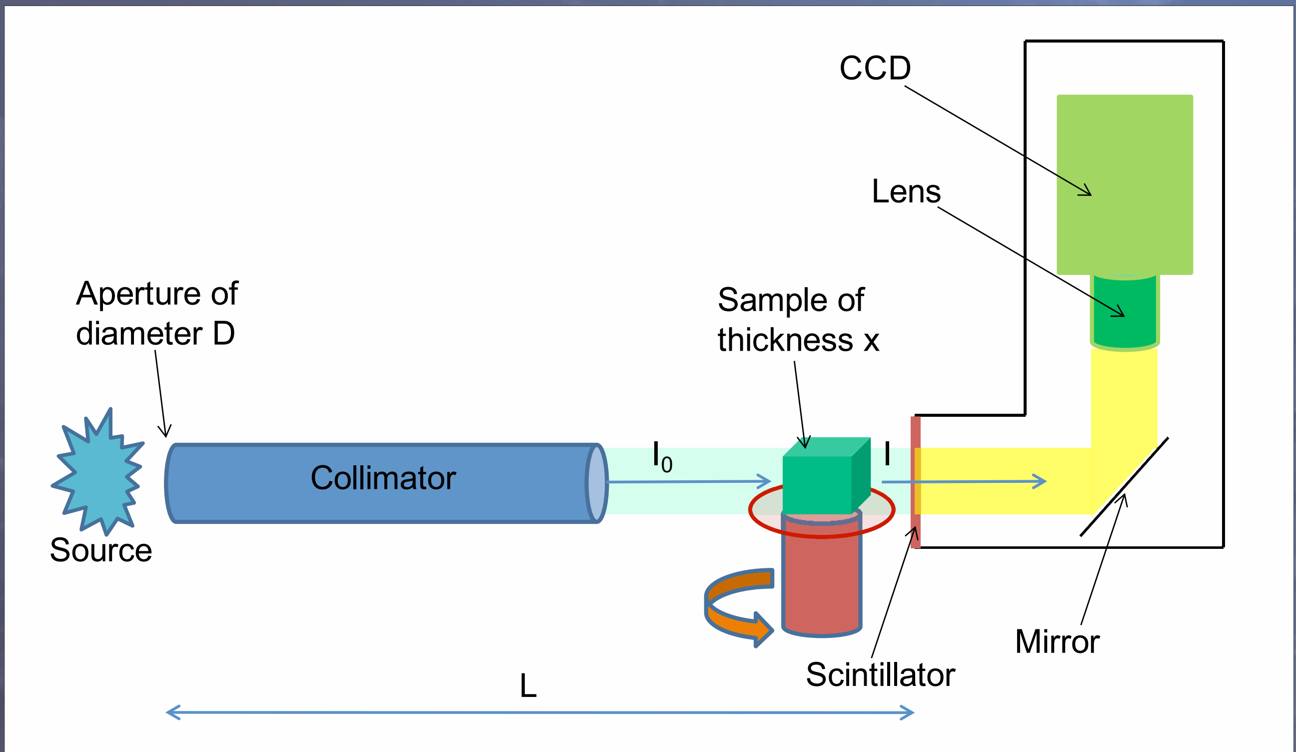
- **Energy materials:**
  - Li/Na diffusion in rechargeable batteries
  - Ion-diffusion in solid electrolytes (fuel-cells)
  - Hydrogen ad-/de-sorpion for H-storage
  - Catalysis reactions





Neutron Imaging

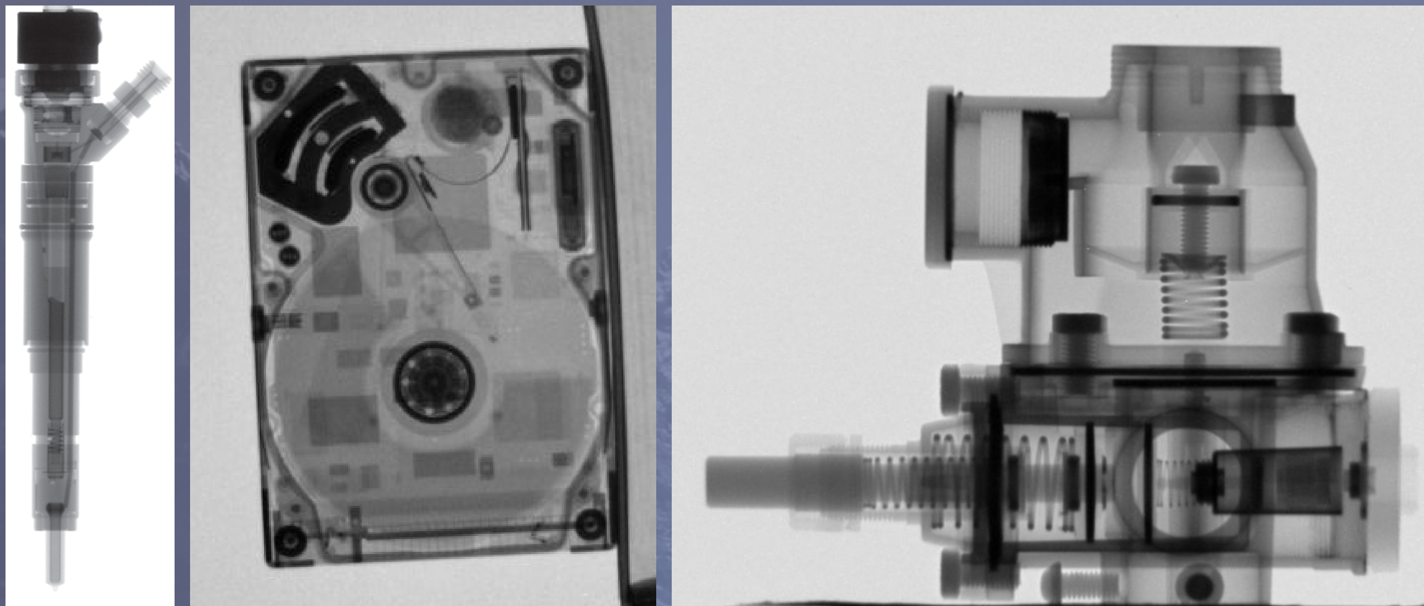
- Similar to an X-ray radiography but technically not a scattering technique
- The resulting image is based on the neutron attenuation properties of the different parts of the imaged object.
- Provide information about the composition and the amount of structure in the sample and changes in them (defects, 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.



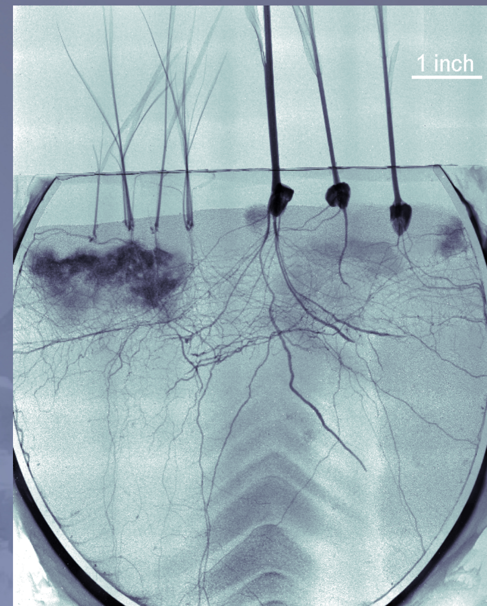
- Modern CCD cameras allow high-resolution on μm scale
- Stroboscopic measurements allow to study slow dynamics
- Possible to make tomography to obtain a 3D image of the object's internal structure
- Non-destructive testing of large objects!

