The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1866-9

School on Pulsed Neutrons: Characterization of Materials

15 - 26 October 2007

Accelerator generated Probes as Tools for Materials Science

Kurt Clausen

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PAUL SCHERRER INSTITUT

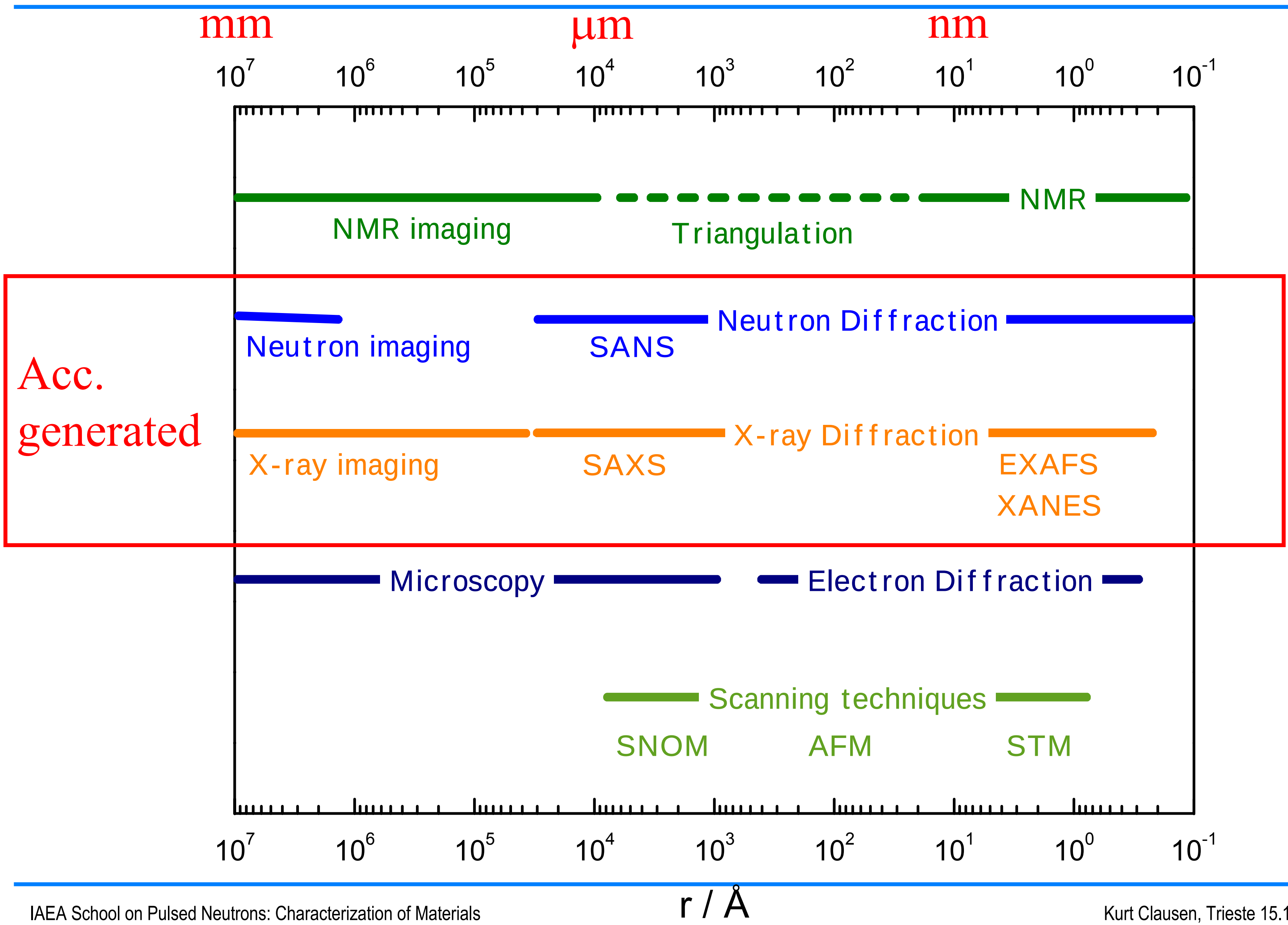
Accelerator generated Probes as tools for Materials Science

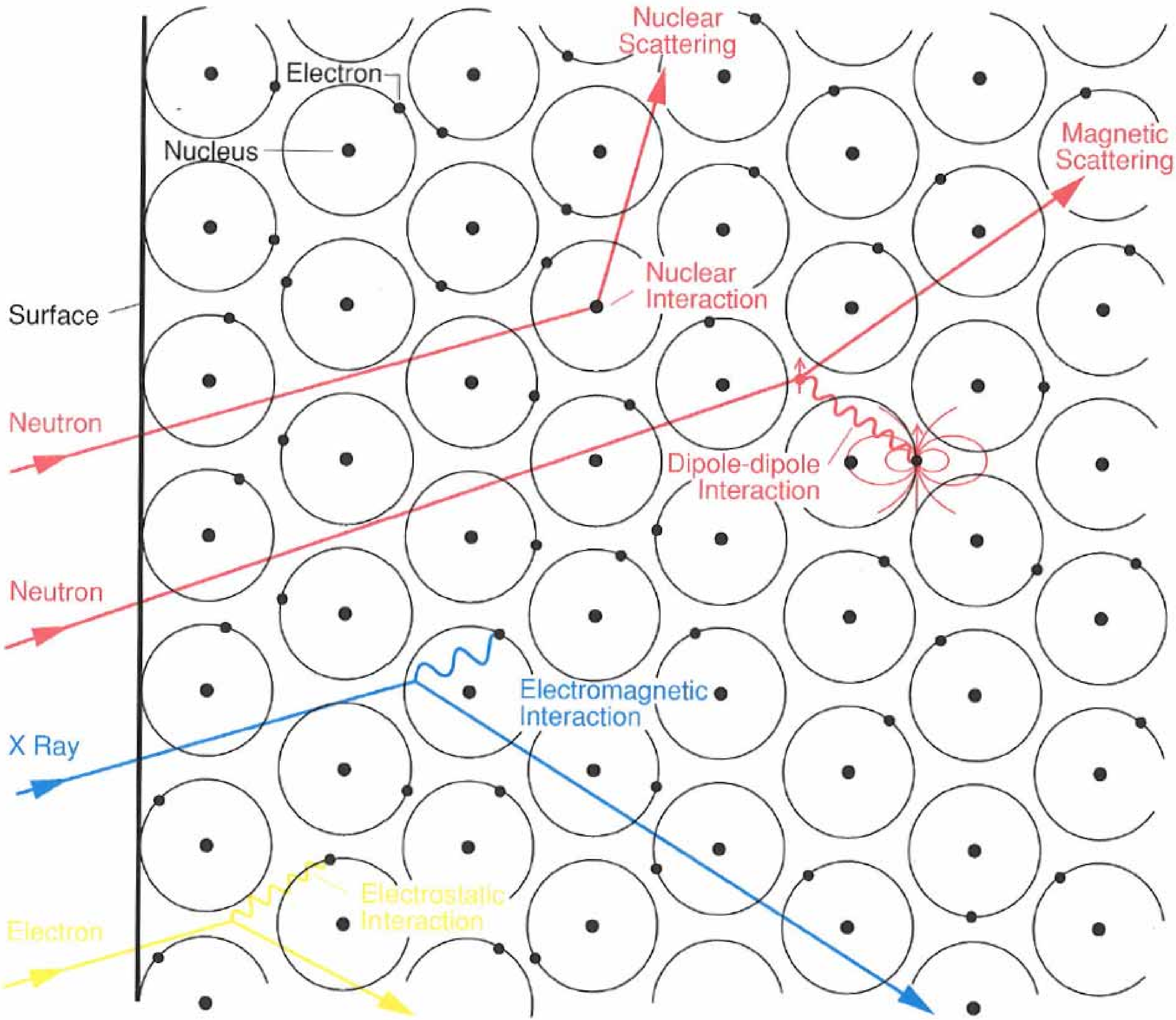
IAEA School on Pulsed Neutrons:

Characterization of Materials

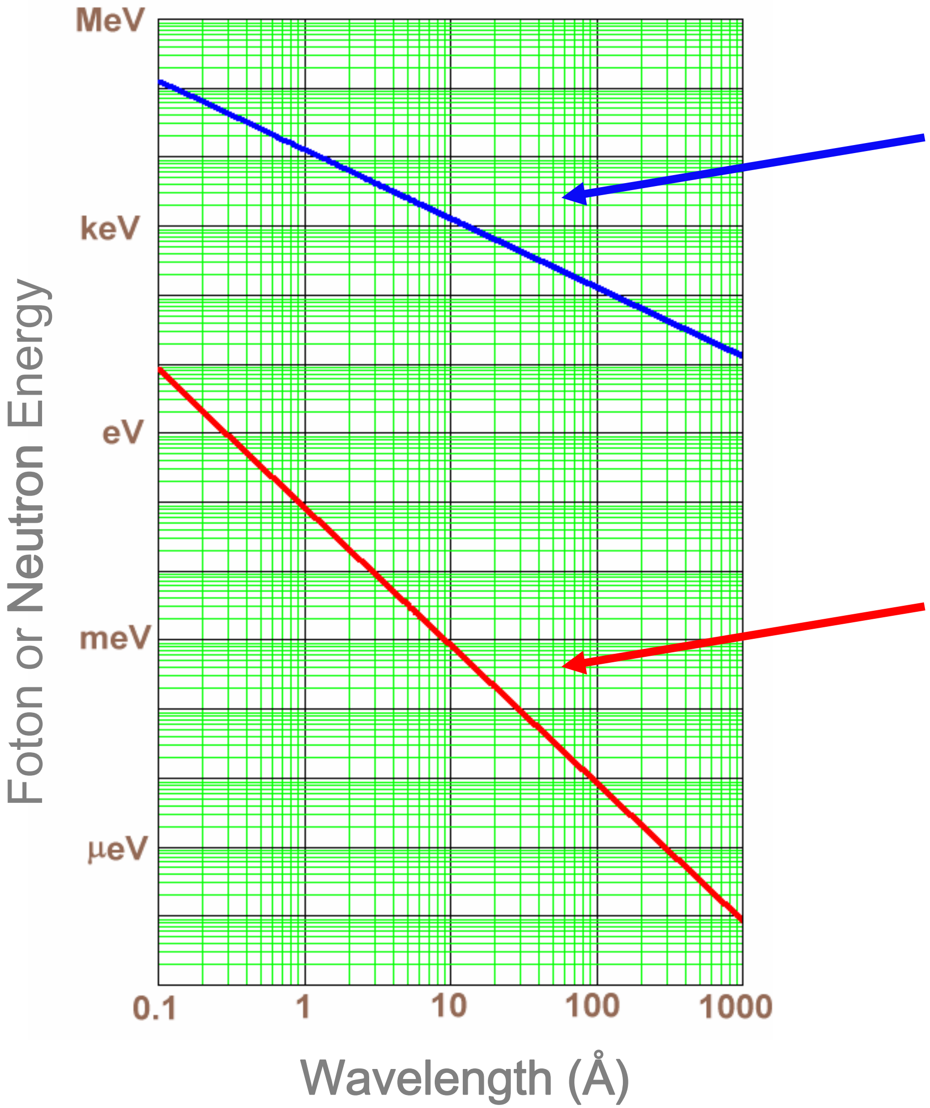
Kurt N Clausen
Condensed Matter Research with Neutrons and Muons
Paul Scherrer Institut
Switzerland

Imaging, Microscopy, Diffraction → *Structure*




Nuclear Scattering
Electron
Nucleus
Magnetic Scattering
Nuclear Interaction
Surface
Neutron
Dipole-dipole Interaction
Neutron
Electromagnetic Interaction
X Ray
Electrostatic Interaction
Electron

Energy wavelength relation



Fotons:

$$E = \frac{h \cdot c}{\lambda}$$

$$(h \cdot \nu)$$

$$E = \hbar\, \omega$$

Neutrons:

m = 1.67 10^{-27} kg ~ m_{proton}

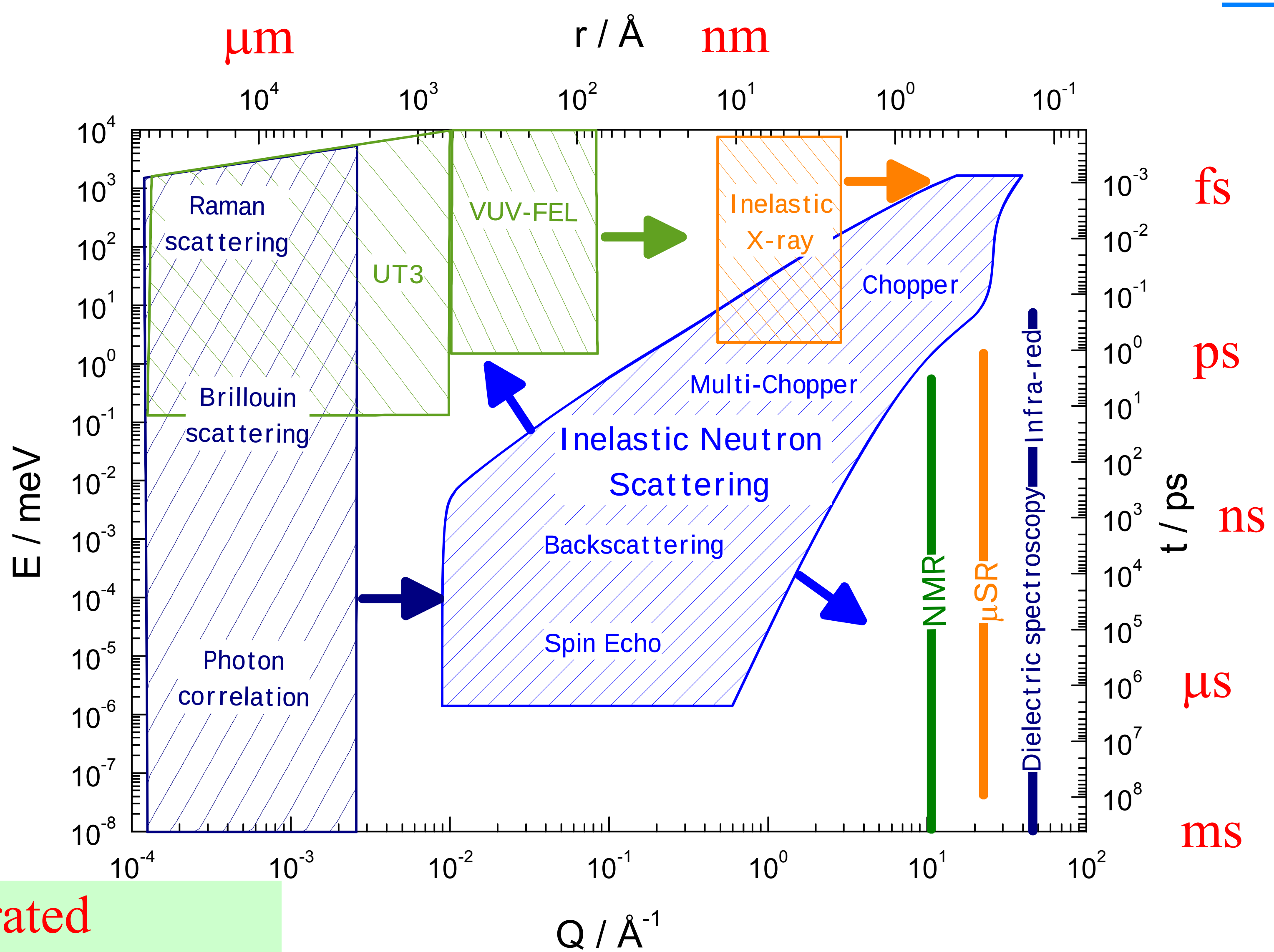
Spin = ½

Charge = 0

$$E = \frac{h^2}{2 \cdot m \cdot \lambda^2}$$

$$\left(\frac{1}{2} \cdot m \cdot v^2\right)$$

Dynamics



Acc. generated Synchrotron X-rays, Neutrons and Muons

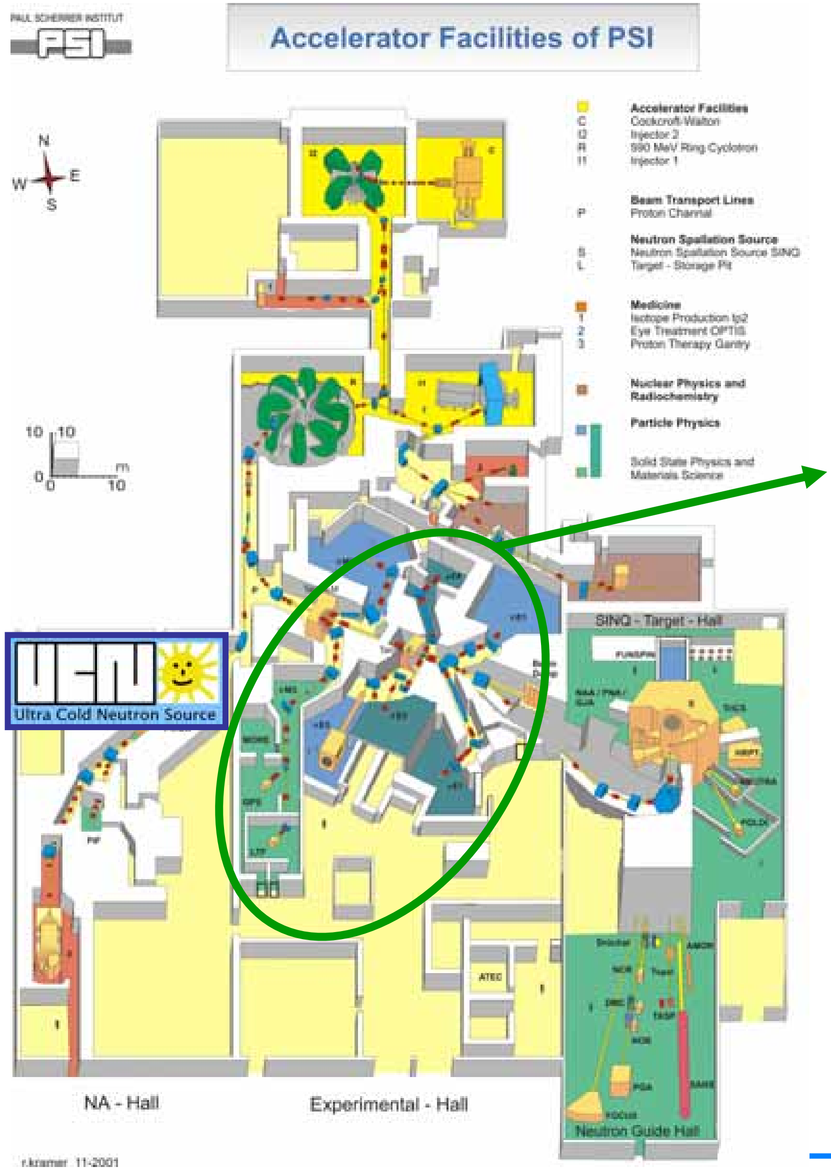
15 October 2007 – outline:

- Muons
    - Sources
    - A local probe
- Fotons – a very short introduction
    - Synchrotron X-rays, X-ray Free electron lasers (XFEL)
    - A few examples – structure – real time experiments → fs

SHORT BREAK

- Neutrons

Proton accelerator Complex PSI



600 MeV proton beam
2 mA proton current,

CW Muon Source at PSI:

2 – 60 mm Graphite target in proton beam.

Generation of Pions that decays into Muons (Pon lifetime 26 ns).

4 sources worldwide, Triumf Canada, J-Parc Japan, ISIS UK and PSI Switzerland

Muon Sources …. (operating, under construction)

Muon lifetime 2.2 μsec

Facility	Energy (MeV)	Freq (Hz)	Pulse - length (nano sec)	Gap if double pulse (nano sec)	Power for Muons (kW)	Proton beam size at Muon target
J-PARC	3000	25	130	598	< 50	> 10 cm^2
ISIS	800	50	80	330	5	few cm^2
TRIUMF	500	CW	CW	CW	< 53	few mm^2
PSI	590	CW	CW	CW	350	few mm^2

CW Source – event rate ~ 40 kHz (1 Muon at a time in the sample)

Ideal Pulsed Source - ~ 2 nsec pulses at ~ 10 kHz

Muons beams generated via pions have pulse length in excess of 26 nsec (pion lifetime)

Pulsed Neutron Sources too low rep rates, too long pulses too large proton beam size

Except for pump probe experiments CW sources are in general preferential

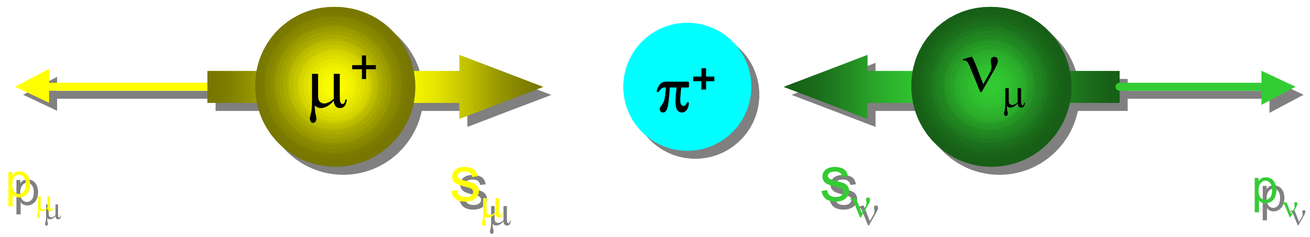
PSI ~10^6 surface Muons/mm^2/sec (at least a factor 100 above competitors)

LEM (Low Energy Muons) basically only feasible at PSI

Potential for microbeam ~ 0.1*0.1 mm^2 (Scanning or very small samples)

Muon production from pions

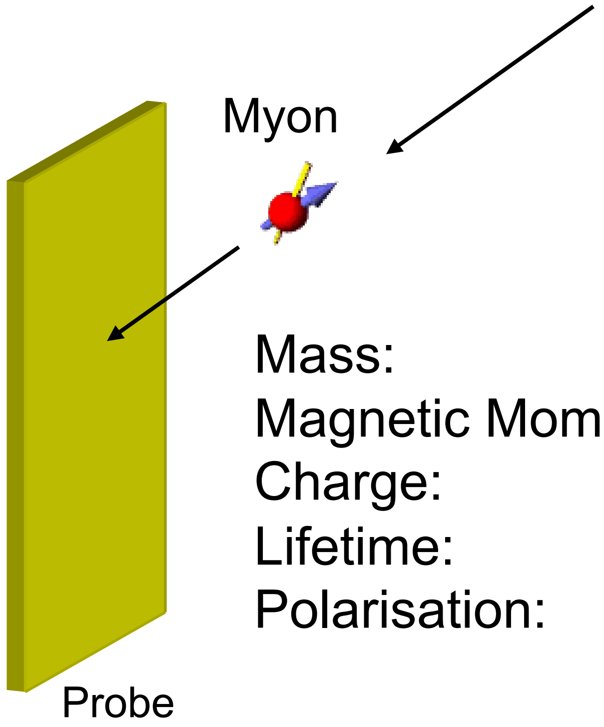
Charge state	π^+	π^-
Mean lifetime (s)	26x10^{-9}	26x10^{-9}
Spin	0	0
Mass (MeV)	139.57	139.57
Decay mode	$\pi^+ \rightarrow \mu^+ + \nu_\mu$	$\pi^- \rightarrow \mu^- + \overline{\nu}_\mu$



100% polarised "*surface*" positive muons (~4MeV) are generally used for condensed matter studies

The principles of a μSR Experiments

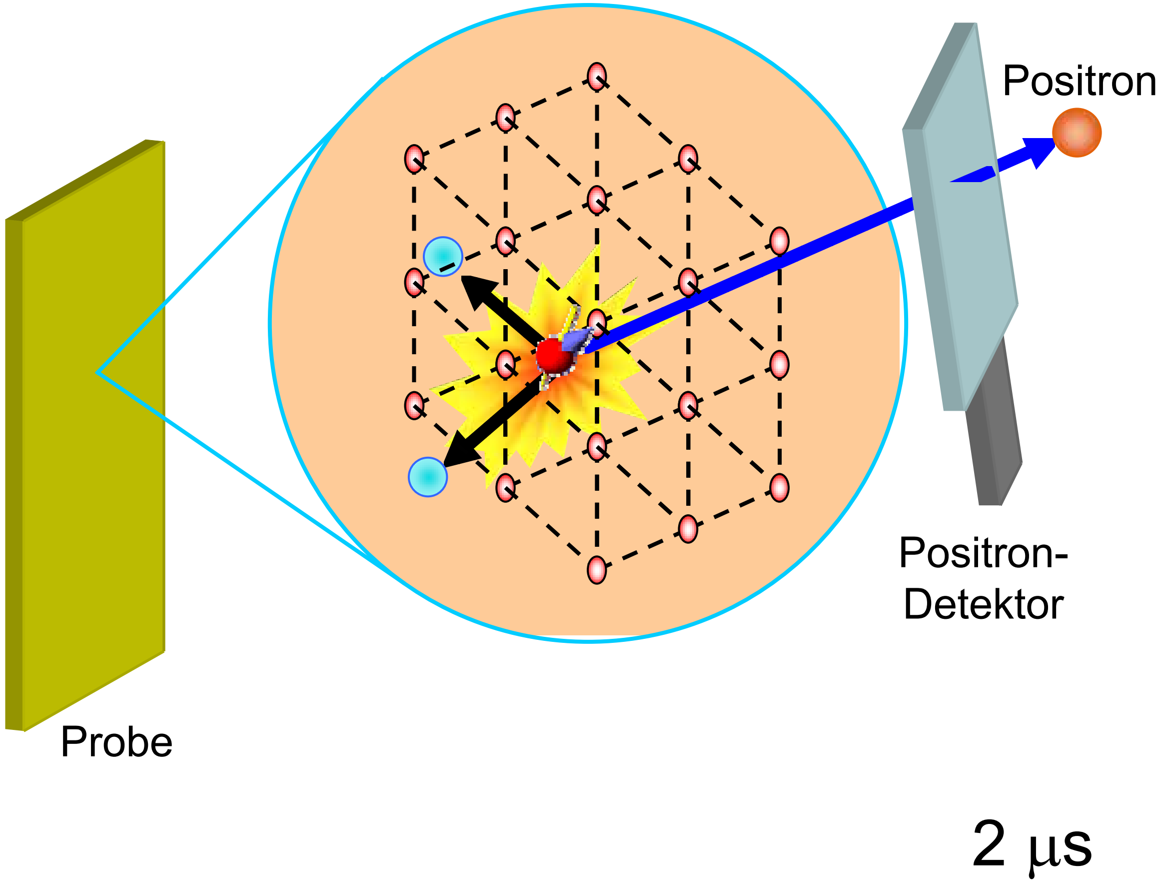
Implantation of Muons in the Probe



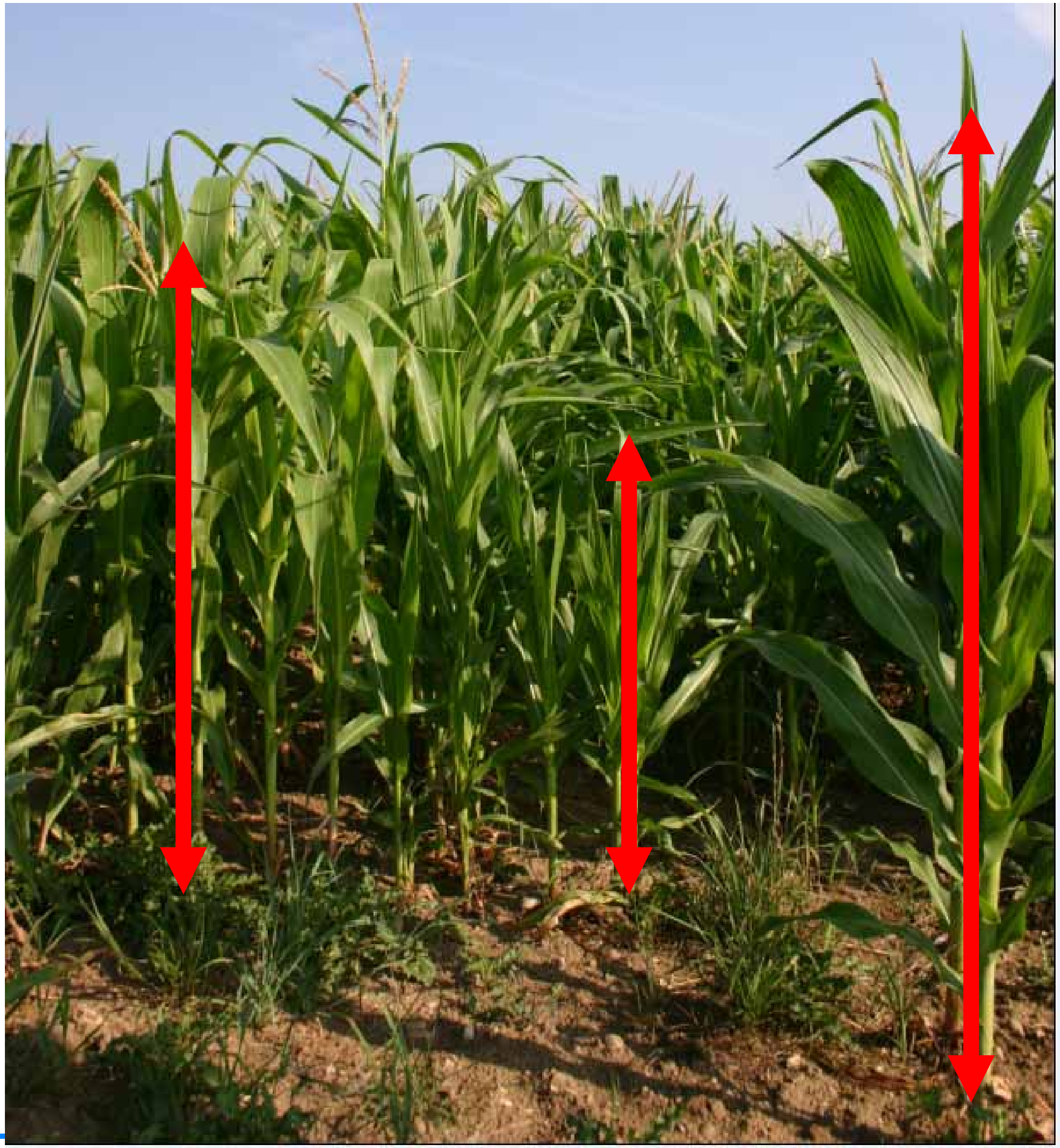
Mass:	$m_\mu \approx 207\ m_e \approx 1/9\ m_p$
Magnetic Moment:	$\mu_\mu \approx 3\ \mu_p$
Charge:	+e
Lifetime:	$t_\mu \approx 2.2\ \mu s$
Polarisation:	100 %

The principles of a μSR Experiments

Detection of the decay positron



Muons – a local probe



Distribution of heights

incl areas with no plants…

μSR - a universal acronym

…..which stands for **Mu**on **S**pin **R**elaxation,
Rotation
Resonance

relaxation describes the time-dependent loss of polarisation of the muon spins by internal fields either in zero applied field or in a field applied parallel to the initial muon spin direction

rotation describes the dephasing of muon spins by local magnetic fields with an applied field transverse to the muon spin direction

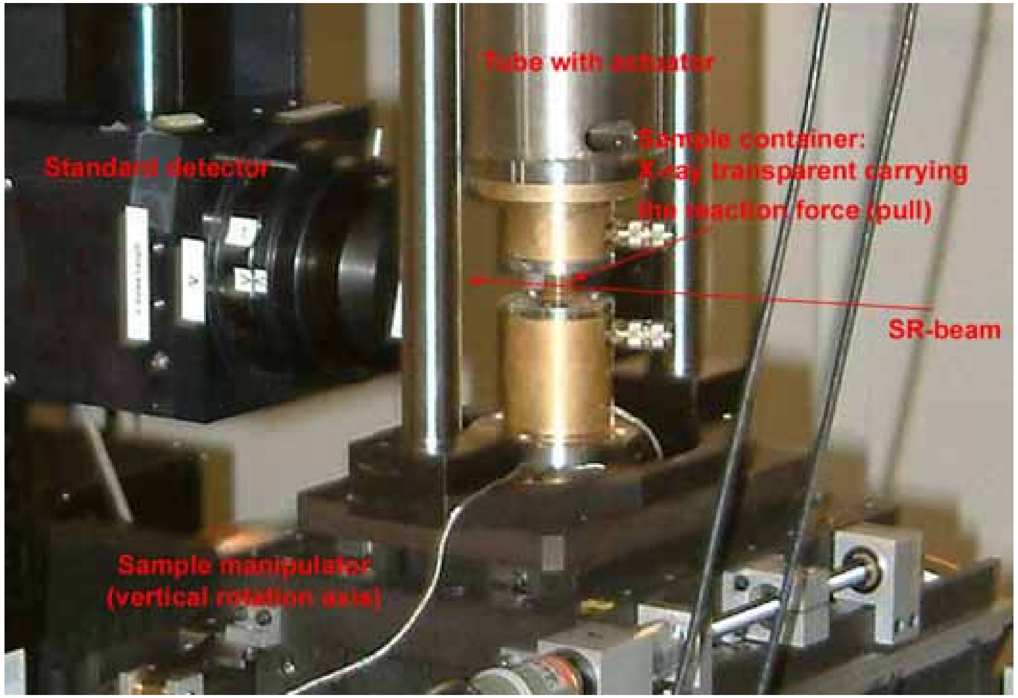
resonance is associated with RF induced transitions (*cf NMR*)

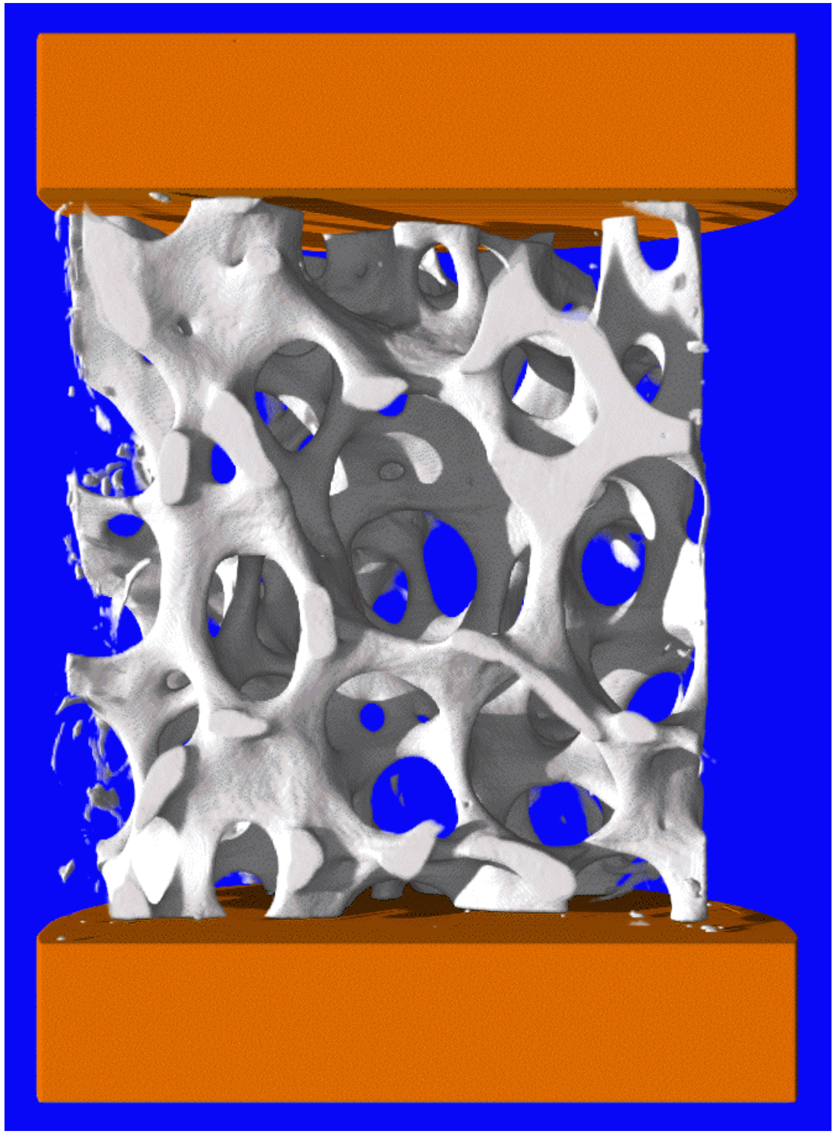
Now on to photons --- X-rays

Wilhelm Conrad Röntgen,
"Father" of X-rays

Hand of Bertha Röntgen
exposure 20 min,
8 Nov 1895

Cracking bones a hundred
years later……

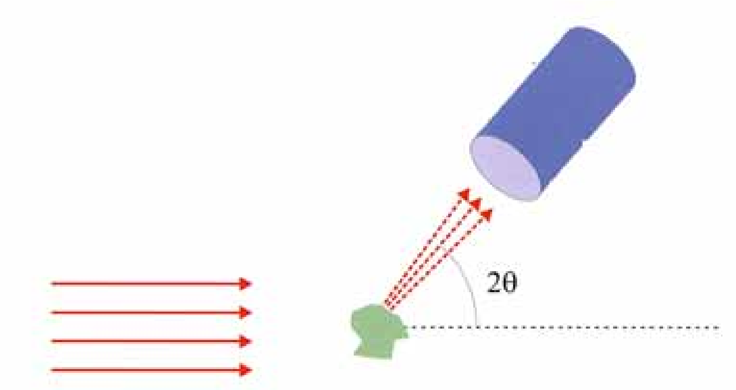




This is called *tomography*

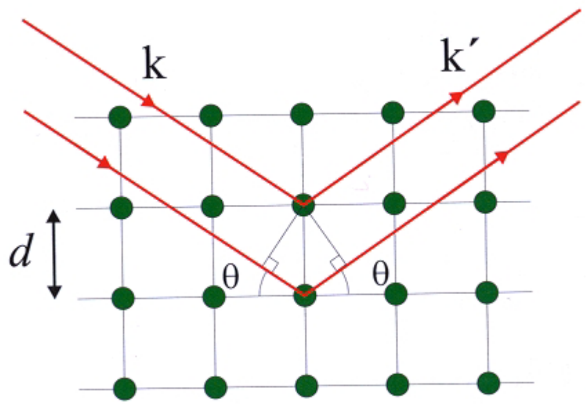
Friso van der Veen, PSI

X-ray diffraction from crystals → structure



Bragg's law:

