EUROPEAN SPALLATION SOURCE

Neutron Science at ESS

A. Hiess

European Spallation Source AB
Neutron Science Division
Lund, Sweden

outline

- Neutrons as a tool for science
- Unique ESS capabilities
- Neutron Scattering Systems and Neutron Science

EUROPEAN SPALLATION SOURCE

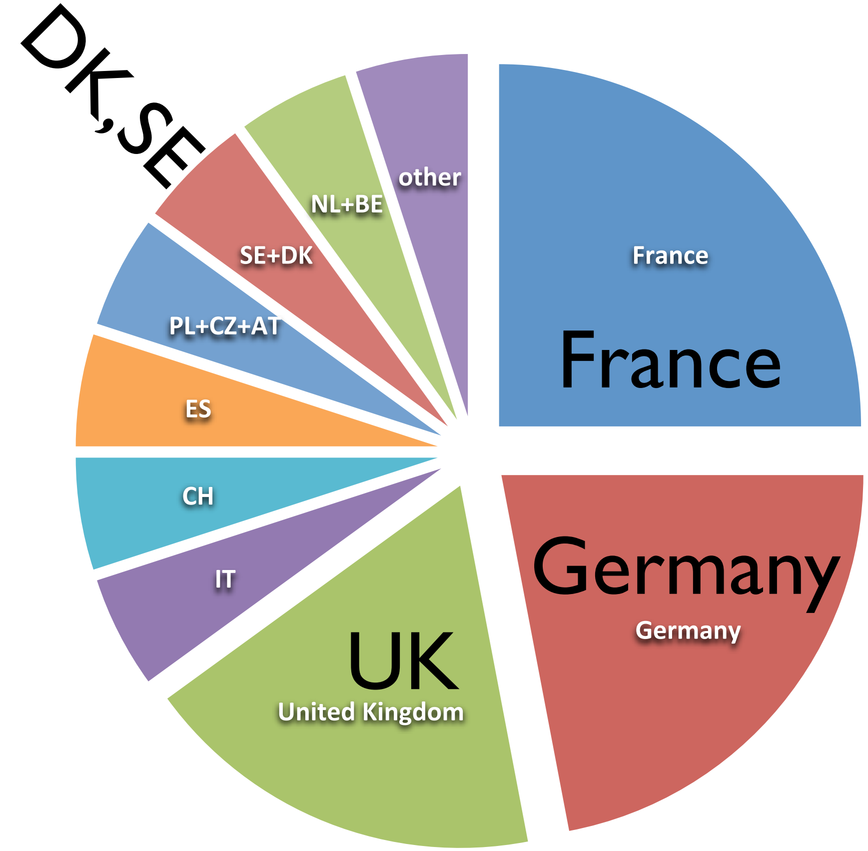
Neutrons

1932: Chadwick discovers "a radiation with the more peculiar properties", the neutron.

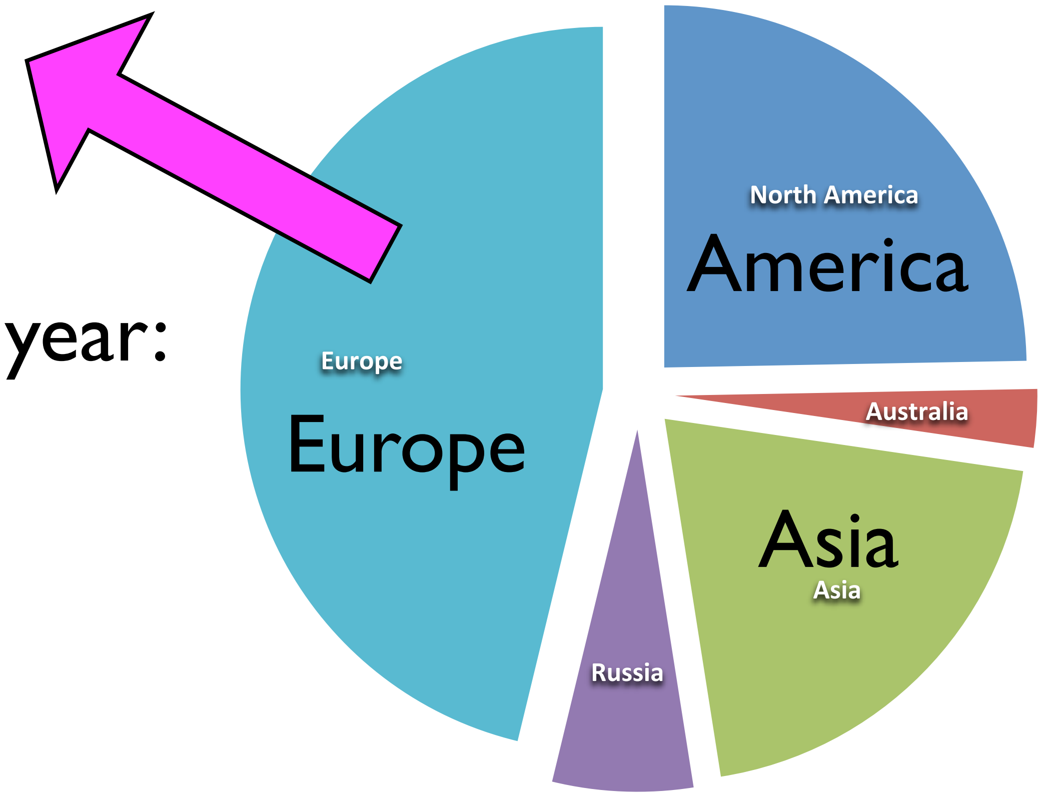
Cliff Shull: where are the atoms ?

Bert Brockhouse: what do they do ?

publications european



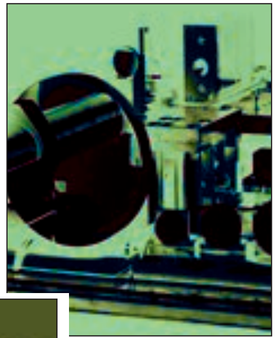
5000 - 6000 researchers
2000 publications per year

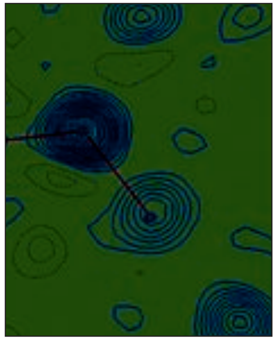


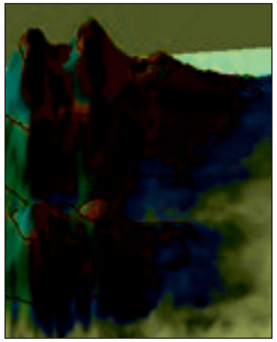
ILL (80M€, 500p) per year:
7500 days requested
3500 days allocated
1000 visitors
1000 experiments
650 publications