Neutron Imaging - Examples

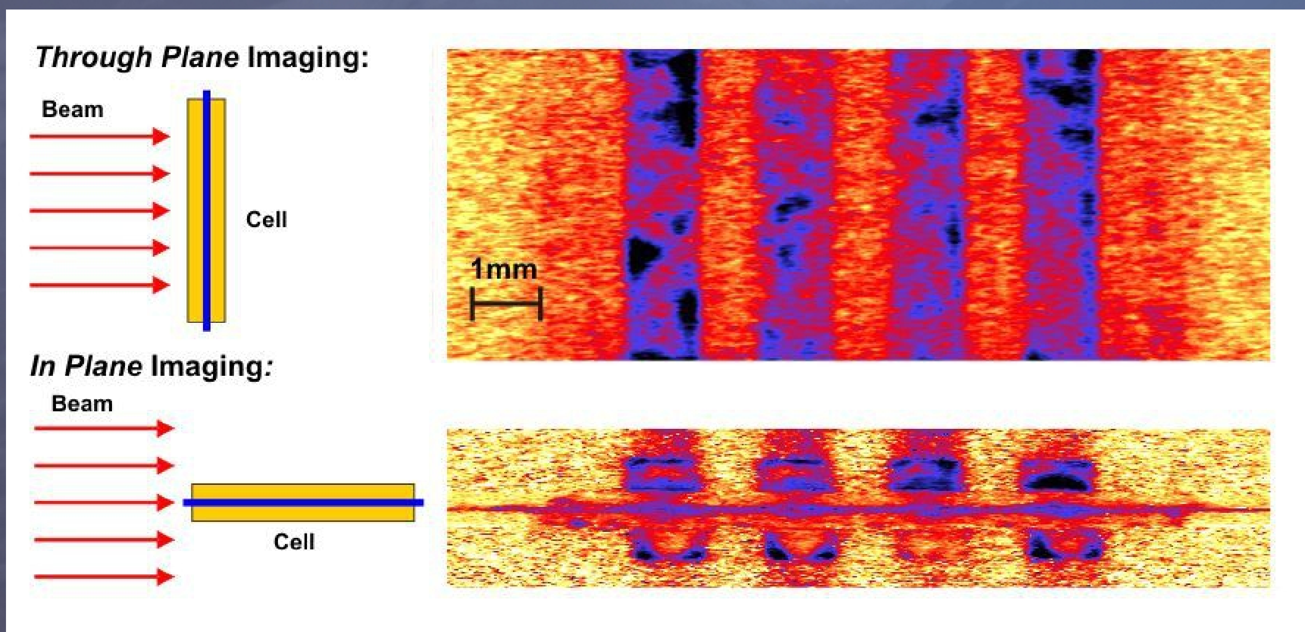
Non-destructive testing of mechanical components



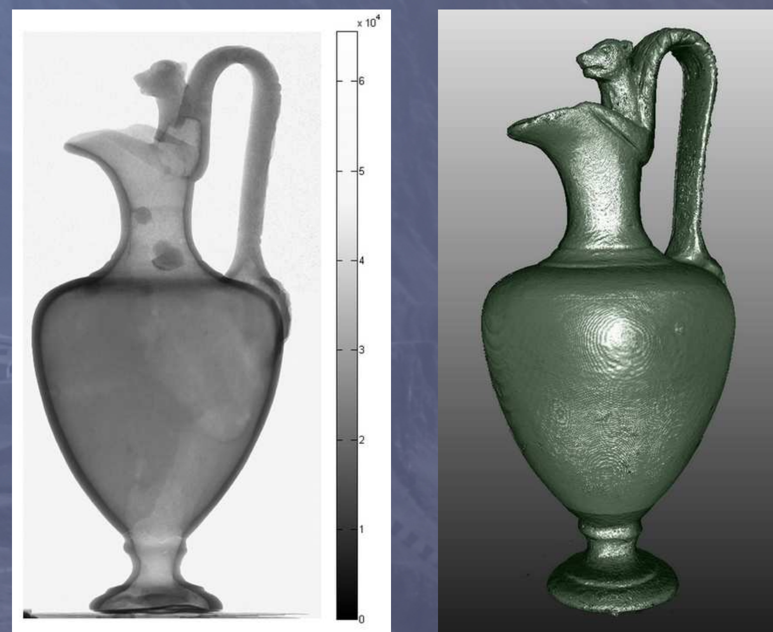
Root-system of plants



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



Radiography / Tomography of archeological artefacts



Neutron Sources of the World

EUROPE

ILL, Grenoble, France
ISIS/RAL, UK
SINQ, PSI, Switzerland
FRM-II, Germany

BER II, HZB, Berlin, Germany (closing !!!)
LLB, Saclay, France (closing 2019 !!!)
IFE, Kjeller, Norway (closed !!!)

OTHER EXAMPLES

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

UNDER CONSTRUCTION

Lund, Sweden — EUROPEAN SPALLATION SOURCE

Dongguan, China — SNS

http://www.neutrons.se/

http://www.neutronsources.org/

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

European Spallation Source (ESS)

- European flagship project with 15 participating countries.
- Sweden and Denmark were selected as host countries 2009.
- Sweden host the actual source and Denmark the data management center.

- Construction cost: 1843 M€ with SE 37.5% / DK 12.5% (+ operations costs)
- First neutrons expected 2022 and user operation 2023 (full 2025)

