Neutron and **X-ray Scattering** of **Quantum Materials**

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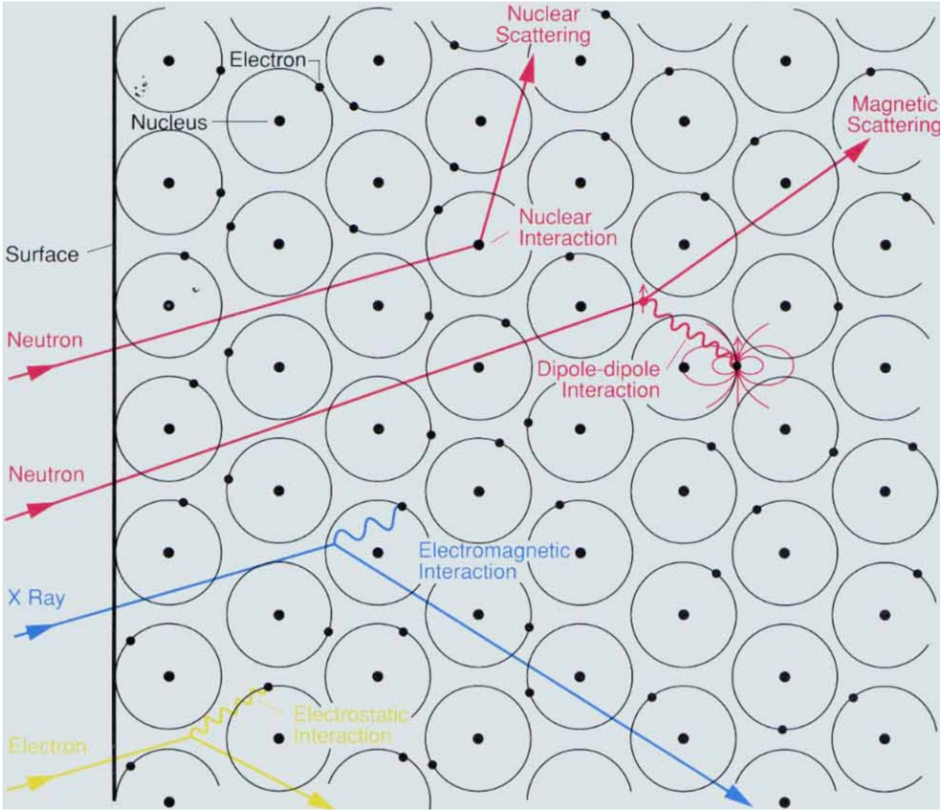
Outline for today

- Introduction to scattering as an experimental tool in general
- Information about the course:
  - Format
  - Contents
  - Expectations
- Introduction to neutron scattering (Chapters 1-2 + 4.1)
  - History
  - How to generate neutrons
  - Facilities
  - Basic scattering theory

Particles as probes in experimental physics

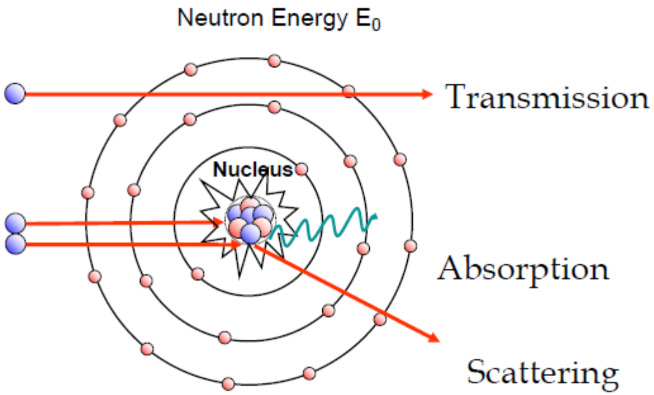
- Neutrons
- X-rays
- Other kinds of light
- Electrons
- Muons
- Ions

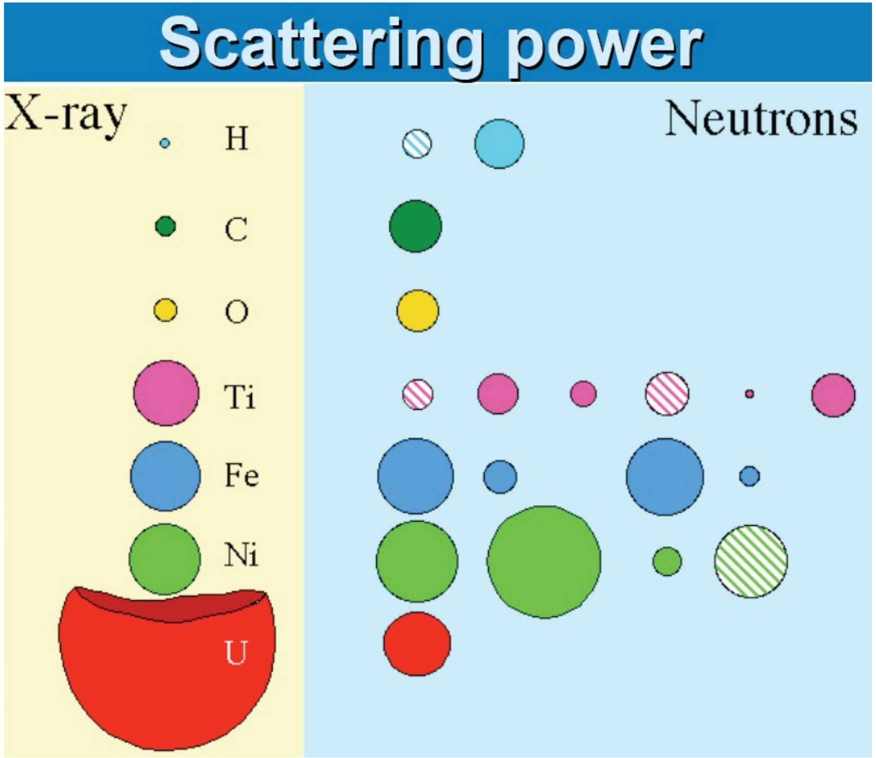
Interaction with matter:
Absorption
Elastic scattering
Inelastic processes