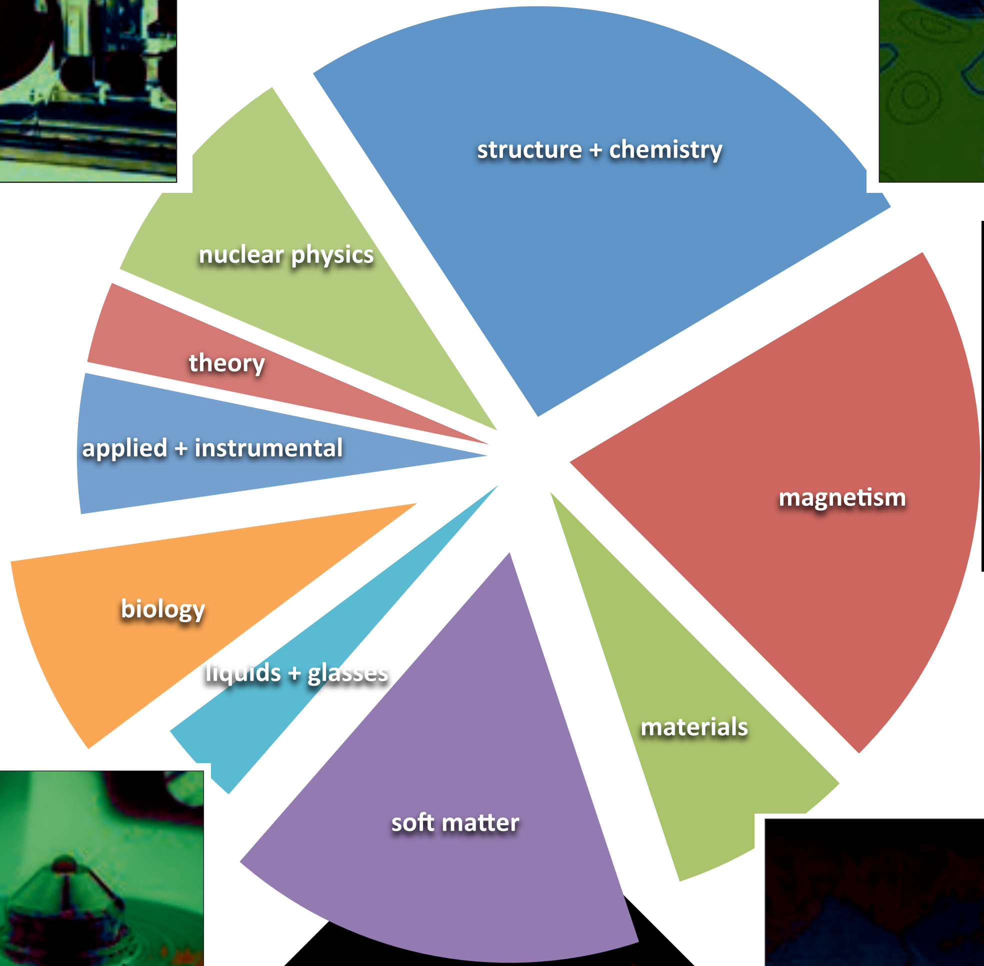
data: ESFRI, KFN

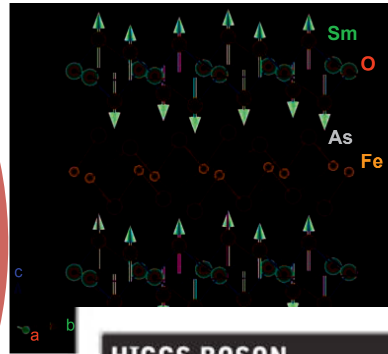
Today's Topics

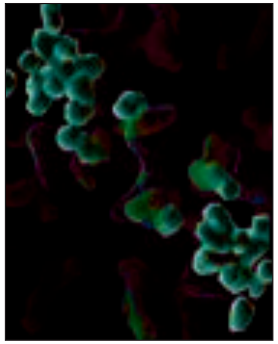


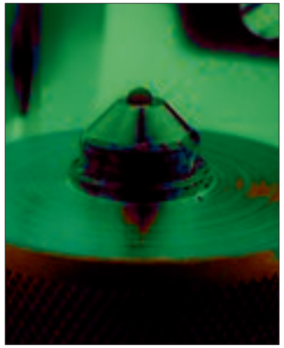


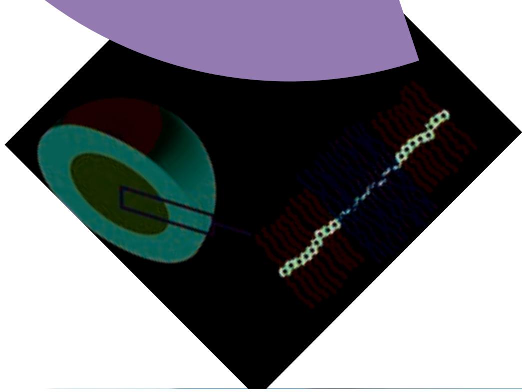


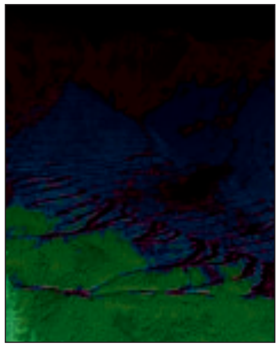






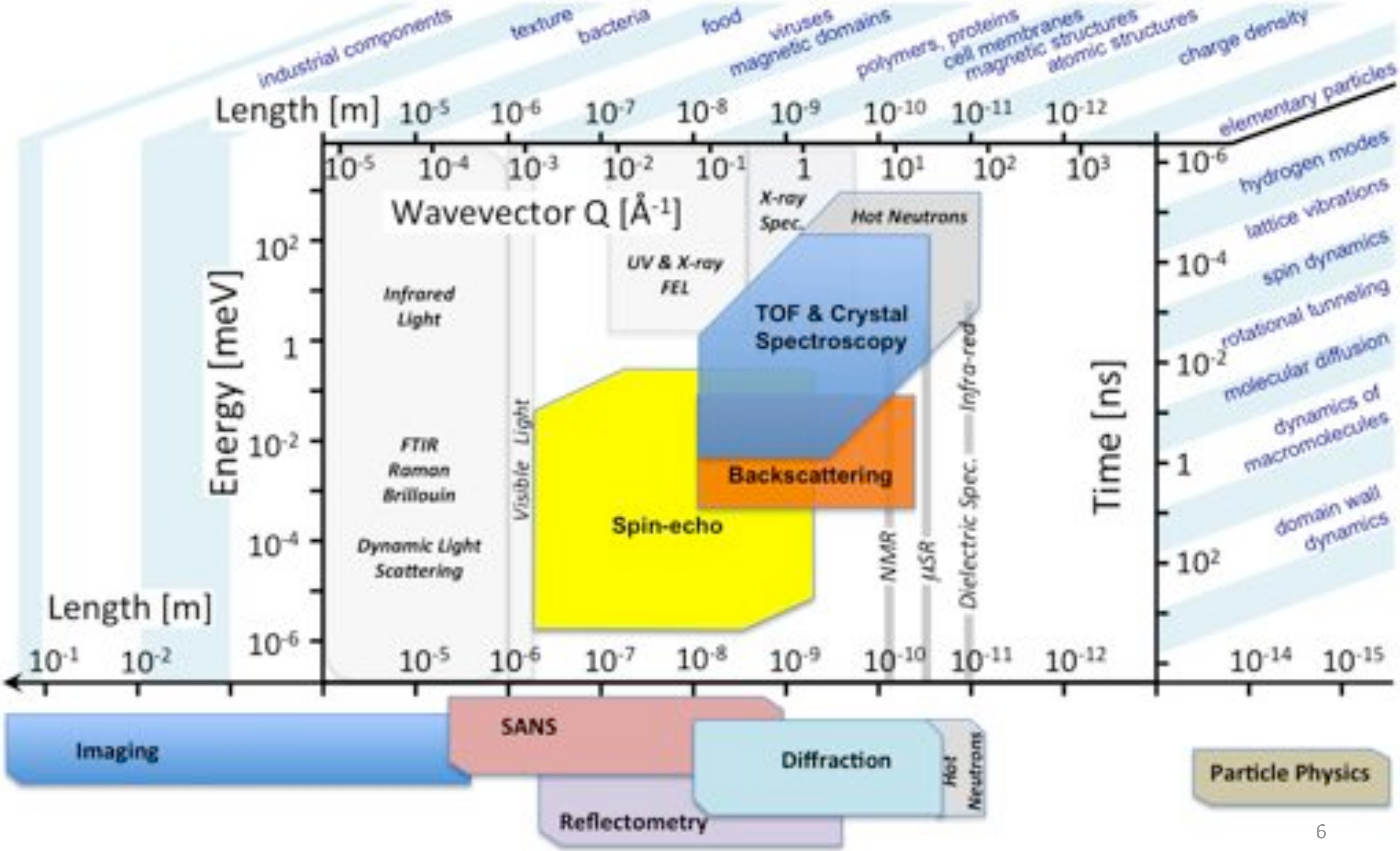






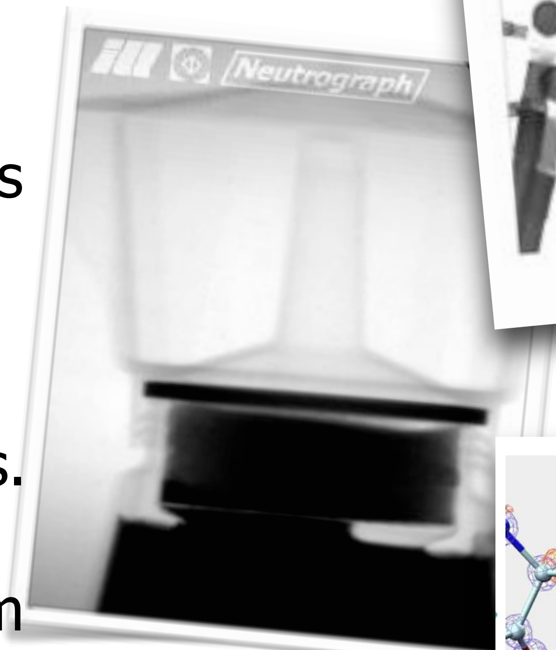
data: ILL

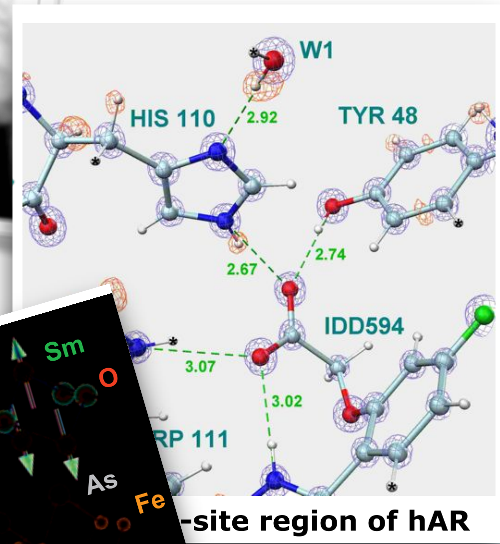
Length and energy scales

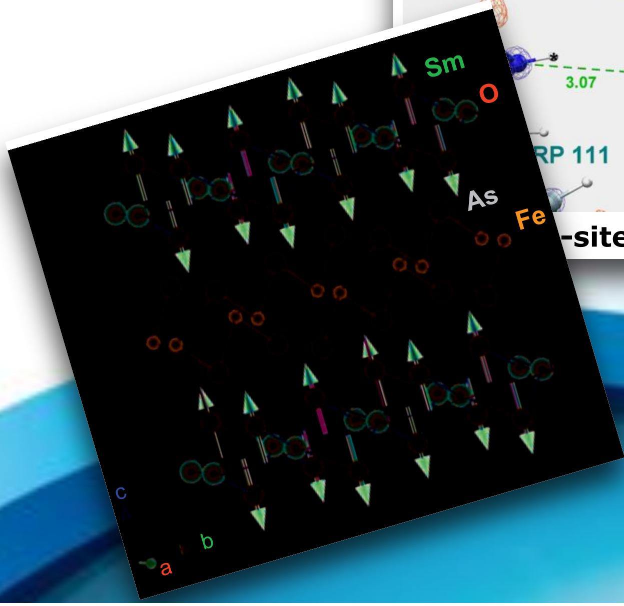