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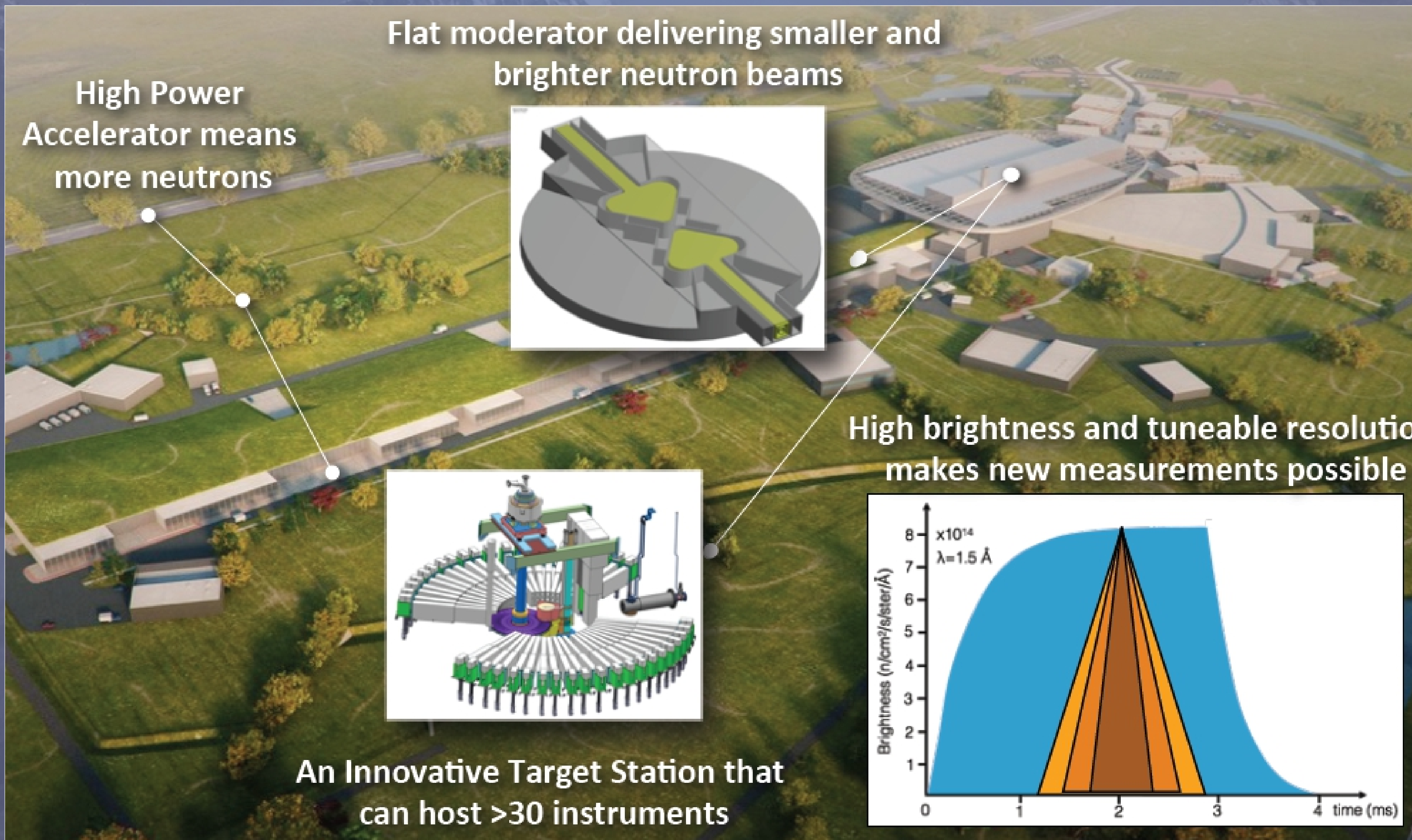

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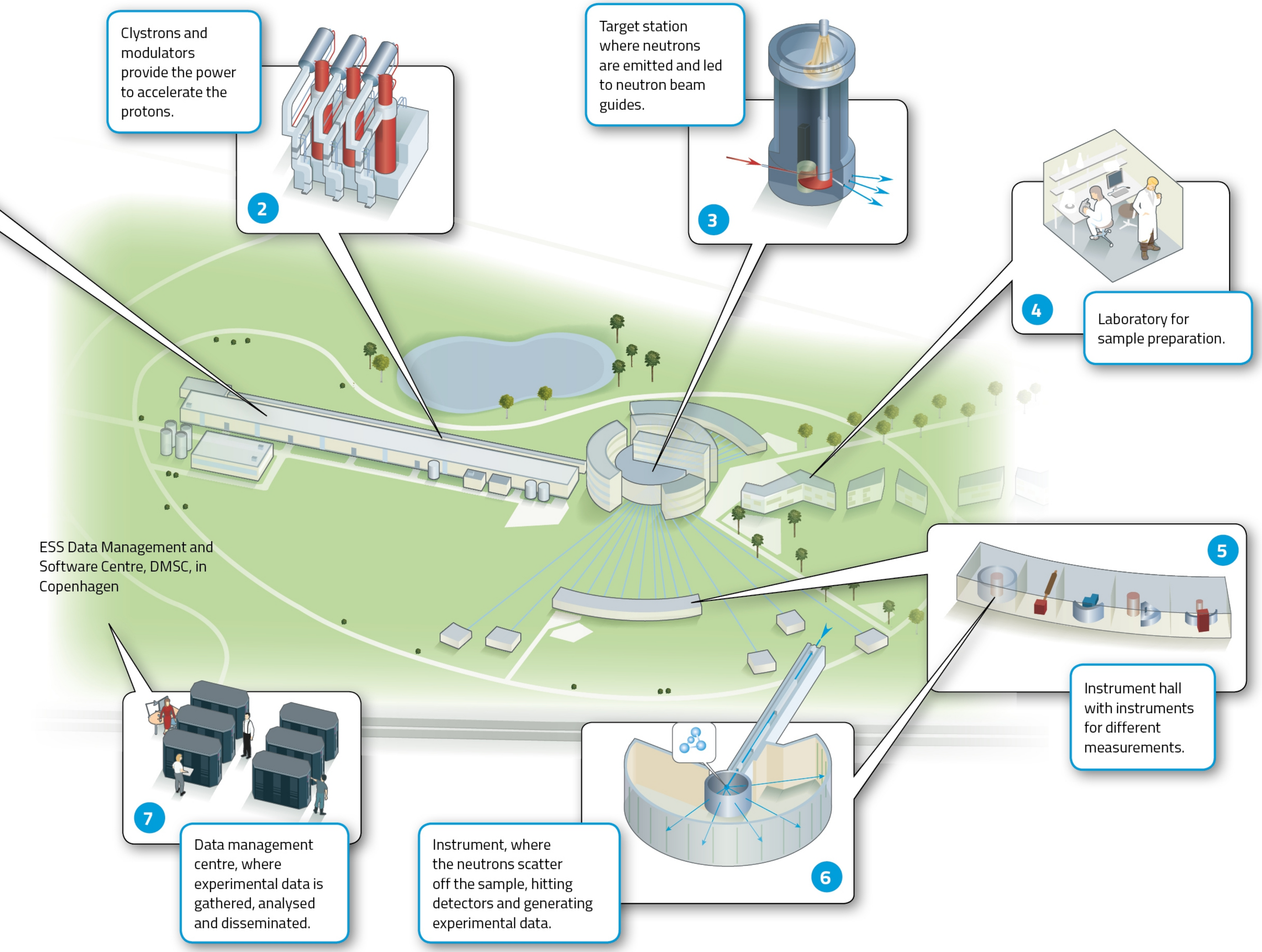
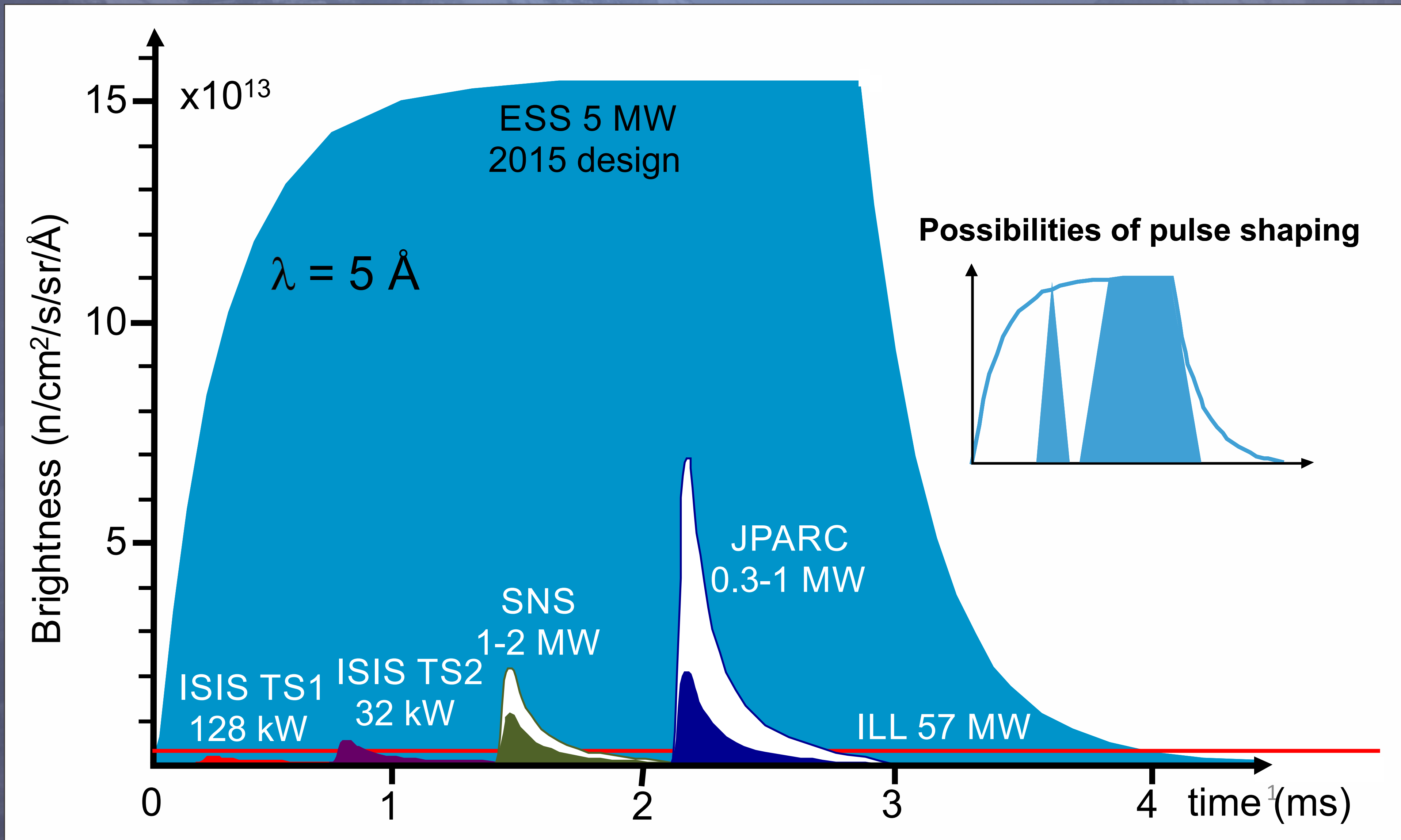
Unique Technology = Next Gen.