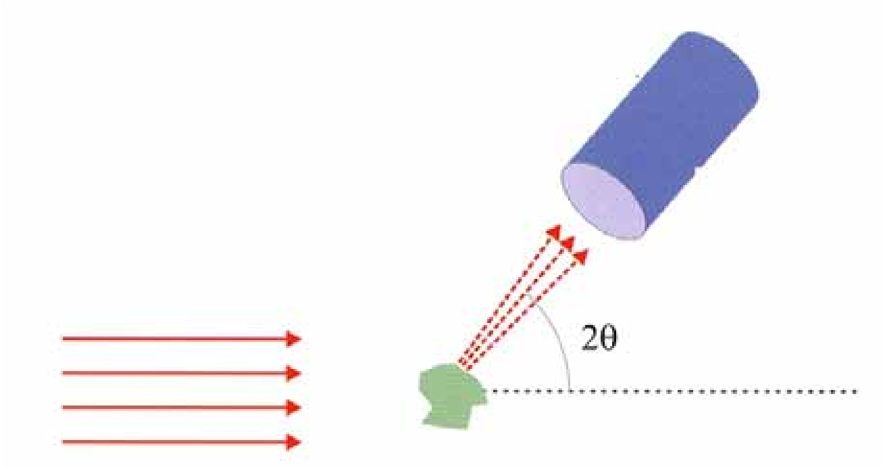
$$m\lambda = 2d\sin\theta$$



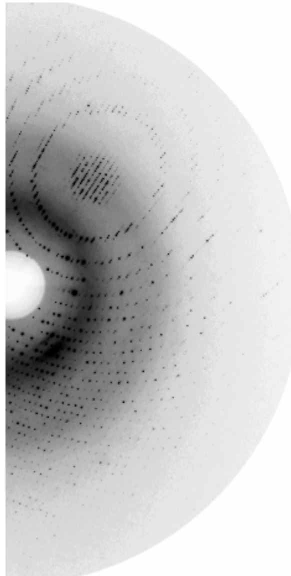
$$k = 2\pi/\lambda$$

J.Als-Nielsen, Des Mc Morrow

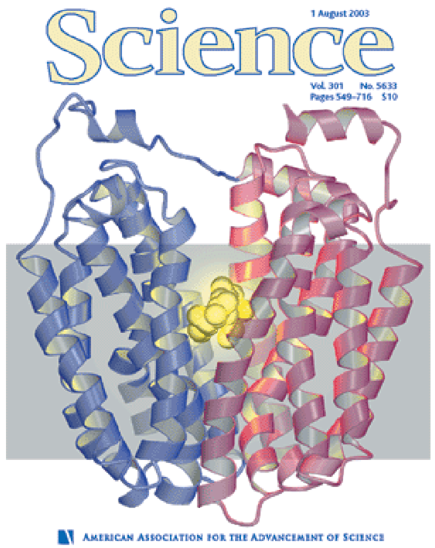
Structural biology



X-ray beam



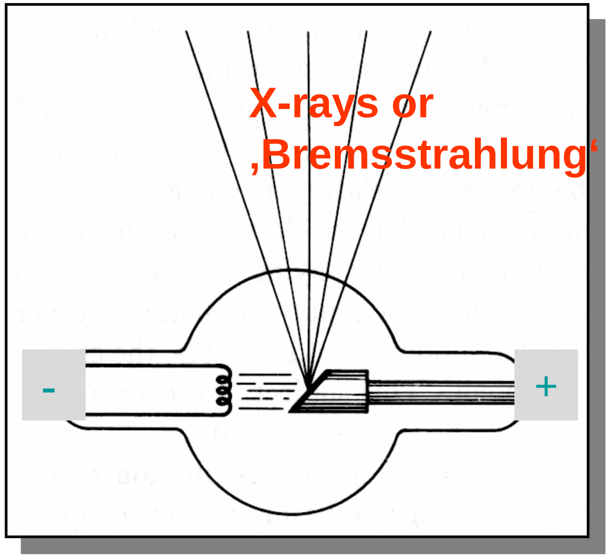
Diffraction pattern



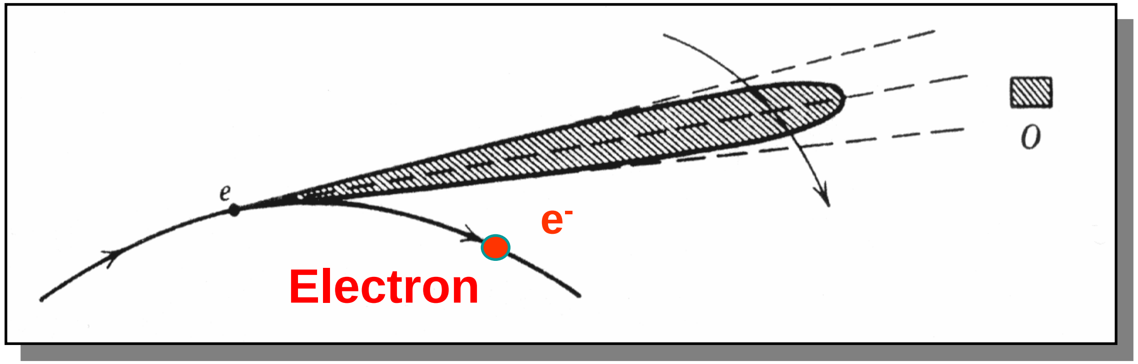
Structure of membrane protein
succinate dehydrogenase (SDH) ,

V. Yankovskaya, S. Iwata et al
Science 299 (2003) 700

Origin of synchrotron radiation



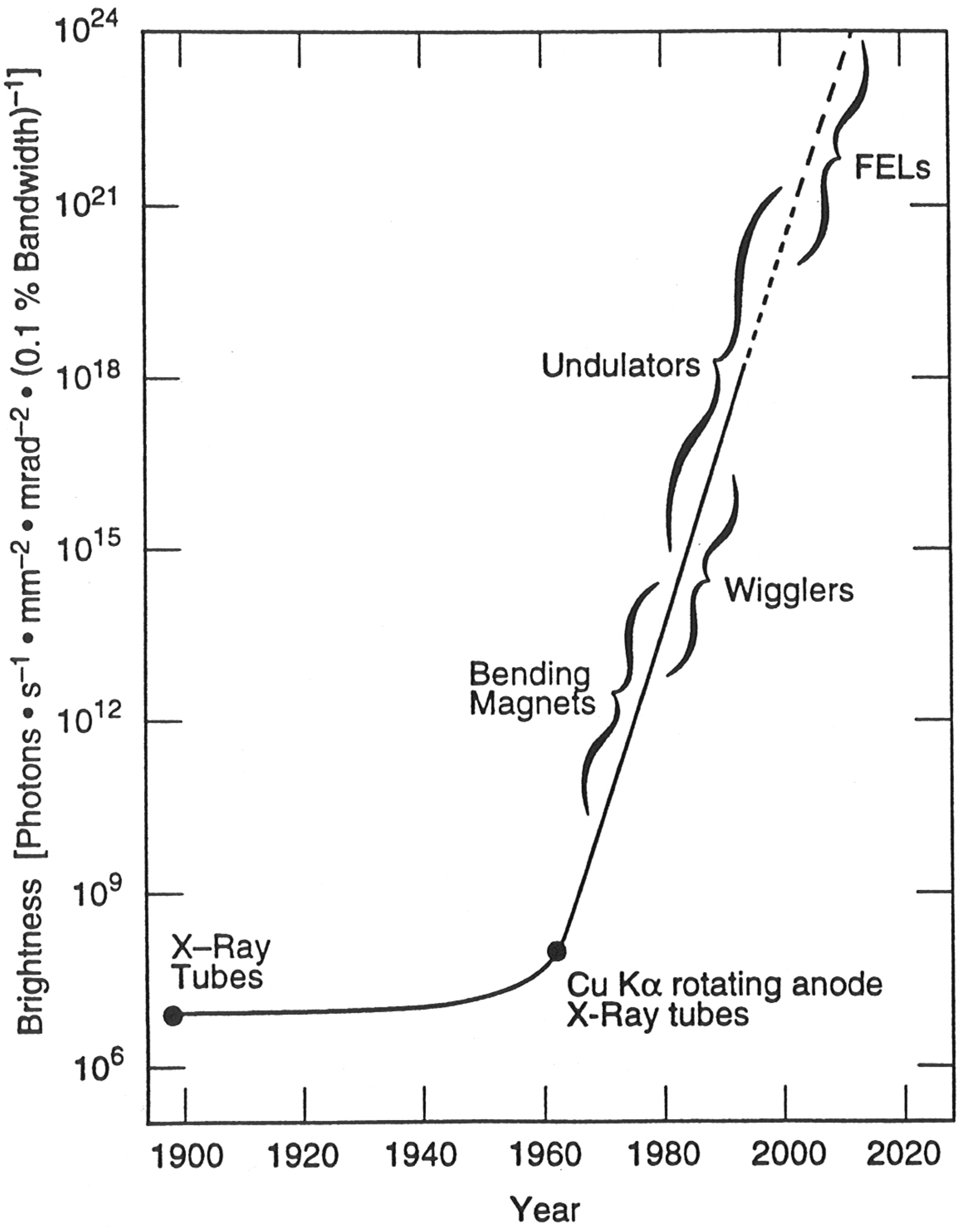
X-ray tube



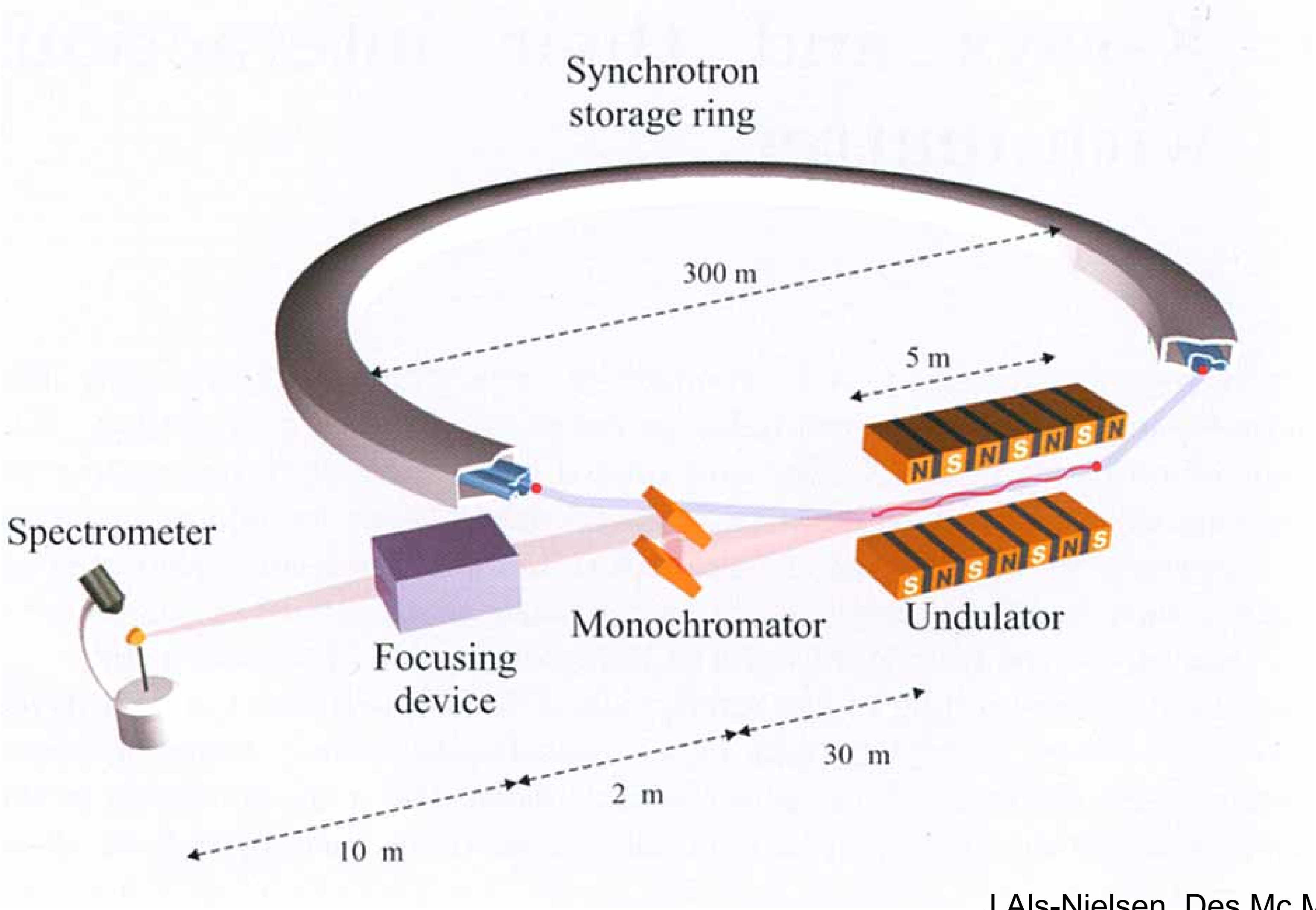
Radiation of charged particle in magnetic field

Brilliant as a lighthouse!

Friso van der Veen, PSI


Brightness [Photons • s−1 • mm−2 • mrad−2 • (0.1 % Bandwidth)−1]
10^24
10^21
10^18
10^15
10^12
10^9
10^6
FELs
Undulators
Wigglers
Bending Magnets
X–Ray Tubes
Cu Kα rotating anode X-Ray tubes
1900
1920
1940
1960
1980
2000
2020
Year

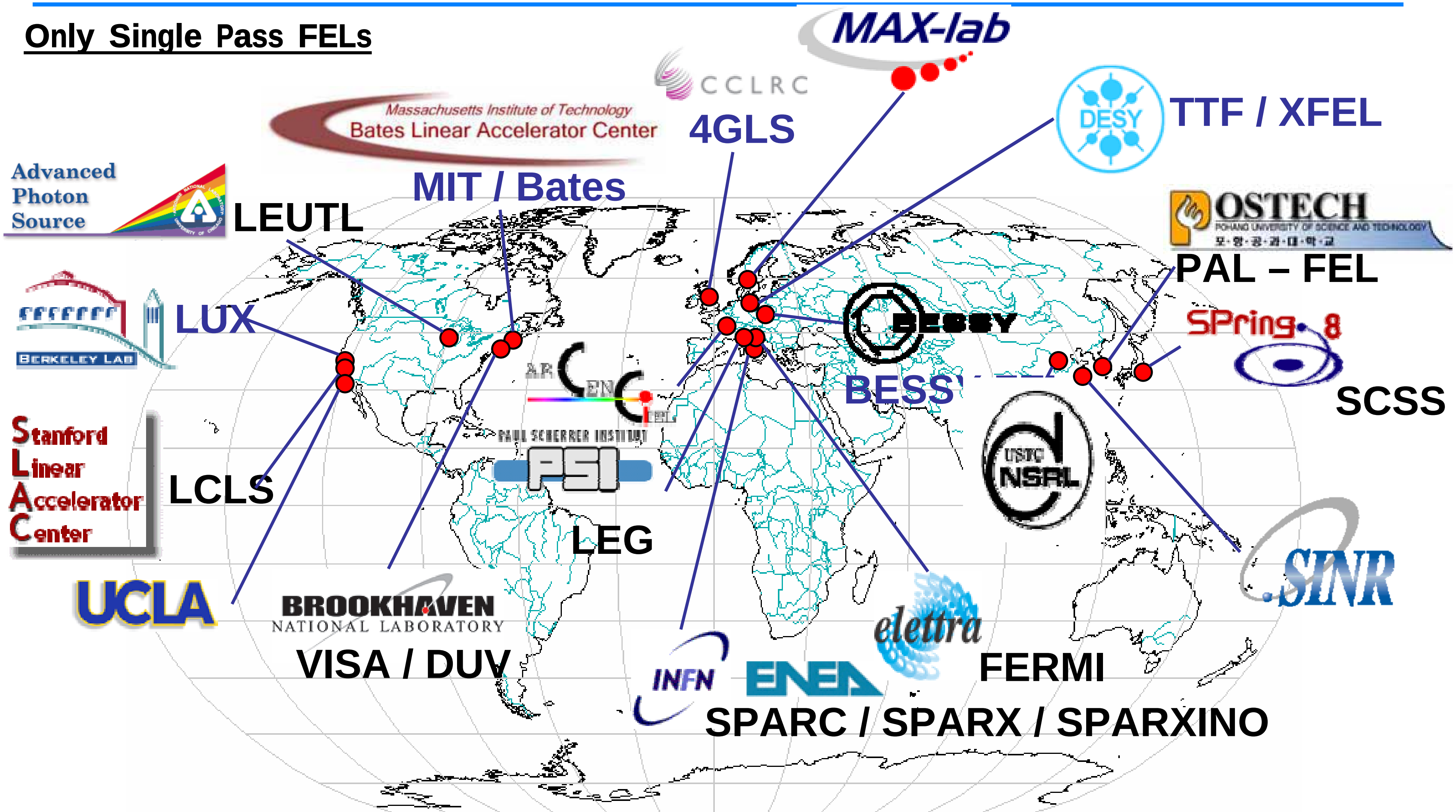
Light from undulators and wigglers



J.Als-Nielsen, Des Mc Morrow

PAUL SCHERRER INSTITUT PSI

Only Single Pass FELs



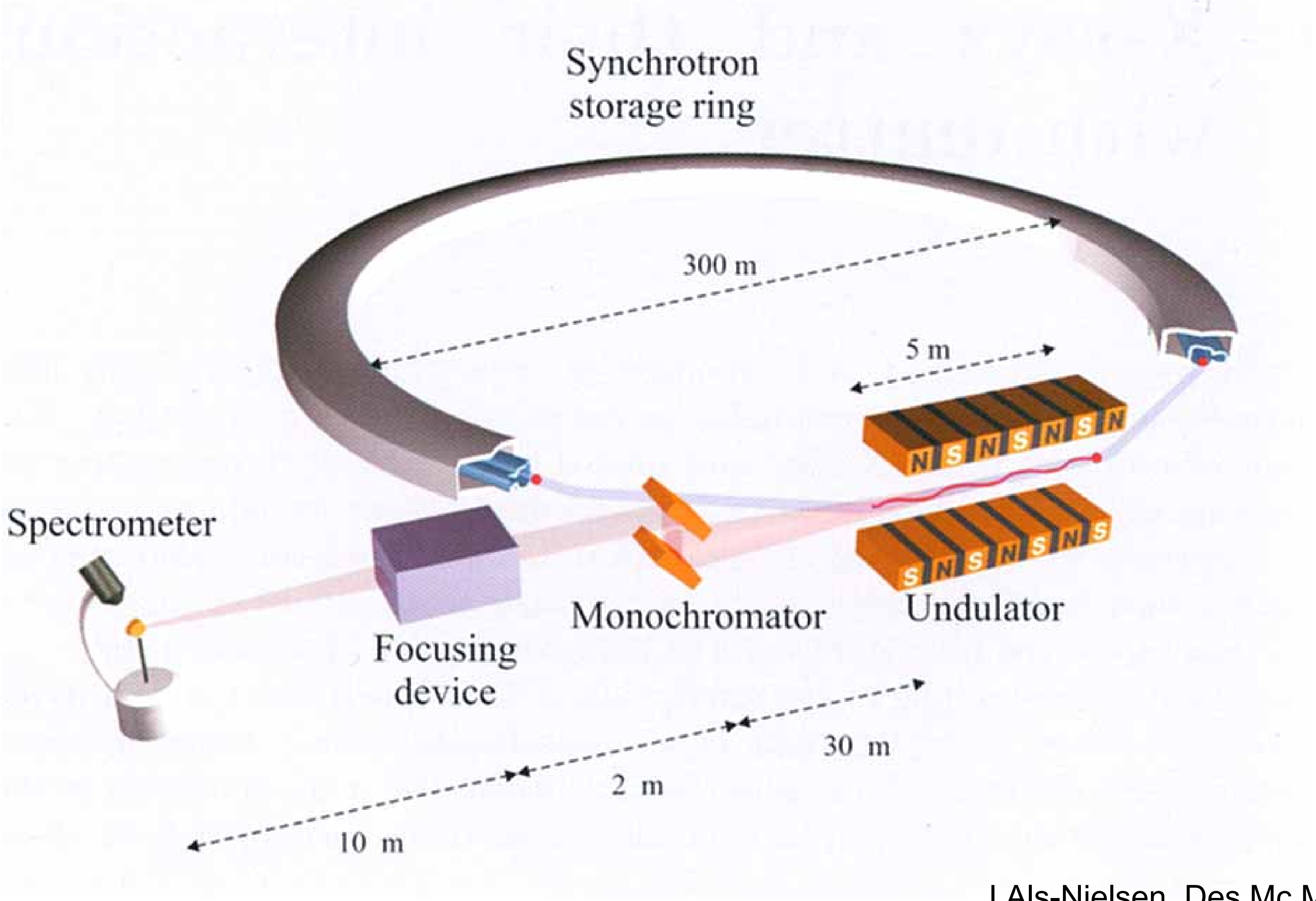
SC technology / NC technology

…

I will not mention --- resonant diffraction, spectroscopy, EXAFS and other abortion techniques and ….

But a few examples of using the pulsed character of the electrons circulating in the synchrotron…

Bunches of electrons in the ring!

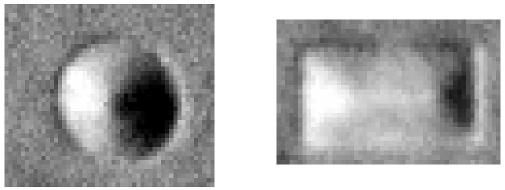


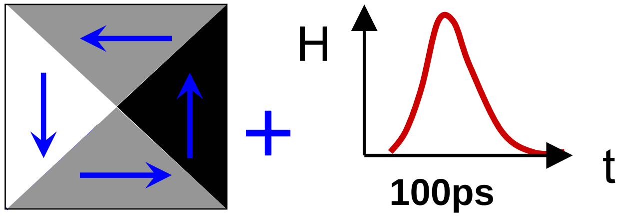
J.Als-Nielsen, Des Mc Morrow

X-ray pulses from single electron bunches in storage ring

Typical duration of electron bunch : 20-60 ps

An example:
Dynamics of nanostructured magnetic objects
Make movies of magnetic particles   μm & sub-ns





J. Raabe, C. Quitmann et al

IBM / HITACHI (2005)
Microdrive, 6 GByte, Pentium IV: 3GHz

Magnetic imaging

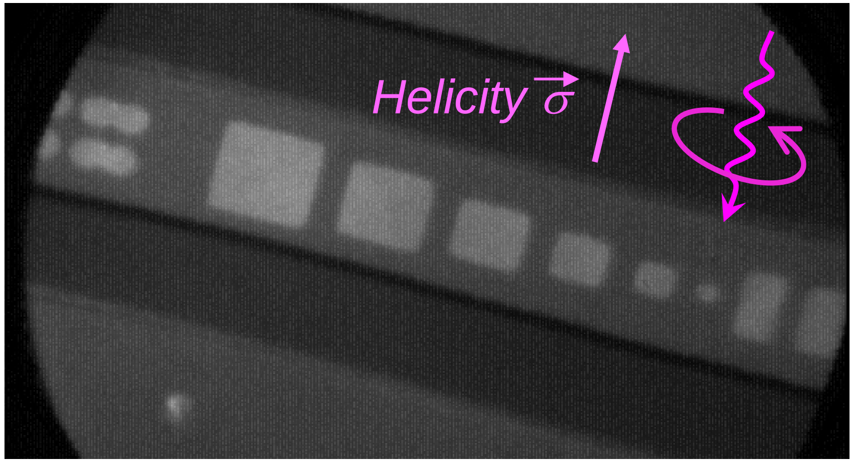


Image 1

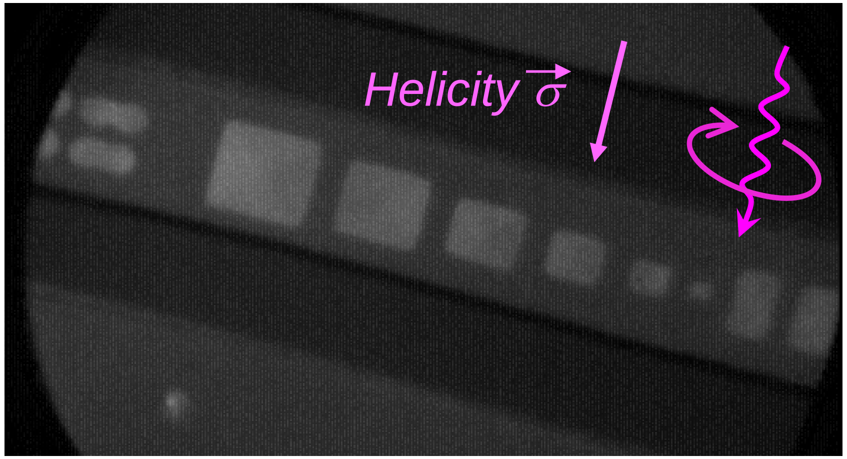
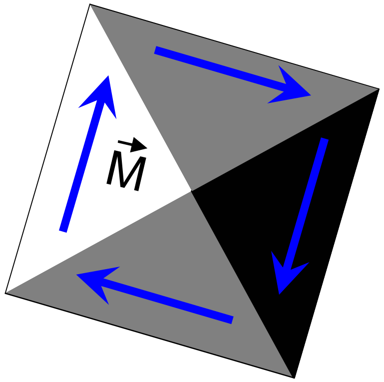


Image 2



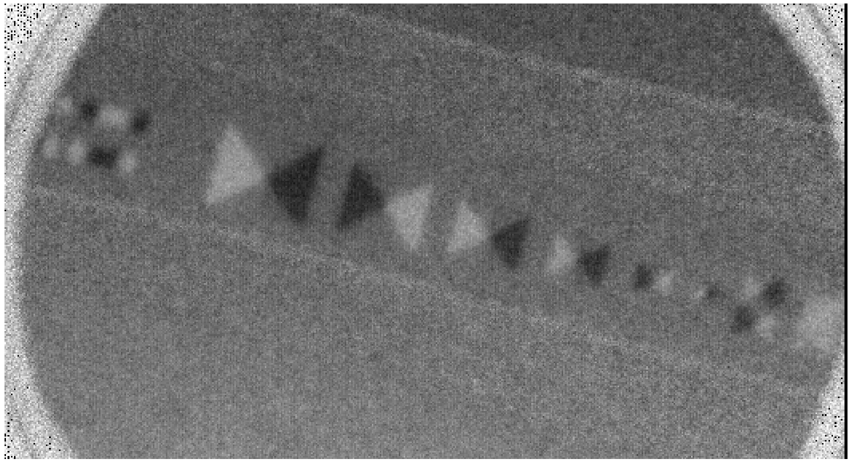
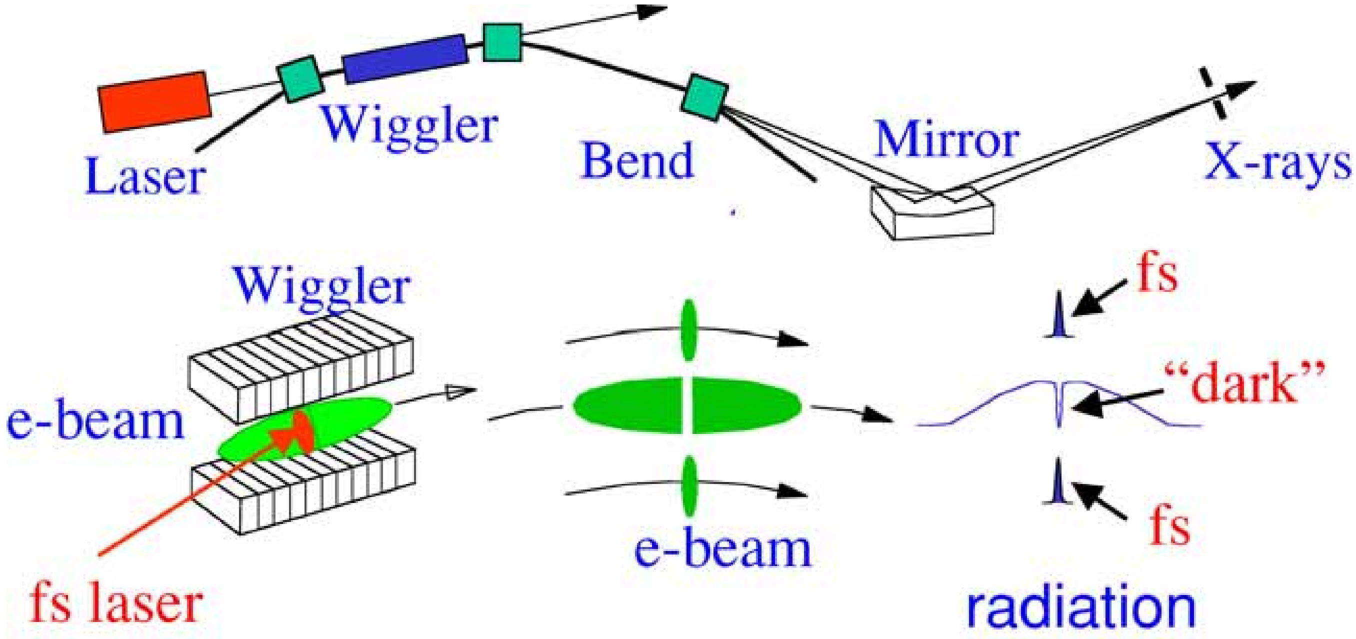


Image 1 / Image 2

Magnetic contrast: $I(\vec{r}) \sim \vec{M}(\vec{r}) \cdot \vec{\sigma}$

Towards shorter X-ray pulses

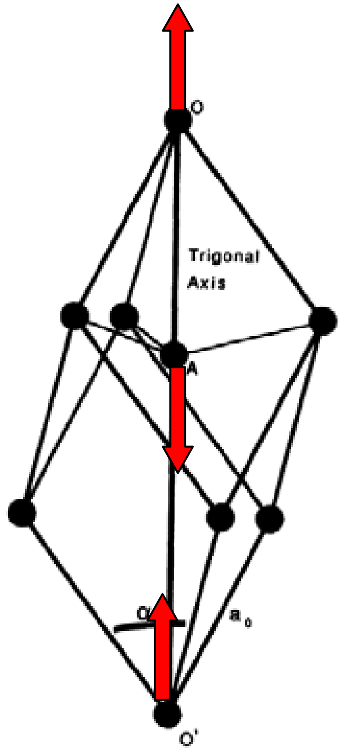
Generating 50-100 fs pulses by electron beam slicing:



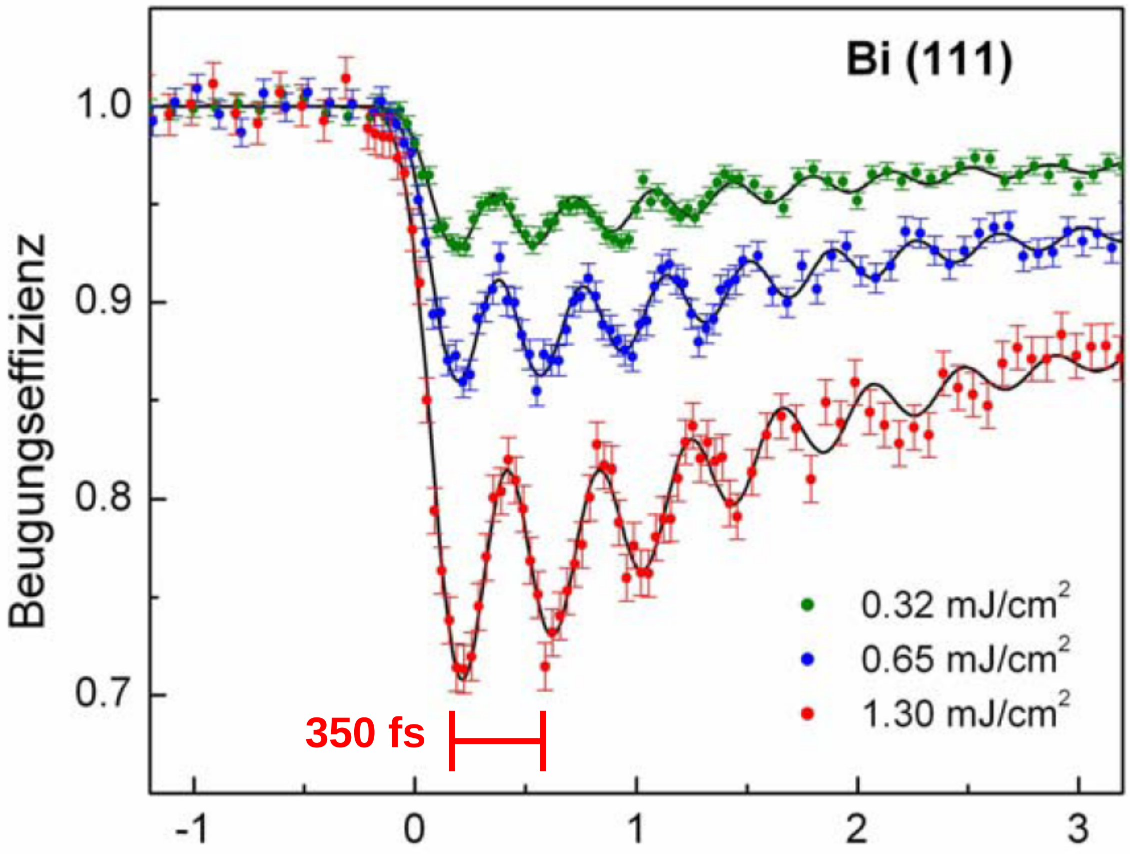
R.W.Schoenlein et al.
Science 287 (2000), 2237

First results from FEMTO beamline

Lattice vibration after excitation



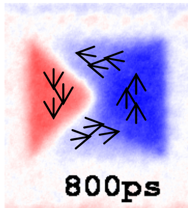
X-ray diffraction from Bi crystal
G. Ingold, S. Johnson *et al*



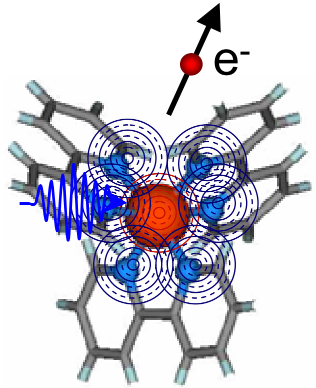
Delay time after excitation [ps]

Images with ever increasing speed

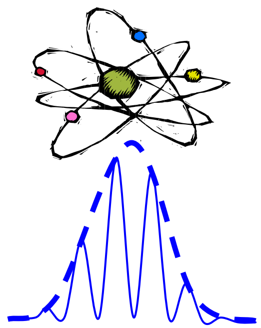
2005: **Movies of magnetic domains. Every 100 picoseconds a new image!**



2006: **Follow vibrations in solids and structural changes in molecules in 1000 times smaller time steps (in femtosecond range).**

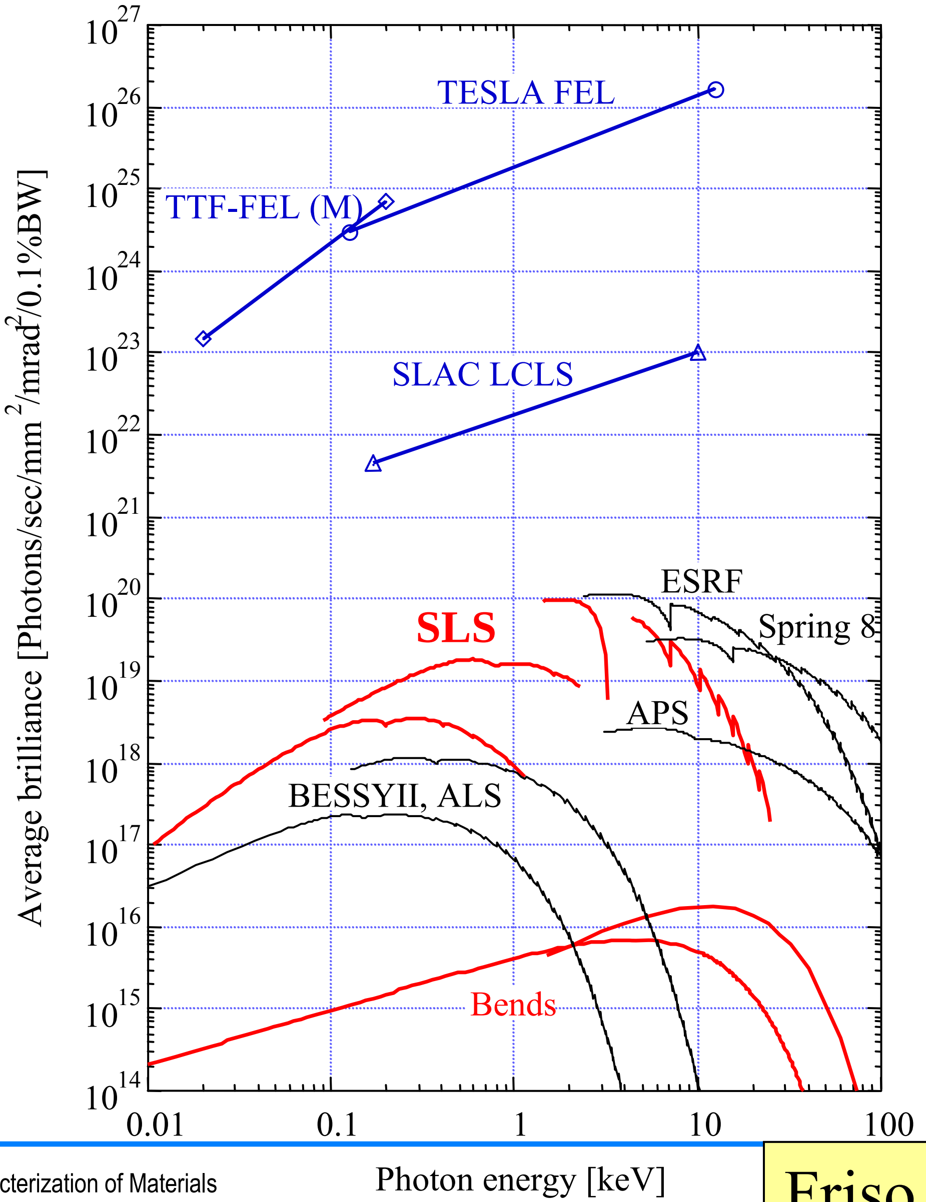


>2010: **DREAM: Use X-ray lasers to image single molecules in a few femtoseconds ???.**



Friso van der Veen and Kurt Clausen, PSI

Brilliance of some sources



Friso van der Veen, PSI

THEORY predicts that intense and short X-ray pulses may allow high resolution imaging of biomolecules

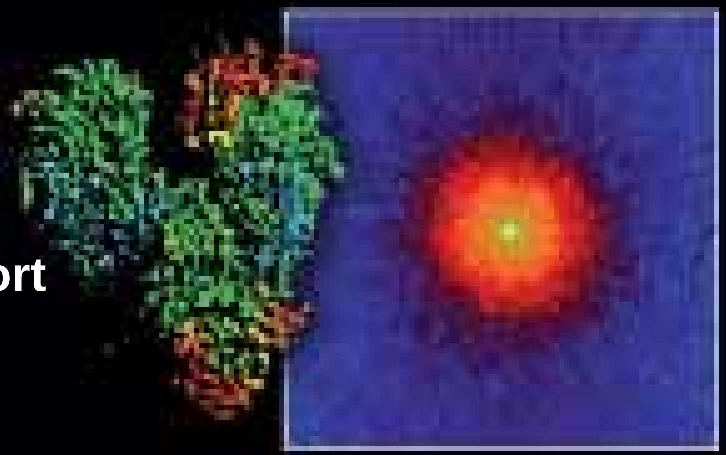
sample injec

eckert, Hajdu

A wonderful dream

but is it realistic?