Neutrons are special

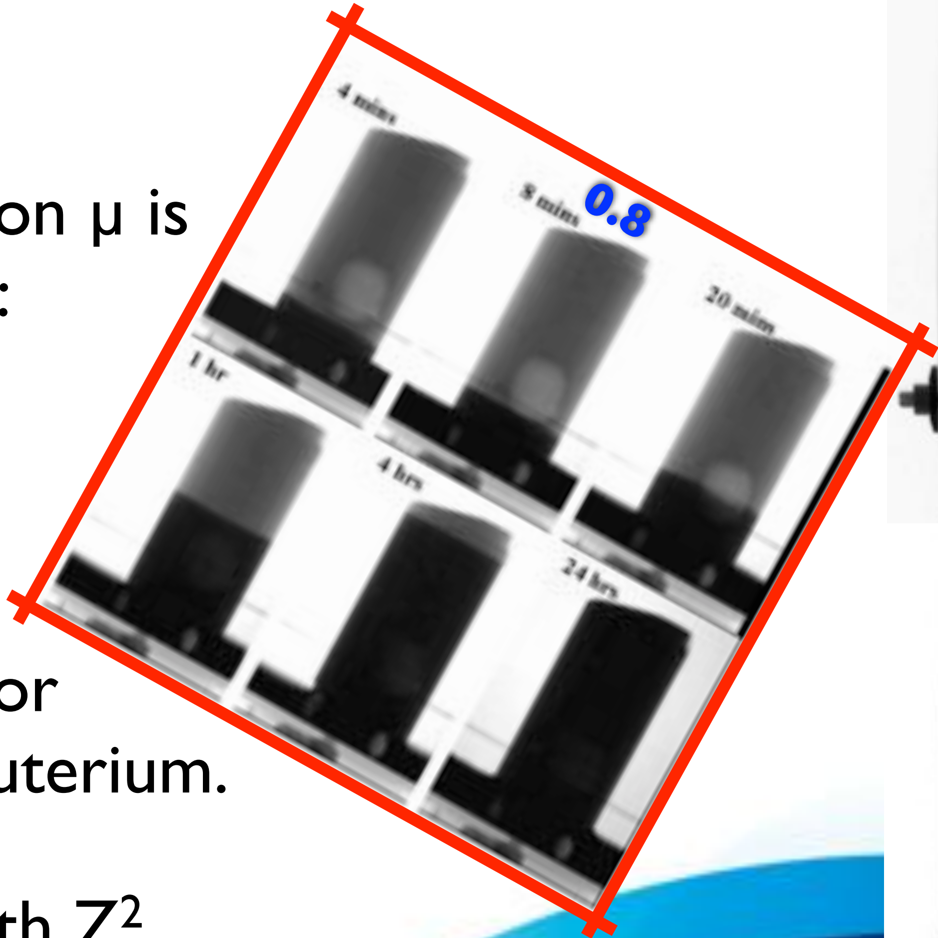
- **charge neutral:** deeply pene-trating ... except for some isotopes
- **nuclear interaction:** cross section depending on isotope (not Z), sensitive to light elements.
- **spin S = 1/2**: probing magnetism
- **unstable** $n \rightarrow p + e + \underline{\nu}_e$ with life time $\tau \sim 900s$, $I = I_0 \; e^{-t/\tau}$
- **mass**: n ~p; thermal energies result in non-relativistic velocities.
  E = 293 K = 25 meV,
  v = 2196 m/s , λ = 1.8 Å