- Not a "copy" of competing sources (SNS/USA, J-PARC/Japan) and a state-of-the-art technological development is being performed

ESS Pulse

- Pulsed source with unique long (3 ms) time structure.
- Highest brightness in the world + highest average neutron flux.
- Flexible by using choppers to shape the pulse.



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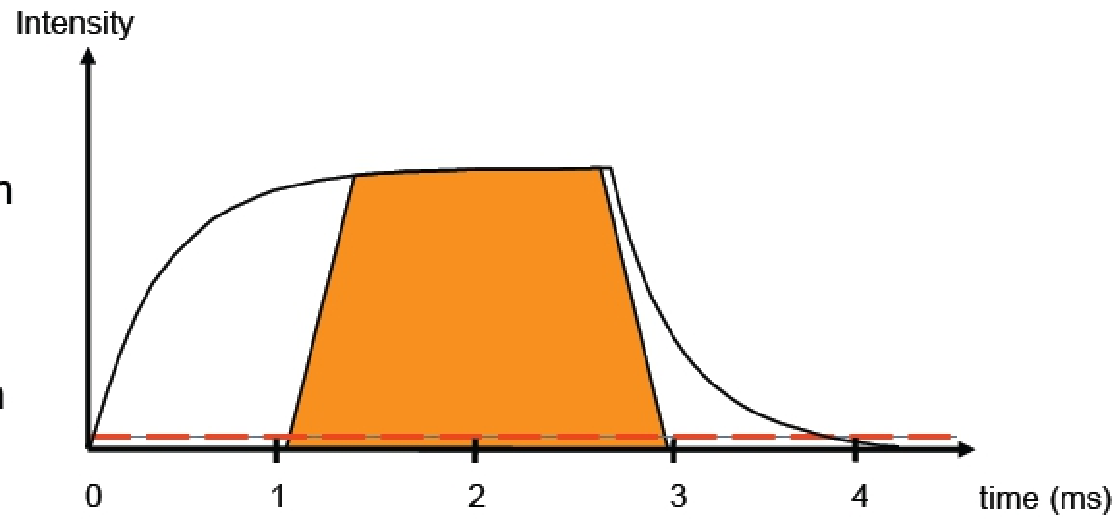
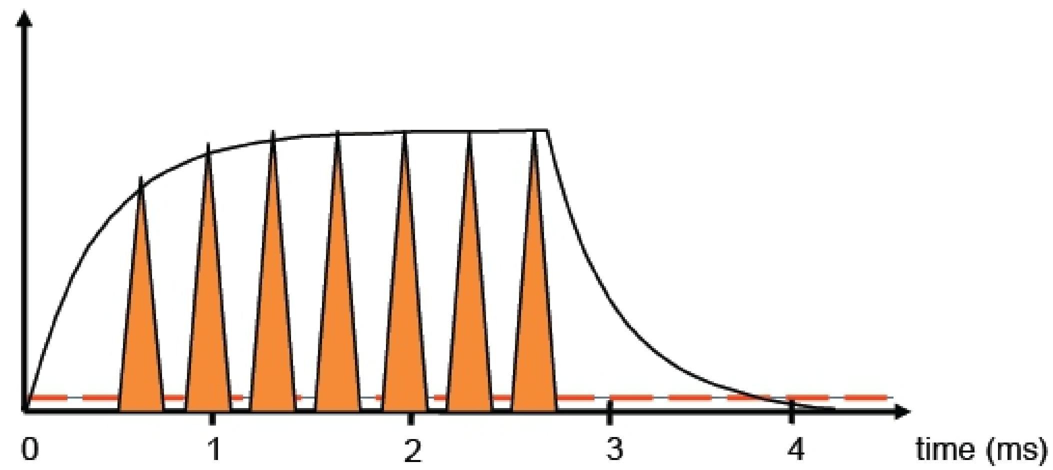
Two Strategies for Neutron Instrumentation at ESS

Use as much as possible of the whole pulse:
Good for low wavelength resolution instruments.
SANS, Reflectometry, single crystal diffraction.
Estimated gains 10-100 times than currently available.