X-fel pulse

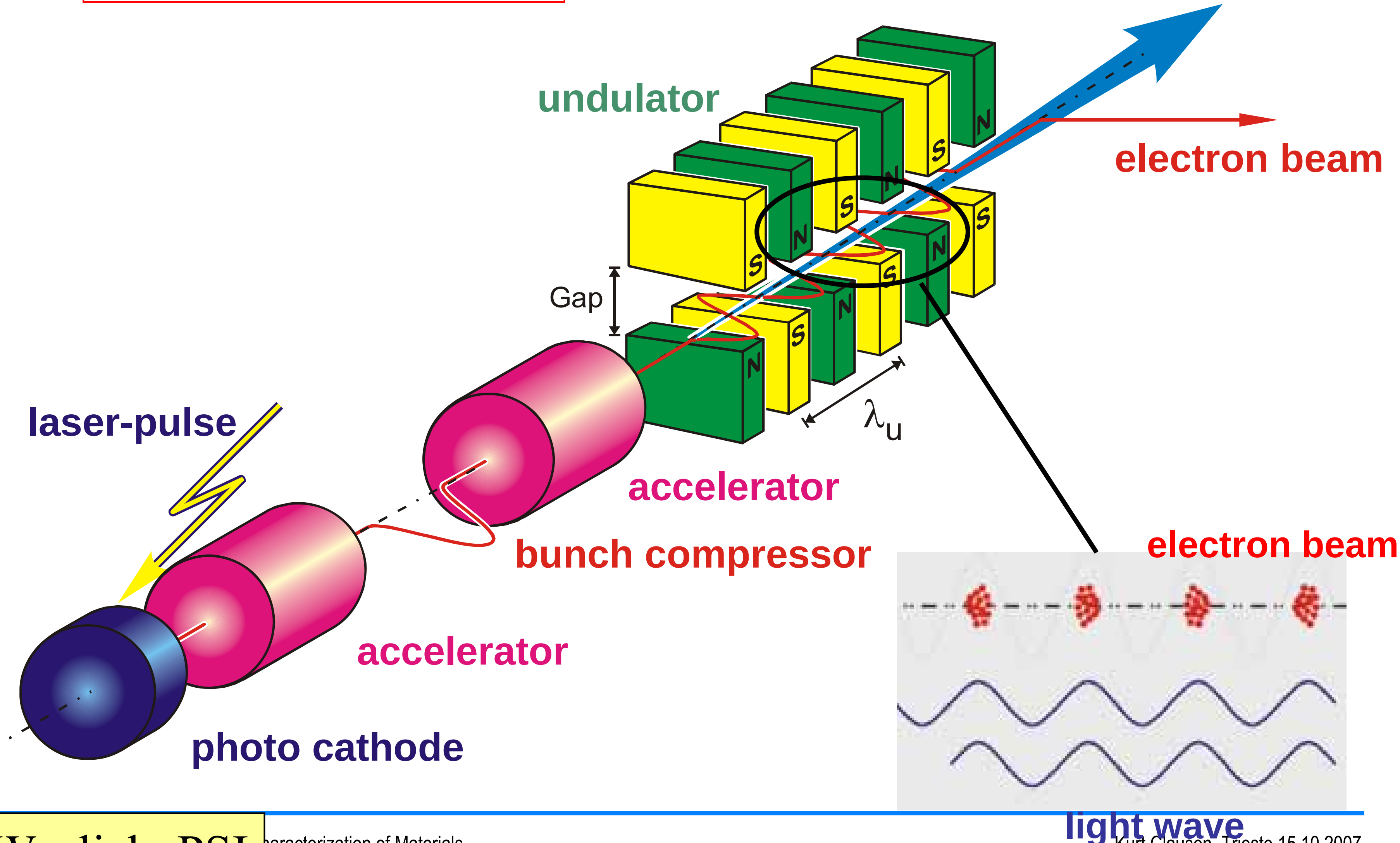


Concept: Capture an image with a short and intense X-ray pulse, *before* the sample has time to respond (explode)

X-ray diffraction pattern

A Wrulich and Kurt Clausen, PSI

FEL Fundamentals

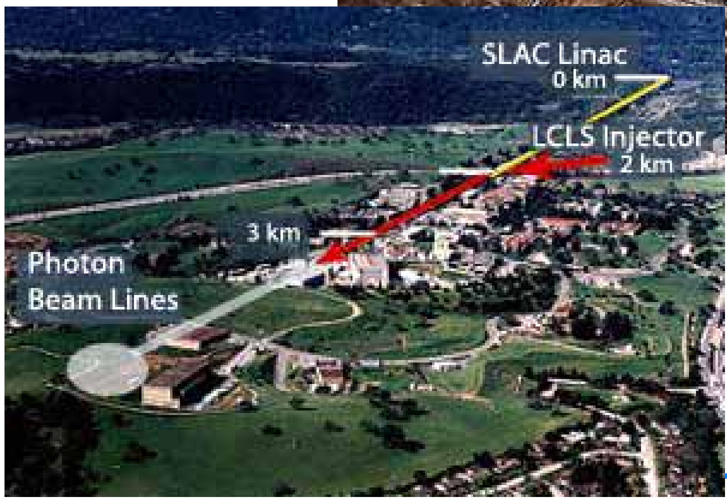


A Wrulich, PSI

X-FEL Facilities

Europe
X-FEL–DESY 2012

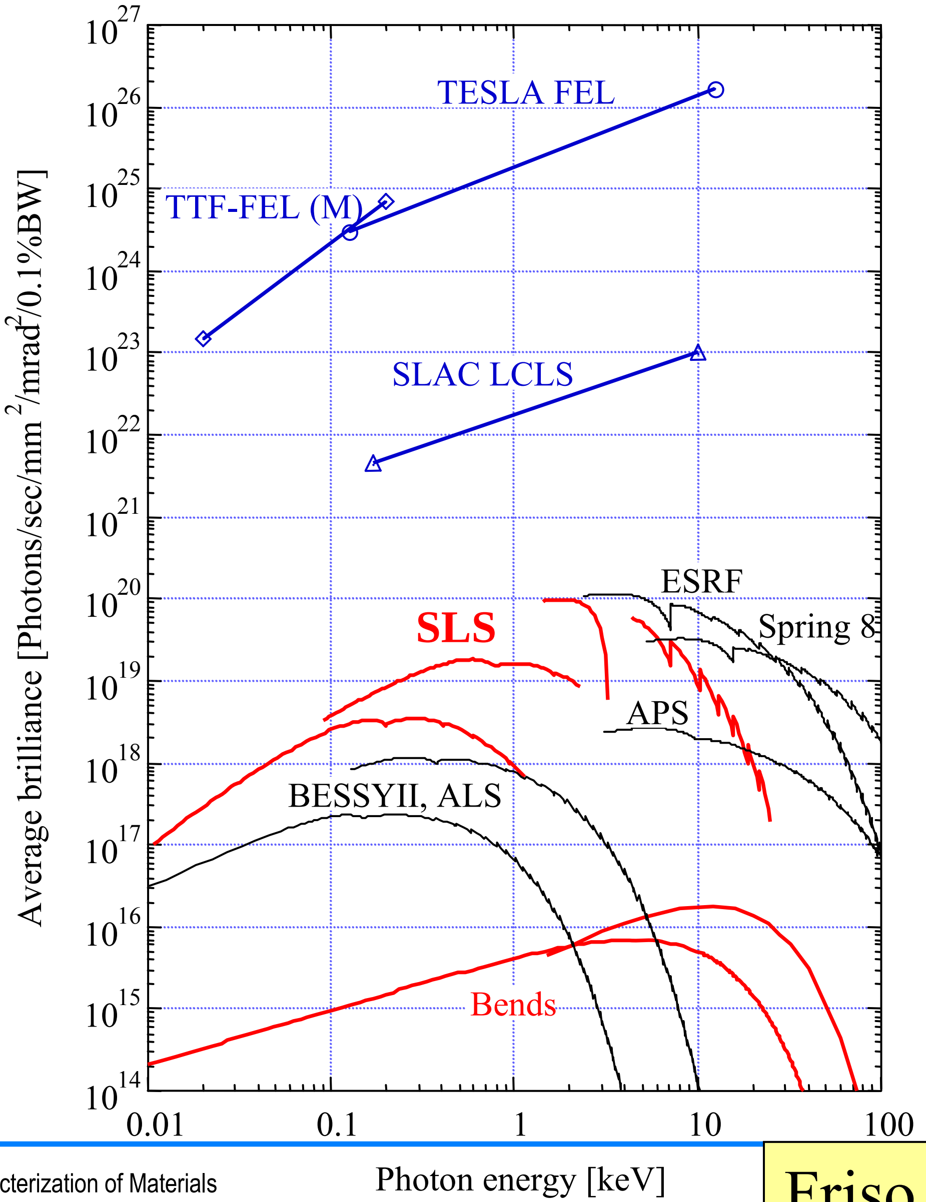
Japan
SCSS–SPring8
2010



USA
LCLS-SLAC
2009

A Wrulich, PSI

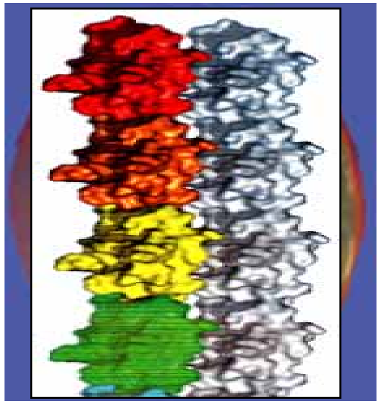
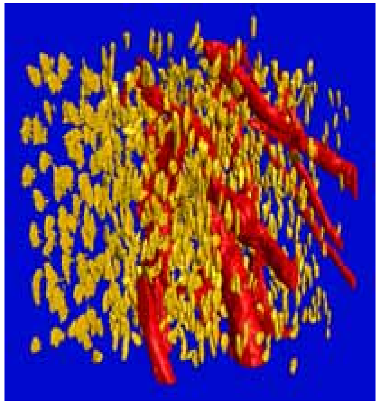
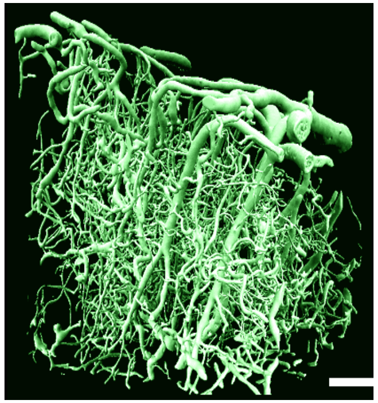
Brilliance of some sources



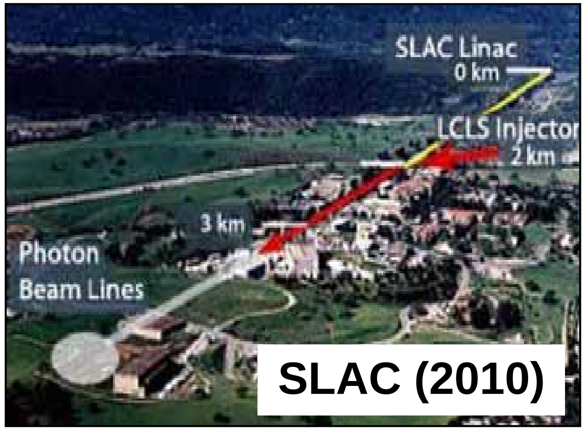
Friso van der Veen, PSI

Coherent X-ray Imaging & Future XFEL Sources

Synchrotron / XFEL | Synchrotron | Laboratory | Laboratory | Hospital

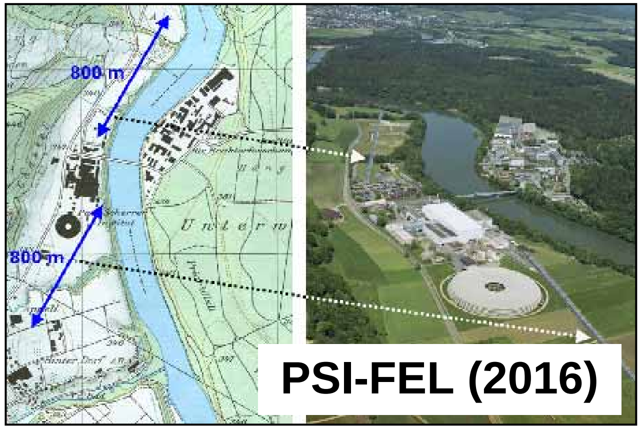




1 Å — 1 µm — 1 mm — 1 m



SLAC (2010)

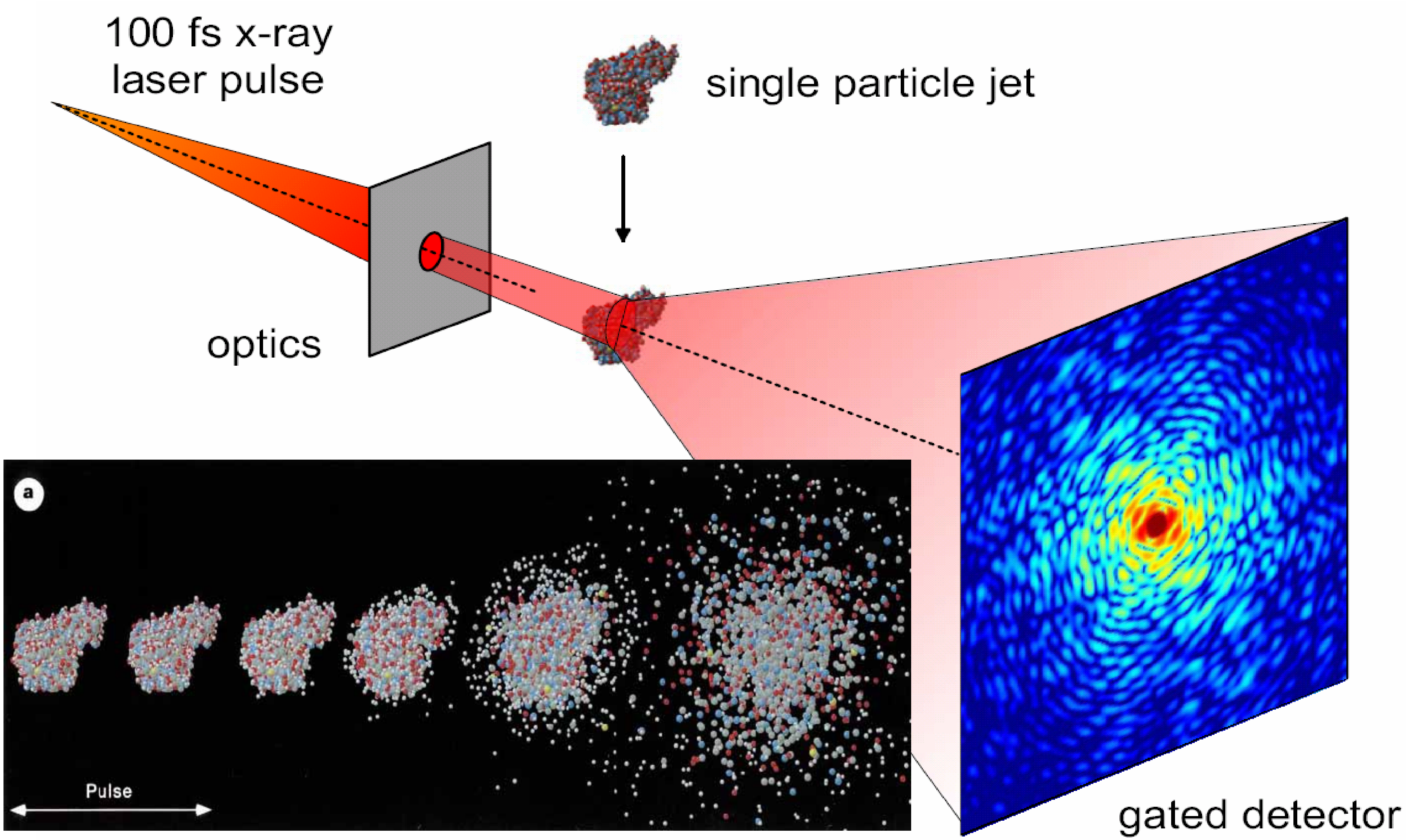

Euro-XFEL (2013)



PSI-FEL (2016)

Franz Pfeiffer, PSI

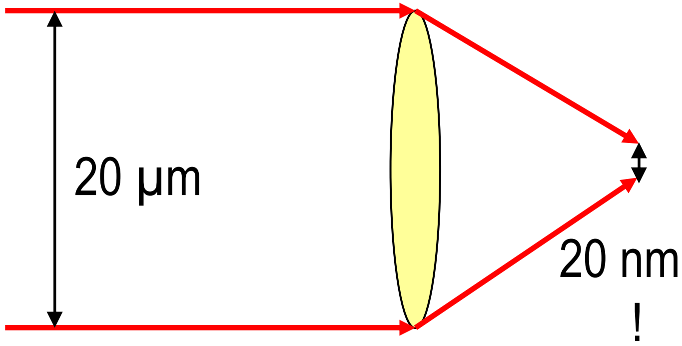
Future: Atomic Resolution from Single Macromolecules ?



R. Neutze et al., Nature 406, 752 (2000); J. Hajdu et al., JSB 144, 219 (2003); H. Chapman et al., Nat. Physics 2, 839 (2007)

Some realistic numbers...

Thomson scattering for a single molecule:



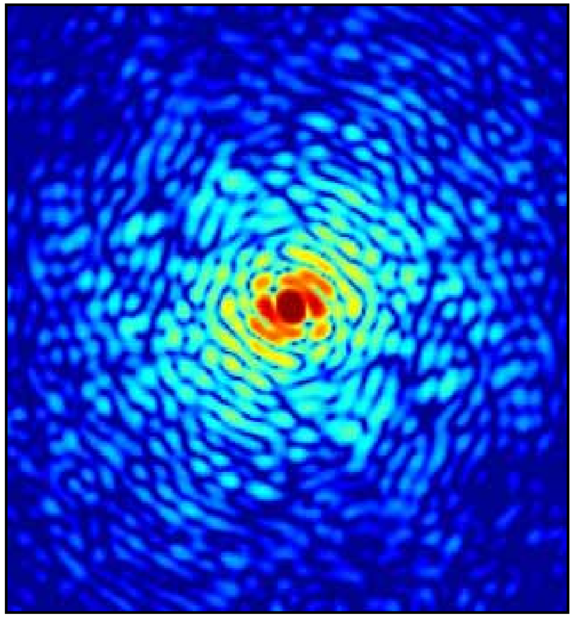
$$I_{scat} = (I_{in}/A_{in})\, \Omega_{det}\, r_e^{\,2}\, N^2$$

I_{in} ~ 2 x 10^{11} ph/pulse, A_{in} = (10 µm)^2 π,

Ω_{det} = 10^{-6} [A_{det} = 1 mm^2, R_{det} = 1 m]

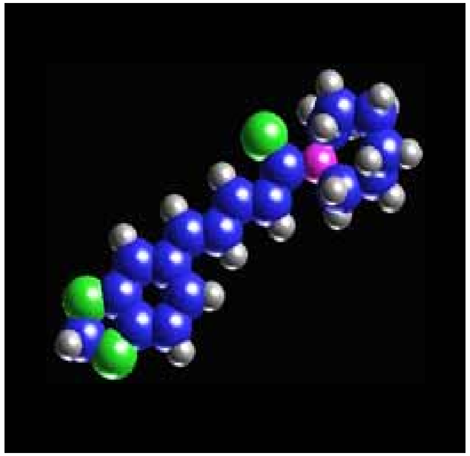
r_e = 2.82 x 10^{-15} m, gain = 2 x 10^5 (optimistic)

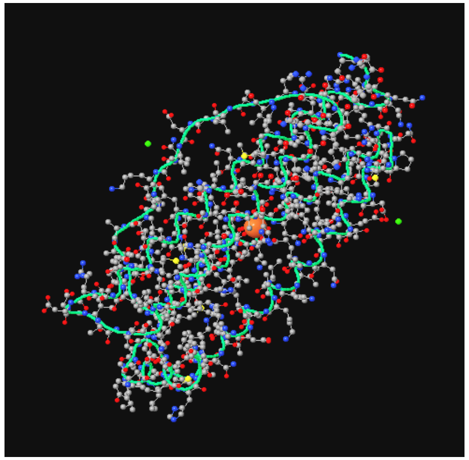
- I_{scat} ~ 5 x 10^{-15} (1 electron) => 1 x 10^{-9}
- I_{scat} ~ 5 x 10^{-9} (10^3 electrons) => 1 x 10^{-3}
- I_{scat} ~ 5 x 10^{-3} (10^6 electrons) => 1 x 10^3
- I_{scat} ~ 5 x 10^3 (10^9 electrons) => 1 x 10^9
  ?

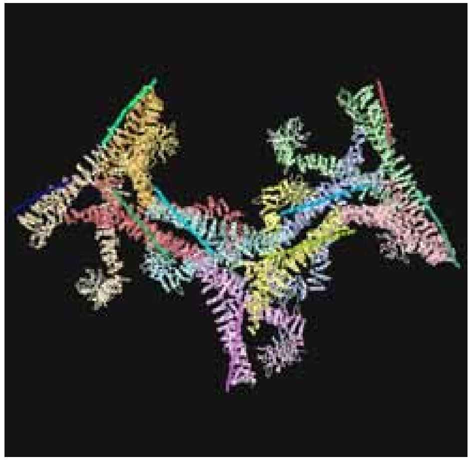


q^{-4} ~ q^{-6} intensity decay !

X-ray Diffractive Imaging of Single Macromolecules

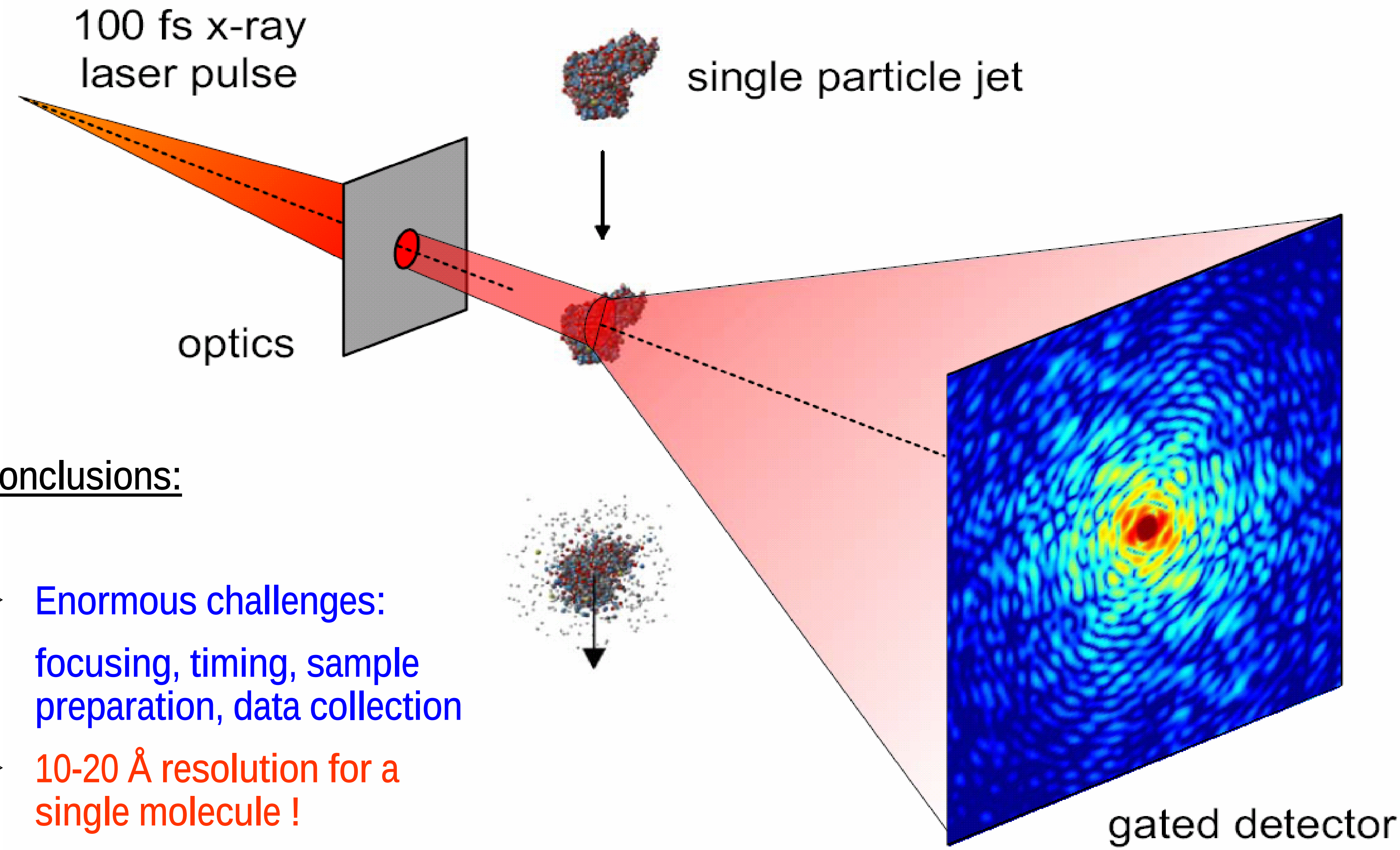

Piperine,
160 e$^-$


Ferritin,
16.789 e$^-$


Clathrin,
91.800 e$^-$

Atomic Resolution from Single Macromolecules ?

10 Å Resolution from Single Macromolecules



Conclusions:

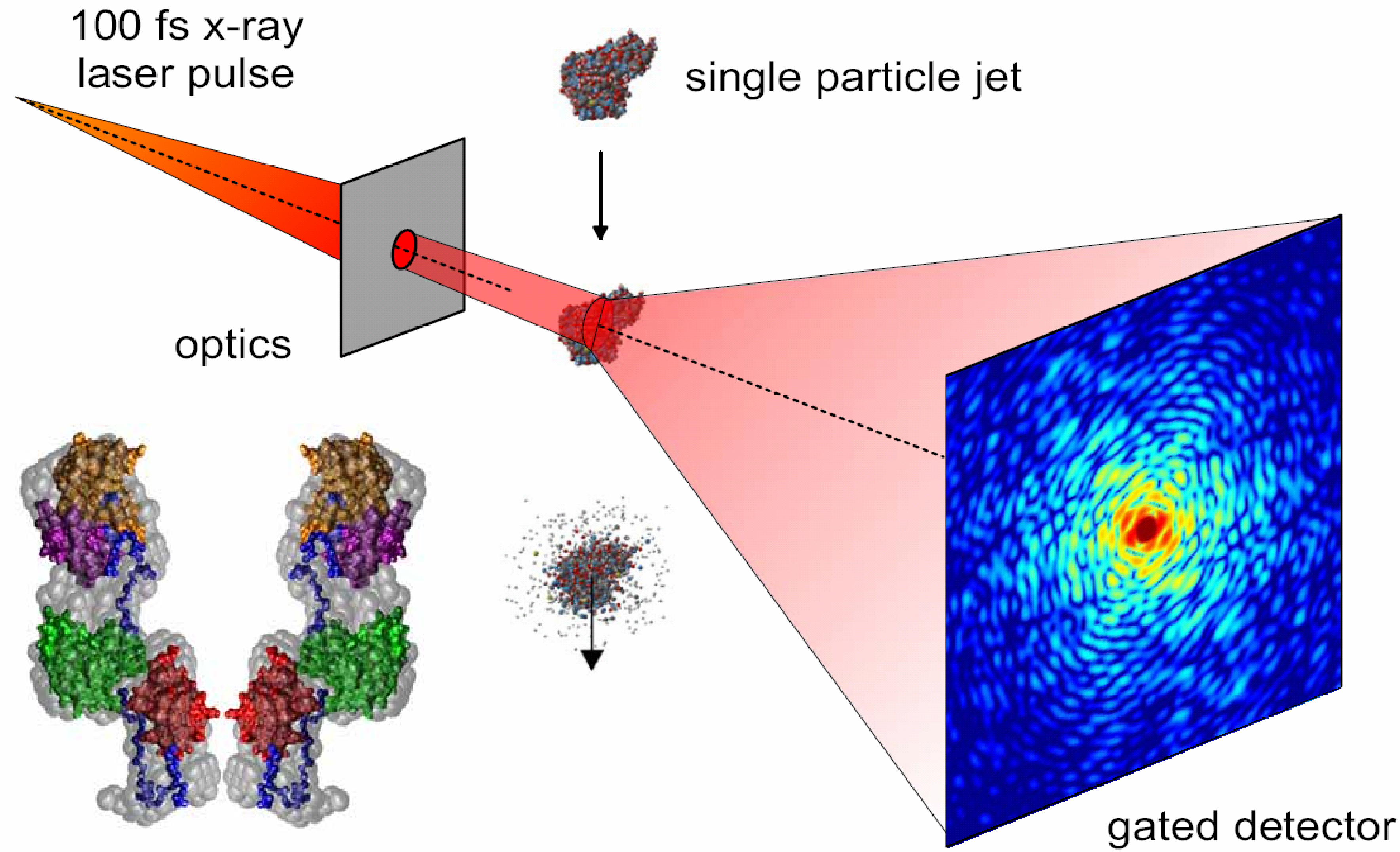
- Enormous challenges:

  focusing, timing, sample preparation, data collection

- 10-20 Å resolution for a single molecule !

R. Neutze et al., Nature 406, 752 (2000); J. Hajdu et al., JSB 144, 219 (2003); H. Chapman et al., Nat. Physics 2, 839 (2007)

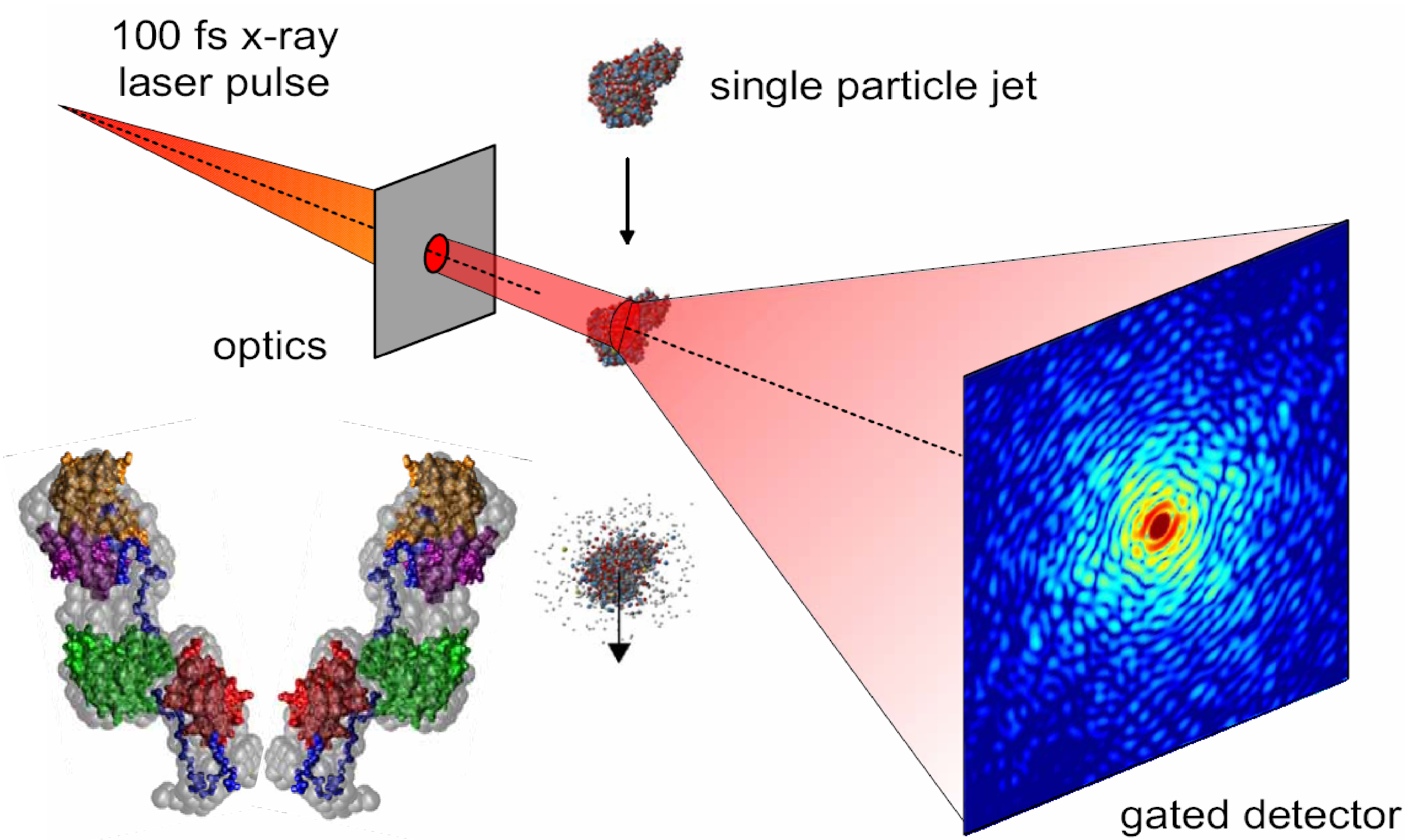
10 Å Resolution from Single Macromolecules



Single particle BioSAXS: Conformational changes in native environment !

Franz Pfeiffer, PSI

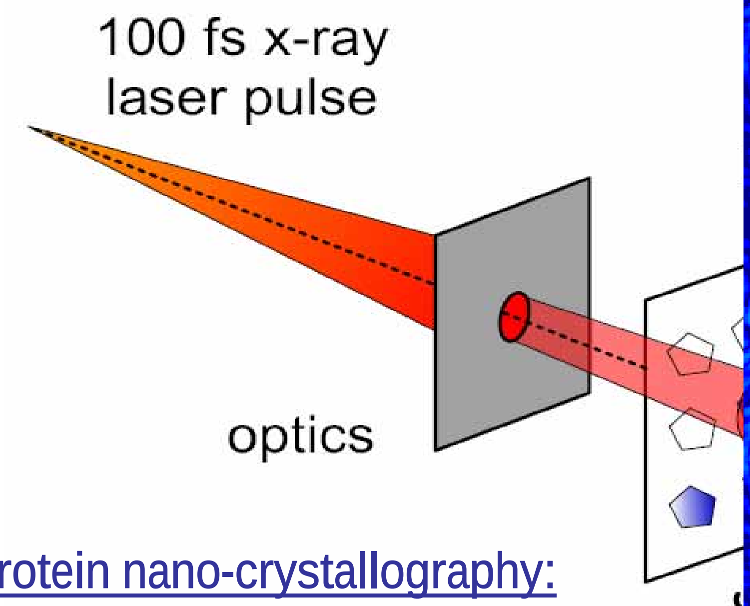
10 Å Resolution from Single Macromolecules

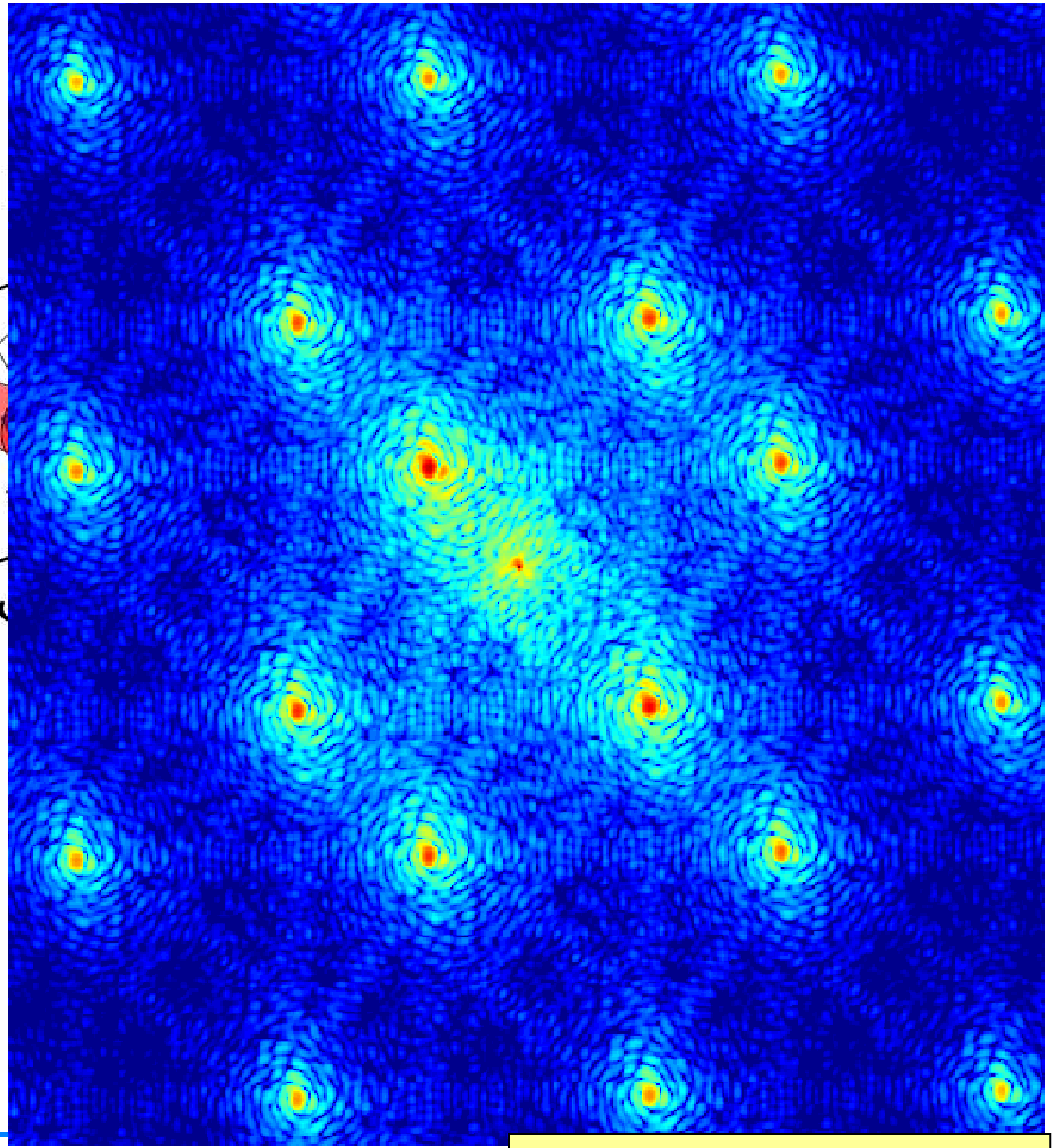


Single particle BioSAXS: Conformational changes in native environment !

Franz Pfeiffer, PSI

Atomic resolution from protein nano crystals ?



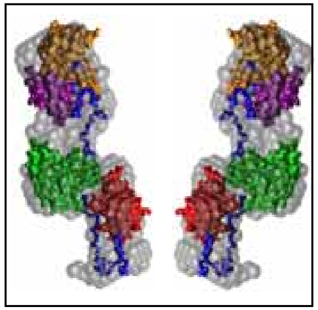


Protein nano-crystallography:

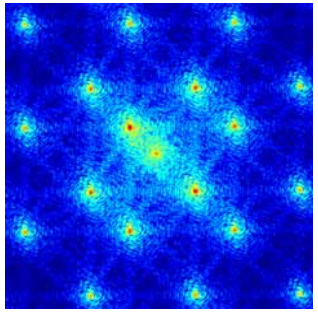
- Combines 'classical' PX with coherent diffractive imaging
- Potential for atomic resolution from sub-micron protein crystals
- fs-experiments can potentially overcome radiation damage

Franz Pfeiffer, PSI

X-FEL - some conclusions



- Diffractive x-ray imaging of single macromolecules could provide insight into conformational changes of known sub-structures at 10-20 Å resolution (Atomic resolution NOT achievable)



- Coherent protein nano-crystallography could provide atomic resolution and overcome existing limitations due to radiation damage (sub micron i.e nano size crystals)

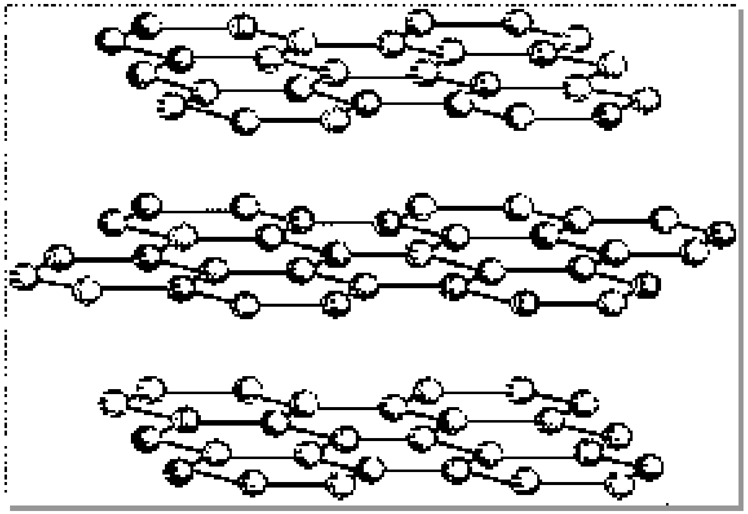
- X-FEL in other fields – science case still in its infancy …
  - Plasma state YES,
  - fs processes?