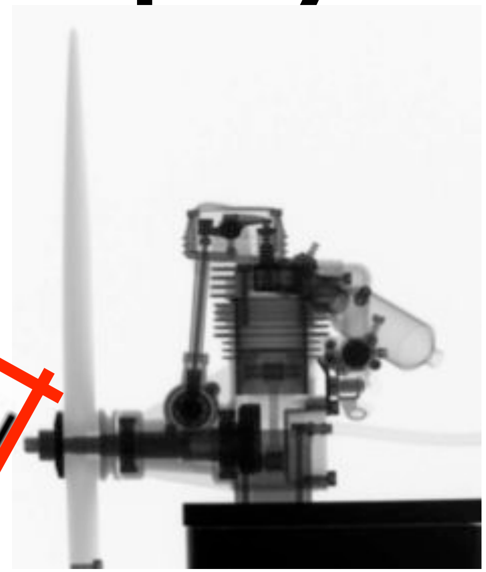


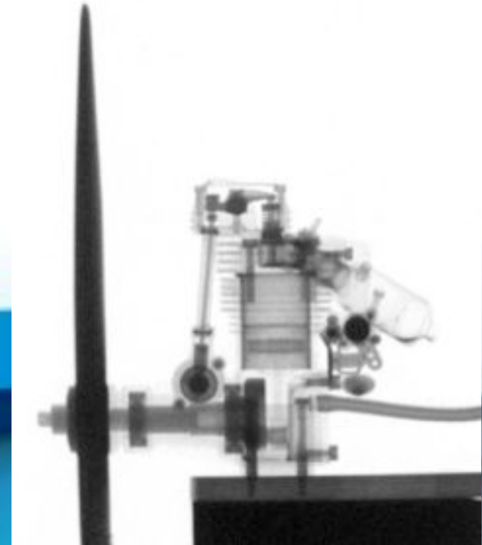




neutron radio- and tomography



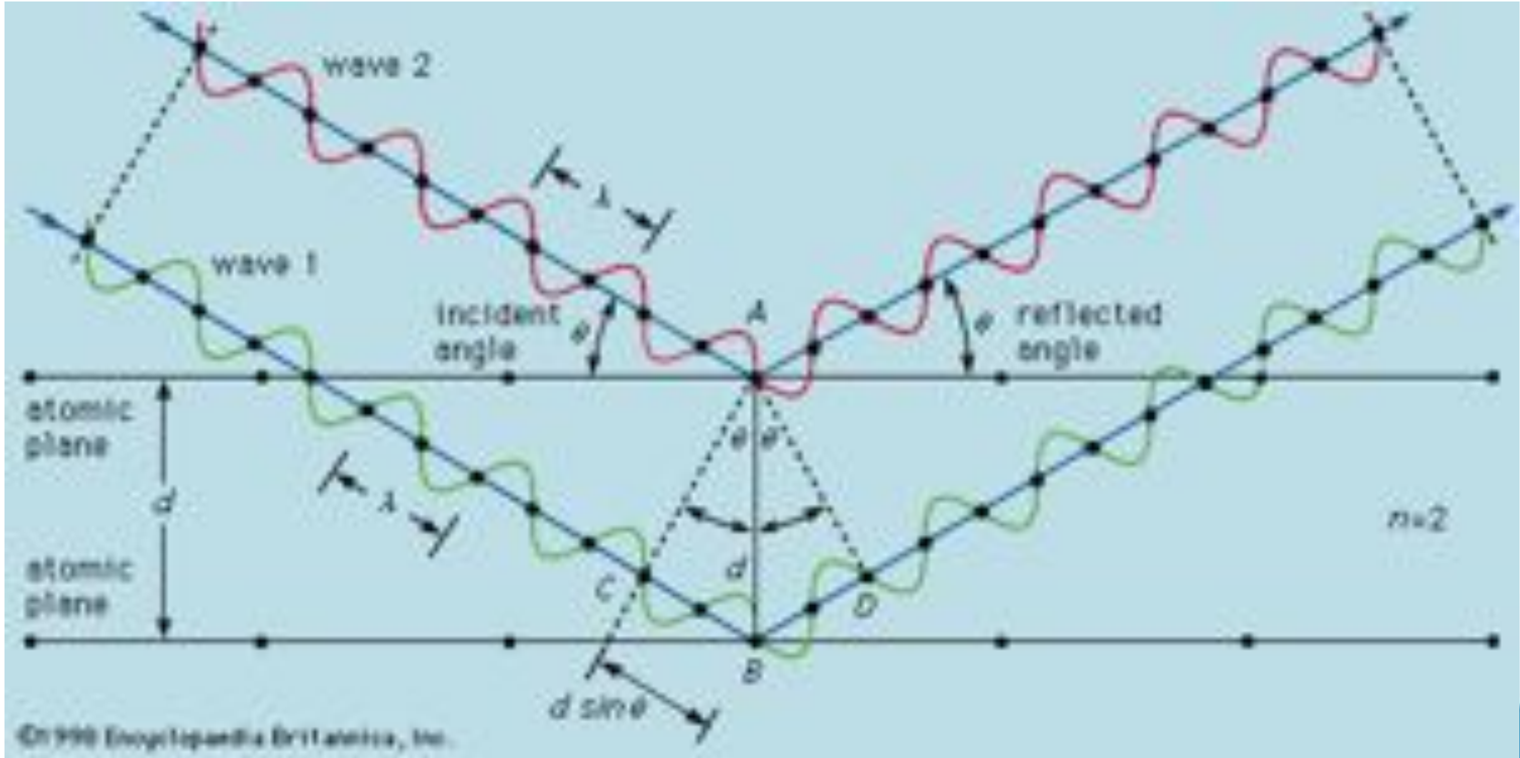




- neutron absorption μ is different to x-ray: $I = I_0 e^{-\mu.d}$
- Strong contrast for hydrogen and deuterium.
- not increasing with Z^2

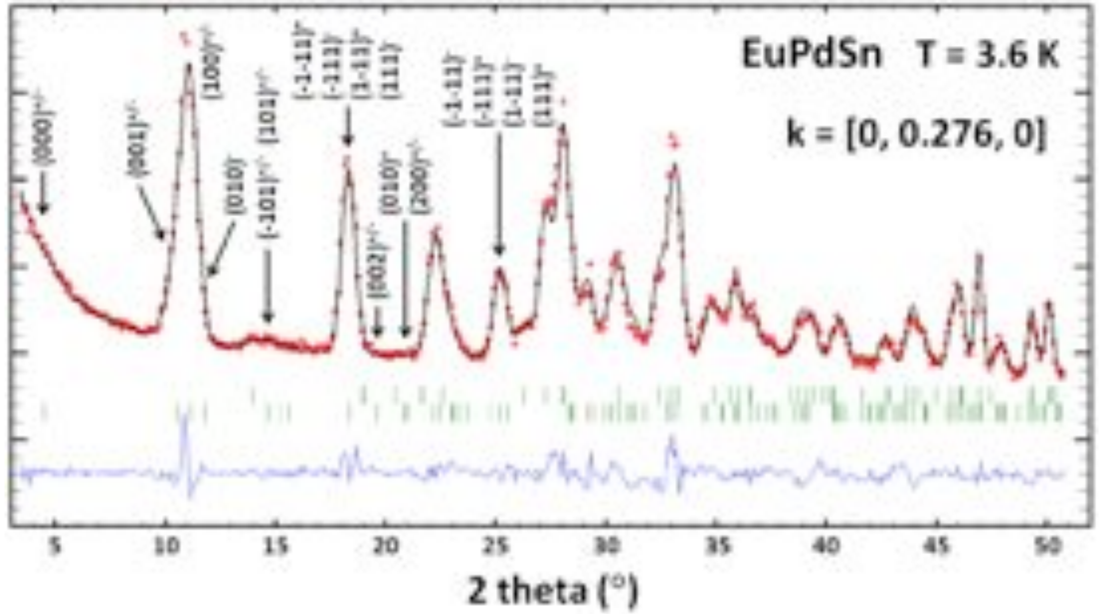
WExpertenforum/talks/TUM-Industrietag_Schillinger.pdf

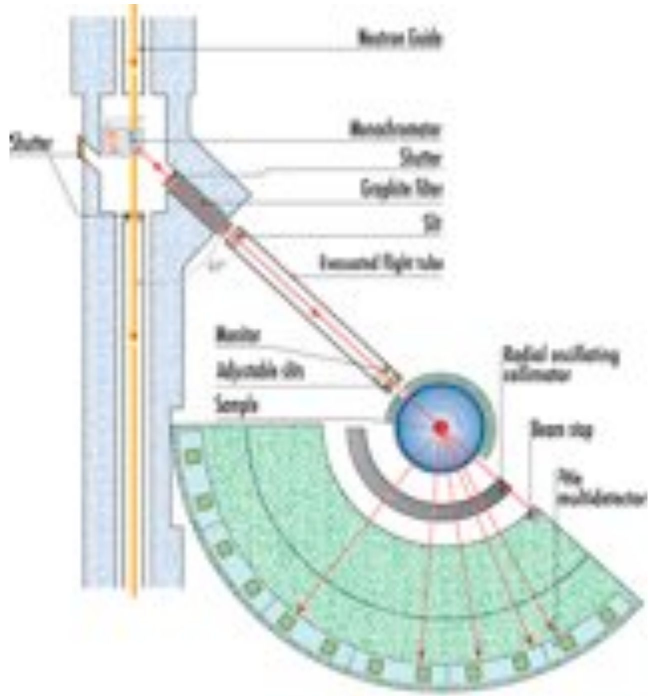
Bragg law



wave 2
wave 1
incident angle
reflected angle
A
atomic plane
atomic plane
d
d
C
D
B
d sin θ
n=2
©1998 Encyclopaedia Britannica, Inc.