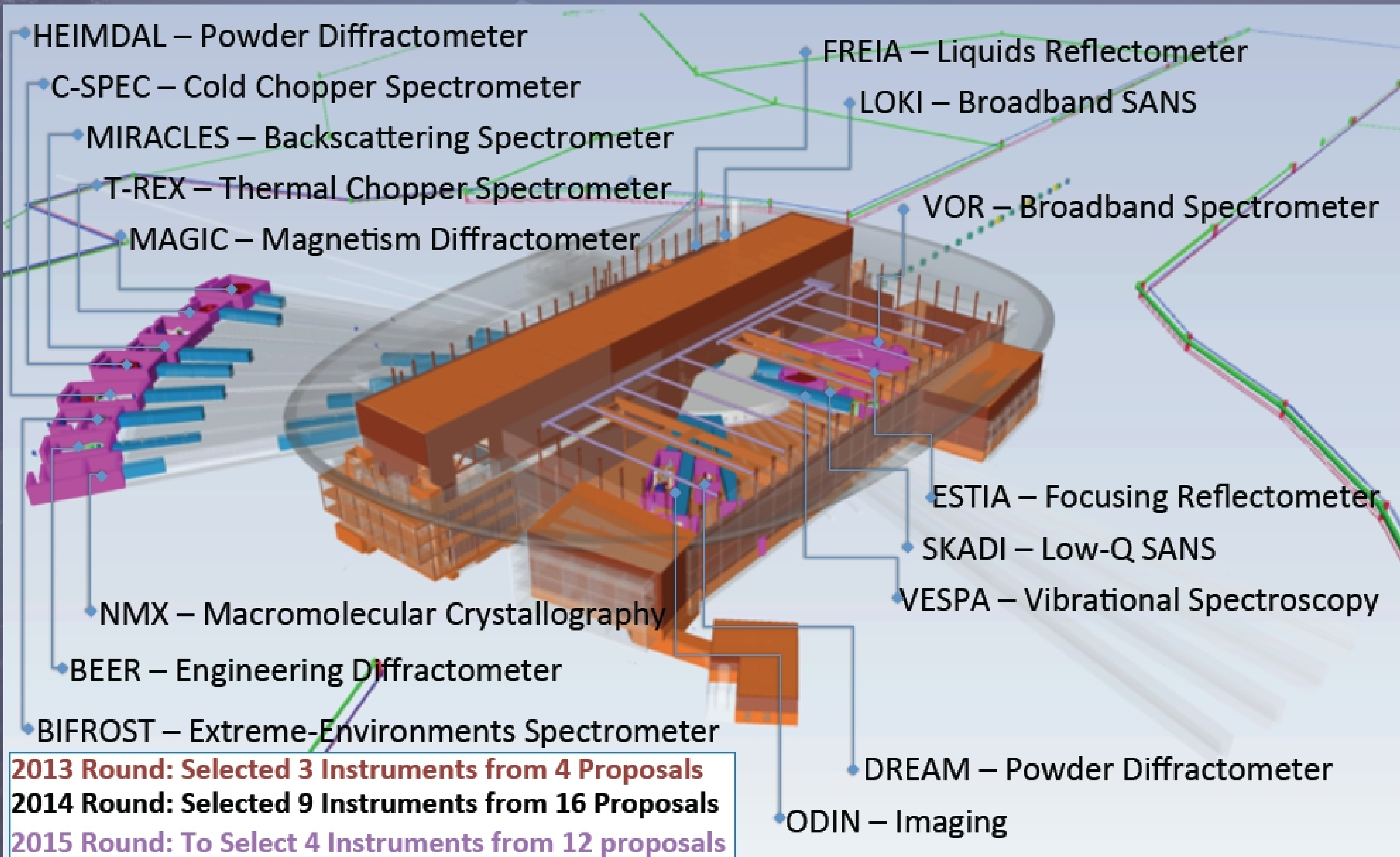


Cut the long pulse into smaller pulses:
Good for higher wavelength resolution instruments
Diffraction, cold/thermal spectrometers.
Long Instruments (80-100 m)
Estimated gains 10-30 times than currently available.
Thermal gains lower.