15 October 2007 – outline:

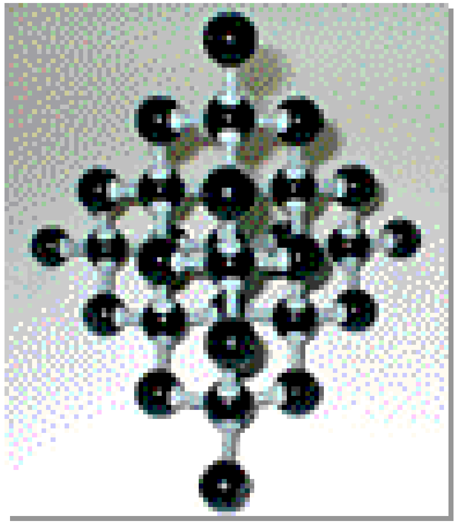
- A short repetition
- Why Neutrons – sources are weak and expensive but properties unique
- Why spallation sources
- Spallation Sources – status and projects
  - ISIS → TS2
  - PSI
  - SNS
  - J-PARC
  - ESS

Structure determines properties

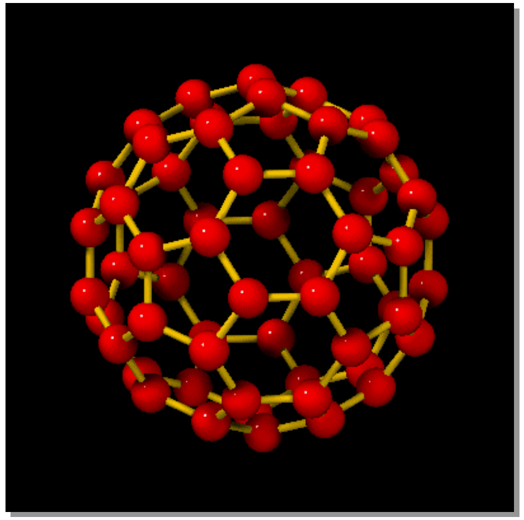
Three forms of carbon – very different materials



Graphite



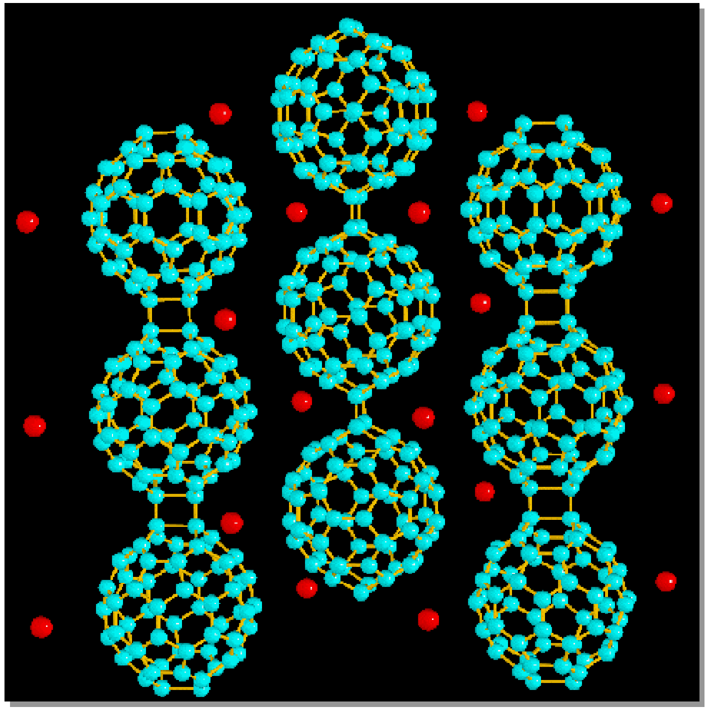
Diamond

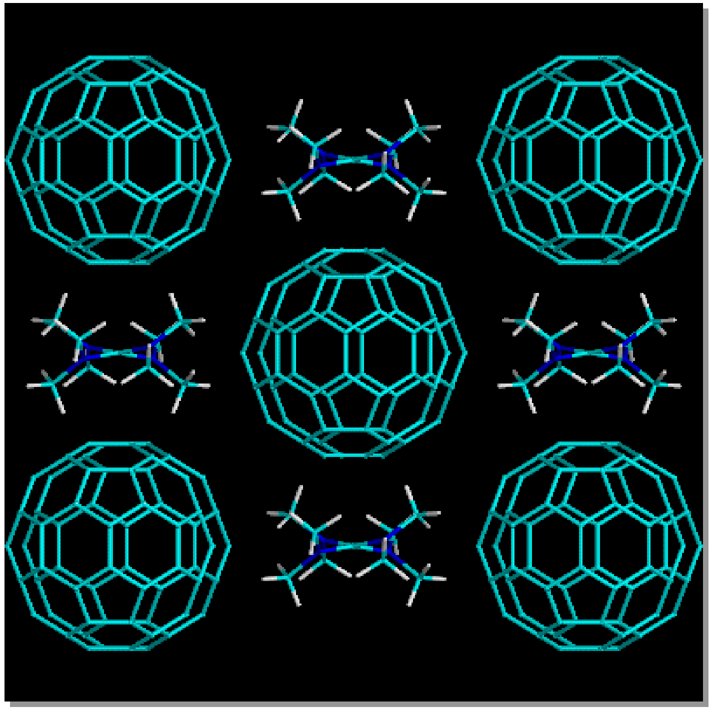


Buckyballs

T Mason, SNS

Structure and dynamics determines "function"





Superconductors or organic ferromagnets

T Mason, SNS

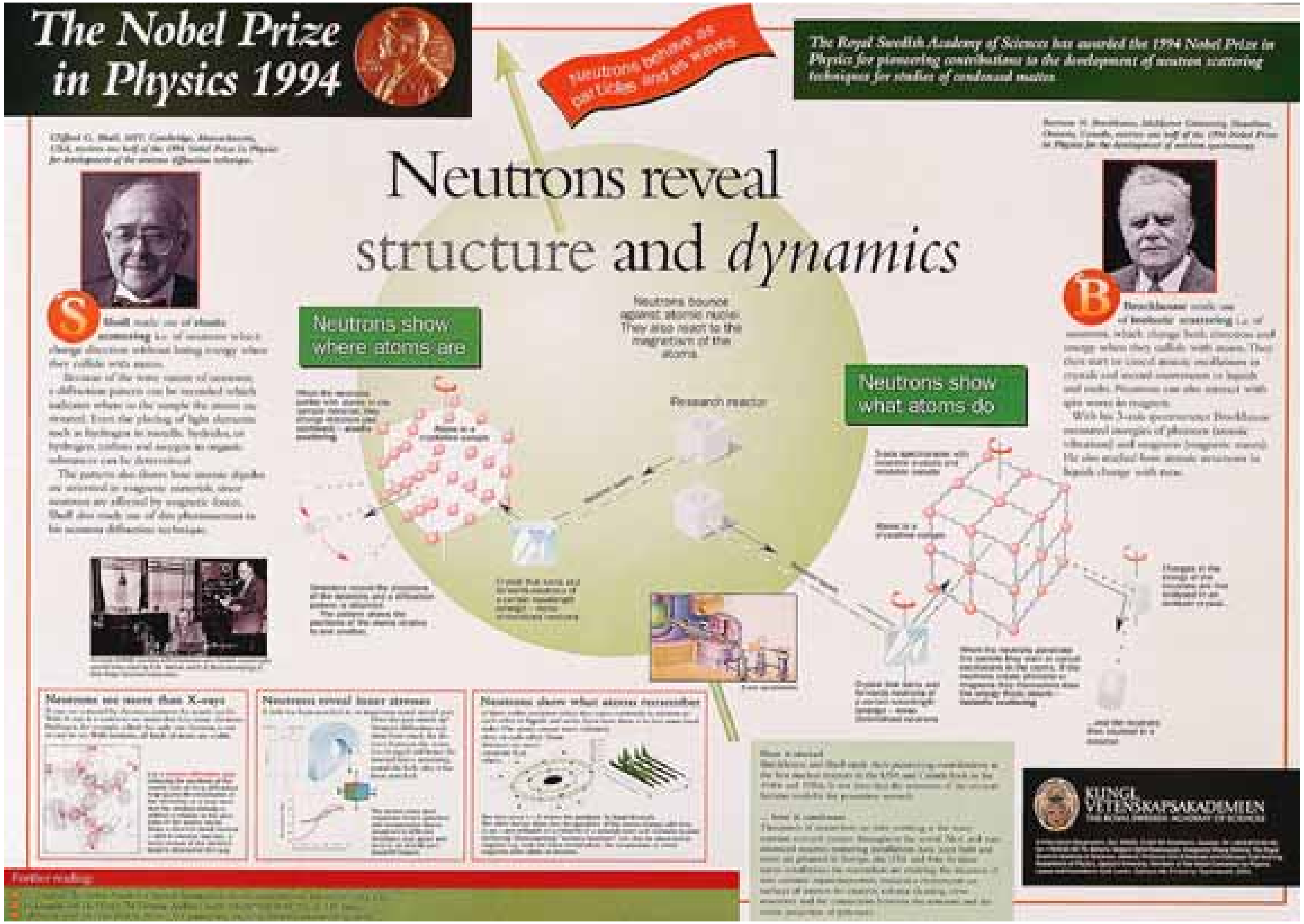
Neutrons and Neutron Sources

1932
The neutron was discovered in by Chadwick in the UK

1936
Coherent neutron diffraction (Bragg scattering by crystal lattice planes) was first demonstrated by two groups in Europe in order to better understand neutrons themselves

> 1945
The possibility of using the scattering of neutrons as a probe of materials developed with the availability of copious quantities of slow neutrons from reactors. Enrico Fermi's group in Chicago used Bragg scattering to measure nuclear cross-sections.

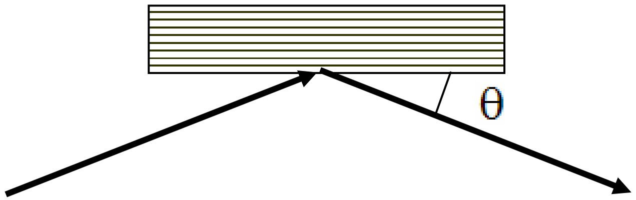
1994
Nobel Prize in Physics – B Brockhouse and C Shull

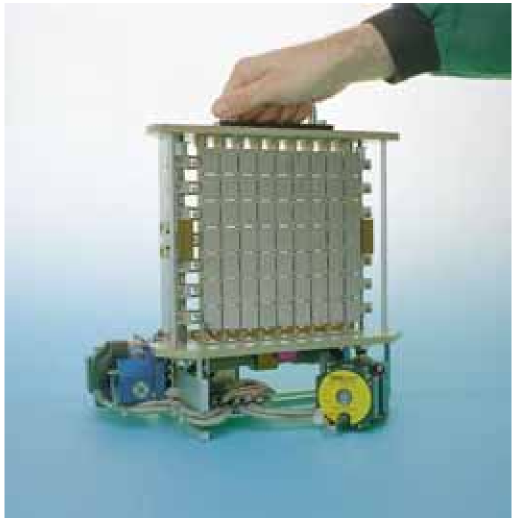

The Nobel Prize in Physics 1994
The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter
Neutrons behave as particles and as waves
Neutrons reveal structure and dynamics
Neutrons show where atoms are
Neutrons bounce against atomic nuclei. They also react to the magnetism of the atoms.
Research reactor
Neutrons show what atoms do
S
B
KUNGL. VETENSKAPSAKADEMIEN

1994

Determination of k_i and k_f

Using crystals





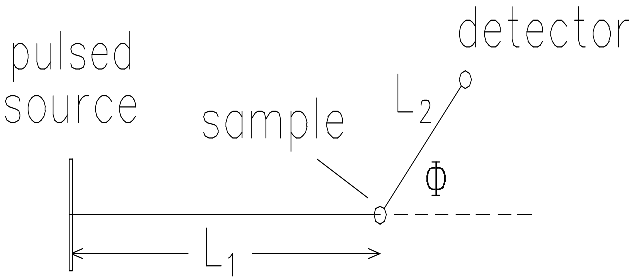
$$\lambda = 2 \cdot d \cdot \sin(\theta)$$

$$|\underline{k}| = \frac{2 \cdot \pi}{\lambda}$$

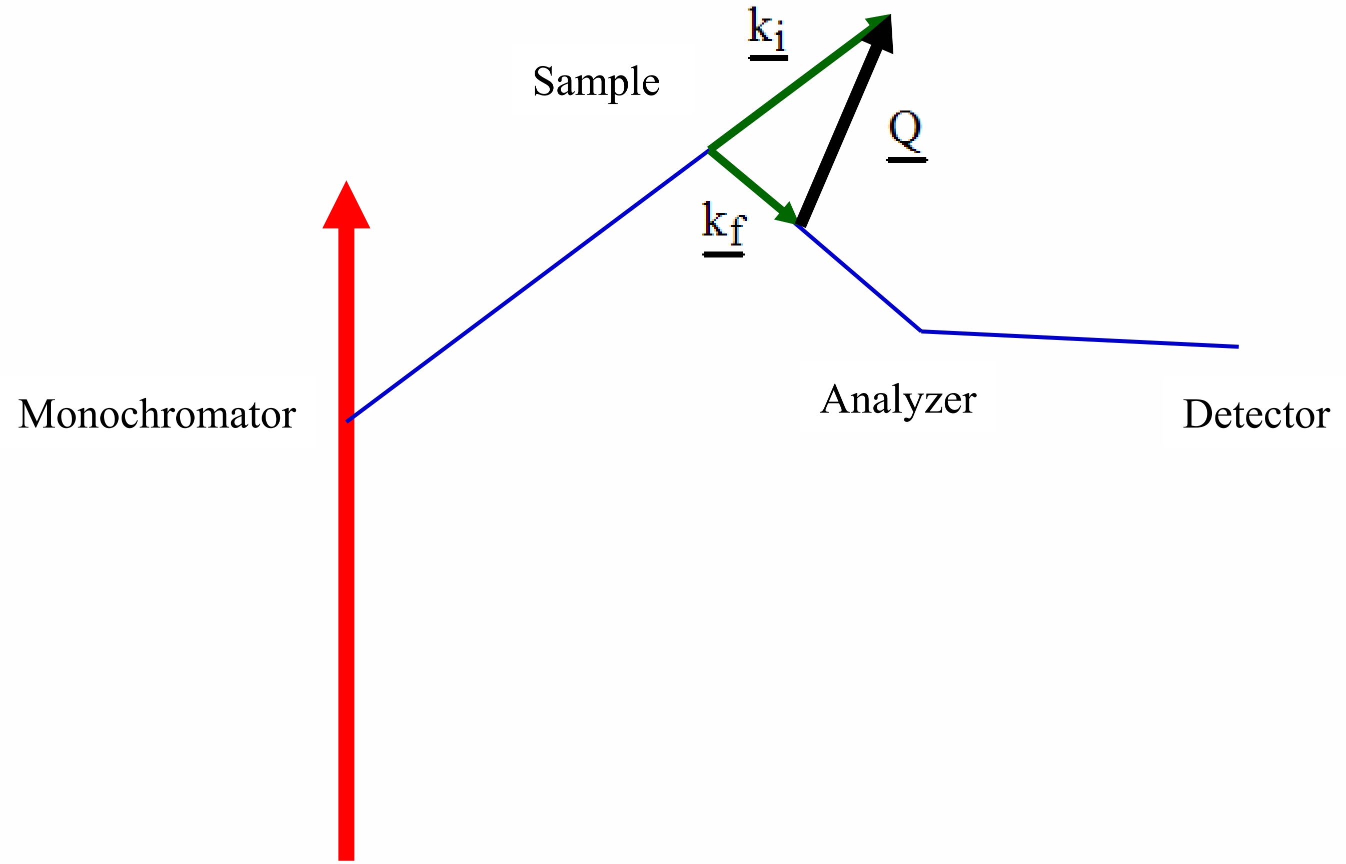
Using time of flight

$$\lambda = \frac{h}{m \cdot L} \cdot t$$

$$|\underline{k}| = \frac{2 \cdot \pi}{\lambda}$$



A generic spectrometer



$$|\underline{k}| = \frac{2\cdot\pi}{\lambda}$$

$$E_i = \frac{\hbar^2 \cdot \underline{k}_i^2}{2\cdot m}$$

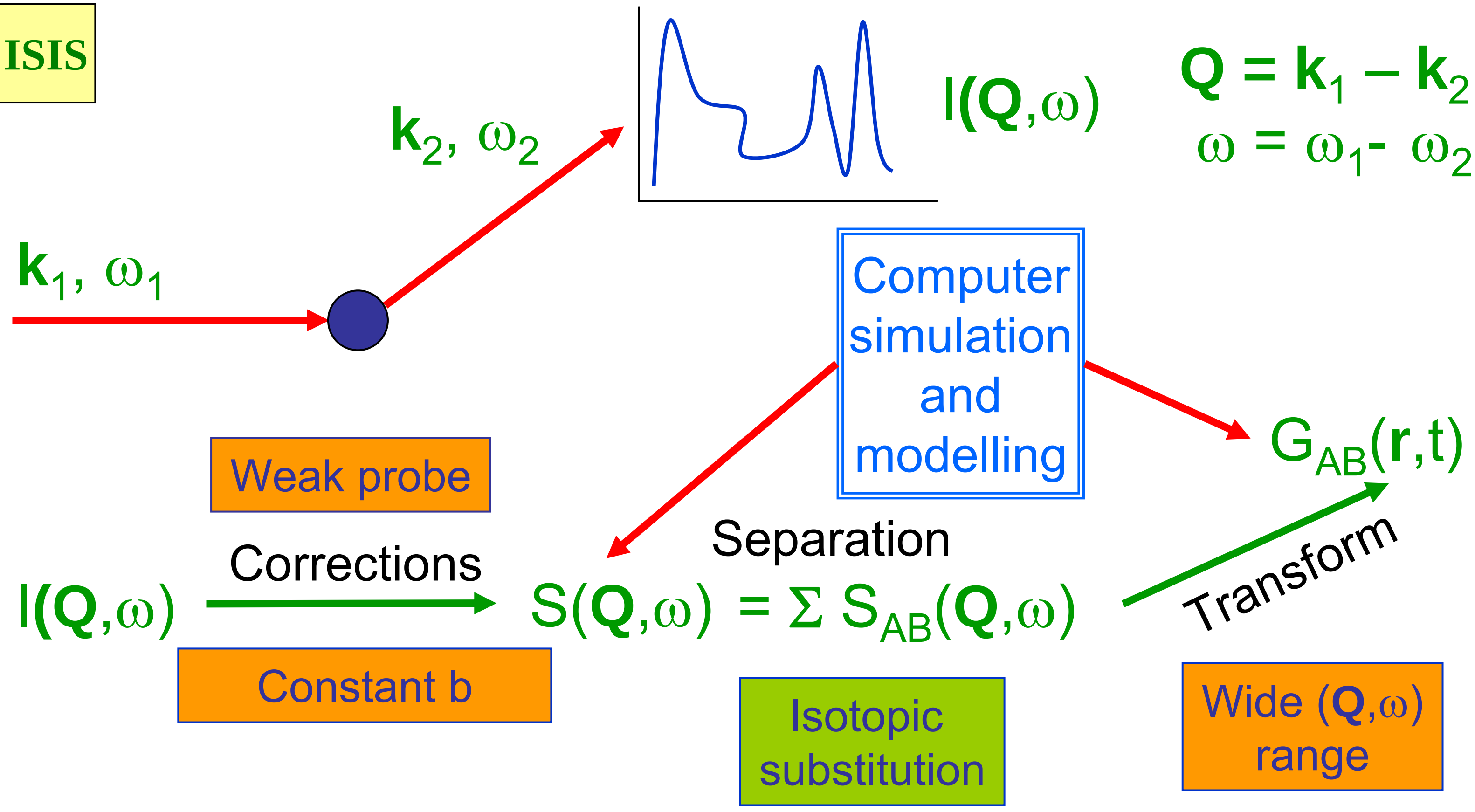
$$E_f = \frac{\hbar^2 \cdot \underline{k}_f^2}{2\cdot m}$$

$$E = \hbar\,\omega$$

Energy transfer to sample $E = \frac{\hbar^2}{2\cdot m}\left[\underline{k}_i^2 - \underline{k}_f^2\right]$

Wave vector transfer to sample $\underline{Q} = \underline{k}_i - \underline{k}_f$

R McGreevy, ISIS



Measurement → Understanding

PAUL SCHERRER INSTITUT

Neutron scattering is an intensity limited technique

The same number of fotons/neutrons will be emitted from:

- 1 W *light bulp* of 2 eV visible light
- 6 kW conventional *X-ray source* of 12 keV radiation
- 100 MW *nuclear reactor* (200 MeV per neutron)

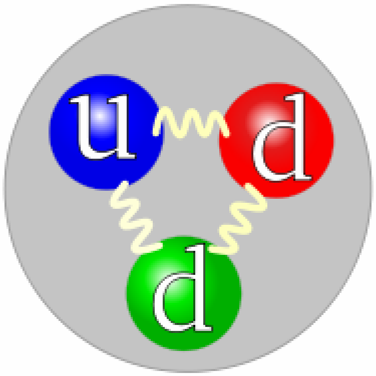
The source size for the reactor is of dimensions m^3 for the others mm^3.

A large number of presentations in the following two weeks will demonstrate that neutrons in many areas are complementary, in some areas competitive and in others unique.

Neutrons : weak source strength – powerful tool for science!

Neutrons

Neutron



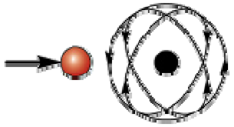
Outside the nucleus, free neutrons are unstable and have a mean lifetime of 885.7±0.8 seconds (about 15 minutes)

$$n \rightarrow p + e^- + \overline{\nu}_e.$$

The quark structure of the neutron.

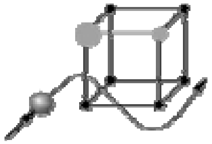
Composition:	one up, two down
Family:	Fermion
Group:	Quark
Interaction:	Gravity, Electromagnetic, Weak, Strong
Antiparticle:	Antineutron
Discovered:	James Chadwick[1]
Symbol:	n
Mass:	$1.674\,927\,29(28) \times 10^{-27}$ kg 939.565 560(81) MeV/c^2 1.008665 u
Electric charge:	0 C
Spin:	½

Uniqueness of Neutrons

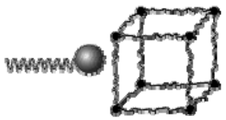


1. Neutrons see the Nuclei

2. Neutrons see Elementary Magnets

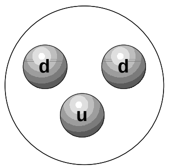


3. Neutrons see light Atoms next to Heavy Ones



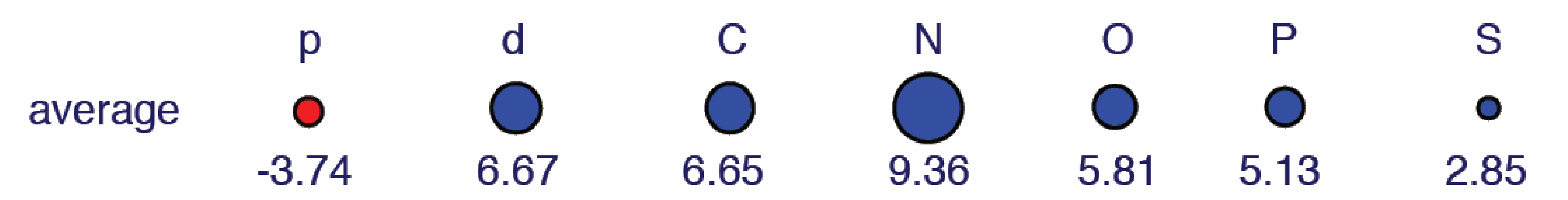
4. Neutrons measure the Velocity of Atoms

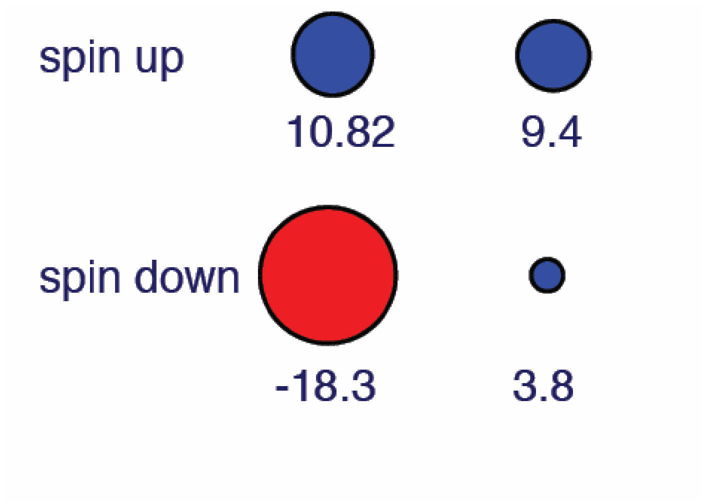
5. Neutrons penetrate deep into Matter



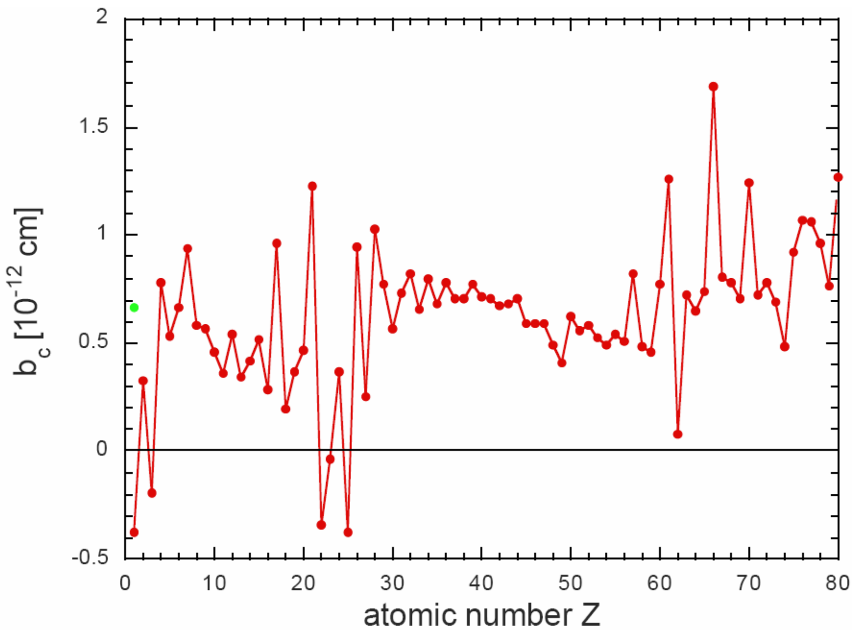
6. Neutrons are Elementary Particles

Neutron Scattering Length [fm]





Spin-dependent scattering lengths

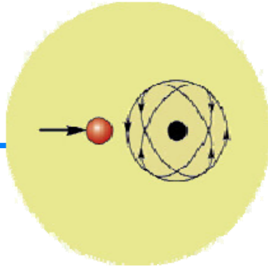


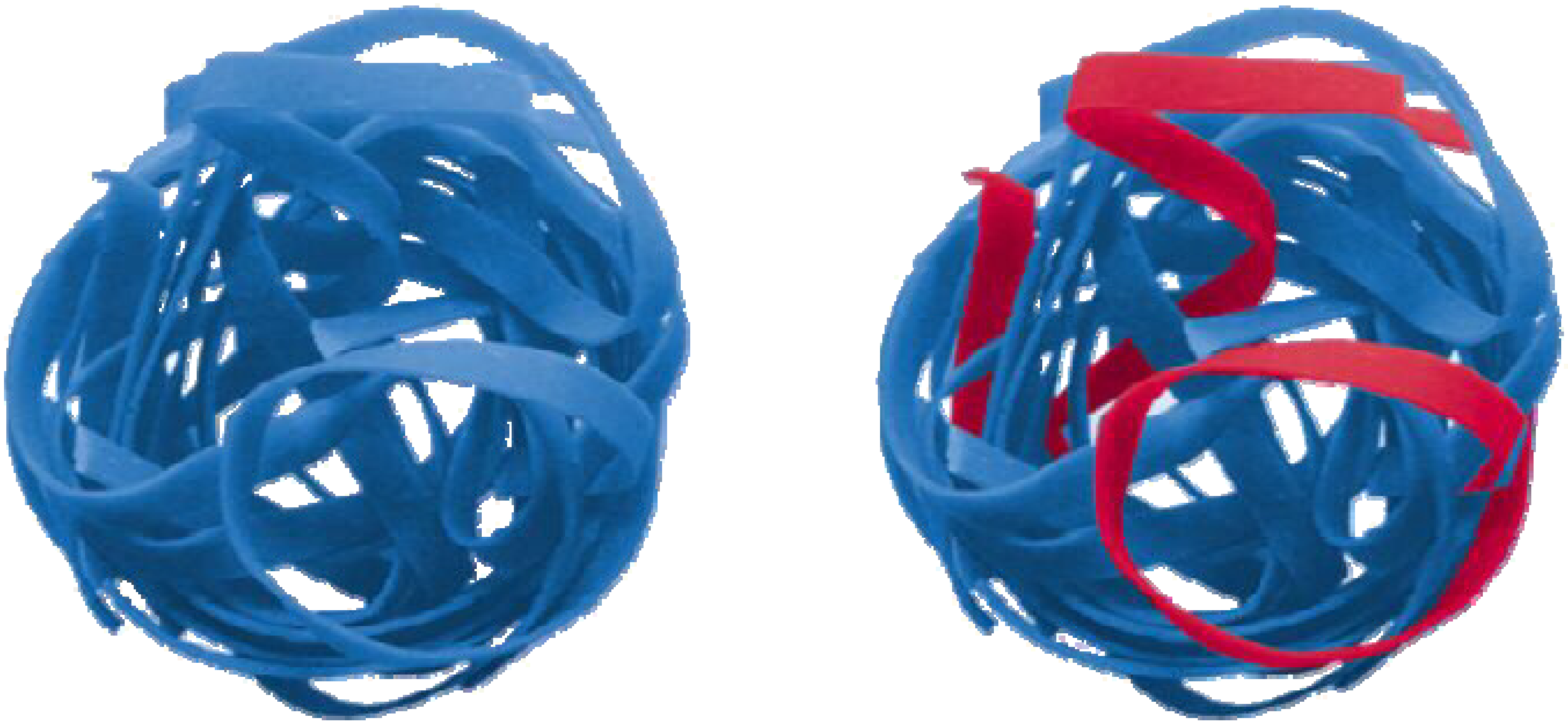
1 fm = 0.1×10^{-12} cm

Contrast Variation

J Kohlbrecher PSI

Neutrons see the Nuclei



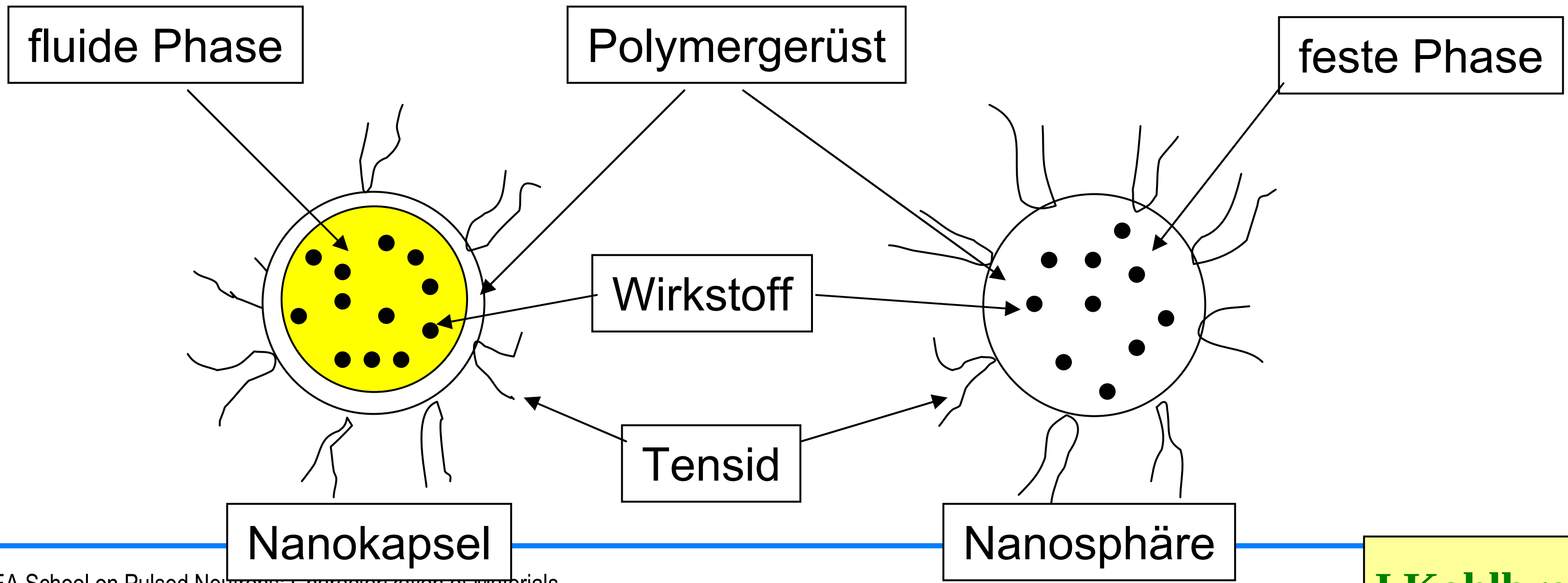


Isotopic contrasting.