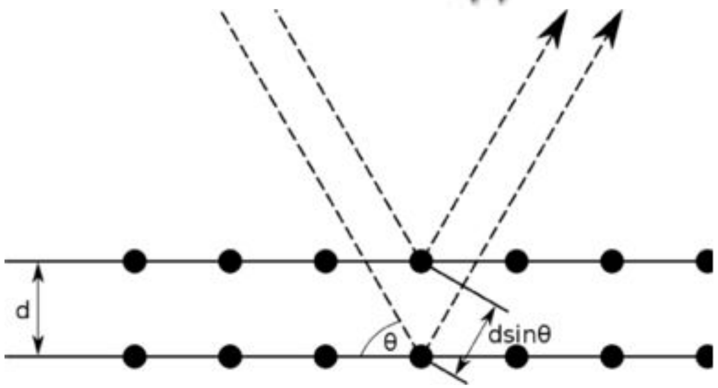
diffraction





$$I(Q) \sim |F_N|^2 + |F_M|^2$$

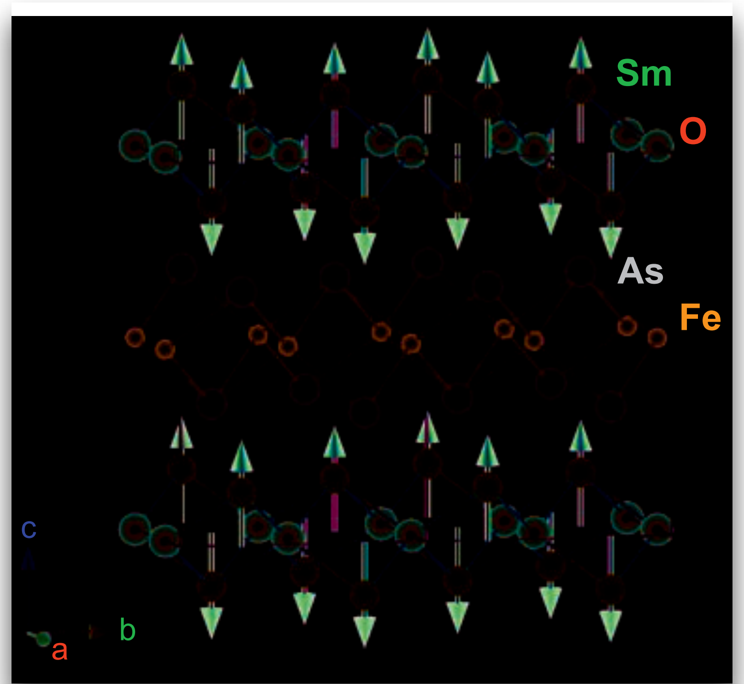
$$F_N = \sum b \exp(i\,Q\,r)$$



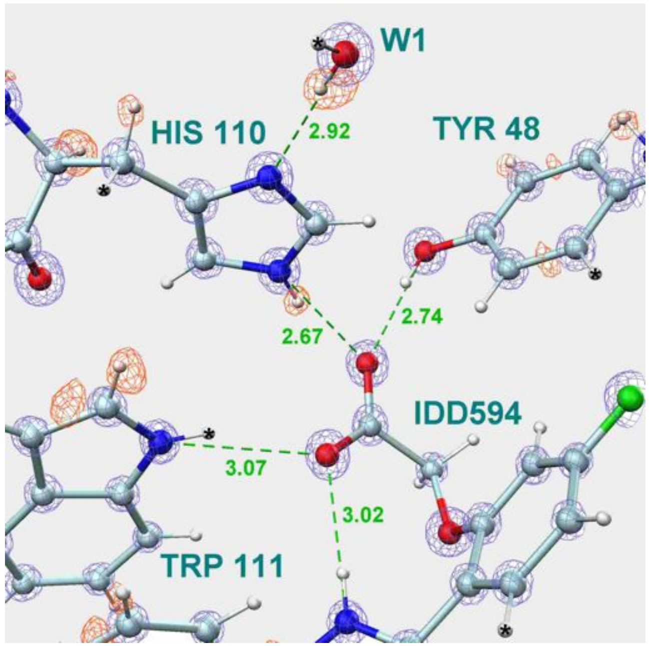
$$\lambda = 2d\sin\theta$$

http://www.ill.eu/about/movies/animations/science-animations/jdiffraction/

neutron diffraction: elastic scattering



magnetic structures



Active-site region of hAR

hydrogen in organic materials

EUROPEAN SPALLATION SOURCE

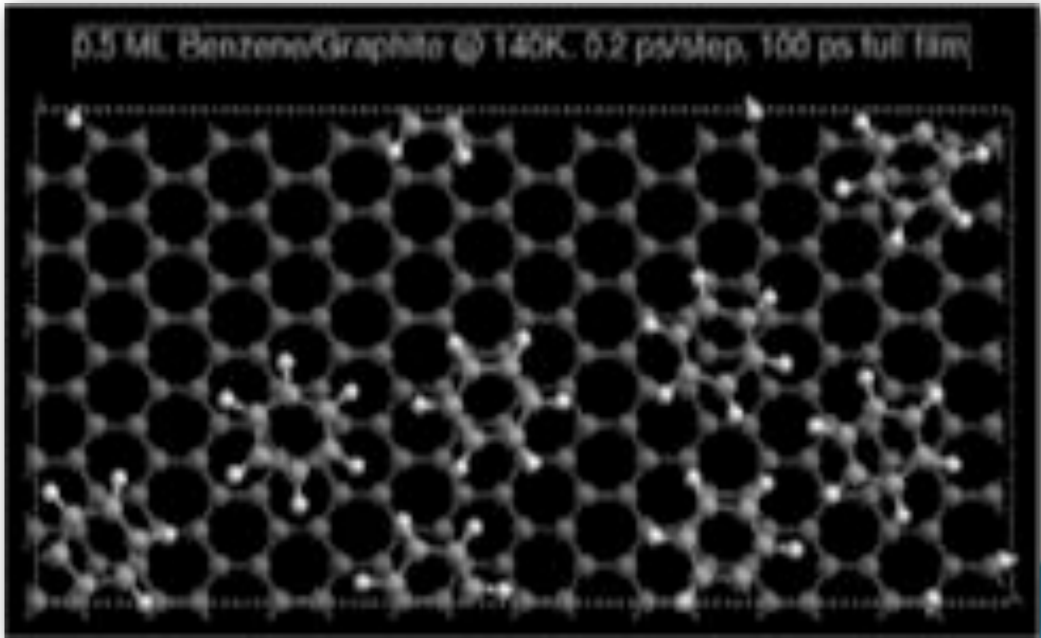
neutron spectroscopy: inelastic scattering

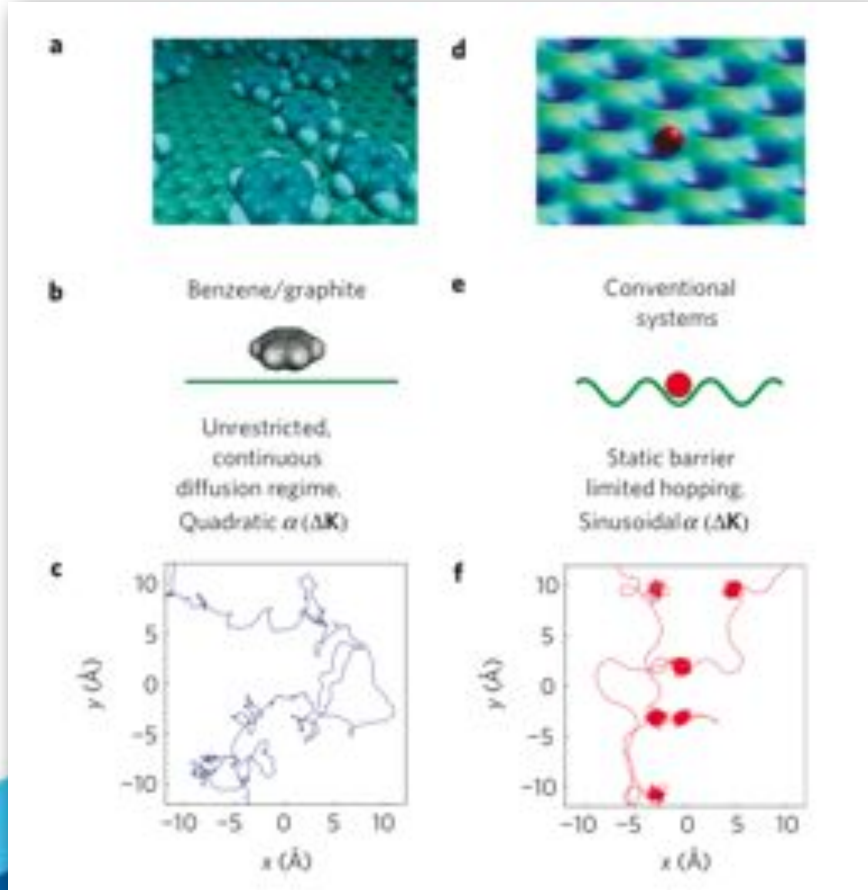
$$I(\mathbf{q},E) \propto S(\mathbf{q},E) = \langle n \rangle \chi''(\mathbf{q},E)$$

- $I(\mathbf{q},E)$: observed neutron intensity.
- $S(\mathbf{q},E)$: scattering function; FT(spin-spin-correlation function)
- $\chi''(\mathbf{q},E)$: microscopic magnetic susceptibility.
- $\langle n \rangle$: temperature (Bose) factor.
    - momentum (Q) and energy (E) dependent microscopic information on the dynamics.

dancing benzene on graphene

- Does the benzene hope from position to position or move freely ?