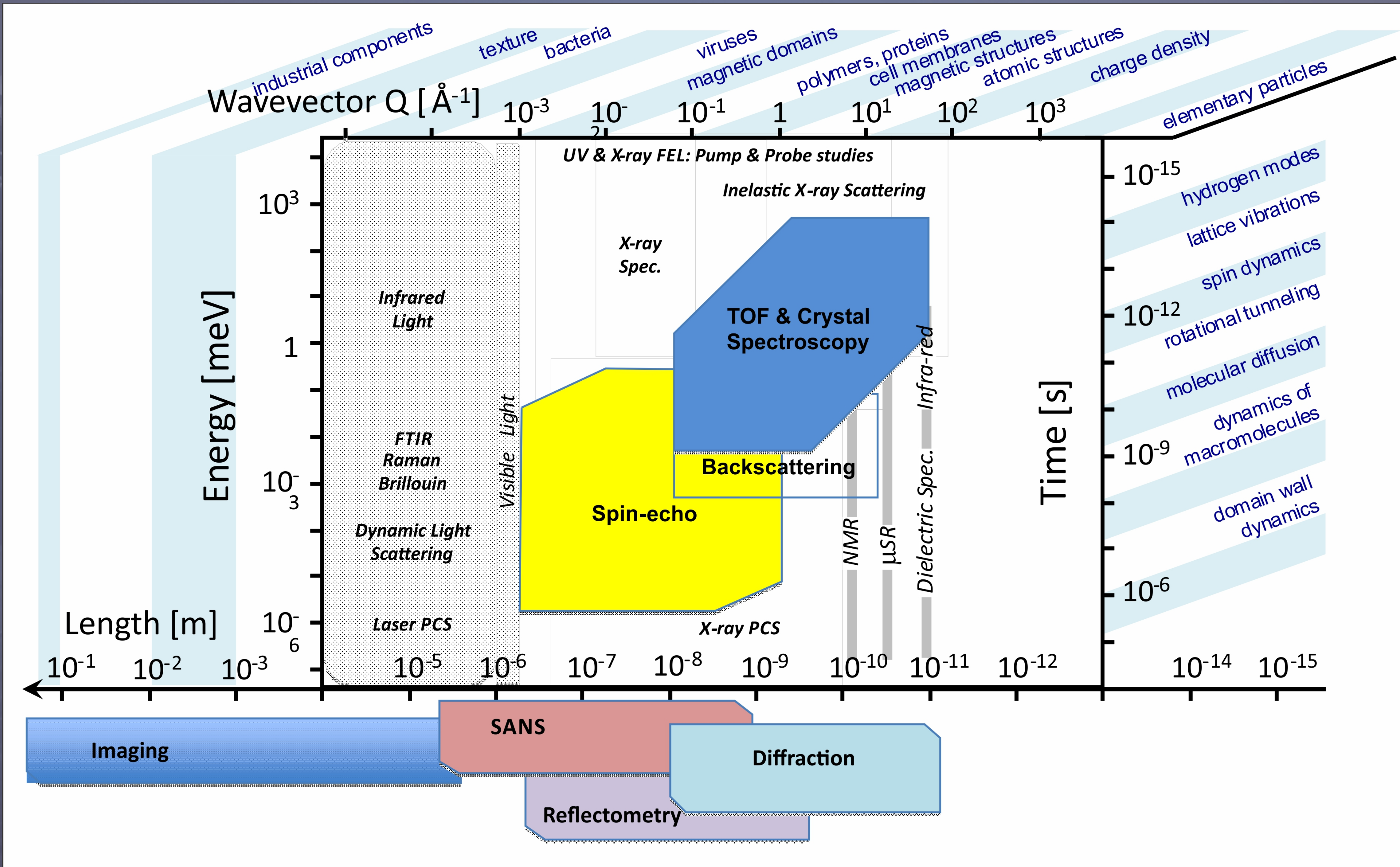


ESS: Instrument Suite

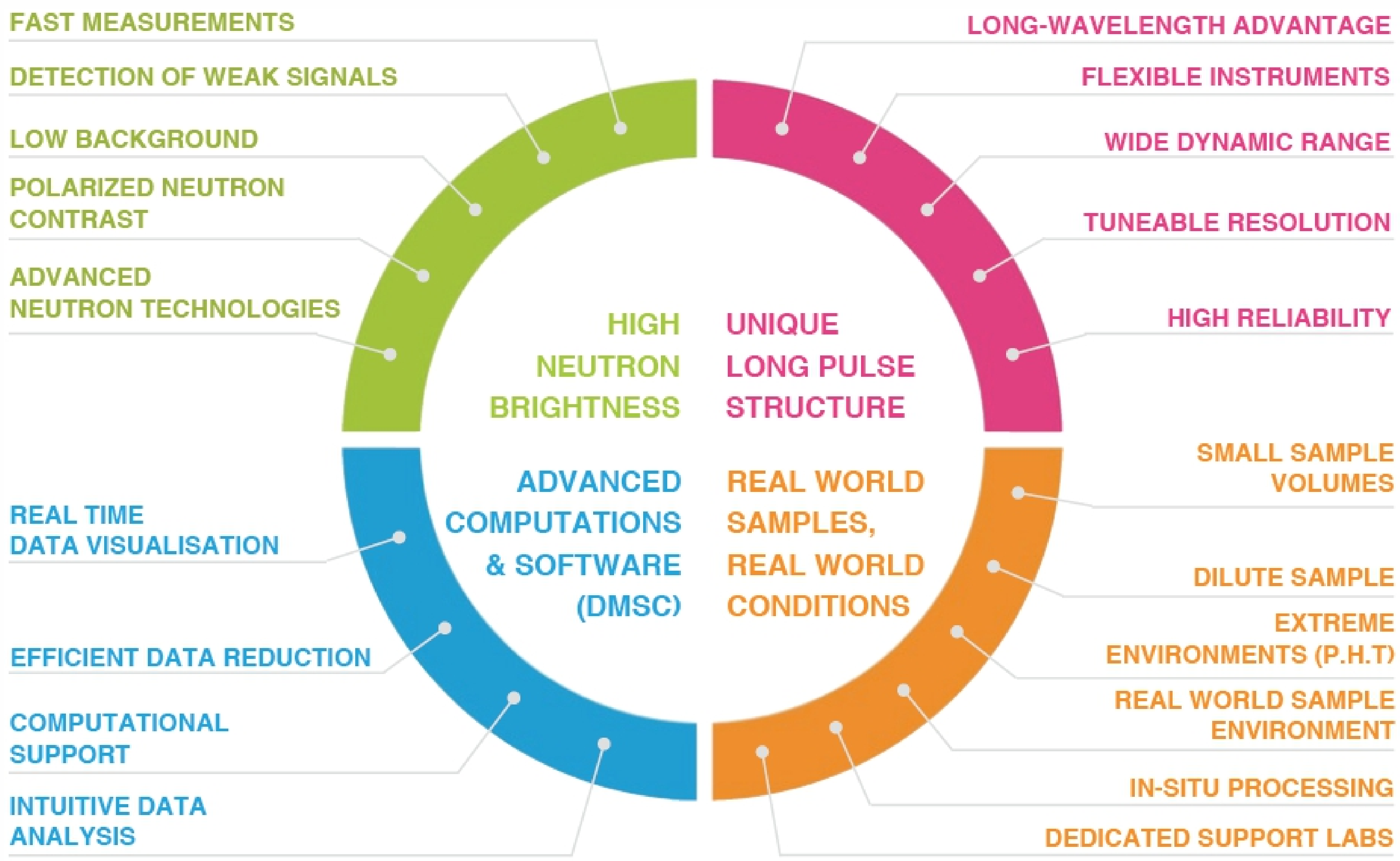
- First 15 (16) instruments have been decided already
- At least another 8 should be planned within the coming years...



ESS: Versatile Neutron Toolbox

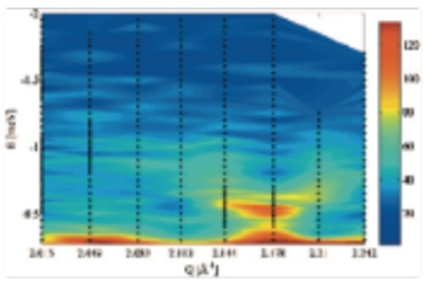
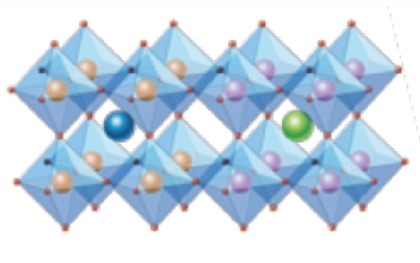
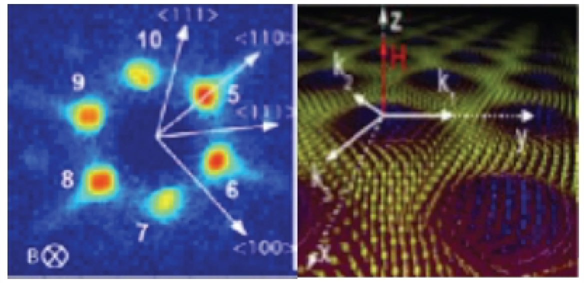