Drug Targeting: Core-Shell Structure of Poly(D,L-lactide) Nanocapsules

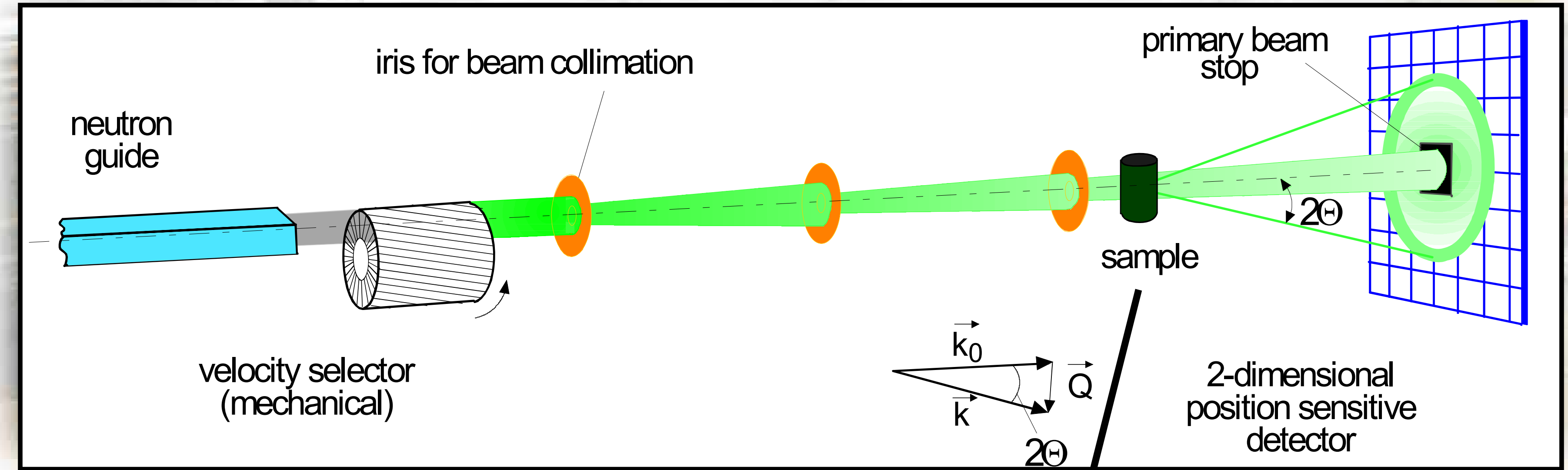
Andrea Rübe[1], Gerd Hause[2], Karsten Mäder[1], Joachim Kohlbrecher[3*]
[1]Institute of Pharmaceutical Technology and Biopharmacy, Martin-Luther-University Halle-Wittenberg
[2]Microscopy Unit, Biocenter of the University, Halle/Saale
[3]Laboratory for Neutron Scattering, Paul Scherrer Institute

- **Einschluss von lipophilen Wirkstoffen in die innere Ölphase möglich**
- **Tensidschicht umgibt Nanokapseln, um sie im Wasser zu stabilisieren**



Small Angle Neutron Scattering

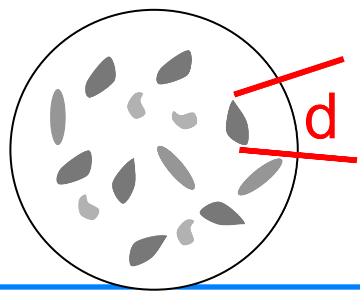
J Kohlbrecher PSI

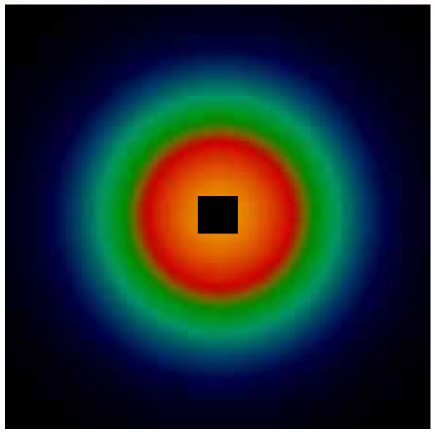


$$\frac{2\pi}{d} = Q = \frac{4\pi}{\lambda}\sin\left(\theta/2\right)$$

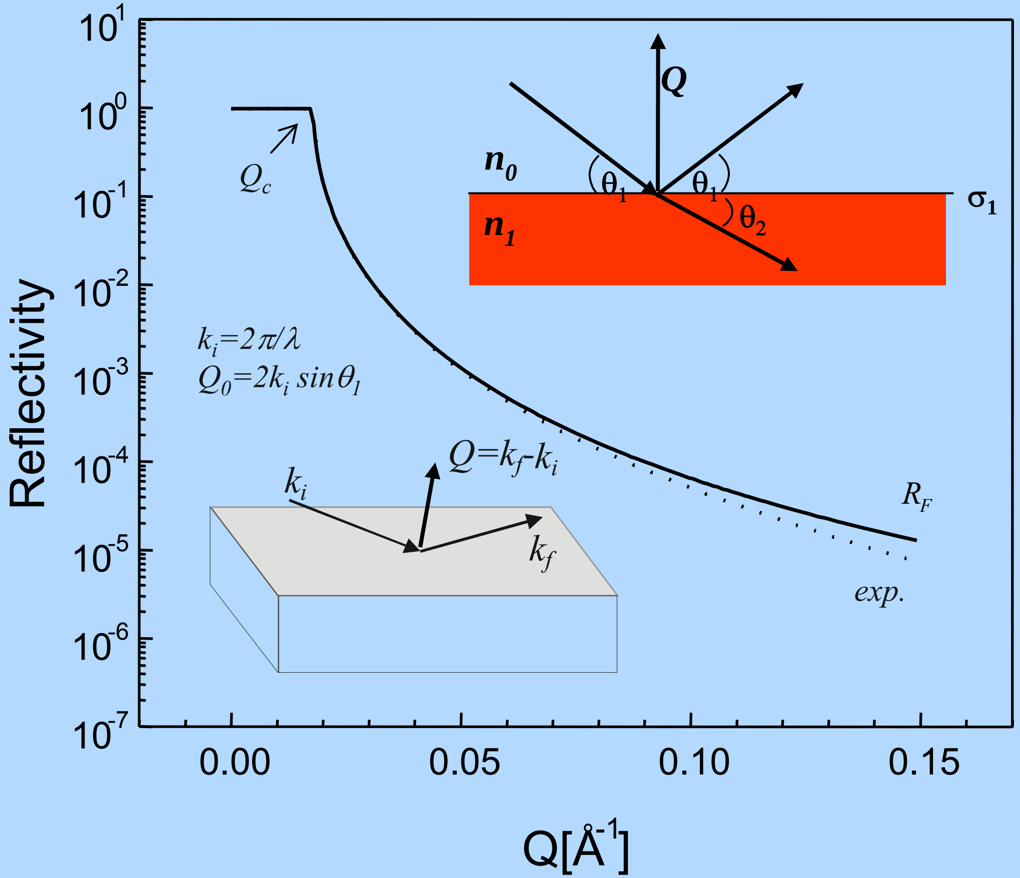
$\lambda \approx 0.5$ nm
d $\approx$ 10 nm

→ $\theta \approx 3$ deg





Biomembranes and Interfaces



Reflectivity of a single interface (Fresnel reflectivity)

$R = r\,r^*$

$r = A'_1/A_1 =$

$(Q_0-Q_1)/(Q_0+Q_1)$ reflection coefficient

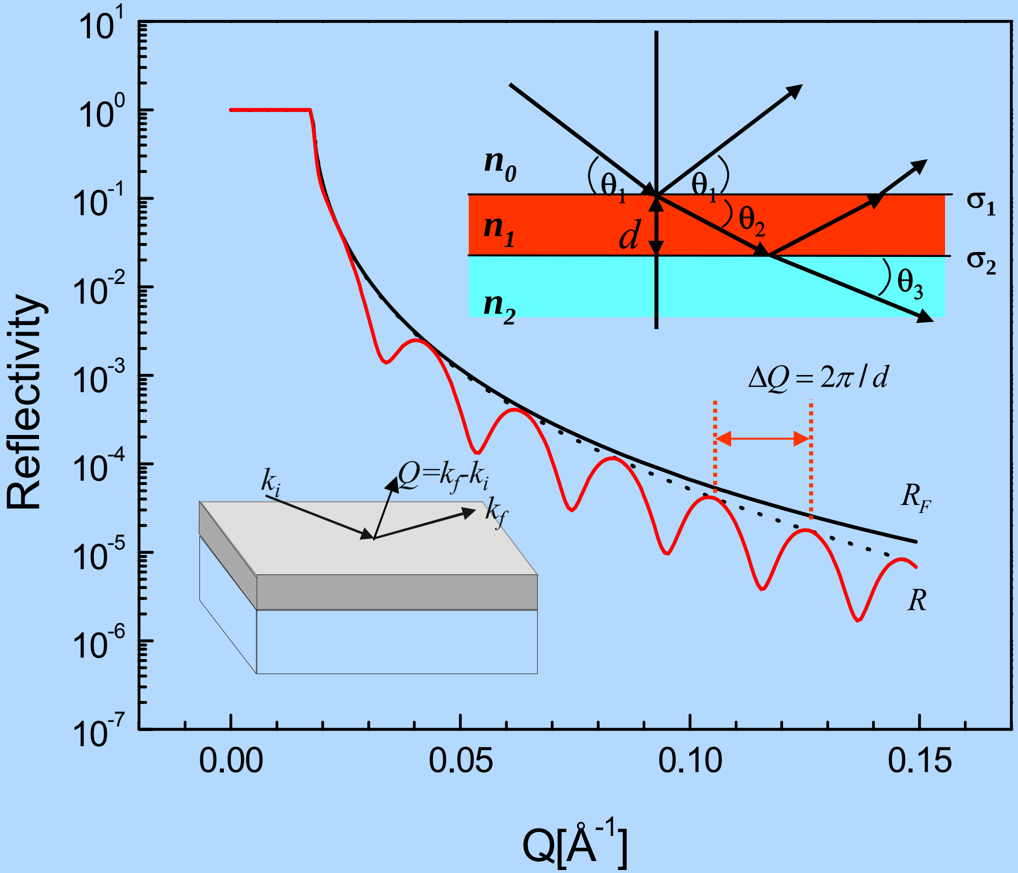
with $Q_i = (Q_0^2-Q_c^2)^{1/2}$

$$R_F(Q) = \left| \frac{1-[1-(Q_c/Q_0)^2]^{1/2}}{1+[1-(Q_c/Q_0)^2]^{1/2}} \right|^2$$

for $Q_0 > Q_c$

$$R_F(Q) \approx (Q_c/Q_0)^4$$

Biomembranes and Interfaces



Reflectivity of two interfaces

$$R(Q) = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos(2Q_1d)}{1 + r_1^2r_2^2 + 2r_1r_2\cos(2Q_1d)}$$

with thickness $d = 2\pi/\Delta Q$

in kinematic theory

$$r = \frac{(k_c^2)^2}{Q_0^4}\left|\int \frac{d\rho}{dz}\cdot\exp(iQ_0z)dz\right|^2$$

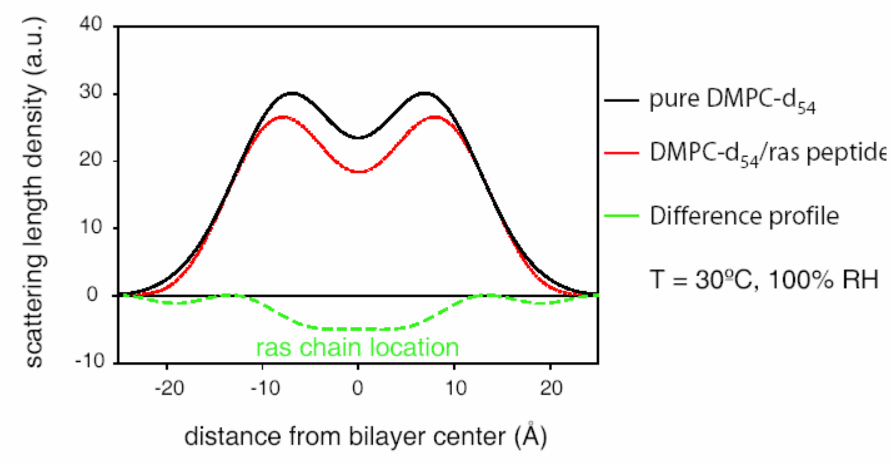
reflectivity of two interfaces

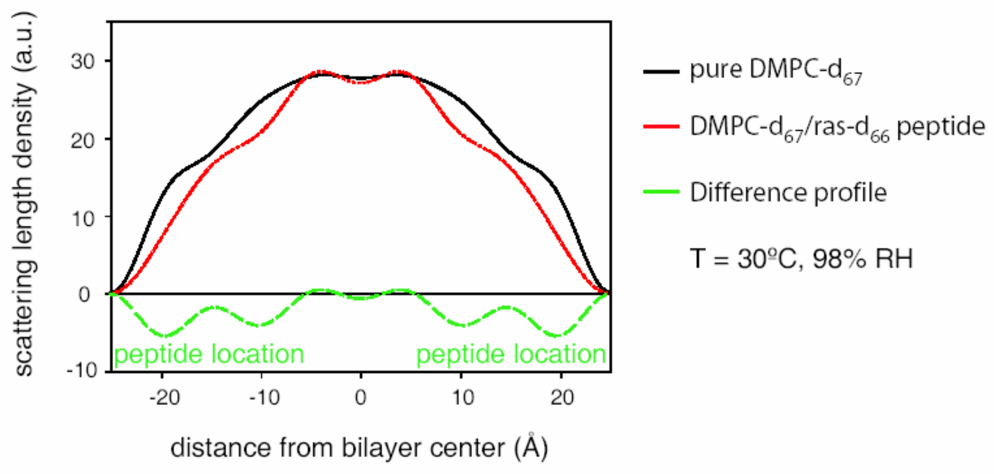
$$R(Q) = \frac{(k_c^2)^2}{Q^4}\left[\begin{aligned}&\Delta\rho_1\cdot\exp\left(-Q^2\sigma_1^2\right) + \Delta\rho_2\cdot\exp\left(-Q^2\sigma_2^2\right)\\ &+\Delta\rho_3\cdot\exp\left(-Q^2\left(\sigma_1^2+\sigma_2^2\right)/2\right)\cdot\cos(Q\mathrm{d})\end{aligned}\right]$$

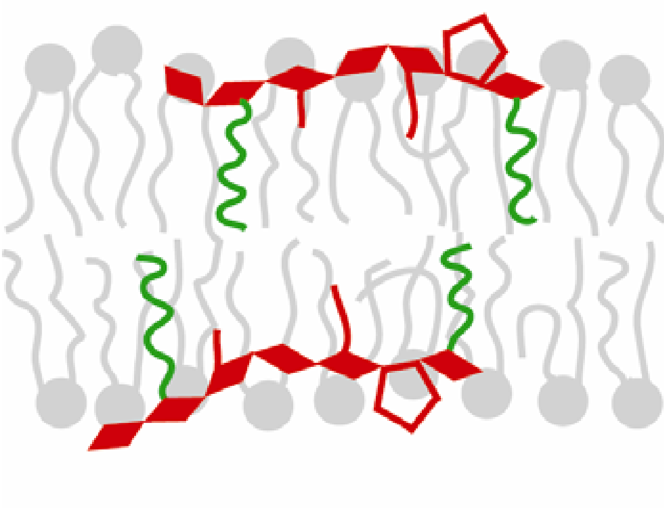
with parameters $d,\ \sigma,\ \Delta\rho$

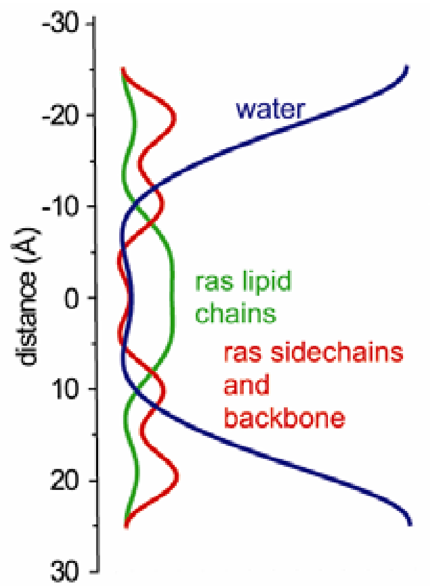
T Gutberlet PSI

Membrane Binding of Lipidated N-ras Peptide





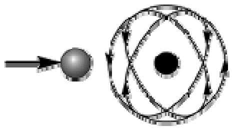




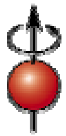
T Gutberlet PSI

(D. Huster et al., JACS, 125, 2003, 4070)

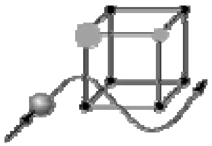
Uniqueness of Neutrons



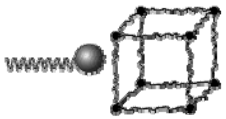
1. **Neutrons see the Nuclei**



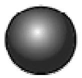
2. **Neutrons see Elementary Magnets**



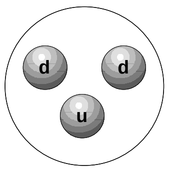
3. **Neutrons see Light Atoms next to Heavy Ones**



4. **Neutrons measure the Velocity of Atoms**

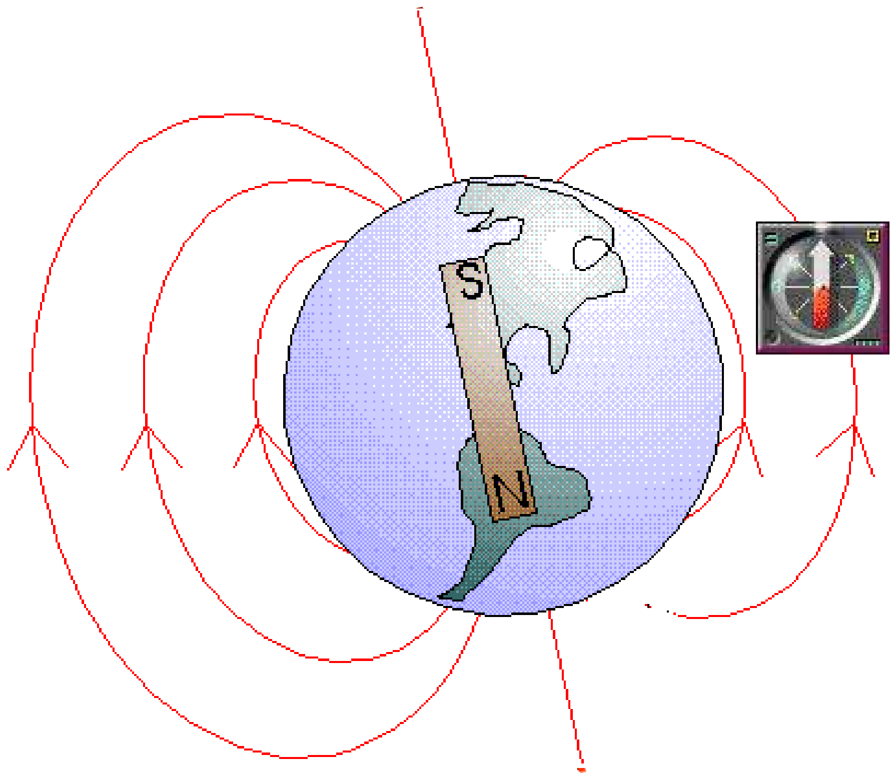


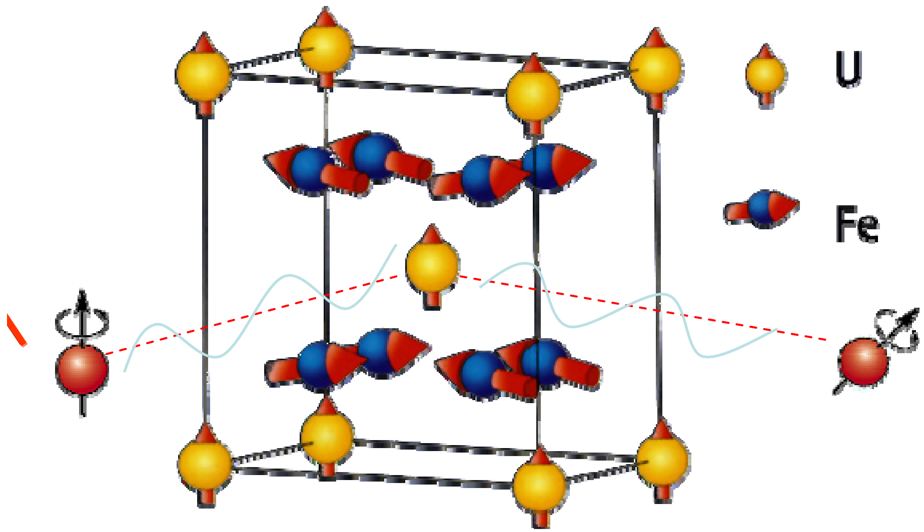
5. **Neutrons penetrate deep into Matter**



6. **Neutrons are Elementary Particles**

Neutrons see Elementary Magnets

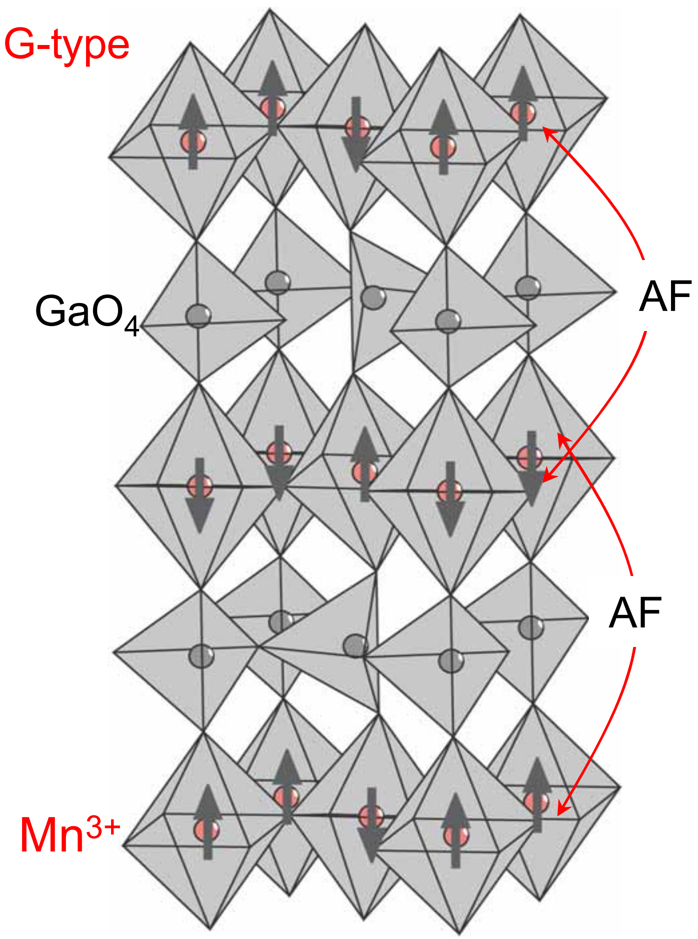




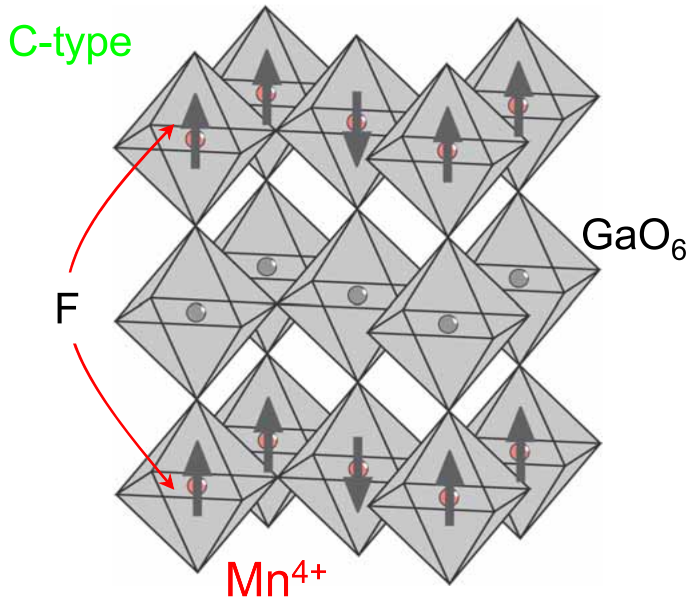
Nearly all what we know about magnetic structures comes from neutrons.

Magnetic and crystal structures

Sr_2MnGaO_5



$Sr_2MnGaO_{5.5}$

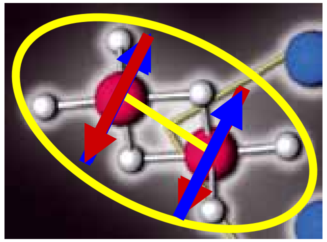


Pomjakushin,V.Yu., Balagurov,A.M., Elzhov,T.V., Sheptyakov,D.V., Fischer,P., Khomskii,D.I., Yushankhai,V.Yu., Abakumov,A.M., Rozova,M.G., Antipov,E.V., Lobanov,M.V., Billinge,S. "Atomic and magnetic structures, disorder effects, and unconventional superexchange interactions in A2GaMnO5+x (A=Sr,Ca) oxides of layered brownmillerite-type structure", Phys. Rev. B 66, 184412 (2002)

V. Pomjakushin PSI

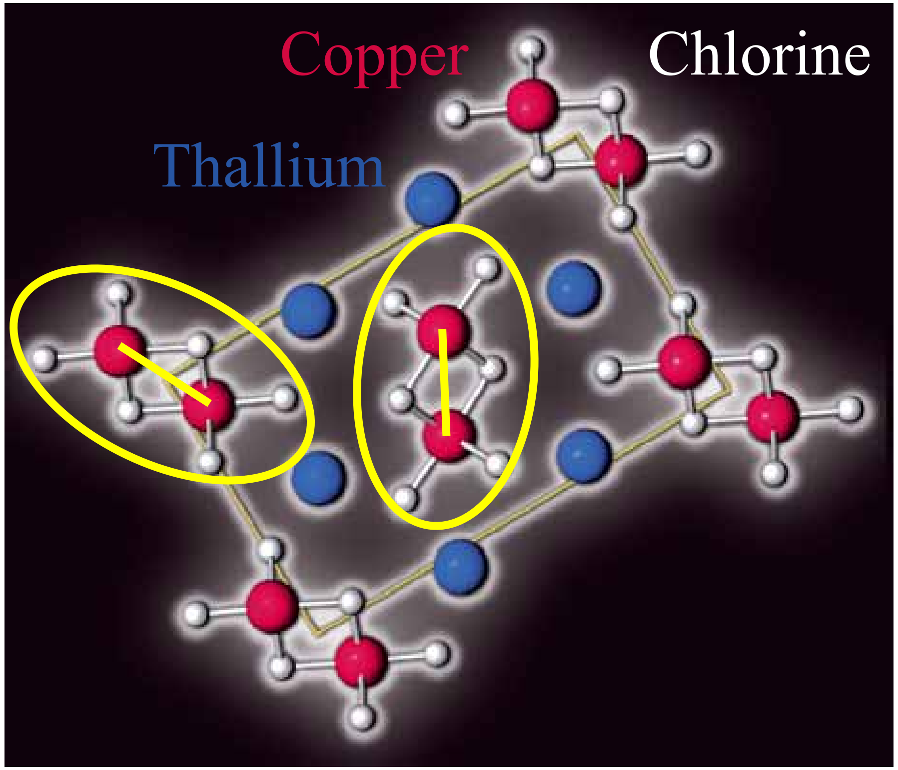
Our quantum model system

<u>Dimer spin system $TlCuCl_3$</u>



- antiferromagnetic
- fluctuating moments
- no magnetic order
- “singlet” ground state

SPIN LIQUID



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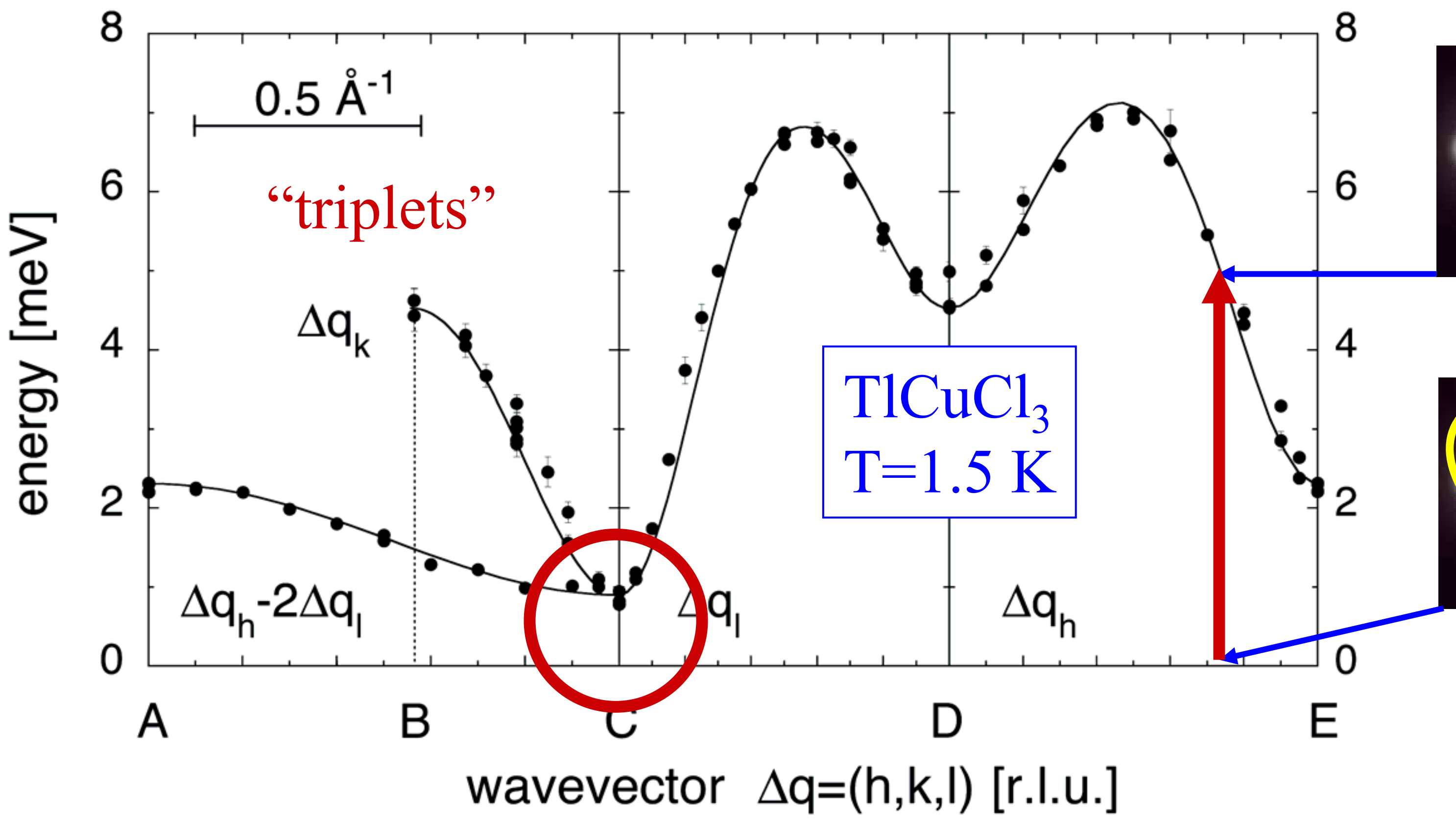
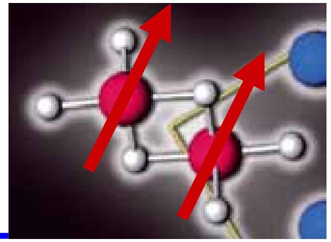
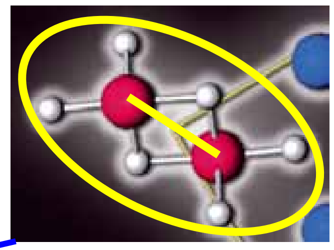
Magnetic excitations







- N. Cavadini et *al.*, Phys. Rev. B **63**, 172414 (2001)
- N. Cavadini et *al.*, J. Phys.: Condens. Matter **12**, 5463 (2000)

Physicist’s Lego

H Luetkens PSI

Magnetic properties

P

FM

AFM

CMR

MF

Electric properties

M | I

FE | SC

AFE

Combinations

Fundamental Science

- Competition of ground states
- Coexistence of ground states
- Coupling of different ground states
- (Giant) proximity effects
- Electric field effects (2D-electron gas, ...)
- …

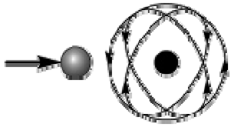
Applications

- Spintronics (Switching of currents with magnetic fields)
- Sensors (Magnetism, pressure, temperature, gases, …)
- Actuators
- Non-volatile memory (MRAM, …)
- …

IT and quantum devices

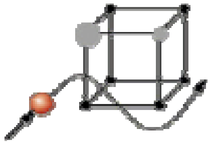
- Giant magnetoresistance and exchange bias for spintronics and high density data storage
- Hard thin film magnets for micro-motors, -switches and -sensors
- Understanding magnetic roughness and phase diagrams - towards better electronic devices
- Understanding quantum complexity

Uniqueness of Neutrons

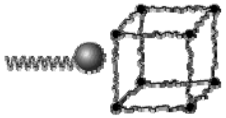


1. Neutrons see the Nuclei

2. Neutrons see Elementary Magnets

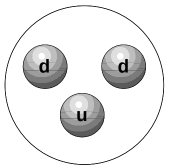


3. Neutrons see Light Atoms next to Heavy Ones



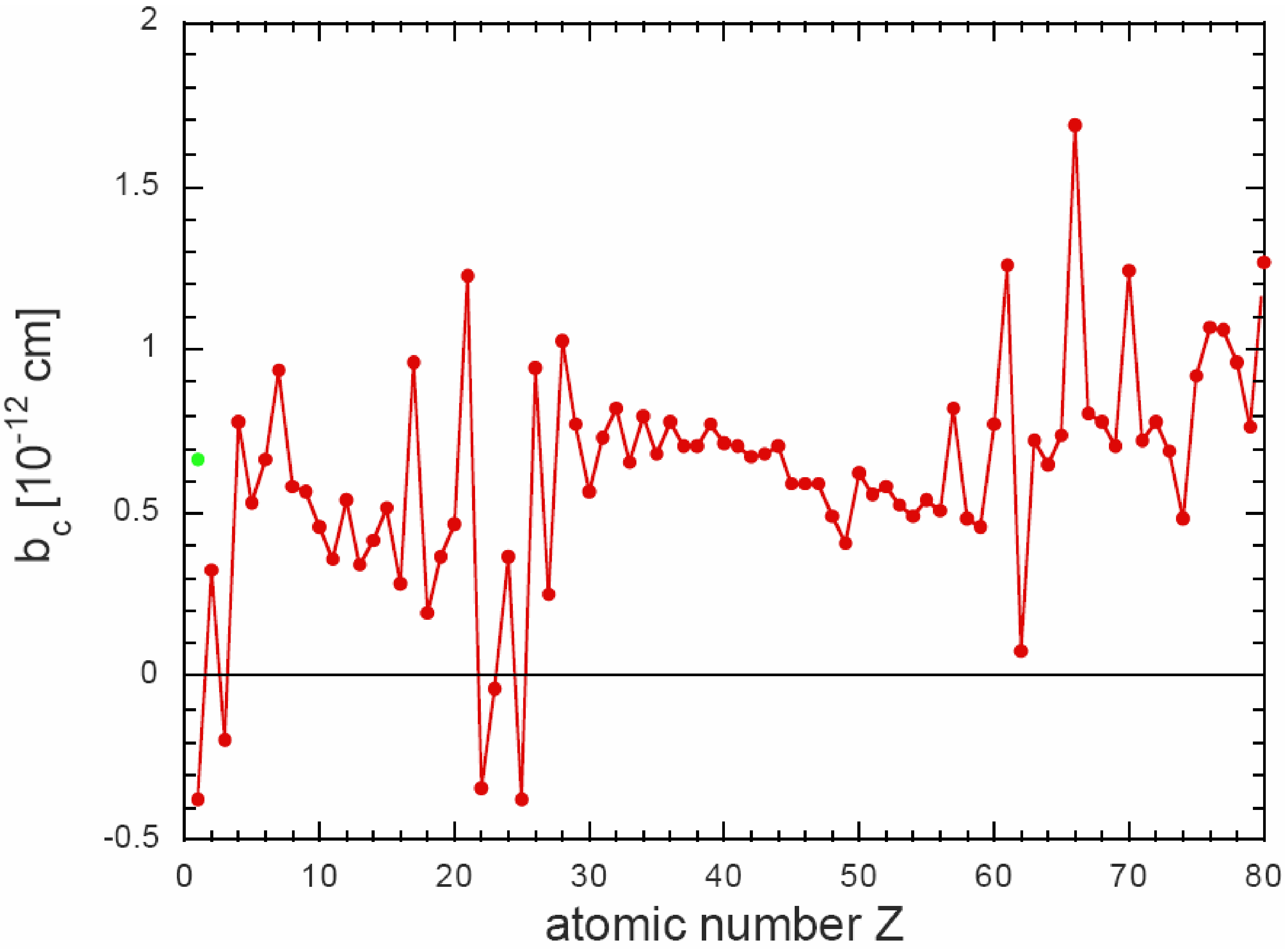
4. Neutrons measure the Velocity of Atoms

5. Neutrons penetrate deep into Matter



6. Neutrons are Elementary Particles

Coherent Neutron Scattering Length [fm]



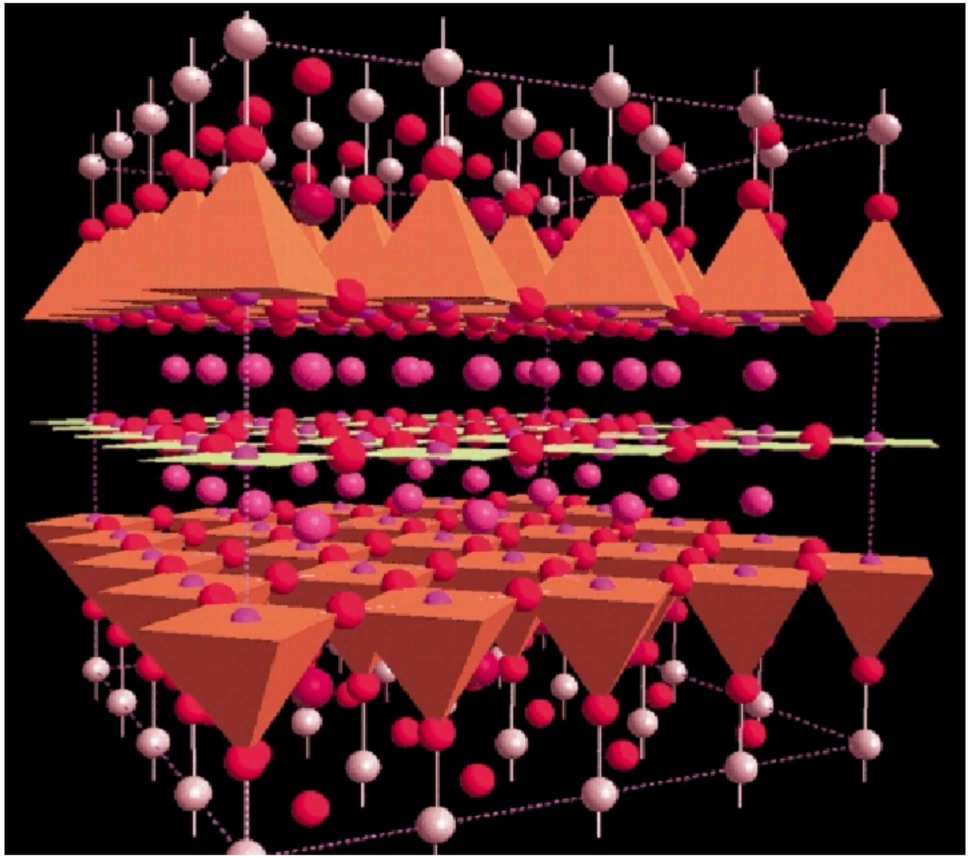
Scattered Intensity proportional to b^2

For X-rays:

$b \propto Z$

$I \propto Z^2$

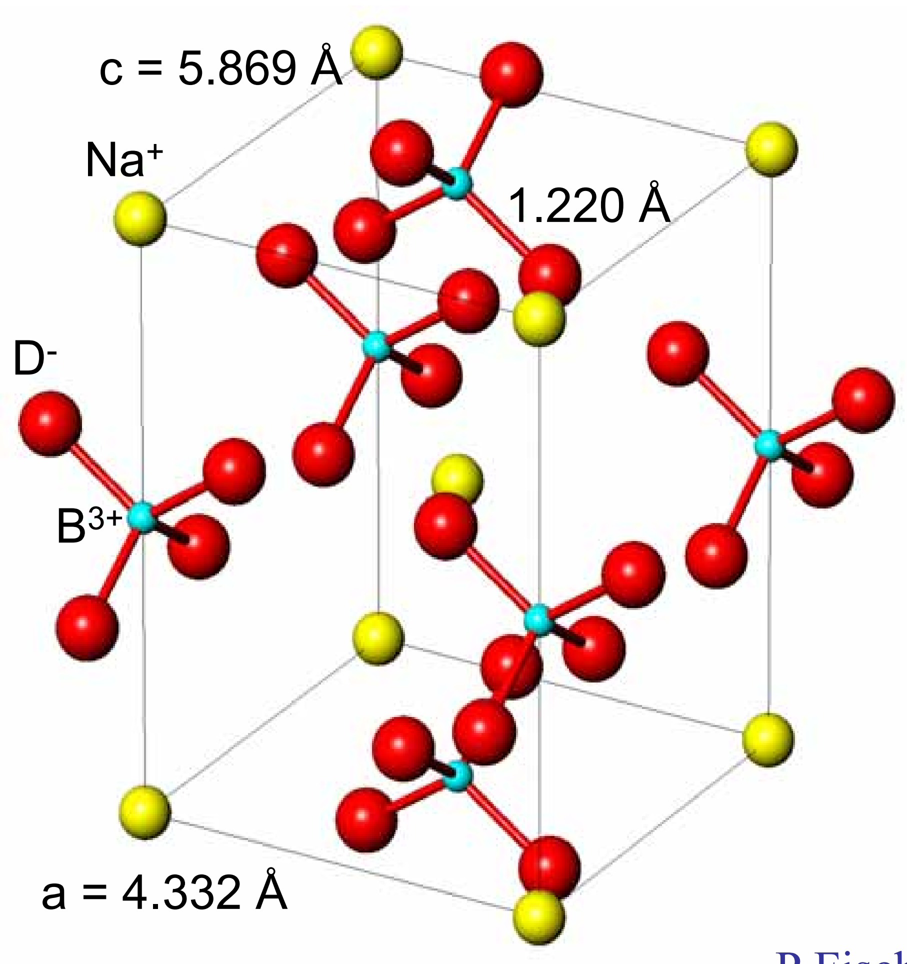
Neutrons see Light Atoms next to Heavy Ones



Crucial oxygen positions revealed by neutrons

High temperature superconductors for the technology of tomorrow.