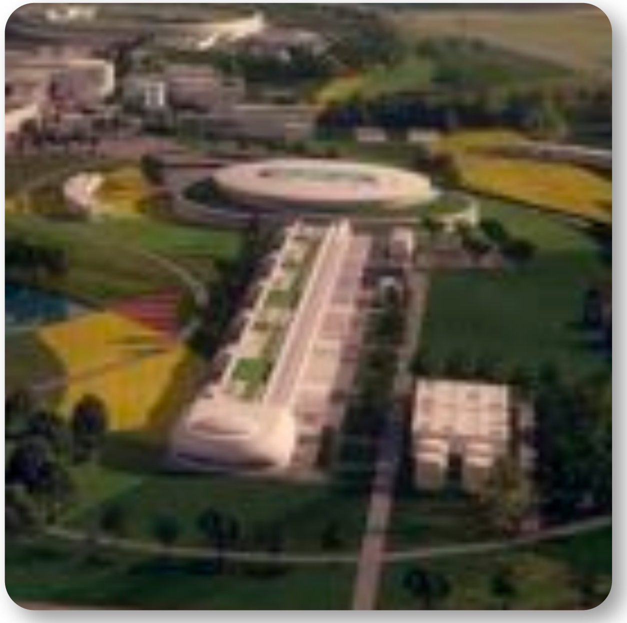




by P. Fouquet

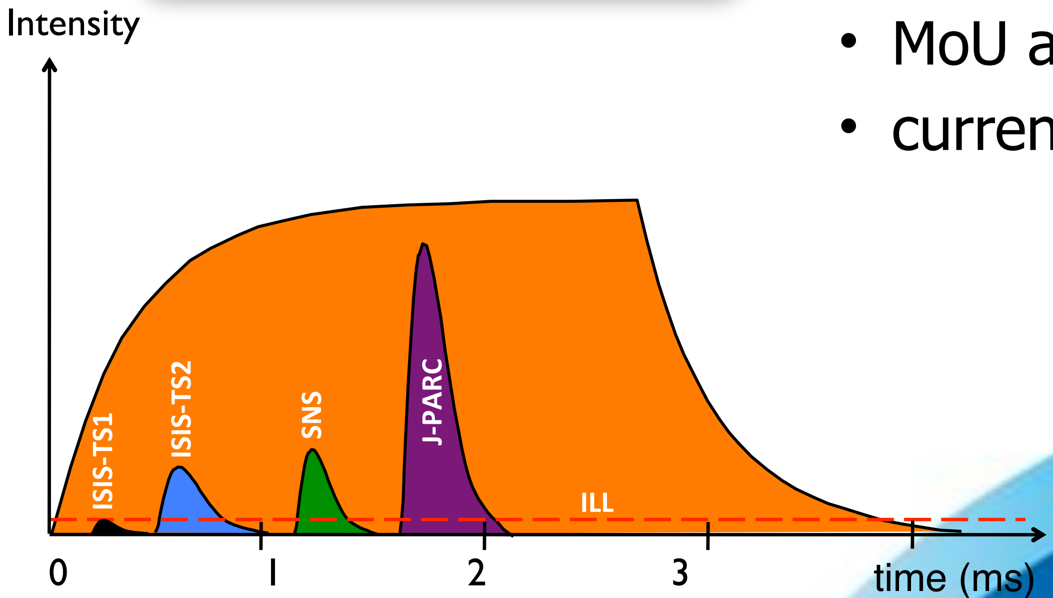
EUROPEAN SPALLATION SOURCE

ESS project: key facts

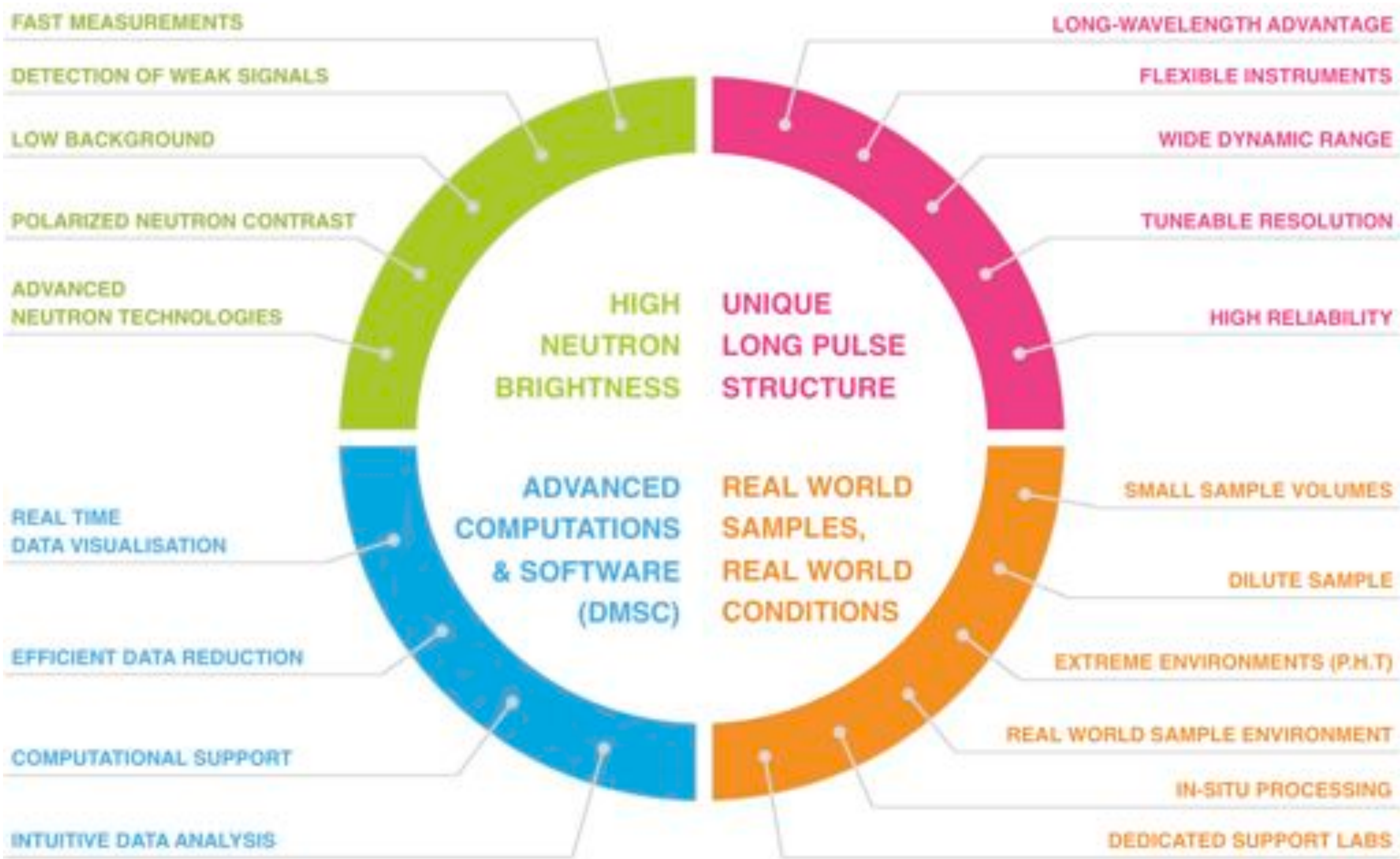


- 5MW long-pulse neutron source.
- First neutrons in 2019 on 7 instruments.
- 22 instruments by 2025
- ESS will be user facility.

- Total cost 1478 M€; funding negotiation
- MoU agreed with 17 european countries
- currently in pre-construction phase