ESS: New Tech = New Possibilities



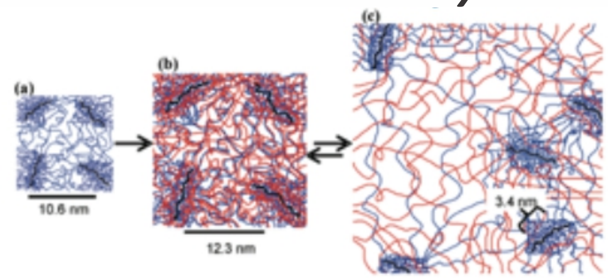
ESS: New Tech = New Possibilities

Complex Interfaces

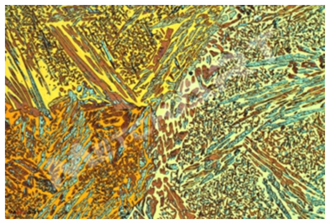




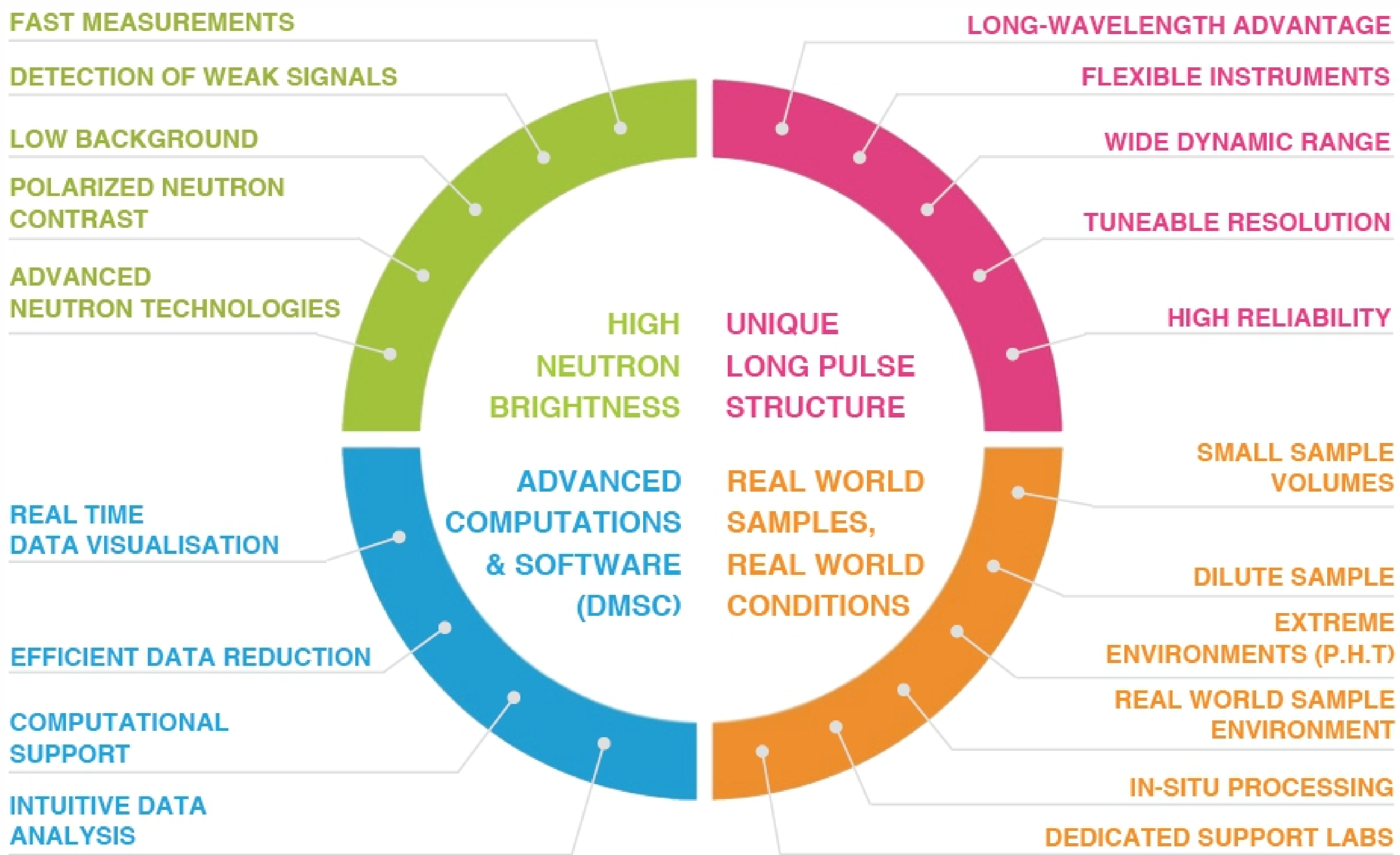
Charge and Spin transport

Multi-scale structure & dynamics

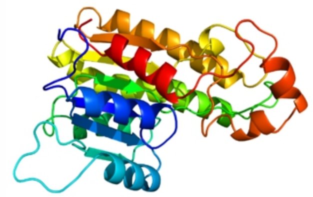


Advanced Engineering Materials

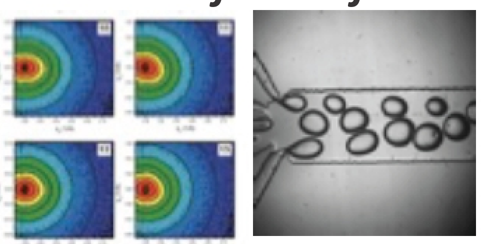



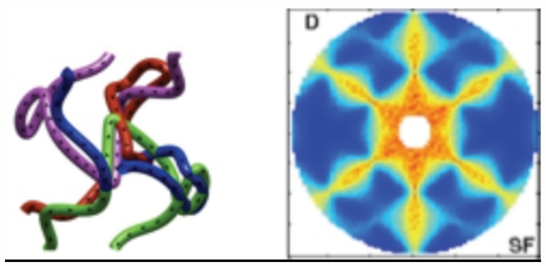



Life-Science



Kinetics of microfluids





New states of matter

In operando studies

Prof. Martin Månsson, KTH Royal Institute of Technology, condmat@kth.se

ESS Construction Phase

ESS Construction Phase

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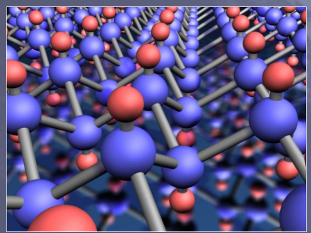
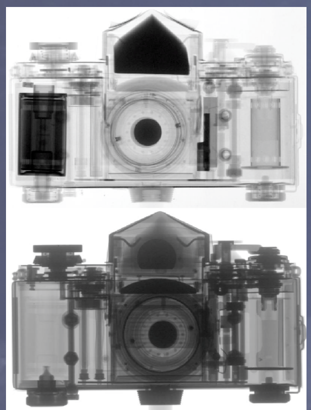
Neutrons & X-rays

- 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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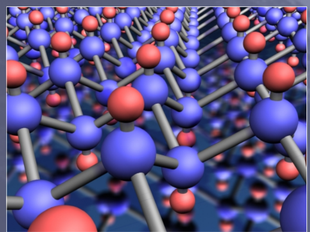

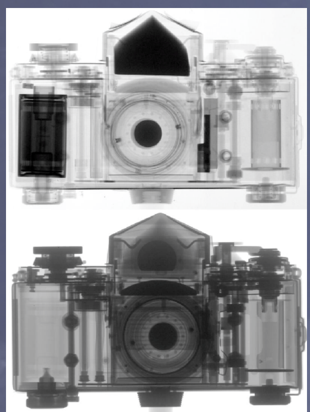

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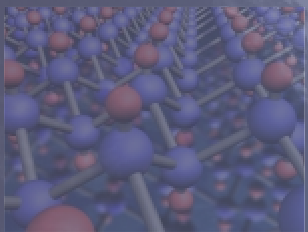

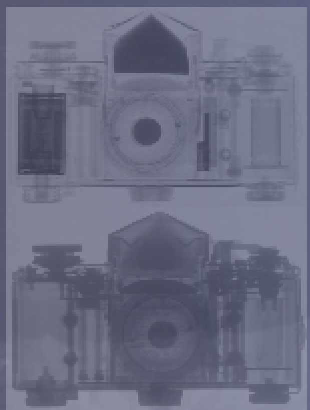

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- Contras ... aphy techniques.
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Swedish Beamline @ PETRA III

Neutrons vs. X-rays

NEUTRONS	X-RAYS
Low Intensity	High Intensity
Slow Measurement	Fast Measurement
Bulk properties	Not always bulk properties
Extreme Conditions /In operando	"Difficult"
No beam damage	Potential beam damage (bio/organic)
Access to light elements Isotope Sensititive / Labelling	No access to light elements or Isotope labelling (especially H/D)
Better energy resolution	Worse energy resolution
Direct access to magnetism	No direct access to magnetism
Difficult to manipulate beams	Easy to manipulate beams

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!)