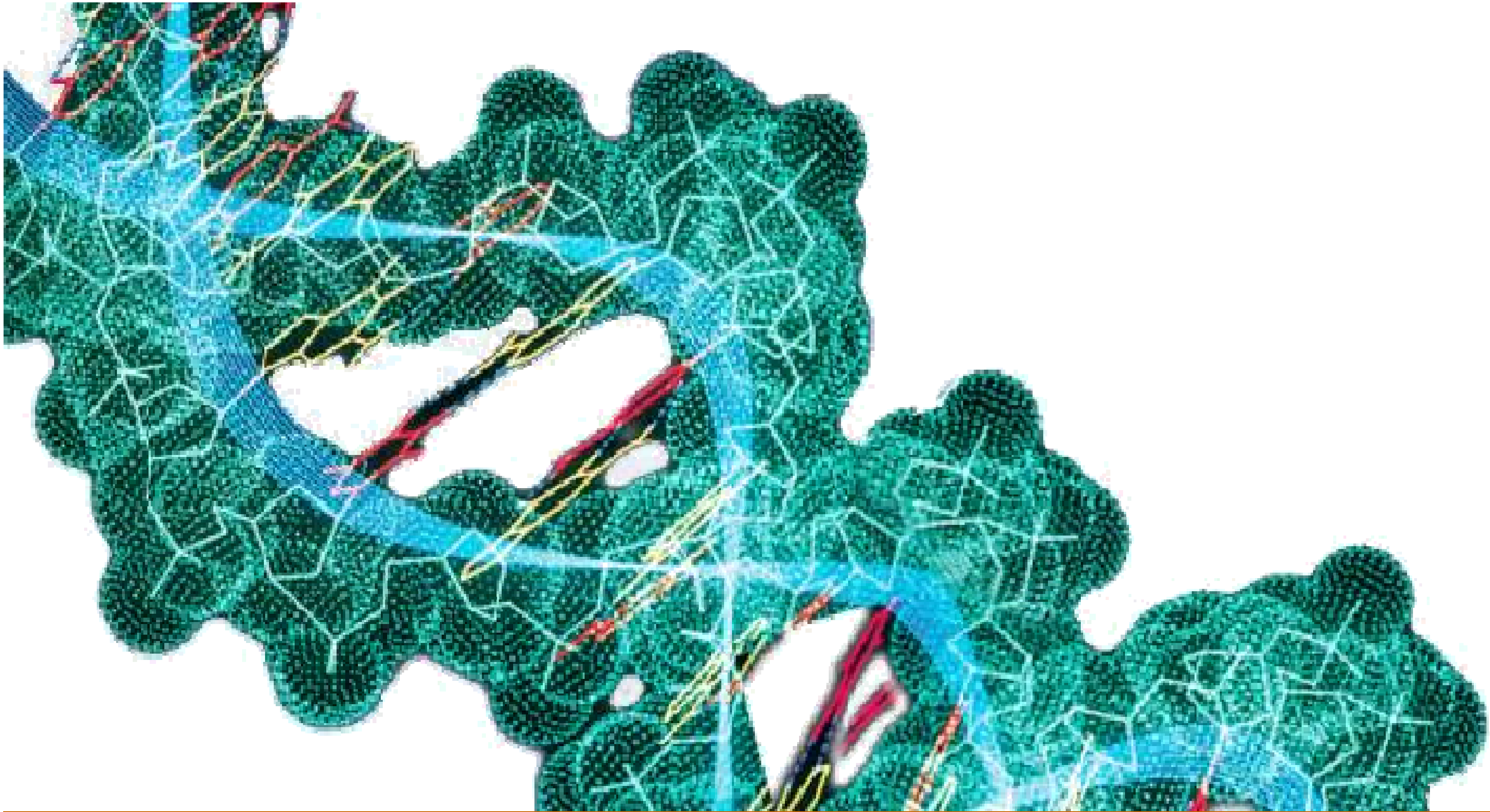
Order-Disorder phase transition due to reorientation of BD_4^- tetrahedra in **$NaBD_4$**



V. Pomjakushin PSI

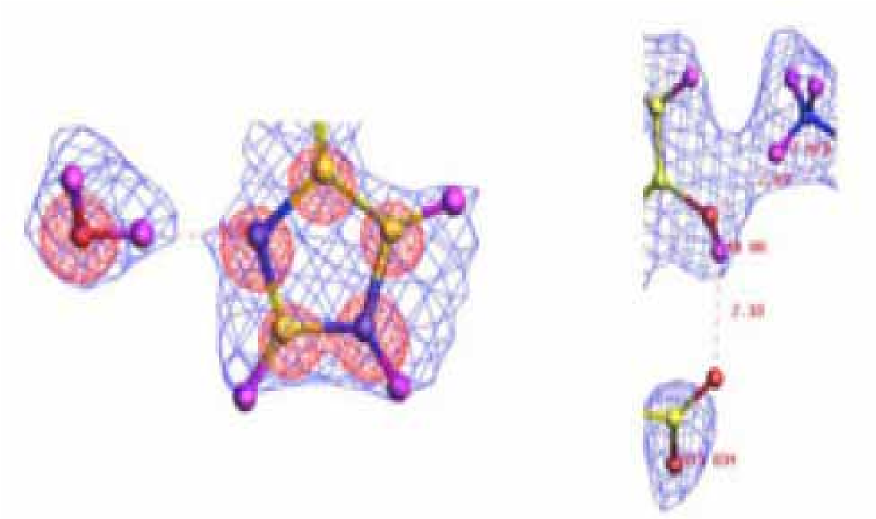
P.Fischer, A. Züttel (2004)

Neutrons see Light Atoms next to Heavy Ones

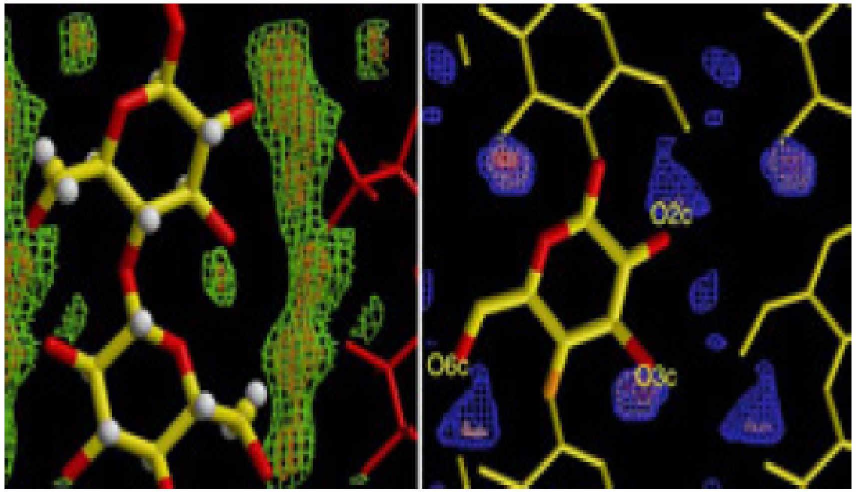


Only neutrons see H-bonds and catalytic H positions.

Locating Hydrogen



Density maps showing the positions of hydrogen atoms in protein crystals as determined by neutron crystallography

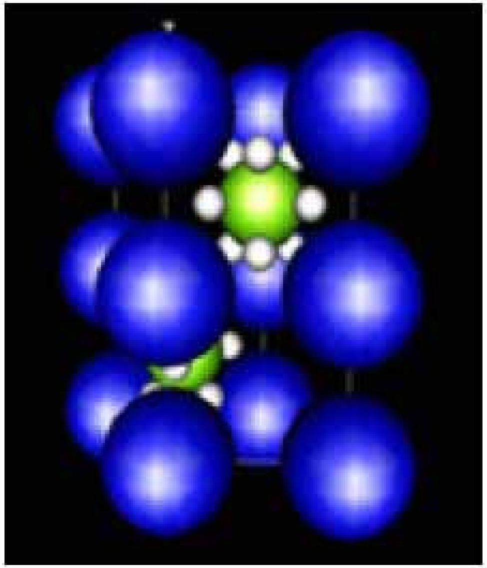


Density maps from neutron high-angle fibre diffraction reveal the hydrogen bonding network in cellulose.

Hydrogen storage materials and batteries

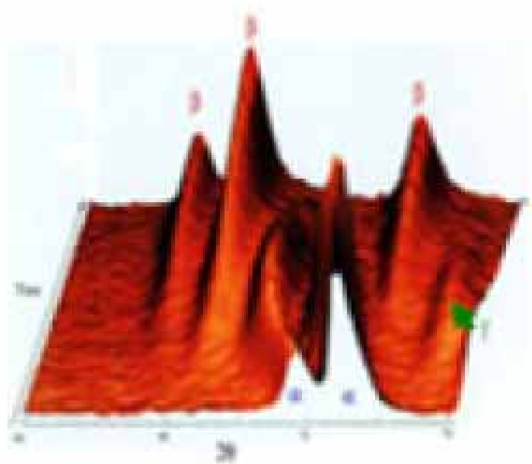
Energy for the future

- Hydrogen storage materials.
- Fuel cell components; oxide ion conductors.
- Clathrate hydrates for energy sources.
- Light, high energy density batteries.
- Energy efficient transport; superalloys, ceramics, fuel additives.



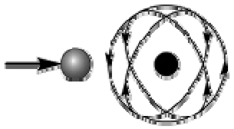
The crystal structure of Mg_2FeH_6

In situ studies of functioning H storage or Battery.



In-situ neutron diffraction during charging of a Ni-MH battery

Uniqueness of Neutrons



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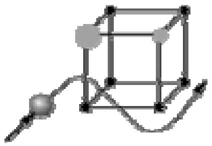

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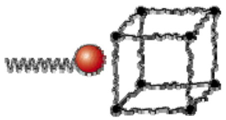
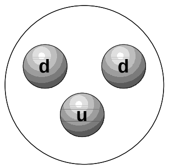


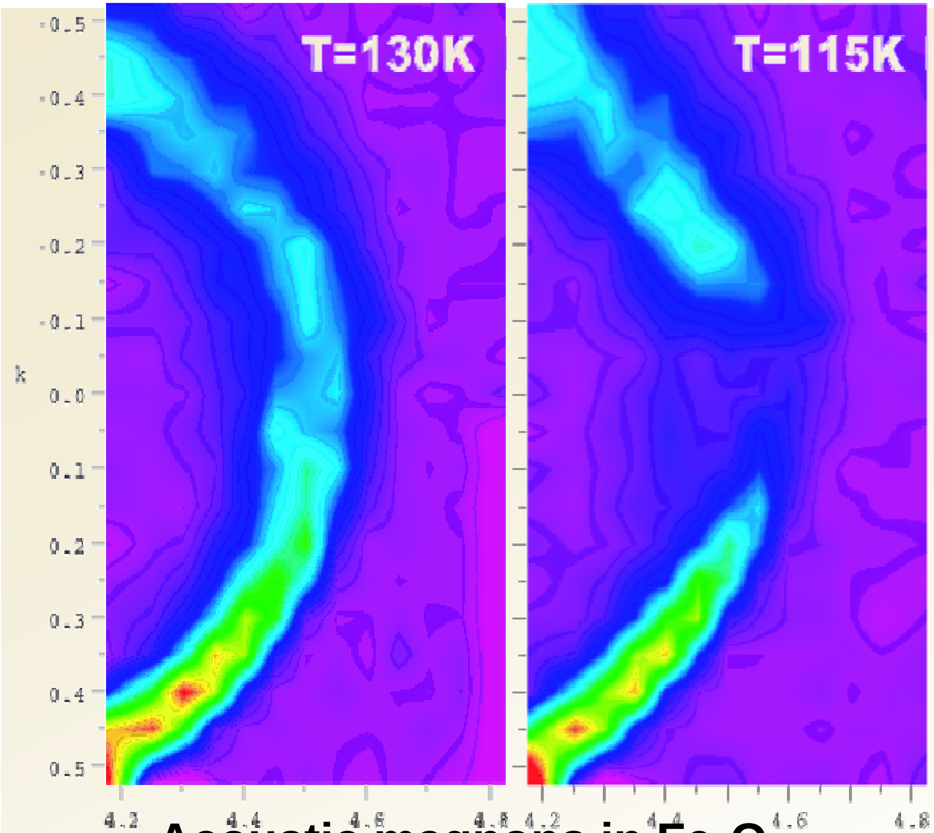
4. **Neutrons measure the Velocity of Atoms**

5. Neutrons penetrate deep into Matter



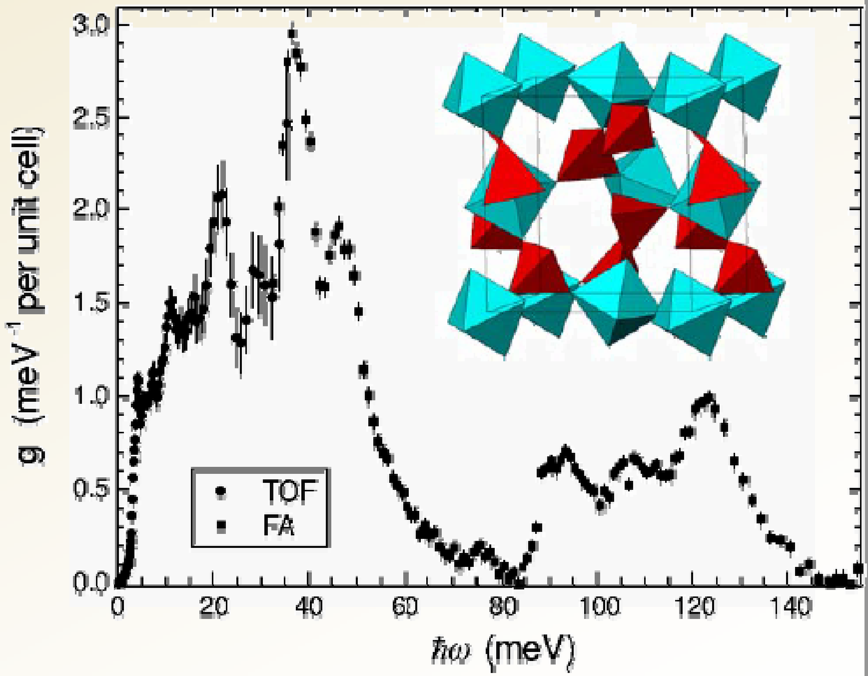
6. Neutrons are Elementary Particles

Inelastic scattering



Acoustic magnons in Fe_3O_4

(h,k,0) grid at constant energy transfer = 42.5 meV



Phonon density of states of ZrW_2O_8

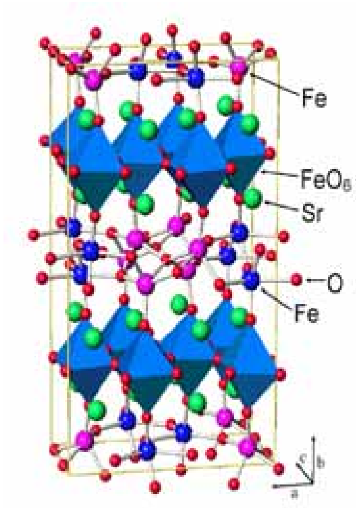
T Mason, SNS

Ionic Conducting Materials: SOFCs, Ceramic Membranes

Rietveld Analysis:
performance relationship to composition, crystal structure, phase transitions (order-disorder), microstrain, texture, …

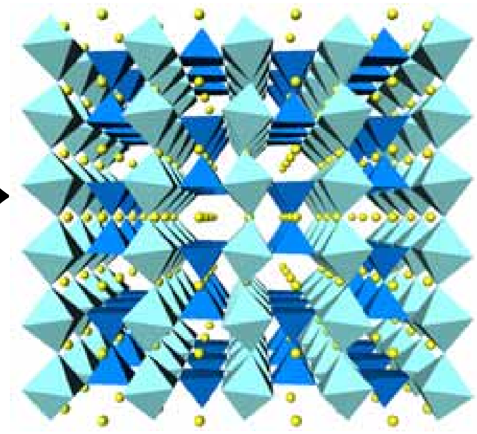
Max-Entropy Analysis:
real space imaging of proton and oxide-ion conducting pathways,

High-Temperature Furnace with Automated Gas Flow Controllers:
dynamic in-situ experiments under realistic conditions (extreme ΔpO_2 and ice formation expts)

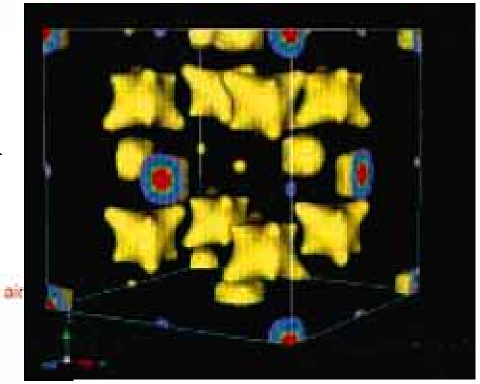


$Sr_2(Fe_{1-x}Co_x)_3O_{6+\delta}$

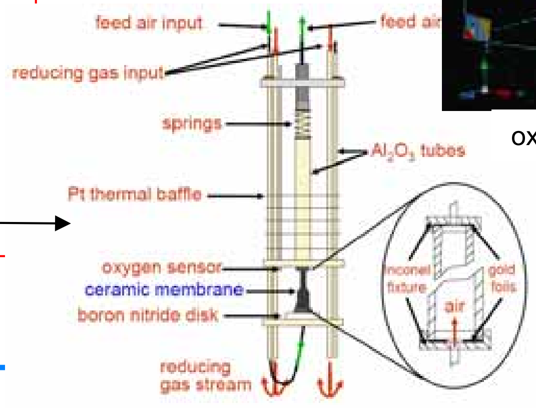
↔



$Sr_4(Fe_{1-y}Co_y)_4O_{12}$

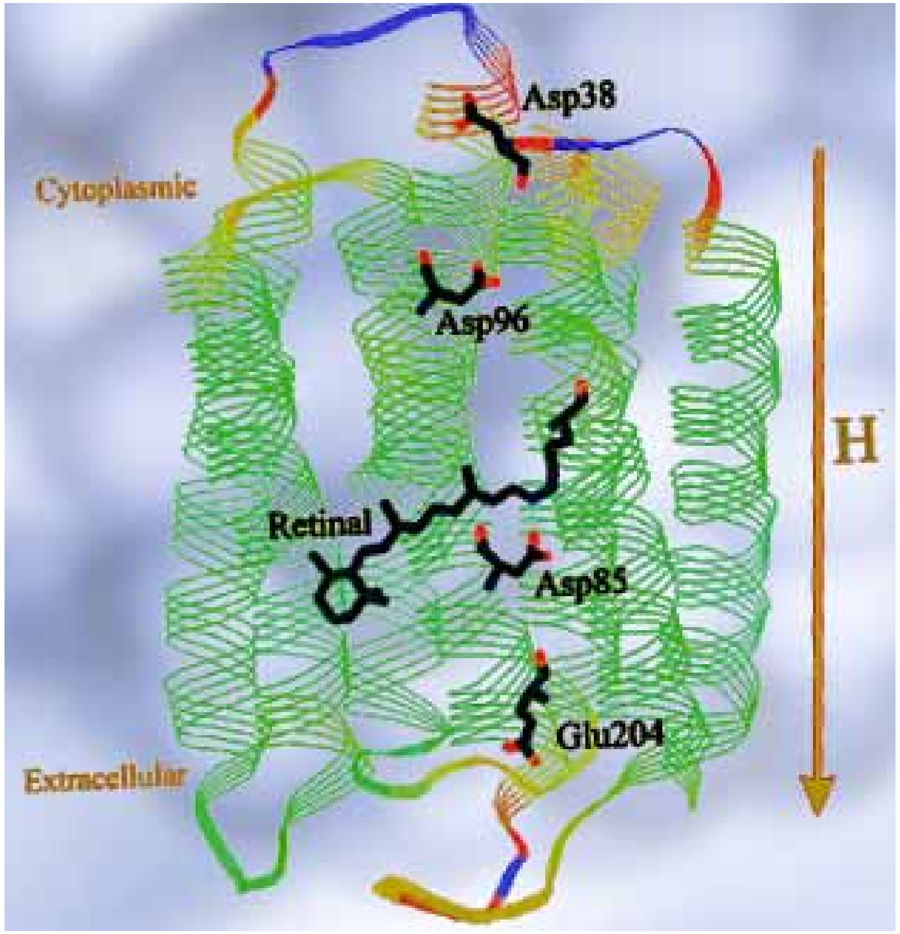


oxide-ion migration in CeO_2 (1497°C)
Appl. Phys. Lett., Vol. 84, No. 4, 26



T Mason, SNS

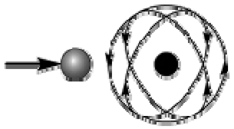
Neutrons measure the Velocity of Atoms



Mechanism of proton pumping

Transport through a biological membrane.

Uniqueness of Neutrons



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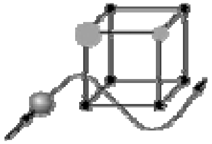

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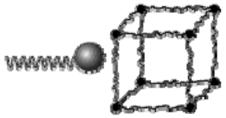

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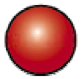

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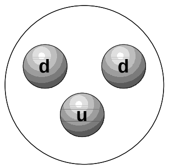
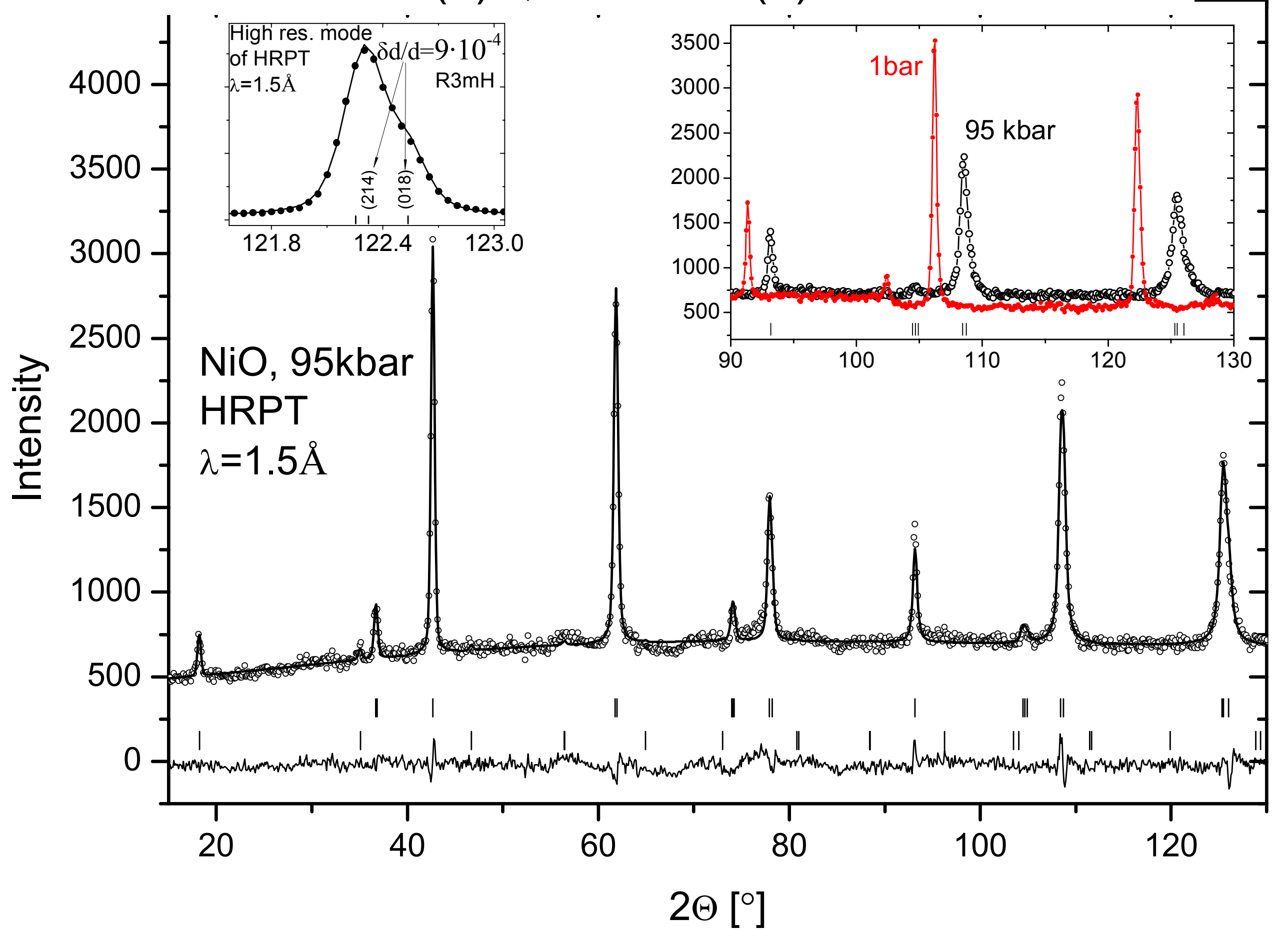


6. Neutrons are Elementary Particles

PAUL SCHERRER INSTITUT

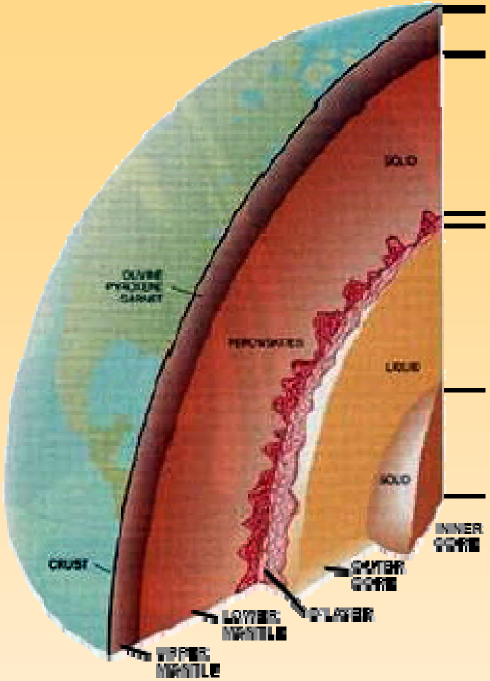
Lattice distortion and magnetic structure in NiO under high pressures (up to 130kbar)

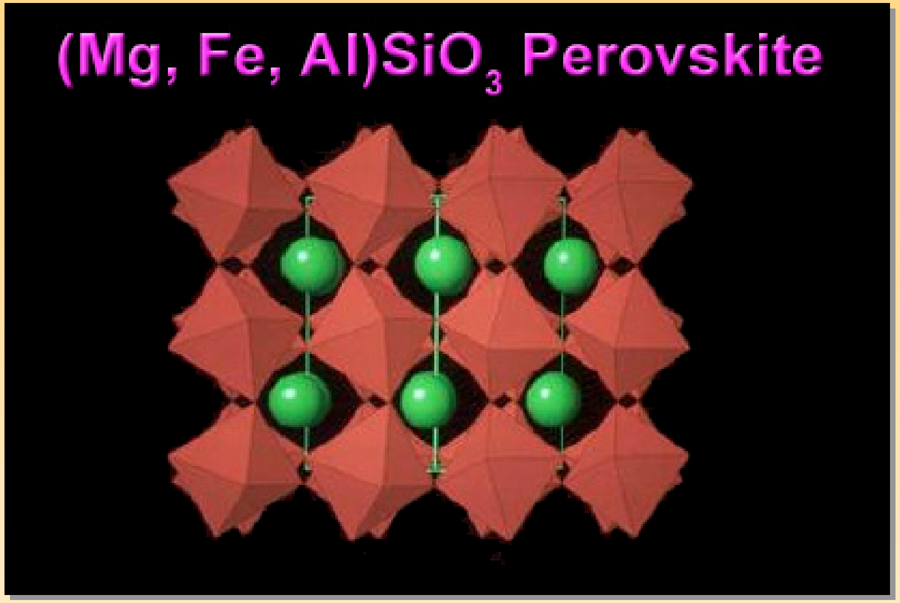
@ p=1bar: μ_{Ni}=1.73(9) μ_B, k =[½ ½ ½] in *Fm3m*
R3-m: a=2.9534(2)Å, α=60.061(2)°



S. Klotz, Th. Strässle, G. Rousse, G. Hamel, V. Pomjakushin, *APL 2005*.

V. Pomjakushin PSI





Most abundant mineral in the planet

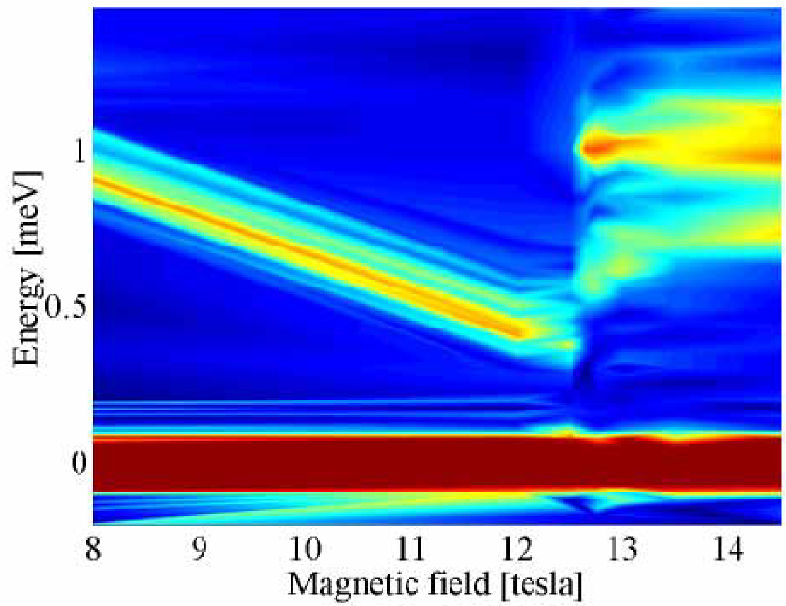
Pressure cell of the type to be employed on SNAP (Spallation Neutrons and Pressure) beamline

T Mason, SNS

Sample environment – Magnetic fields

The neutron is highly penetrating -

enabling studies of samples in containers and complex sample environment…



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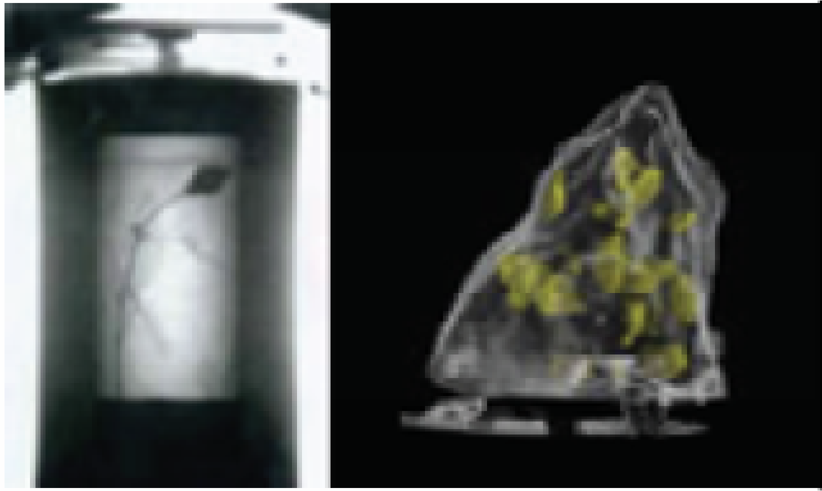
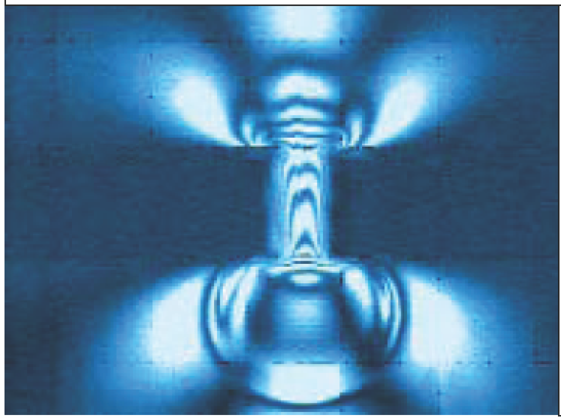
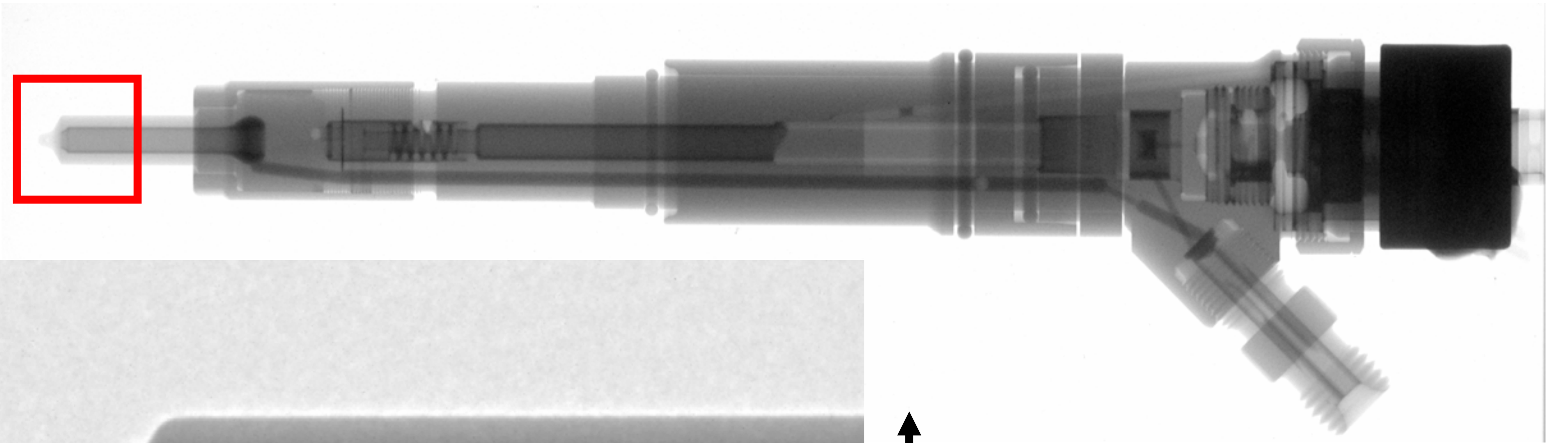
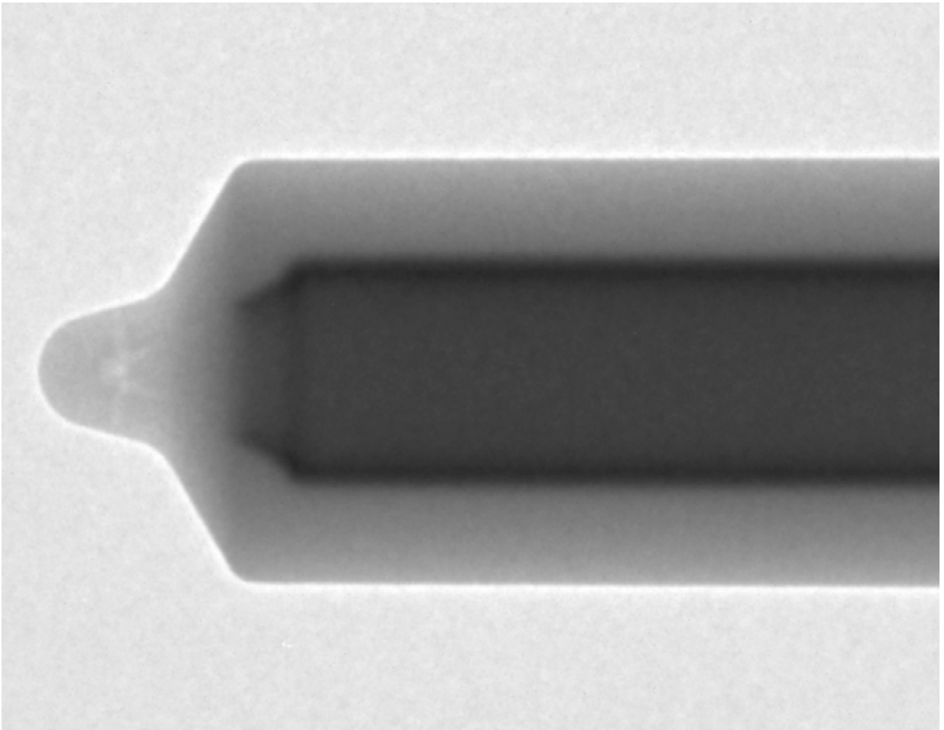


Neutrons can see a red rose inside a lead flask or fossilized Arauc leaves inside an Antarctic rock

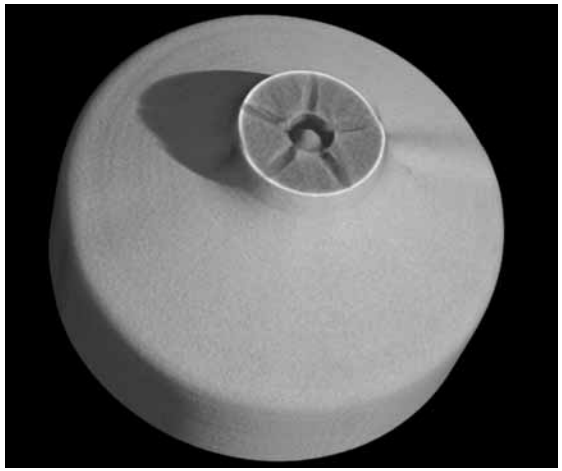
Materials and processing	
	• Processing of soft solids and complex fluids in extruders, mixers, pipe flow and micro-fluidics • Controllable rheology for lubricants and oil extraction • Structural integrity and safety: remediation of residual stresses in alloys, composites and welds • Light weight, high strength, alloys and composites; superconducting wires, bulk amorphous alloys • In-situ measurements to understand materials synthesis, processing and treatments

diesel injection nozzle



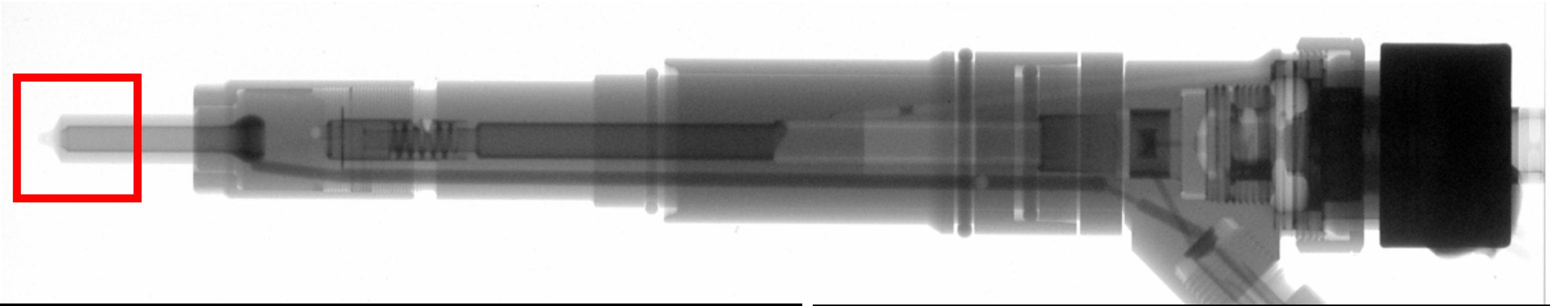


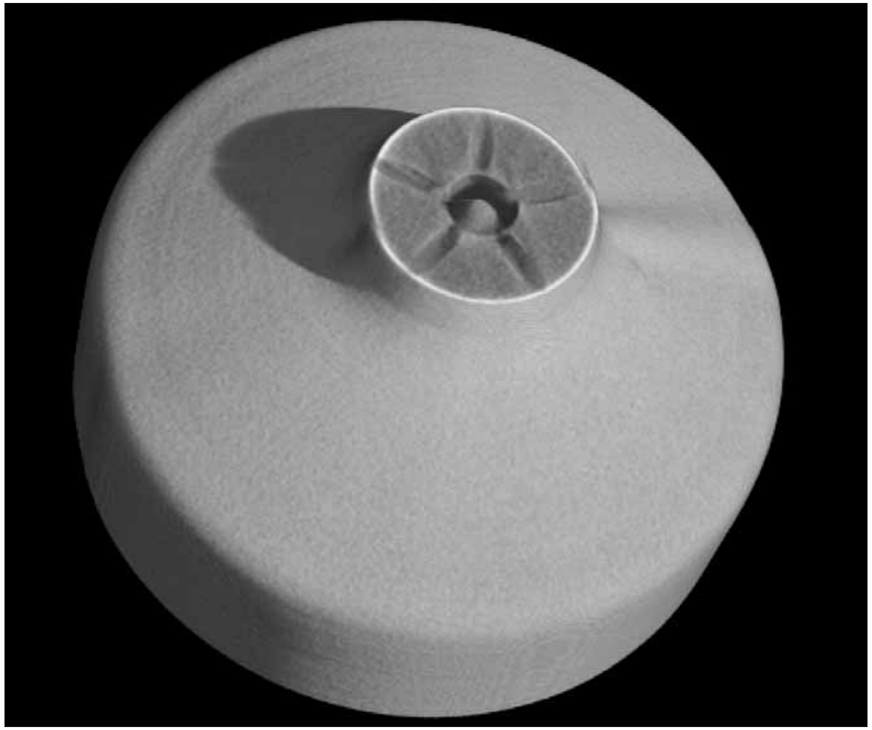
7 mm

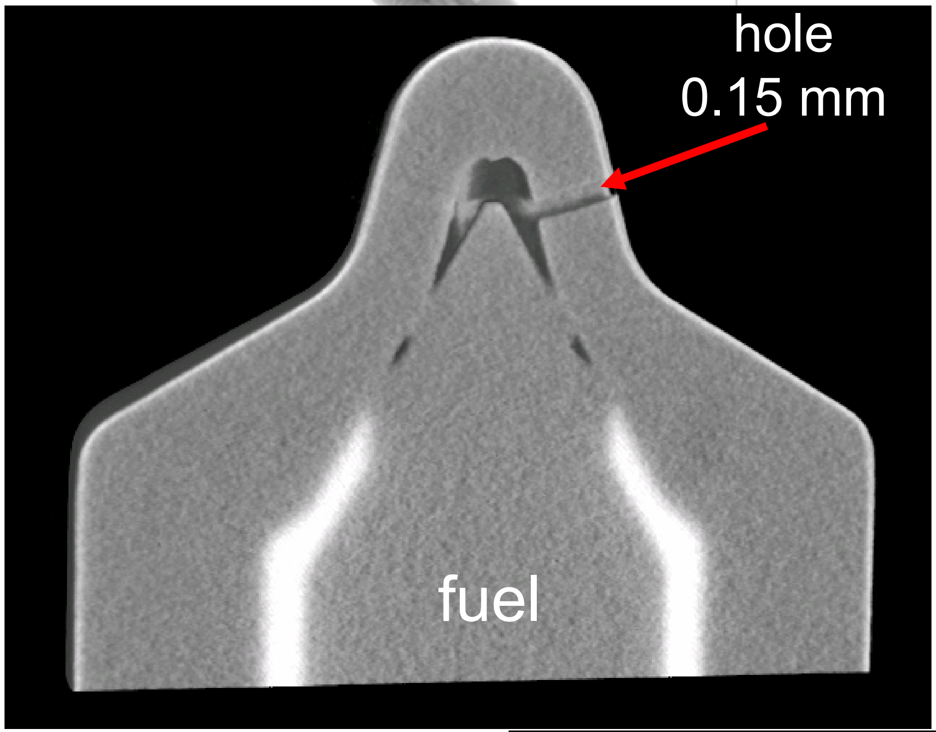


Kuehne/Lehmann PSI

tomography data – diesel injection nozzle

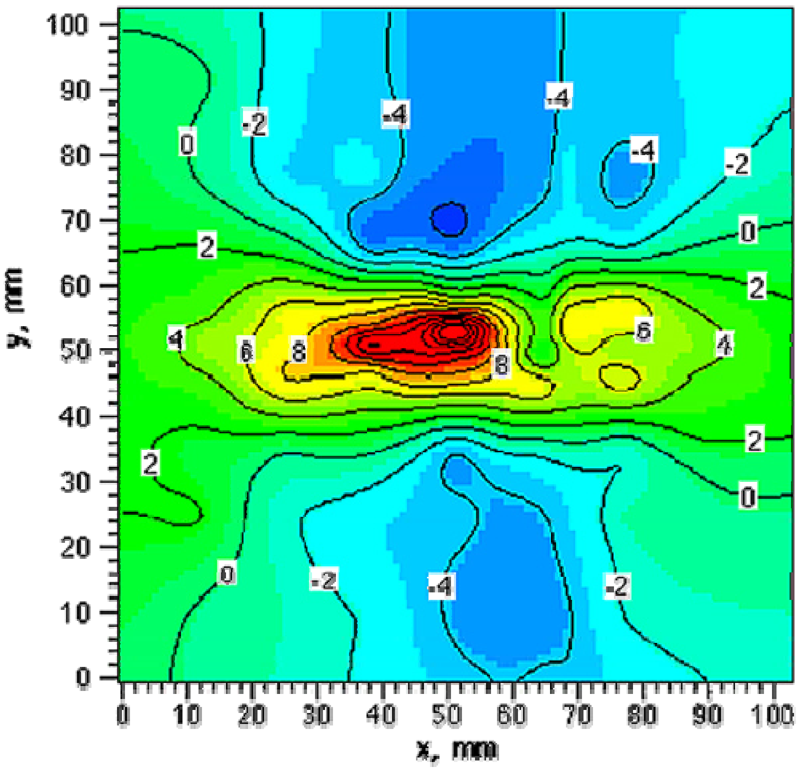






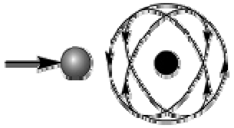
Kuehne/Lehmann PSI

Neutrons penetrate deep into Matter



The aircraft of tomorrow: welding instead of rivets.