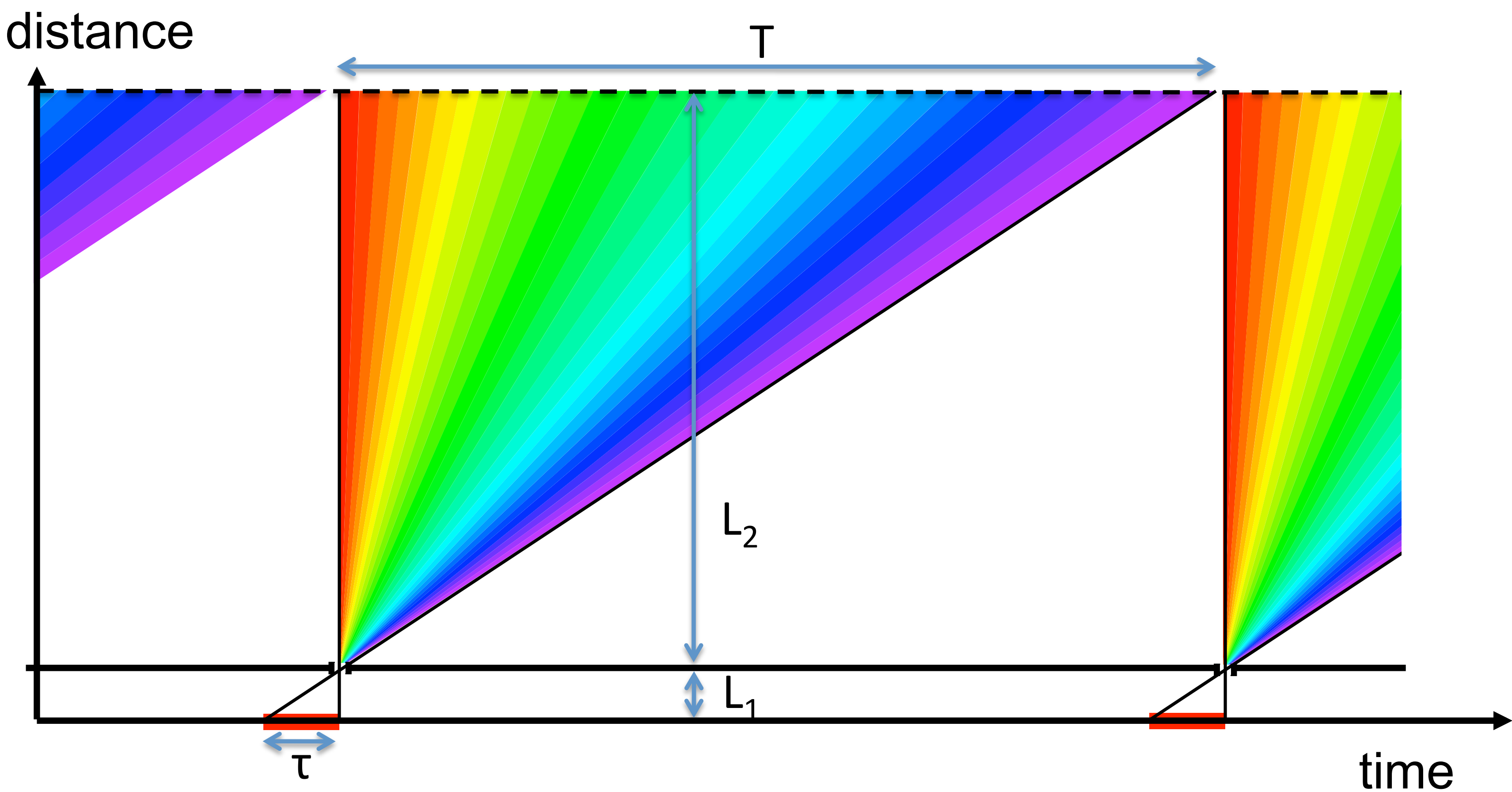


unique capabilities of ESS

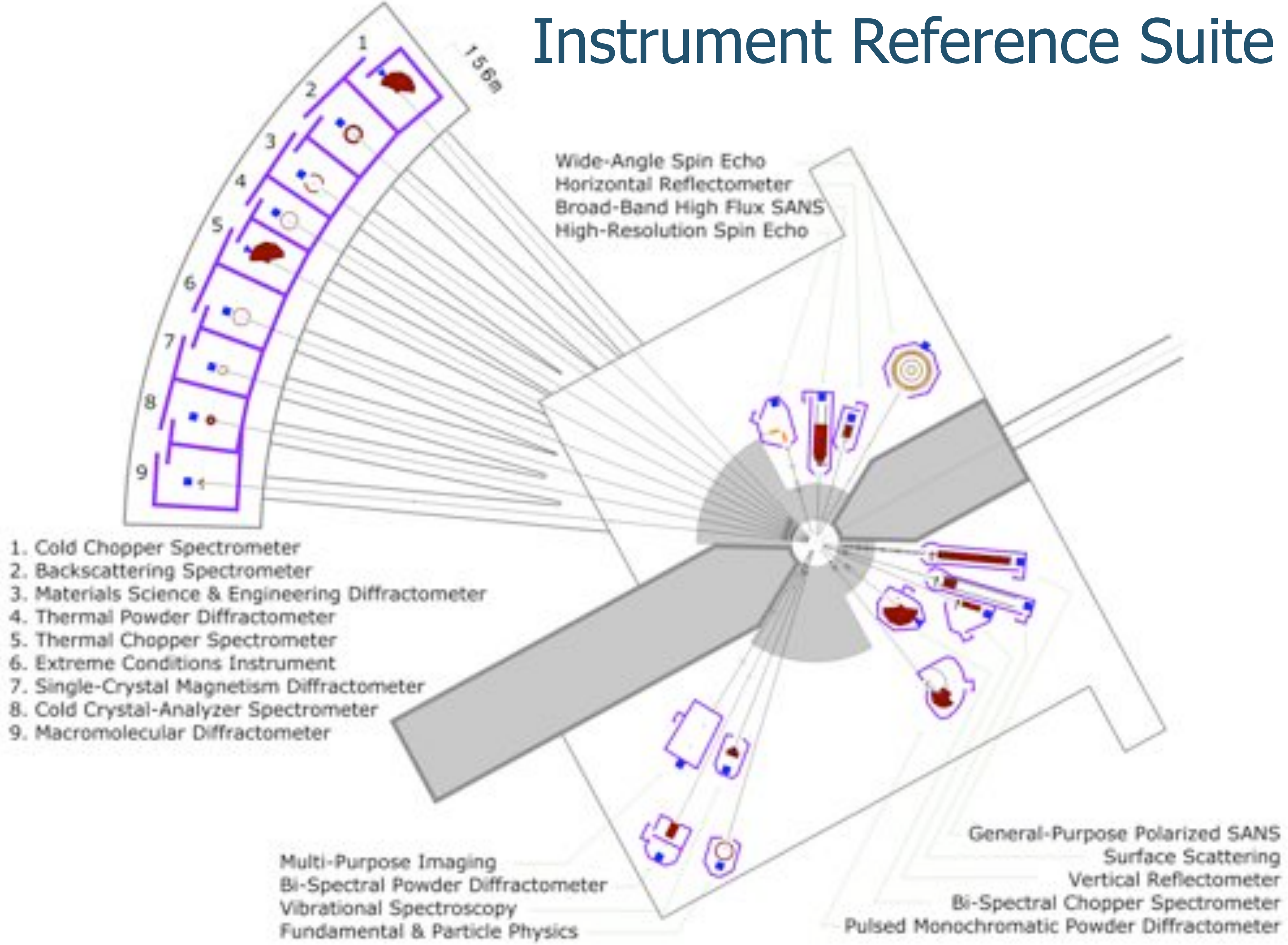


Time distance diagram

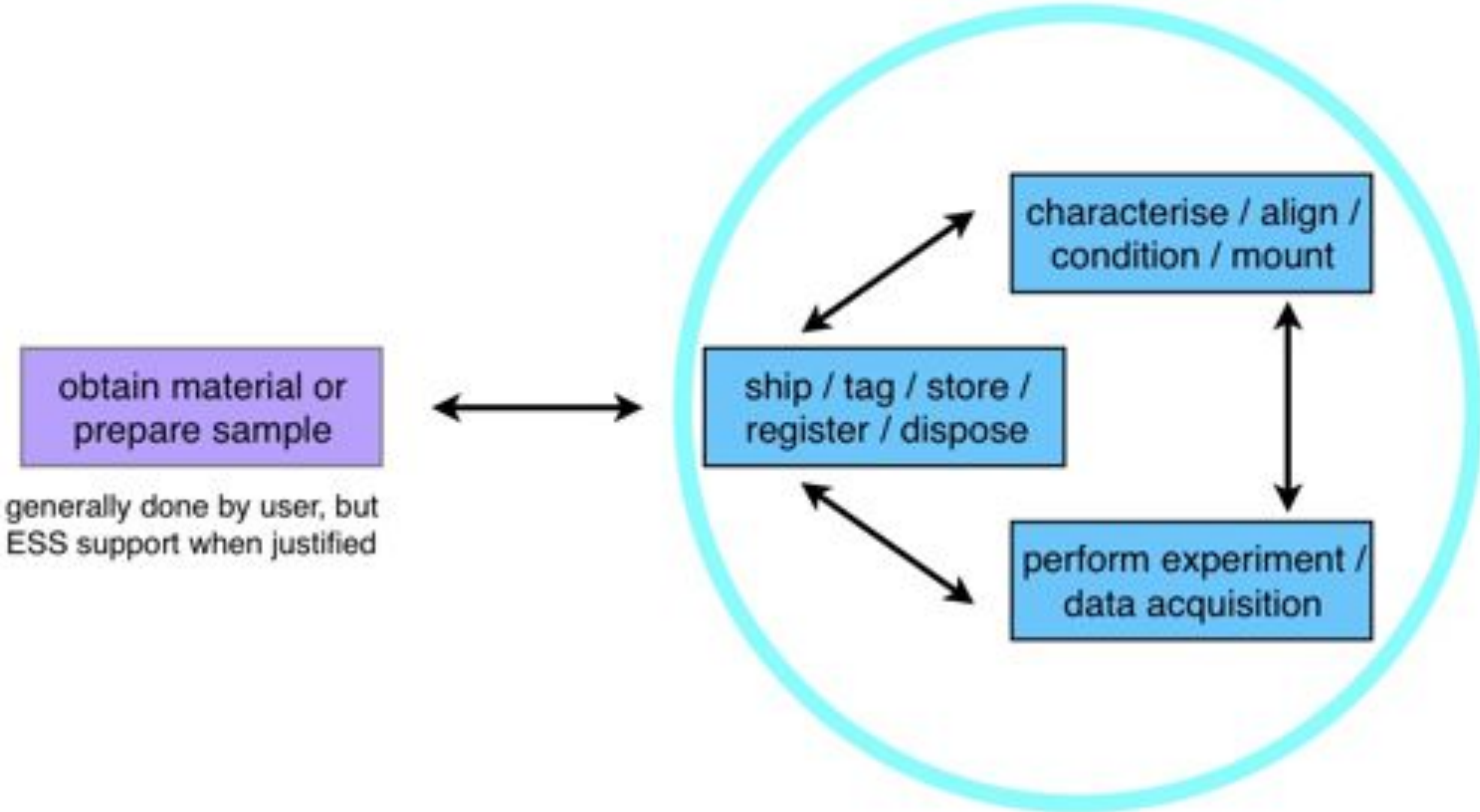
- Time distance diagram of white beam instrument with Pulse shaping chopper .