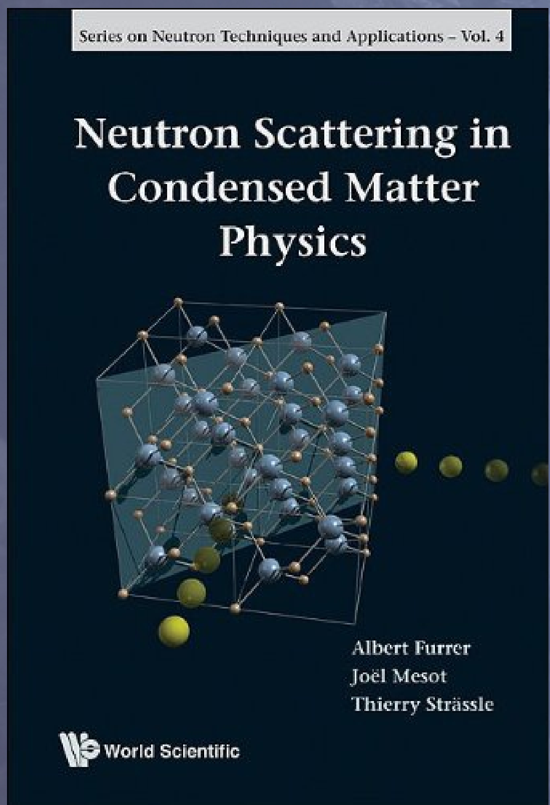
Neutron References

Swedish Neutron Scattering Society
www.snss.se

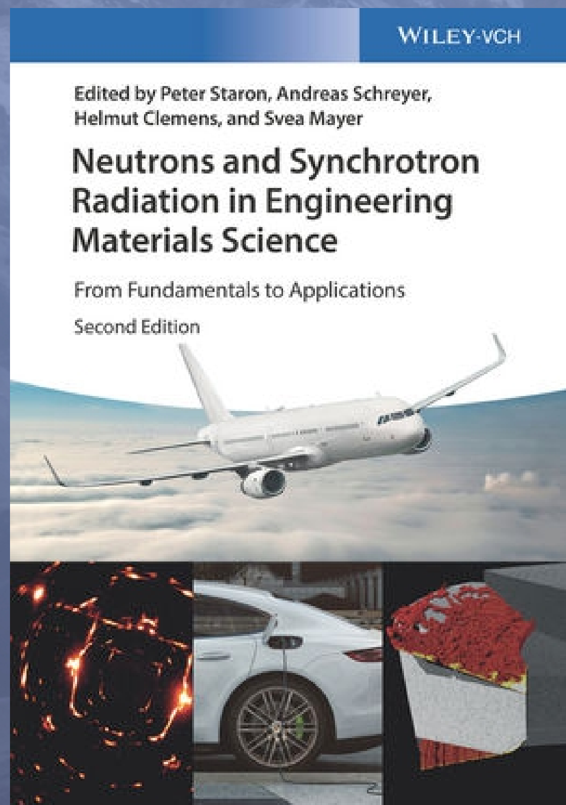
http://www.SNSS.se/

http://www.SwedNess.se/

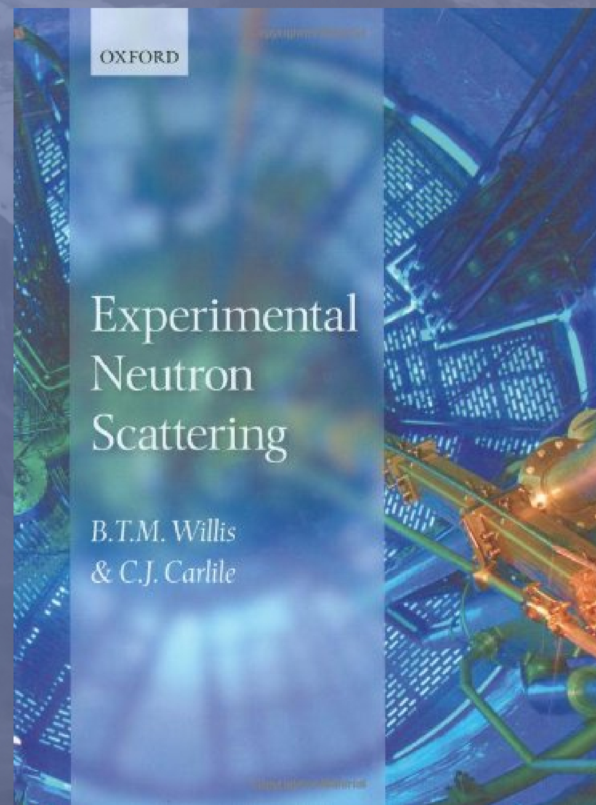
Lecture series given by Prof. Roger Pynn, Indiana University, USA
https://www.indiana.edu/~sesame/WebSite/TeachingResources.html



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



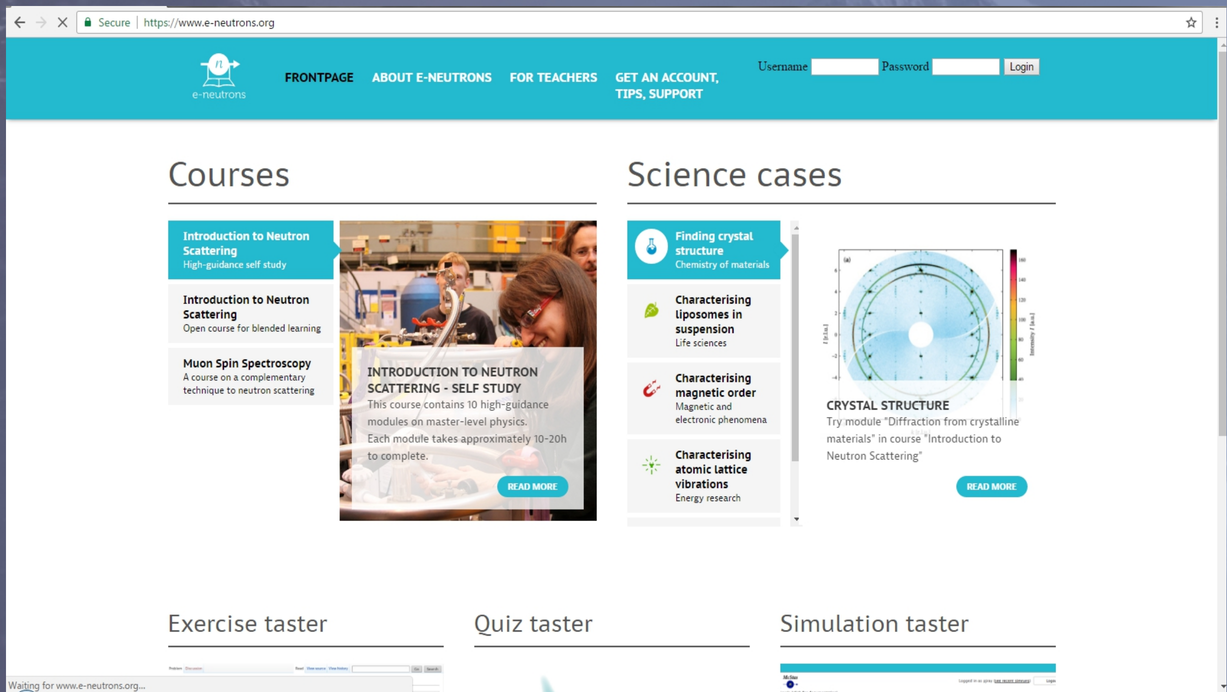
"Neutrons and Synchrotron Radiation in Engineering Materials Science"
P. Staron, A. Schreyer, H. Clemens & S. Mayer



Experimental Neutron Scattering
Willis and Carlile

e-Learning for Neutrons

- As a complimentary tool e-learning could work very well together with traditional lectures and exercises.



- Already existing initiative that includes both preparatory work, virtual neutron instruments etc.

e-neutrons.org

- Assoc. Prof. Linda Udby, Niels Bohr Institute Copenhagen, Denmark

- Will also adapt/extend the platform for NNSP/SwedNess
- Such development will be there also for future generations (SwedNess contribution/funding under discussion)
- Denmark, Norway and Sweden are currently working together to develop Tartu + e-neutrons into a Massive Open Online Course (MOOC).

Conclusions

- Neutron scattering is the most versatile & poweful experim. techniques 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 **2023**.
- 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 !!!
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