Uniqueness of Neutrons



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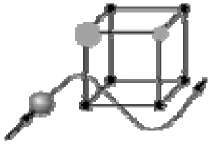

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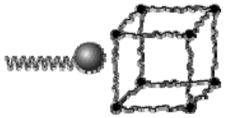

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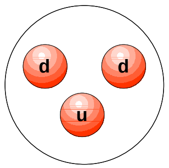

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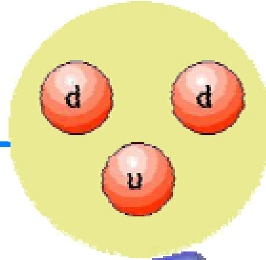

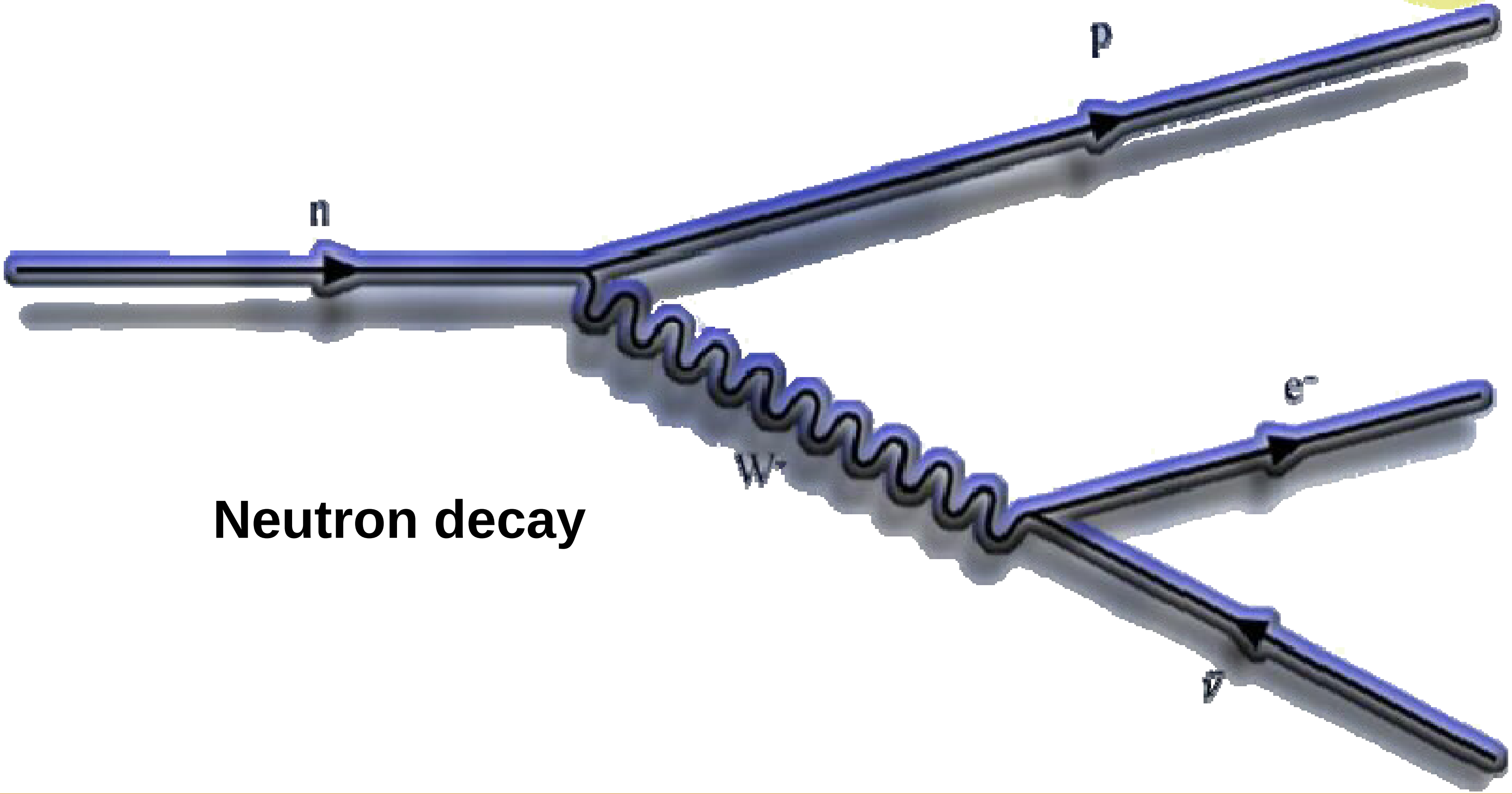

Neutron physics elucidates elementary forces of nature.

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Why not just build better sources?

A free neutron only survives about 1000 sec. $n \rightarrow p^+ + e^-$

To use neutrons we must first get them out of a nuclei, there are basically 3 methods:

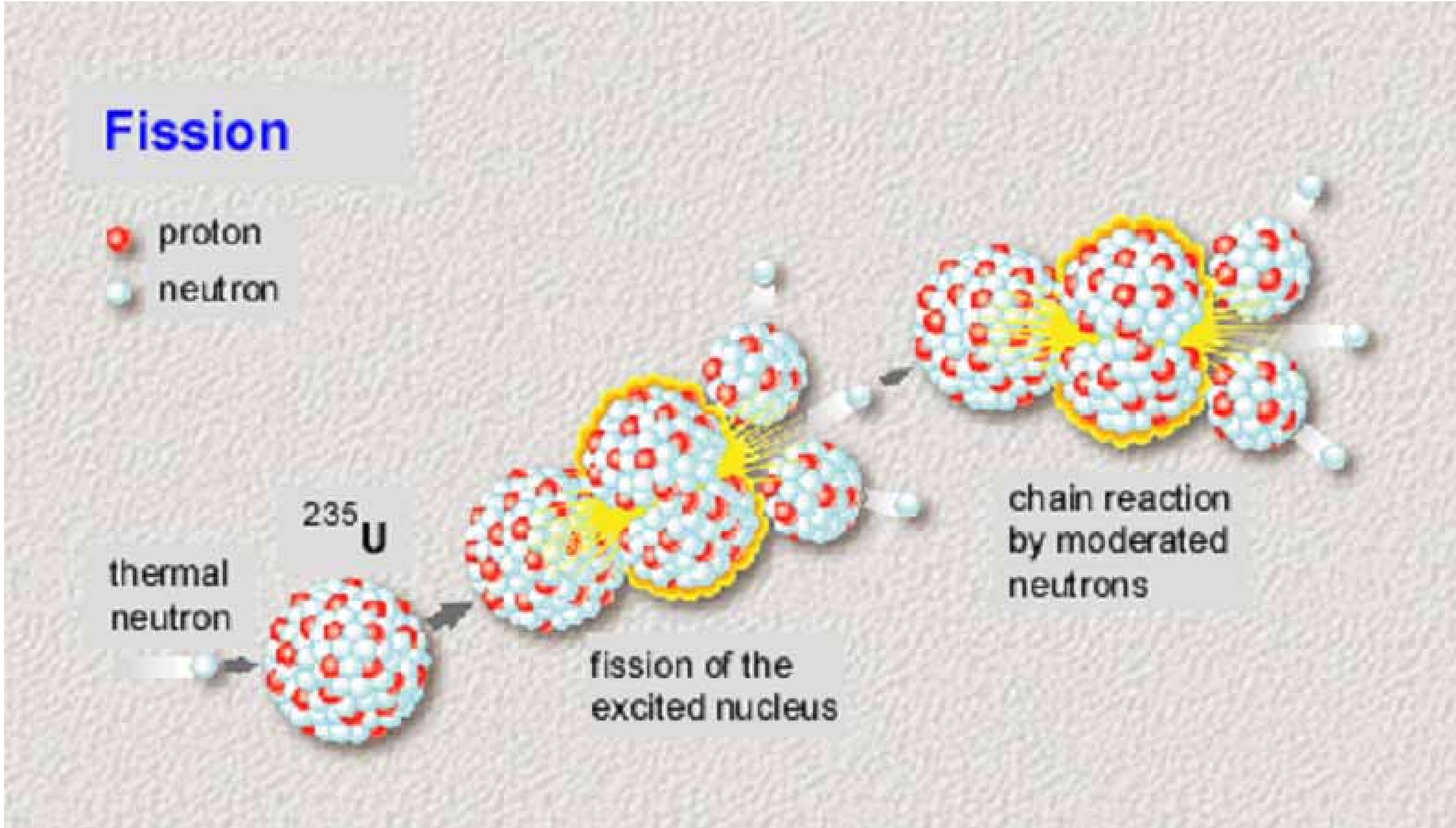
1. Fission
2. Spallation
3. Fusion

In all these cases neutrons are released with high kinetic energy ~ MeV

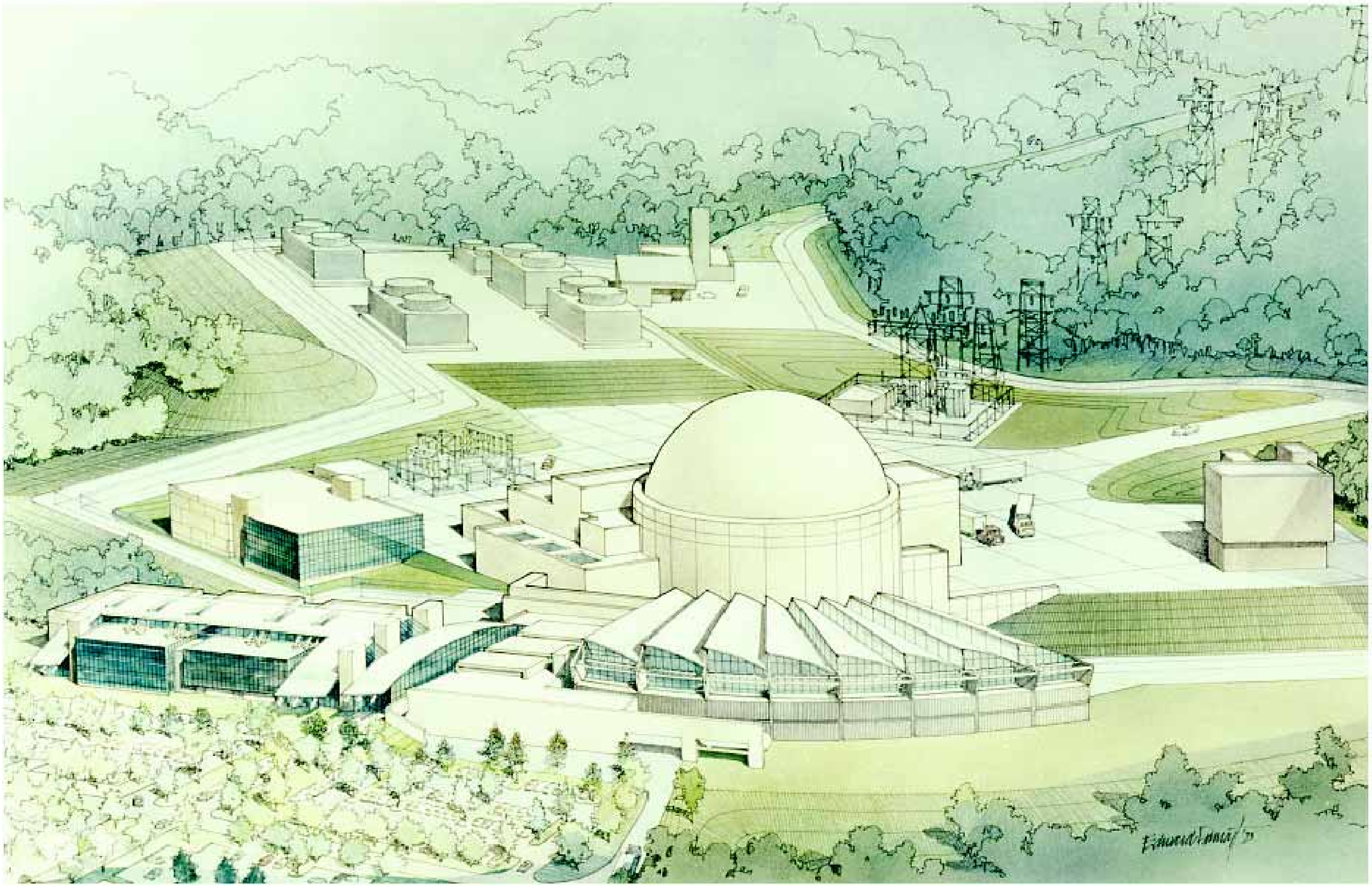
Fission

180-200 MeV/useful neutron

In general for a Continous Source



ANS – Advanced Neutron Source Oak Ridge - USA



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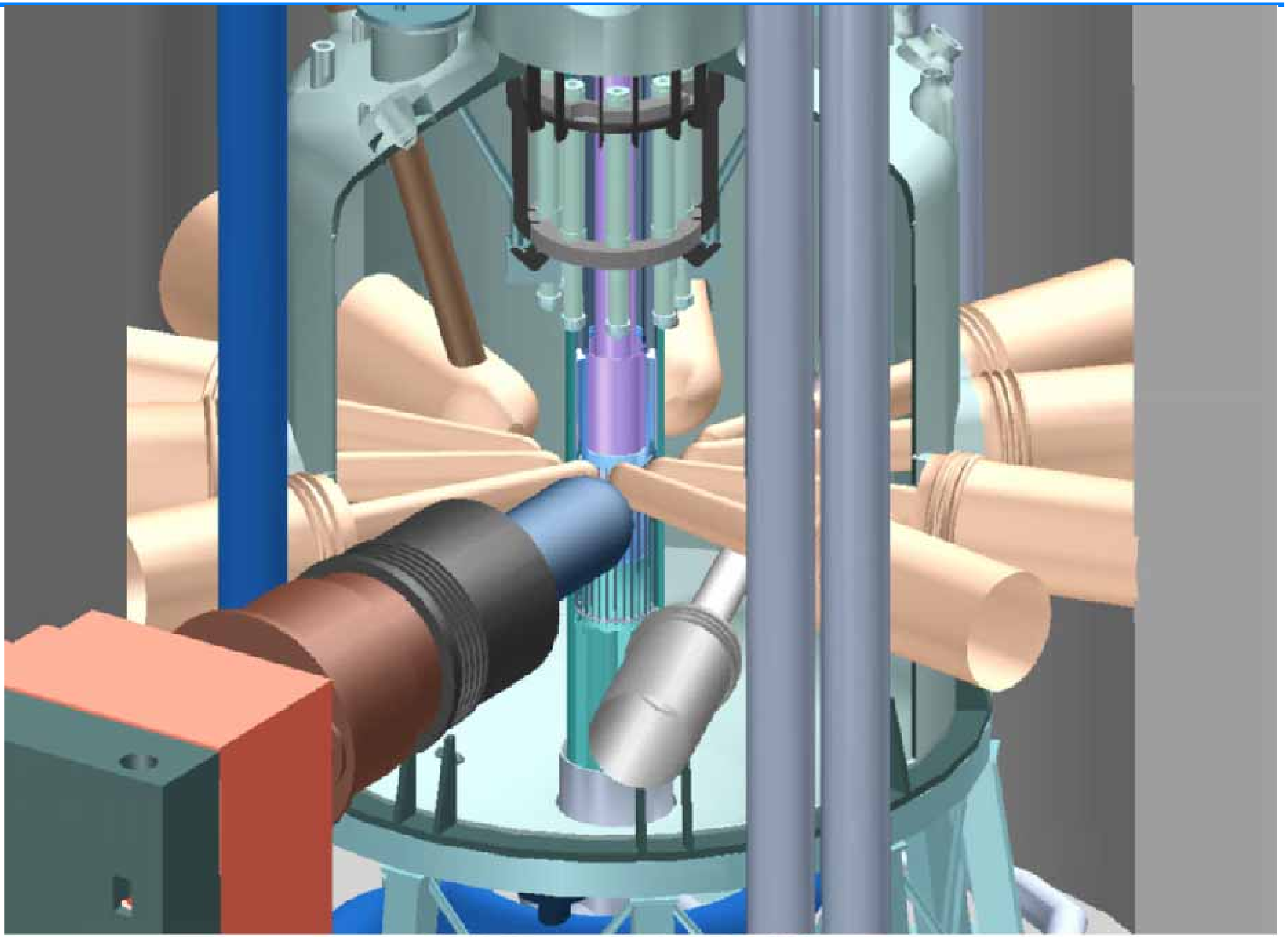


ANS Beam Tube Facilities

ANS parameters -1

Table 2.1. Key reactor physics parameters

Parameter	Reference value
Reactor power	
MW (deposited in fuel and primary coolant)	303
MW (fission)	330
Core life (full power days)	17
Core average thermal power density (MW/L)	4.5
Peak reflector thermal flux	
BOC ($m^{-2}s^{-1}$)	7.19×10^{19}
EOC ($m^{-2}s^{-1}$)	7.40×10^{19}
Flux efficiency at EOC ($m^{-2}s^{-1}MW_f^{-1}$)	2.24×10^{17}
Core fissile loading at BOC (Kg ^{235}U)	15.1
Fuel burnup (Kg ^{235}U)	7.0

ANS parameters - 2

Parameter	SI units	Alternate units
Primary coolant flow rate:		
Total (through pump)	2.01 Mg/s	29,100 gal/min
Through active core (fuel)	➡ 1.83 Mg/s	26,500 gal/min
Reactor assembly inlet pressure	3.5 MPa	508 psia
Fuel inlet pressure	➡ 3.2 MPa	464 psia
Secondary coolant flow rate	4.96 m^3/s	78,600 gal/min
Primary loop design pressure	4.0 MPa	580 psi

ANS:

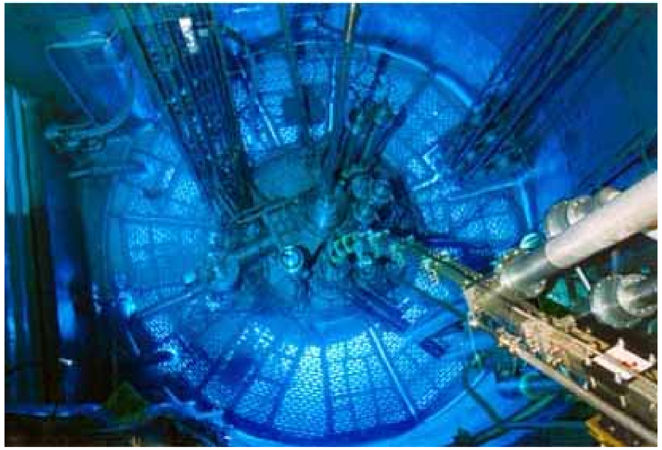
Highly enriched fuel, substantial technical risk

Construction and Operation Cost continuously escalating

➔Project abandoned 1995 @ 3 G$

Fission based sources limited by the ability to cool the core!

Operating Fission sources → 1/6 ANS



55 MW thermal

The world's most powerful reactor neutron source.

First operation 1972

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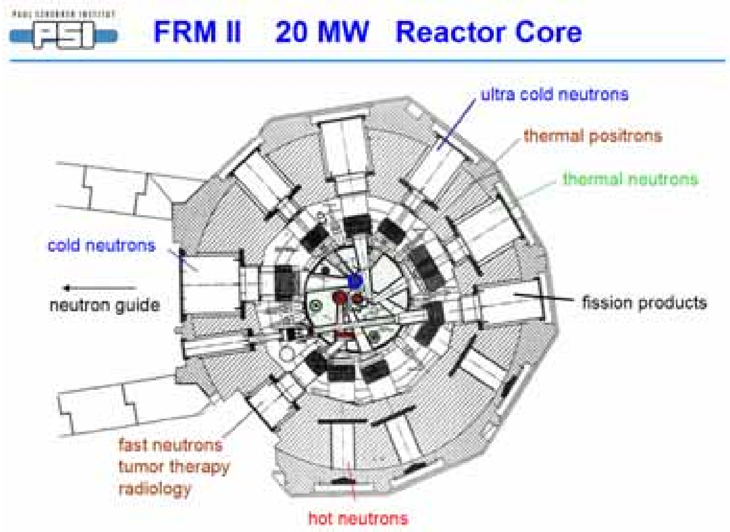
FRM-II



TECHNISCHE UNIVERSITÄT MÜNCHEN

Forschungs-Neutronenquelle

Heinz Maier-Leibnitz

FRM II

Reactor / CW sources – not to be forgotten

still competitive in many areas

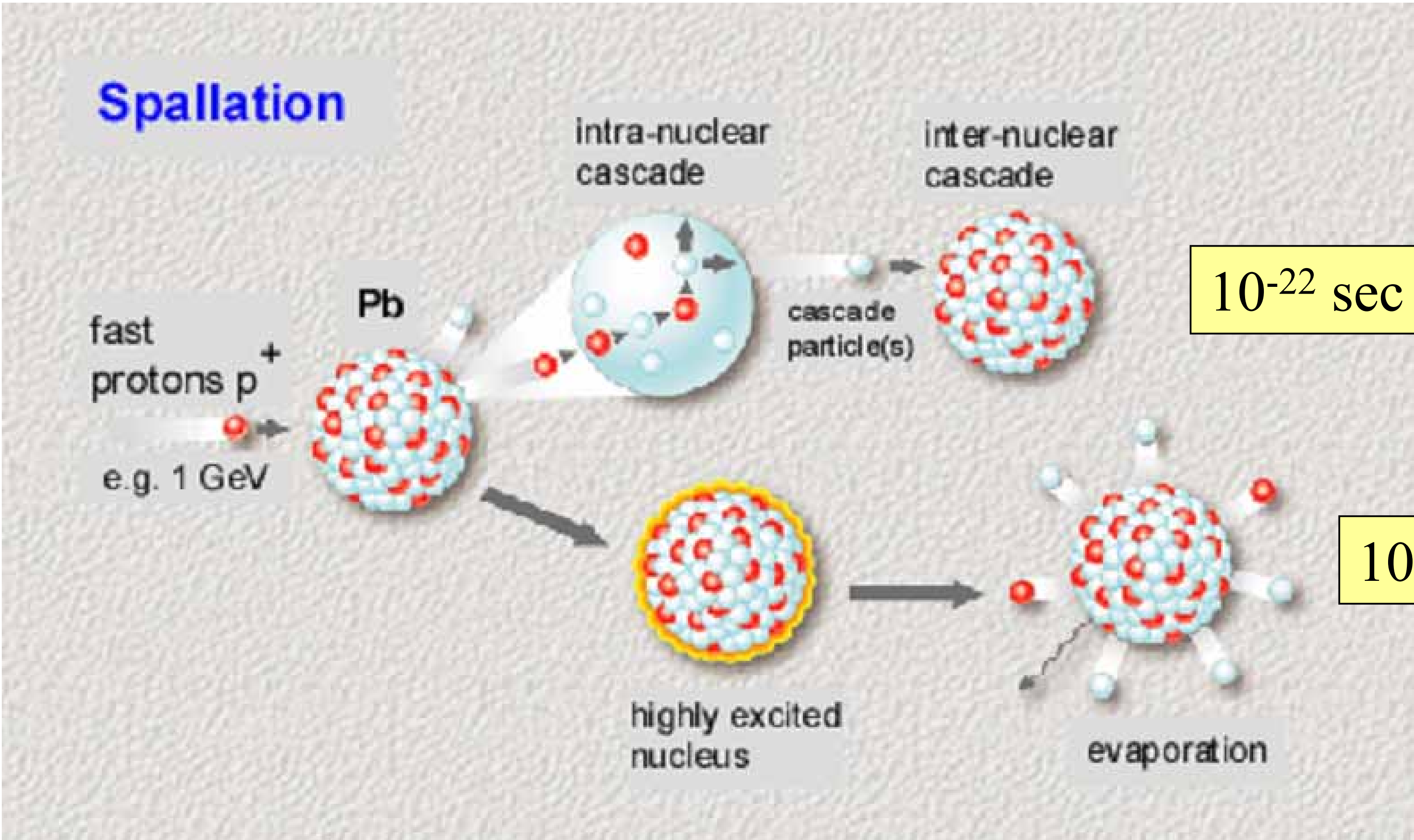
synergy with other applications

Process	Example	Yield	Energy deposition in target (MeV/n)	Average Kinetic Energy carried away by neutron (MeV/n)
Fission	^{235}U	1 n/fission	180	2
Spallation	1.3 GeV protons on Hg	33 - 40 n/proton	30 - 35	2 – 5

Spallation

30 - 35 MeV/useful neutron (Hg 1.3 GeV protons)

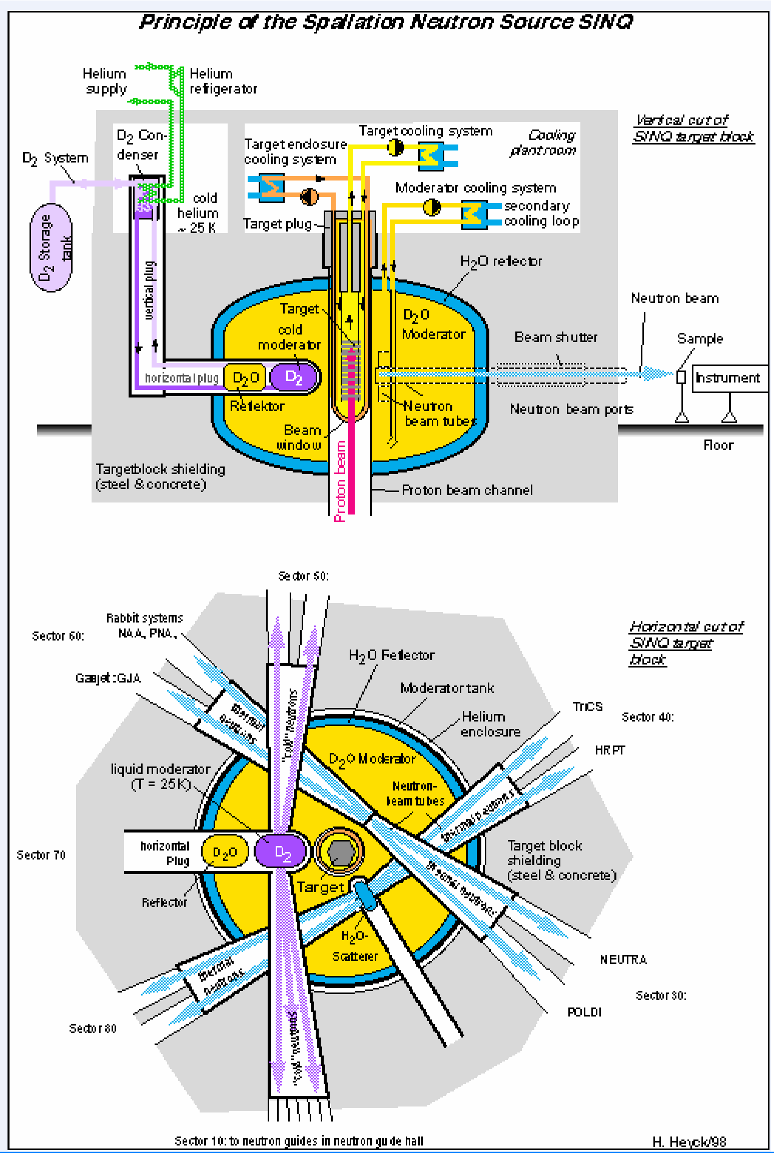
Ideally suited for pulsed operation.

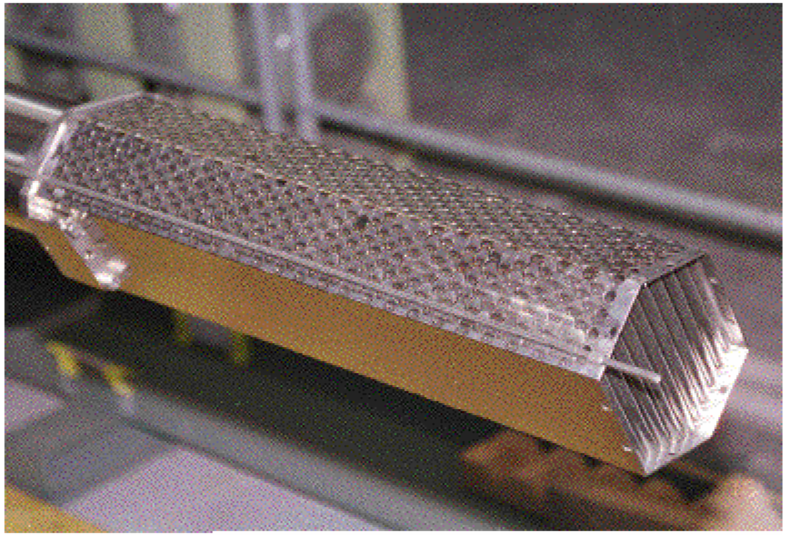


10^{-22} sec

10^{-18} sec

SINQ at PSI





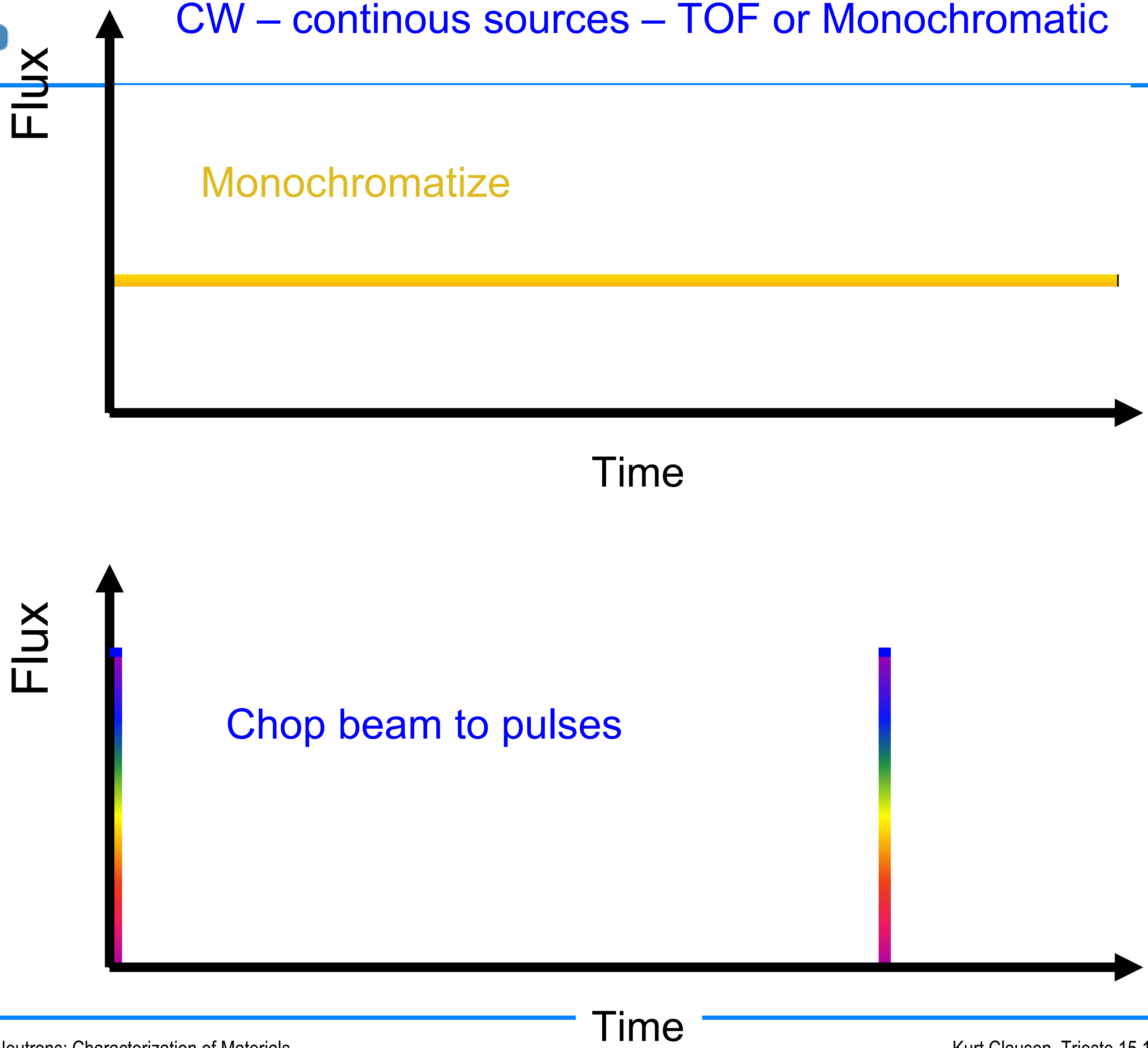
Proton current 1.25 mA

Proton Energy 600 MeV

Beam power 750 kW

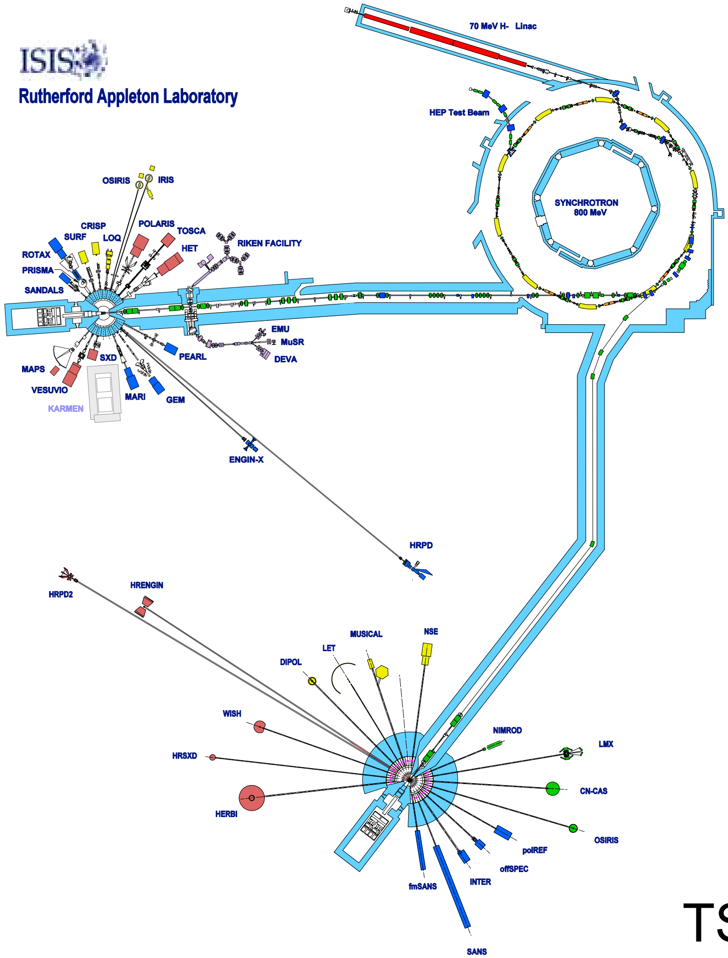
Flux like 10 MW reactor

CW – continous sources – TOF or Monochromatic



ISIS UK – SP spallation source

ISIS SP spallation source



ZOOM	Focusing SANS
LMX	Single crystal
EXEED	Extreme conditions Diffraction
EXESS	Extreme conditions Inelastic chopper
IMAT	Imaging/materials
Chip irradiation	
SPIRAL/LARMOR	SESANS, High Res diffraction, MISANS
NESSIE	Spin-echo