Instrument Reference Suite



users and sample



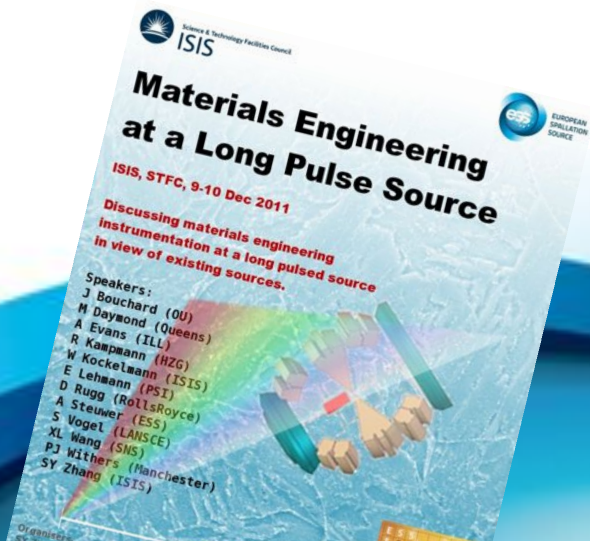
Neutron Scattering Systems and Neutron Science

- BUILDING Neutron Scattering Systems
  - Instrument Concepts: define the ‘best’ instruments to be build
  - Instrument Construction: build the ‘selected’ instruments
  - Neutron Technologies: detectors, chopper, optics, sample environment, electrical engineering
  - Data Management and Software Center
  - Neutron Science Support Facilities

- DOING Neutron Science Activities
  - Science Focus Areas: life science, chemistry, magnetism, engineering, geo-science, fundamental physics
  - Community: science symposia, ESS S&S, sponsoring, outreach
  - Industrial R&D using neutrons
  - Ext. funded Research

Science Symposia

13 Science Symposia
More than 300 people participating
Real Input into the planning of ESS



Topics
Science Symposia

neutrons and art

energy materials

energy strategies

engineering processes

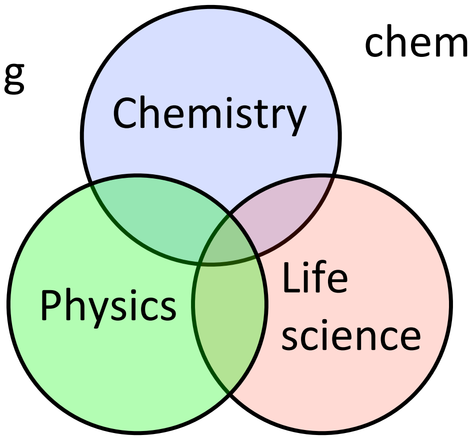
neutrons and NMR

buildingmaterials

in-situ chemistry

materials engineering

neutron technology



Protein xtalo

neutrons and food

imaging

spin dynamics

non-equilib-rium SANS

topological materials

thin films 2D & 3D

biomedical research

ageing concerns

fundamental physics

others ...

Key findings from symposia

- Where is science going and what are the experimental challenges ?
- Which instruments are needed ?
- What else (alternative techniques, infrastructure) ?

summary tables

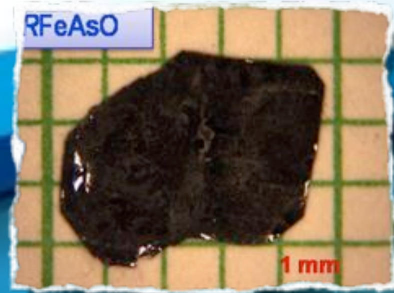
	Scientific challenges	Instrumental requirements	Other techniques and infrastructure requirements
Spin dynamics of correlated systems A Boothroyd Abingdon, UK Feb. 2012	Emergent quasi-particles Small samples under extreme conditions (high B, low T, high p). Users will not all be 'professional users'. Mapping single crystal excitations.	Cold direct geometry chopper spectrometer (super-LET/IN5). Thermal direct geometry chopper spectrometer (super-Merlin). Extreme environment spectrometer. μeV resolution SANS. Polarised neutrons as option on all instruments. Focus on what ESS is good at (avoid doing 'everything'). Avoid 'niche' instruments. Envisage event-mode recording.	Central support facilities. Advanced data analysis. Neutron spectroscopy remains 'standard tool' only complemented by RIXS, IXS and ARPES.
NMR meets neutron scattering H. Bordallo Copenhagen, DK June 2011	Inelastic: rotational tunneling spectroscopy; low frequency excitations in glasses and molecular magnetism. Quasi-elastic scattering: diffusion in soft matter and bio-related molecules; liquids; critical scattering.	Backscattering and NSE instruments to complement TOF instruments for high E resolution. Vibrational spectroscopy (Lagrange or TOSCA type) for high energies.	Scientific support facilities (deuteration). In-situ analysis (x-ray, thermal analysis, bulk measurements). MD modelling efforts.
Neutrons and food W. Bouwman Delft, NL Feb 2012	Nano- to millimeter structural information as a function of external parameters. 'Dirty systems'	Variety of neutron techniques: SANS, reflectometry, SESANS, INS, tomography. Incorporate flow set-up & complementary techniques	Deuteration required. Labs close to instruments. Sample environment. In-situ characterisation. Analysis support. Rapid access. Try first experiments

	Scientific challenges	Instrumental requirements	Other techniques and infrastructure requirements
Off-specular neutron scattering M. Sferrazza Leuwen, BE Jan. 2012	Separating bulk and surface properties in 2D and 3D; nanoscale magnetism and soft matter. Lateral structures	Several complementary SANS instruments; one GISANS; Sergis-type reflectometer with TOF option; polarised neutrons; small samples; Optimise signal to noise. Dedicated instruments (no compromises in combining too much)	Advanced analysis tools.
Materials Engineering Shu Yan Zhang RAL, UK Dec 2011	Nuclear Power Research Advanced materials investigations Strain and imaging Industrial user	Better penetration Better spatial resolution Faster dynamics Detectors: coverage, resolution, small angle Diffraction & Imaging	Automated sample handling More lab space
Neutron Imaging Lehmann Bad Zurzach, CH April 2012	Plant soil systems Concrete and water Battery Research	Flexibility for broad user community High cold intensity Highest spatial resolution Energy resolution	Various sample environment

	Scientific challenges	Instrumental requirements	Other techniques and infrastructure requirements
Non-equilibrium SANS S. Egelhaaf Lund, SE Feb 2012	Sample in more complex situations and non-equilibrium as used in industry processes and in biology. Contrast variation by deuteration and complementary techniques	Instruments for small samples but complex (large) sample environment. Combine SANS with other techniques (light scattering) and neutron methods (imaging...). Large Q range and resolution	Requires external time- and space-dependent 'fields' such as T, B, E, shear. Provide *in-situ* techniques and ex-situ support labs close to instruments. Robotics for sample change. Reliability and reproducibility in measurements.
Topological materials T Fennell Grenoble, FR Oct. 2011	Universality classes in frustrated systems. Quantitative lifetime. measurements. Smaller samples (for new materials); extreme environment. Many experiments will be 'standard' independent of 'scientific fashions'.	Optimse signal to noise. Optimse on current science case but keep flexibility Survey and 'zoom in' Flexible test beamlines for new concepts, non-standard, training	RIXS might cover higher energies, but neutrons for 'standard and high resolution measurements. Advanced analysis and modelling support (theory consortium). Flexible access and in-house research to liaise with university groups. Promote student access and long term visits. Expert groups required for instrument developments. Sociological study to get outside view.

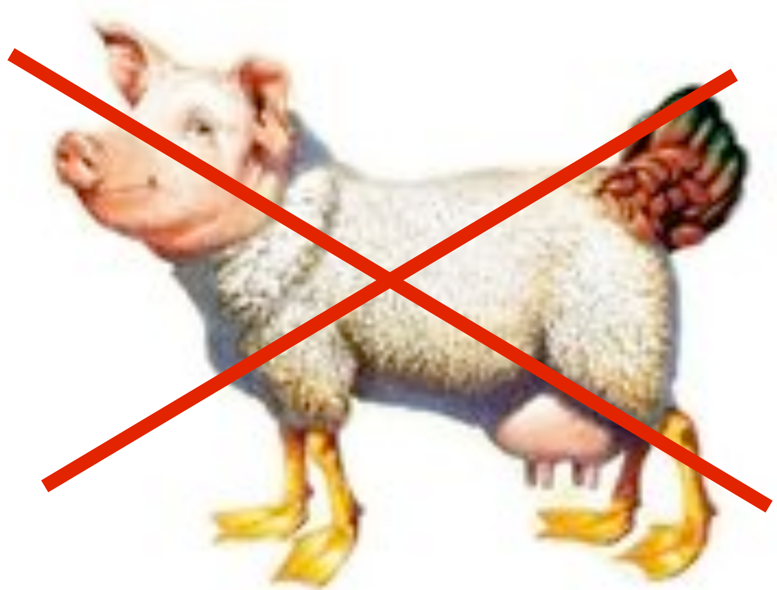
Science and experimental challenges

- ‘real’ samples: diluted, complex, small, bad.
- several length and energy scales; hierarchy
- fast ... reactions, processes, non-equilibrium.
- measure in extreme environment: T, B, p, humidity
- in-frequent *and* strongly engaged users.



Which instruments

- optimize for signal-to-noise
- optimize (not only) for small samples
- polarisation as option (only)
- avoid ‘eierlegende Wollmilchsau’
- avoid niche-only instruments
- focus on what ESS is good at: cold and cold/thermal neutrons
- provide necessary suite for user needs; enable ‘integral’ science.
- easy-to-use and increased flexibility; tune resolution by chopper
- sequential or parallel coverage of S(E,Q): mapping and ‘zooming’ instruments; mulitple E resolutions
- combine other exp. techniques (in-situ and ex-situ)



What else ?

- reliability and reproducibility of experiments
- adequate access modes (rapid, long term, with additional support)
- data reduction, analysis, modeling ... accessible for users in need
- additional scientific support labs
- more support for in-frequent users
- encourage users to get involved (students, visiting scientists)