TS2 will start operation 2008/9

SNS – Short Pulse Spallation Source

The SNS will begin operation in 2006 in Oak Ridge, Tennessee

At 1.4 MW it will be ~8x ISIS, the world's leading pulsed spallation source

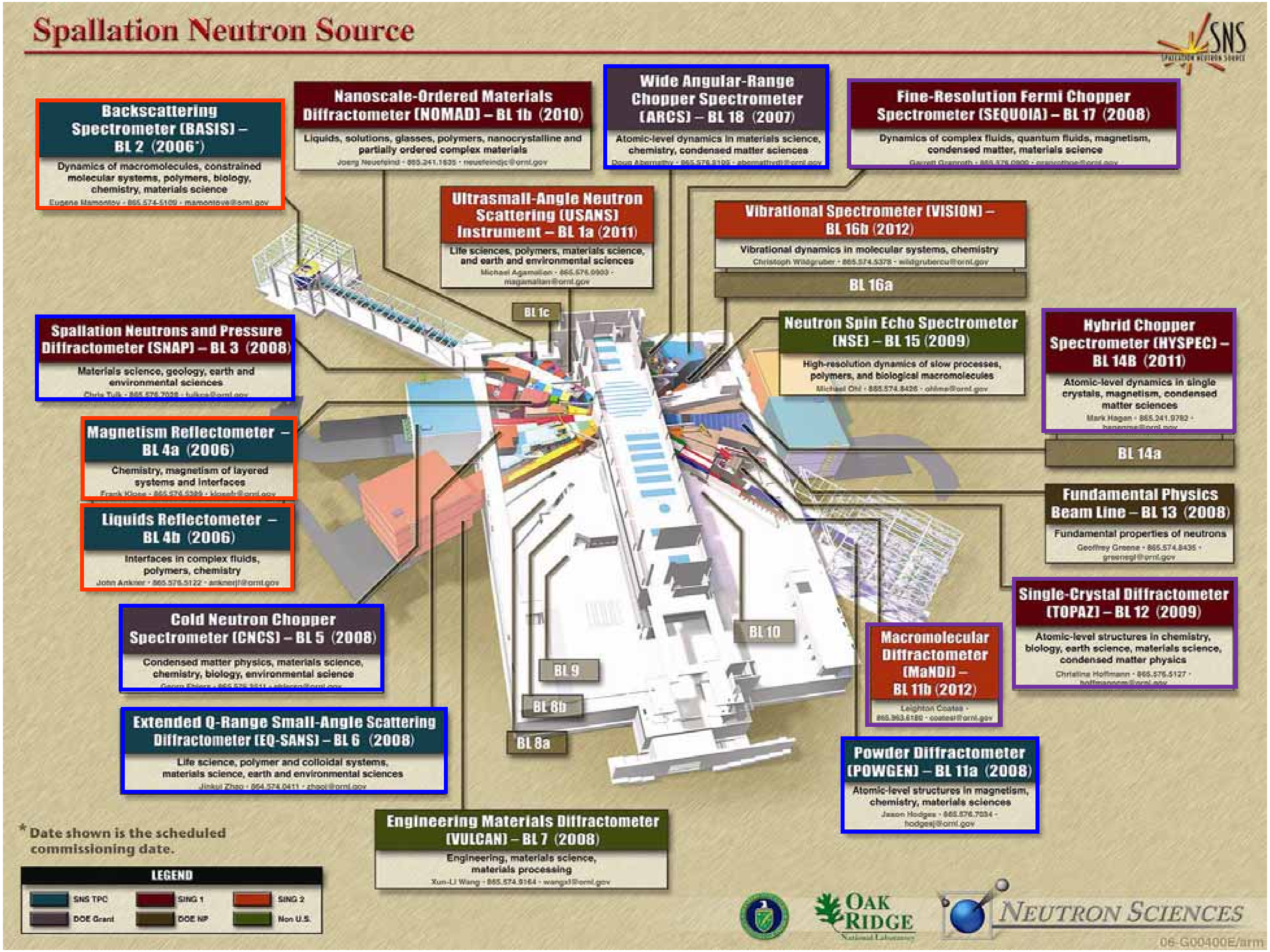
The peak thermal neutron flux will be ~50-100x ILL

Initial facility will have 1 target station with 24 instruments

An upgrade to 3-4 MW and a second target station is planned

ORNL Neutron Scattering Facilities SNS and HFIR

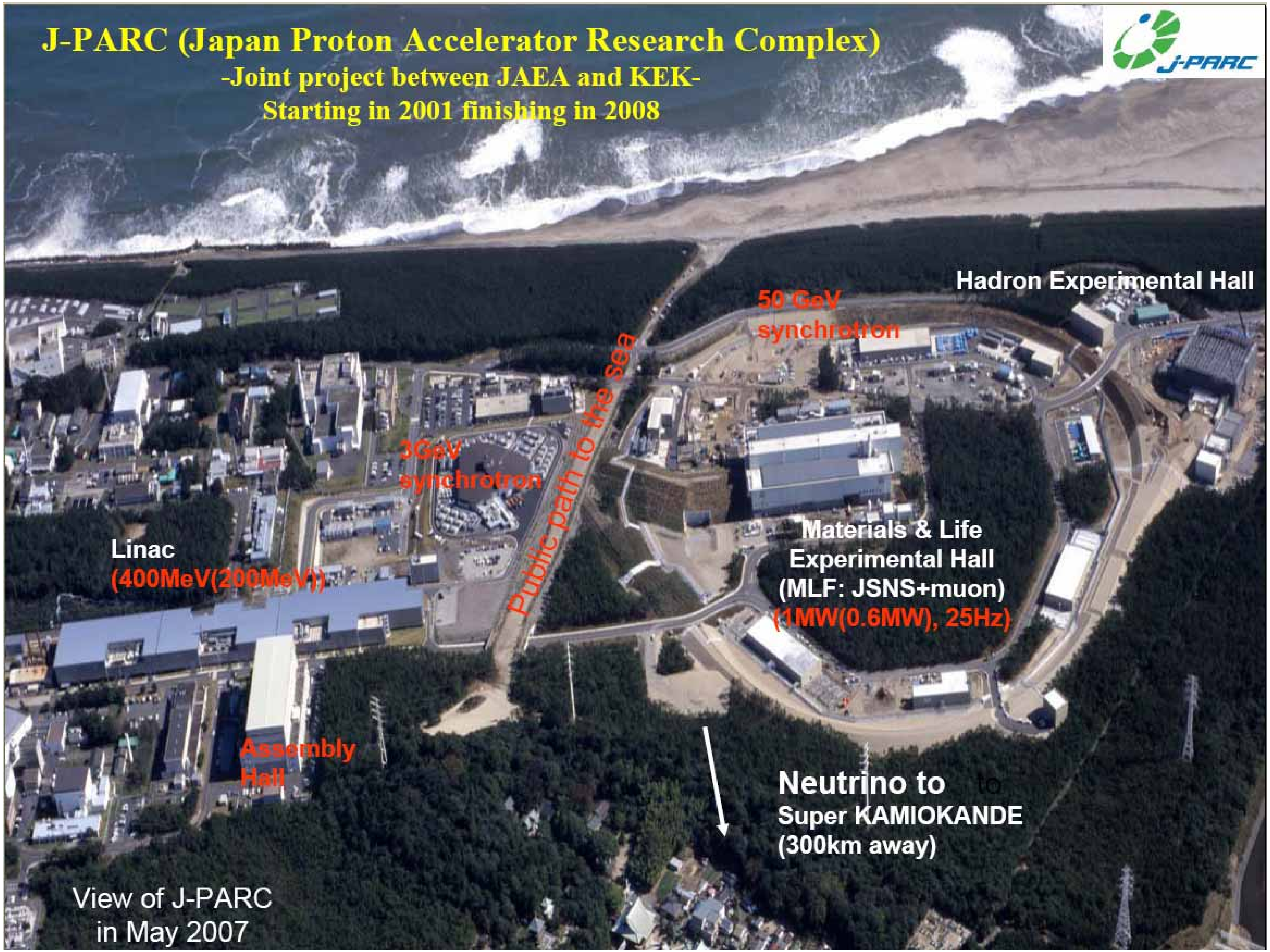
- **SNS construction was completed May 2006, user operations in Fall 2007**
- **At 1.4 MW SNS will be the world's leading pulsed spallation source**
- **Room for eventual 24 instruments spanning physics, chemistry, biology, & materials science**
- **High Flux Isotope Reactor (HFIR) – U.S. highest flux source of continuous neutrons**
- **Restarted with a new cold source in May 2007**
- **Two new SANS instruments in commissioning**


Spallation Neutron Source
SNS
Backscattering Spectrometer (BASIS) – BL 2 (2006*)
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Eugene Mamontov · 865.574.5109 · mamontove@ornl.gov
Nanoscale-Ordered Materials Diffractometer (NOMAD) – BL 1b (2010)
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Joerg Neuefeind · 865.241.1635 · neuefeindjc@ornl.gov
Wide Angular-Range Chopper Spectrometer (ARCS) – BL 18 (2007)
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) – BL 17 (2008)
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Ultrasmall-Angle Neutron Scattering (USANS) Instrument – BL 1a (2011)
Life sciences, polymers, materials science, and earth and environmental sciences
Michael Agamalian · 865.576.0903 · magamalian@ornl.gov
Vibrational Spectrometer (VISION) – BL 16b (2012)
Vibrational dynamics in molecular systems, chemistry
Christoph Wildgruber · 865.574.5378 · wildgrubercu@ornl.gov
BL 16a
BL 1c
Spallation Neutrons and Pressure Diffractometer (SNAP) – BL 3 (2008)
Materials science, geology, earth and environmental sciences
Neutron Spin Echo Spectrometer (NSE) – BL 15 (2009)
High-resolution dynamics of slow processes, polymers, and biological macromolecules
Michael Ohl · 865.574.8426 · ohlme@ornl.gov
Hybrid Chopper Spectrometer (HYSPEC) – BL 14B (2011)
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
Mark Hagen · 865.241.9782 ·
Magnetism Reflectometer – BL 4a (2006)
Chemistry, magnetism of layered systems and interfaces
BL 14a
Fundamental Physics Beam Line – BL 13 (2008)
Fundamental properties of neutrons
Geoffrey Greene · 865.574.8435 · greenegl@ornl.gov
Liquids Reflectometer – BL 4b (2006)
Interfaces in complex fluids, polymers, chemistry
John Ankner · 865.576.5122 · anknerjf@ornl.gov
Single-Crystal Diffractometer (TOPAZ) – BL 12 (2009)
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
Christina Hoffmann · 865.576.5127 ·
Cold Neutron Chopper Spectrometer (CNCS) – BL 5 (2008)
Condensed matter physics, materials science, chemistry, biology, environmental science
BL 10
BL 9
Macromolecular Diffractometer (MaNDi) – BL 11b (2012)
Leighton Coates · 865.963.6180 · coatesl@ornl.gov
BL 8b
BL 8a
Extended Q-Range Small-Angle Scattering Diffractometer (EQ-SANS) – BL 6 (2008)
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
Powder Diffractometer (POWGEN) – BL 11a (2008)
Atomic-level structures in magnetism, chemistry, materials sciences
Jason Hodges · 865.576.7034 · hodgesj@ornl.gov
Engineering Materials Diffractometer (VULCAN) – BL 7 (2008)
Engineering, materials science, materials processing
Xun-Li Wang · 865.574.9164 · wangxl@ornl.gov
* Date shown is the scheduled commissioning date.
LEGEND
SNS TPC
SING 1
SING 2
DOE Grant
DOE NP
Non U.S.
Oak Ridge National Laboratory
Neutron Sciences
06-G00400E/arm

J-PARC (Japan Proton Accelerator Research Complex)

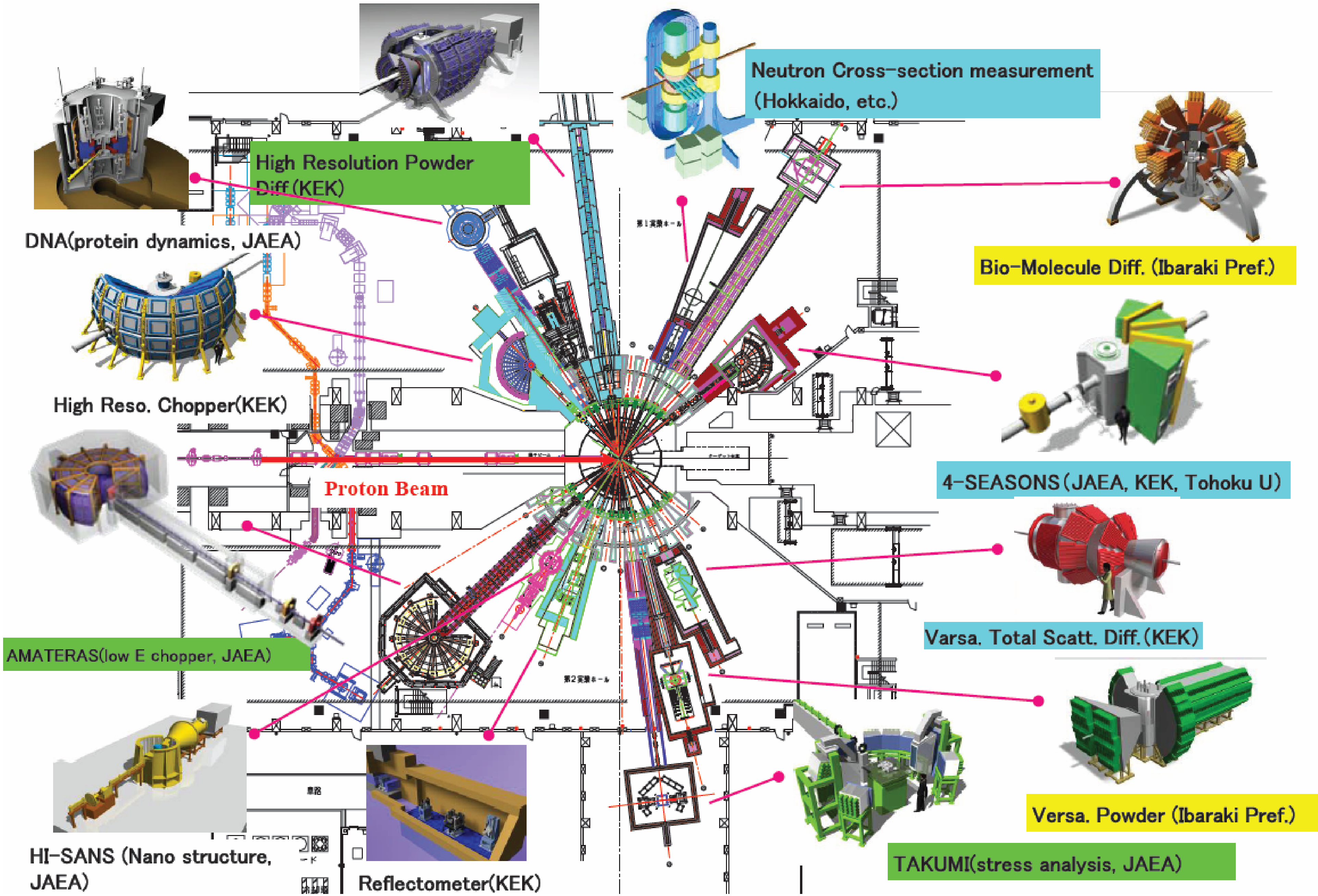
-Joint project between JAEA and KEK-

Starting in 2001 finishing in 2008



Neutron Instruments under construction (color labeled) and planned

JAEA or KEK、 Ibaraki Pref. Grant



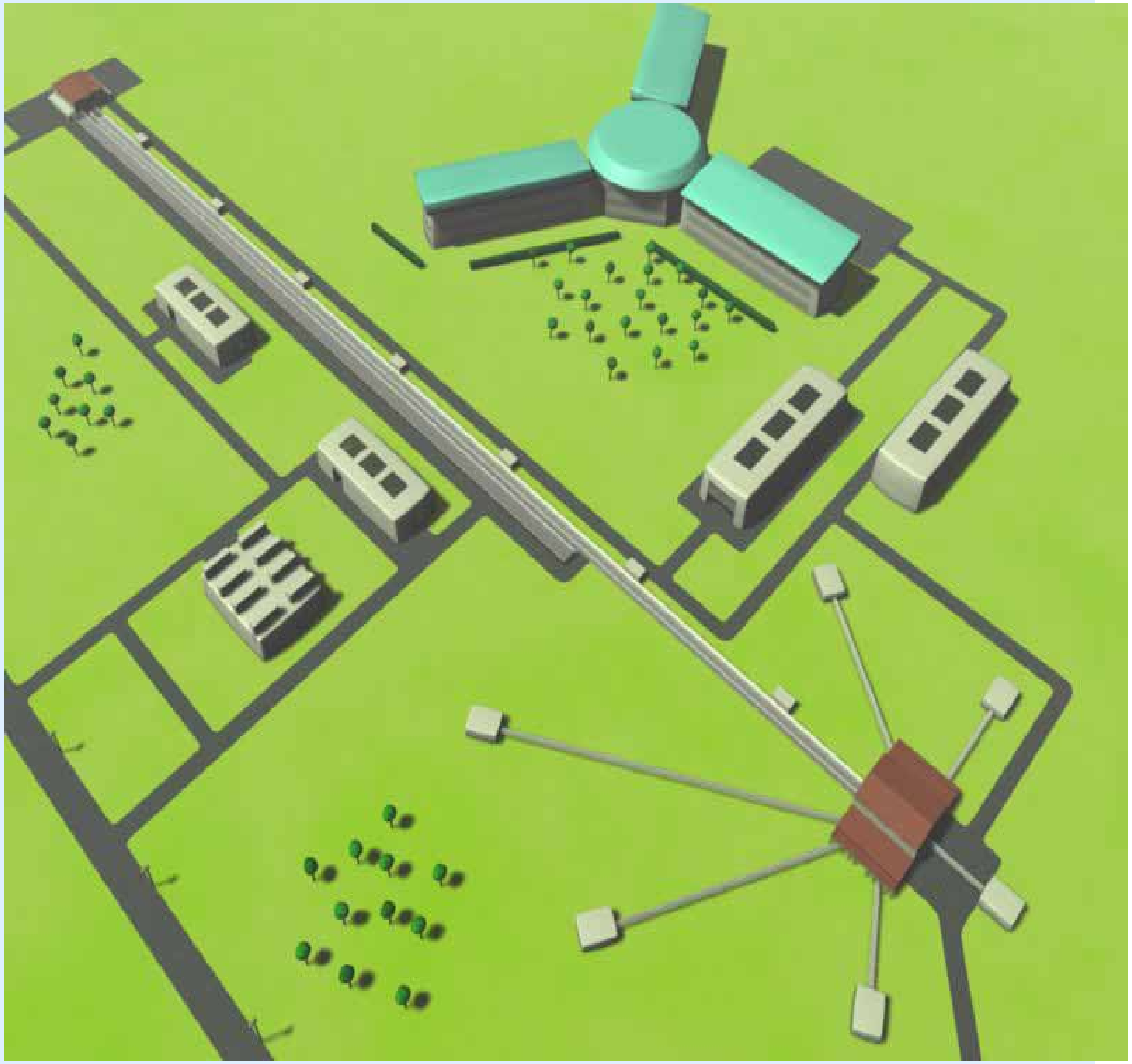
ESS – LP spallation source

5 MW LP (2 msec)
H^+ Linac
Target station with
up to 20+ instruments
(typical length 200 m)

"On ESFRI roadmap"

Superior/Complimentary
to SNS and JPARC

Interest to host
(and fund substantial part)
Lund Sweden
Bilbao Spain
?? Hungary



Process	Example	Yield	Energy deposition in target (MeV/n)	Average Kinetic Energy carried away by neutron (MeV/n)
Fission	^{235}U	1 n/fission	180	2
Spallation	1.3 GeV protons on Hg	33 - 40 n/proton	30 - 35	2 – 5

Fusion – when will it be interesting?

Let us first forget the repetition rate and only look at the required flux:

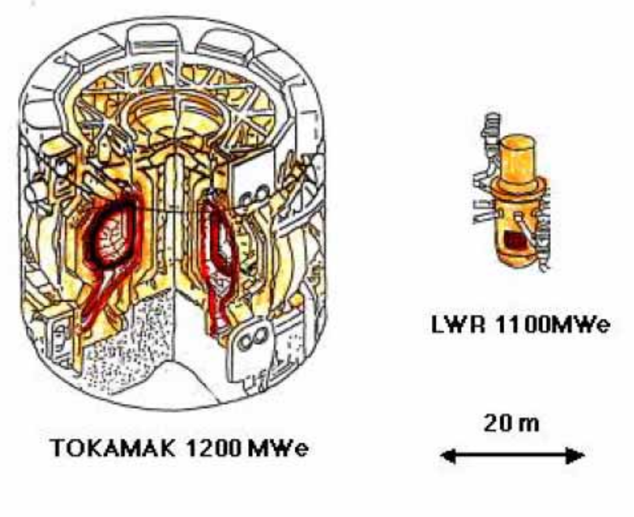
The best present sources delivers about 10^{18} neutrons/sec

For fusion to be competitive it must

- either be much cheaper than fission or spallation
- or provide a neutron production rate of > 10^{18} neutrons/sec within a volume of the order of 50 dm^3 !

We can forget about thermonuclear fusion

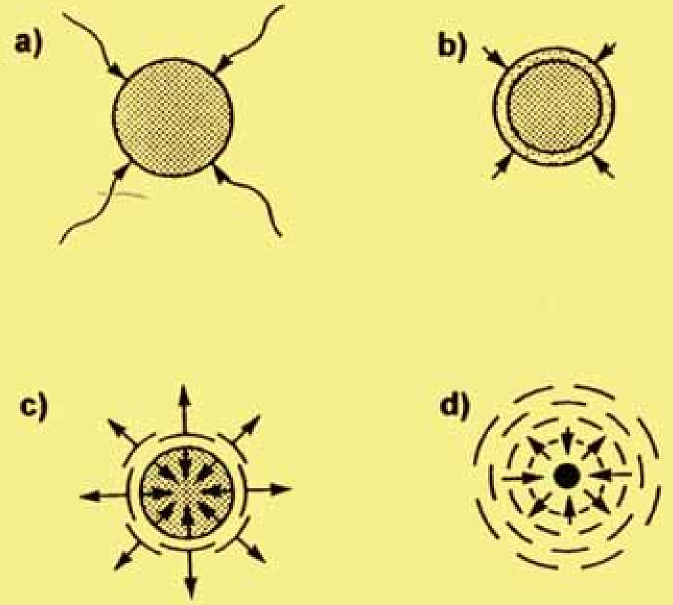
- neutron production in too big a volume
- Geometry incompatible with neutron scattering



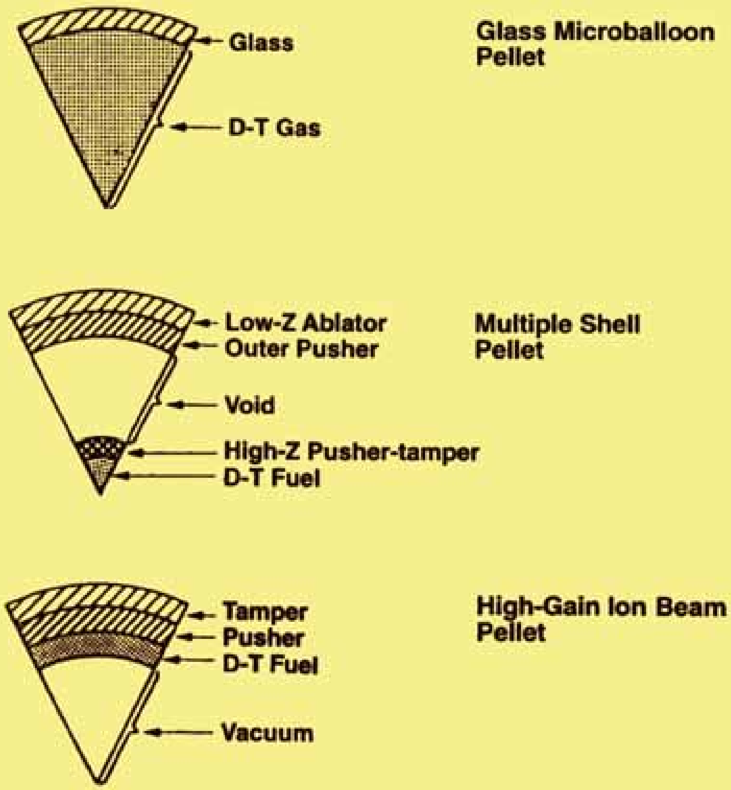
[Comparison of reactor size]

Process	Example	Yield	Energy deposition in target (MeV/n)	Average Kinetic Energy carried away by neutron (MeV/n)
Fission	^{235}U	1 n/fission	180	2
Spallation	1.3 GeV protons on Hg	33 - 40 n/proton	30 - 35	2 – 5
Fusion DT solid target	400 keV Deuterons on T in titanium	4.0 10^{-5} n/D	10’000	14.1
Fusion DT inertial confinement	D + T fusion in laser or ion-beam imploded target	1 n/fusion	3.5 + 0.1	14.1

Inertial confinement fusion



Stages associated with inertial confinement fusion: (a) irradiation with high intensity beams, (b) corona formation, (c) ablation and compression, (d) heating, fusion, and disassembly.



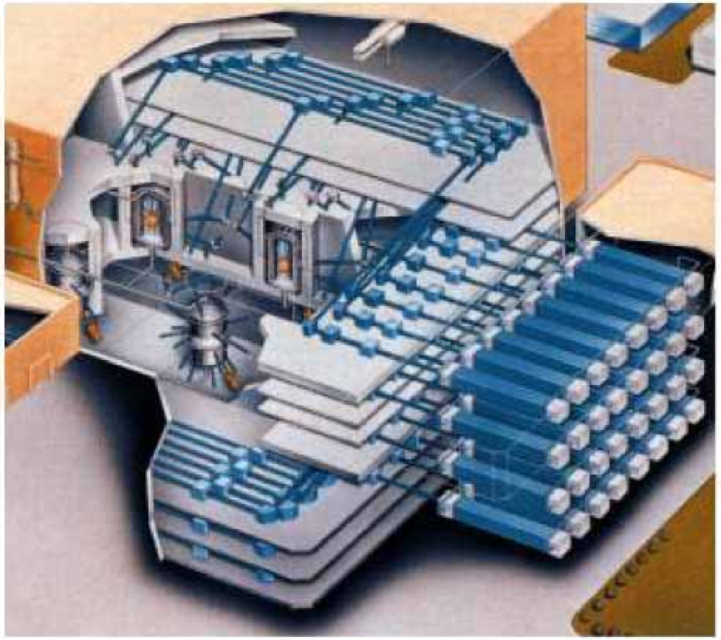
Cross section of selected pellets for inertial confinement fusion.

Laser fusion – demo at the earliest 2030

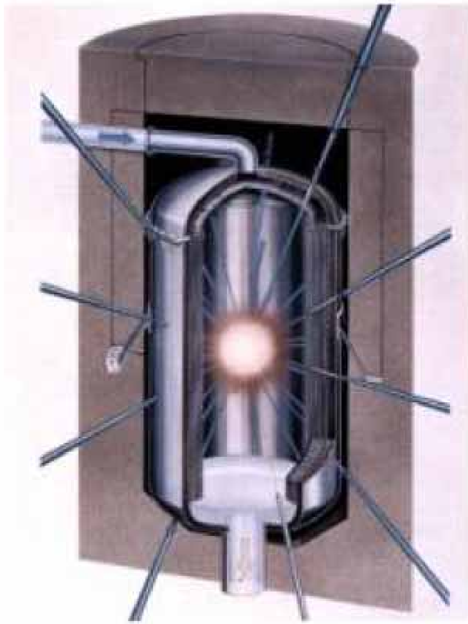
Characteristics of laser fusion power plnts

ILE OSAKA

1. Separabillity of major system and high potential for modular plants
2. Pulse power and pulse repetition plants
3. Potential for small size plants, simple reactors



Laser fusion power plant KOYO
4 reactor modules (700 MWe x 4)



Liquid wall reactor modules

Ca 10 m

Energy deposition

$$_1D^2 + {_1T^3} \rightarrow {_2He^4} + {_0n^1}$$

$$3.5\ \text{MeV} + 14.1\ \text{MeV} = 17.6\ \text{MeV}$$

Heat to be removed by water (pre-)moderator around the Fusion source (to match existing sources or sources under construction):

> 17.6 MeV/n * 10^{18} n/sec = 2.8 MW plus heating from laser beams

If we want the source to be the next generation beyond existing sources then we should have a pulse sequence of 10 to 50 Hz and 10^{19} n/sec in total production within 50 dm^3!

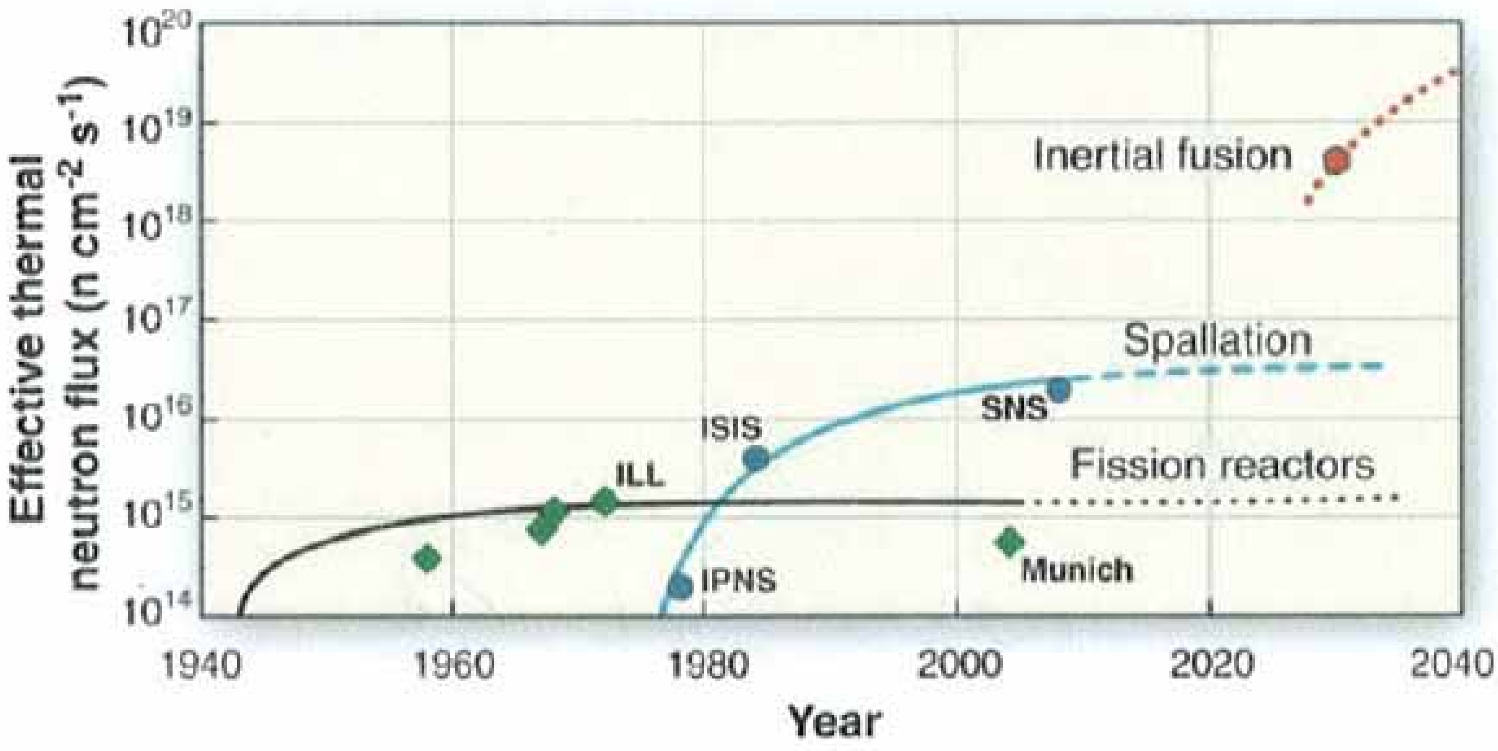
This technology is not available now and will not be so in the next many years to come!

SURPRISE!

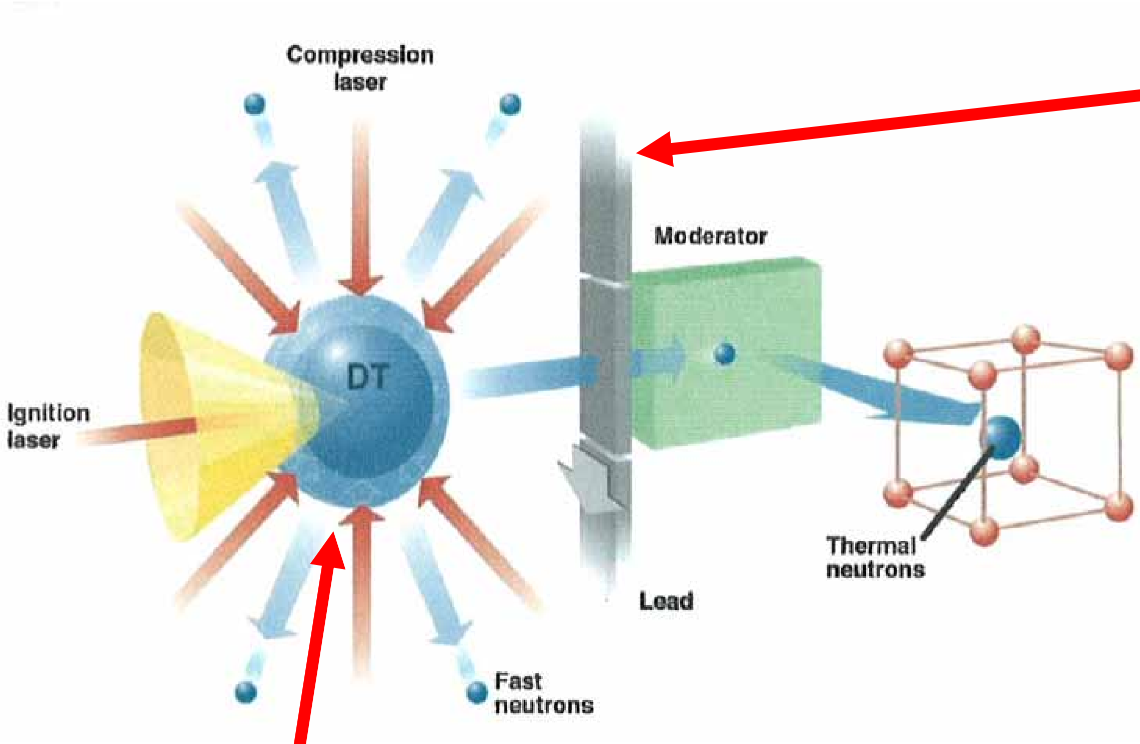
23 FEBRUARY 2007 VOL 315 **SCIENCE** www.sciencemag.org

A Route to the Brightest Possible Neutron Source?

Andrew Taylor,[1*] Mike Dunne,[1] Steve Bennington,[1] Stuart Ansell,[1] Ian Gardner,[1]
Peter Norreys,[1] Tim Broome,[1] David Findlay,[1] Richard Nelmes[2]



Some "minor" problems!



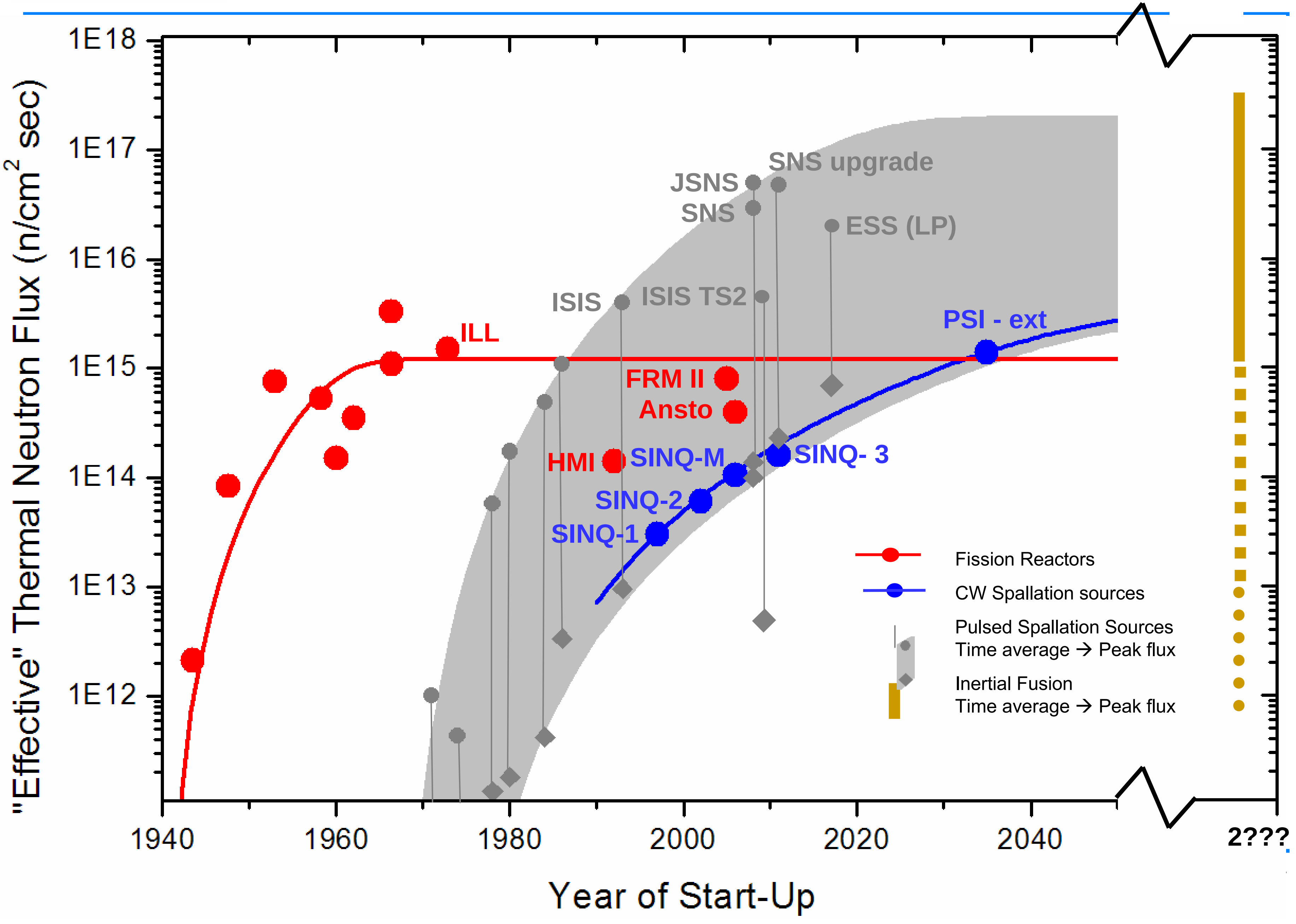
2160 metric tons of (radioactive) lead per moderator that need to be handled daily.

An operational source will at most be a factor of two beyond a spallation source

10 kg of Tritium per year in the form of 864.000 encapsulated Tritium pellets per day.

Furthermore experience show that it takes ca 30 years from first demonstrator to dedicated neutron source – fusion demonstrator ….far away

SPALLATION IS THE ONLY WAY!



Acknowledgement – thanks to:

The ESS project: D Richter, G Bauer, R McGreevy, CPT, …….
http://neutron.neutron-eu.net/n_documentation/n_reports/n_ess_reports_and_more

SNS – Oak Ridge, USA: T Mason, N Holtkamp, I Anderson, http://www.sns.gov/

J-SNS Japan: M. Arai, … http://jkj.tokai.jaeri.go.jp/

The UK Neutron Strategy Document: www.neutrons.cclrc.ac.uk/Activity/ScienceCase

PSI: W Wagner, S Janssen, Joachim Kohlbrecher, Thomas Gutberlet, E Lehmann, F. Pfeiffer, F van der Veen, C. Quitman, M Stampanoni, V. Pomjakushin, Christian Rüegg, Henrik Ronnow, R Bercher, H Luetkens plus LNS and LMU
http://www.psi.ch
http://www.psi.ch/forschung/benutzerlabor.shtml

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