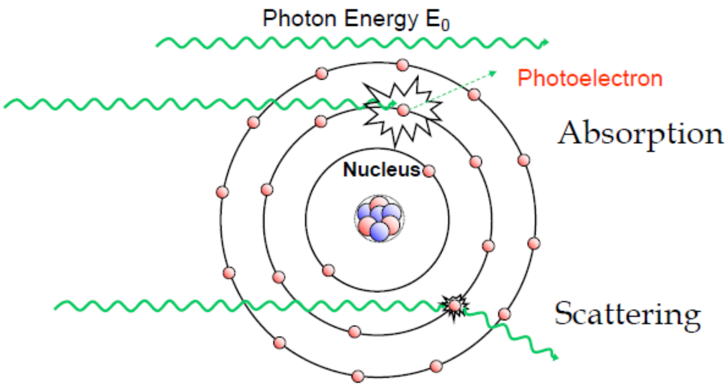


Neutrons interact with the nucleus

X-rays interact with the electrons

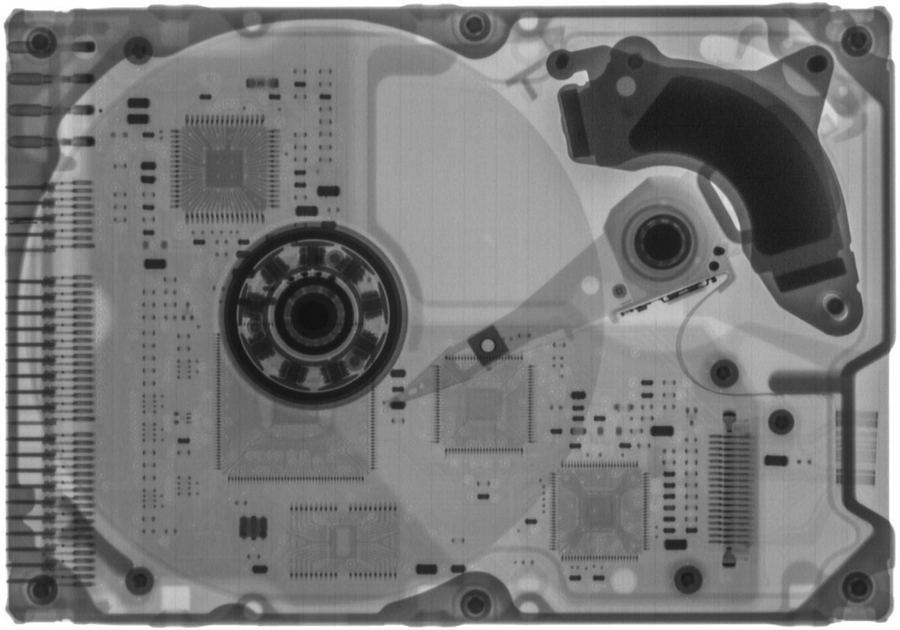






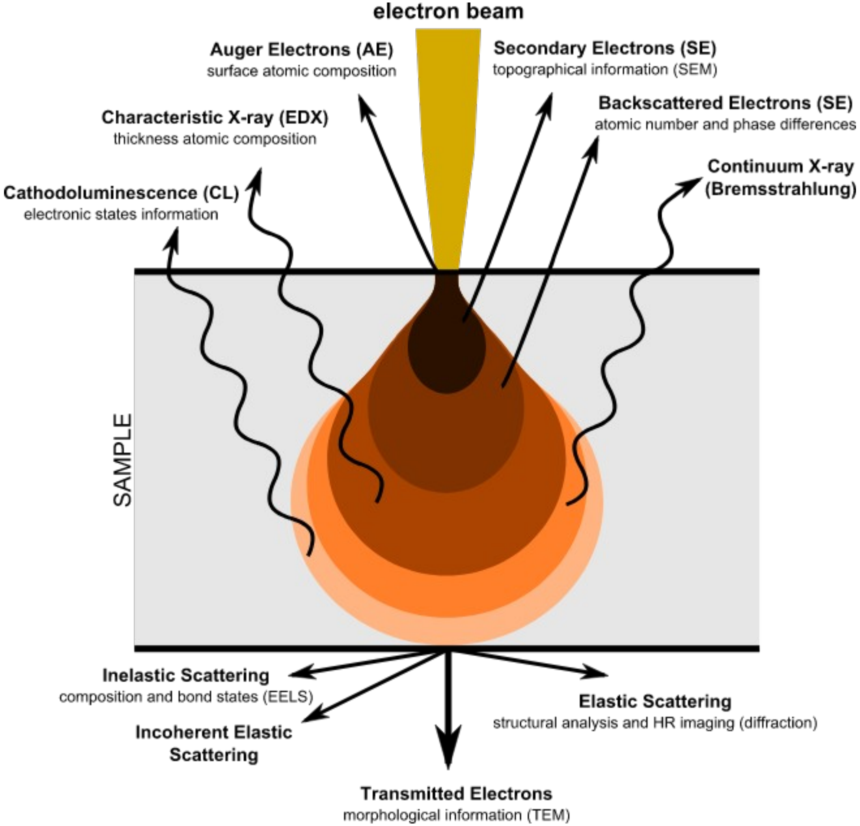
Neutrons and X-rays are complementary techniques

X-ray image of an old hard drive

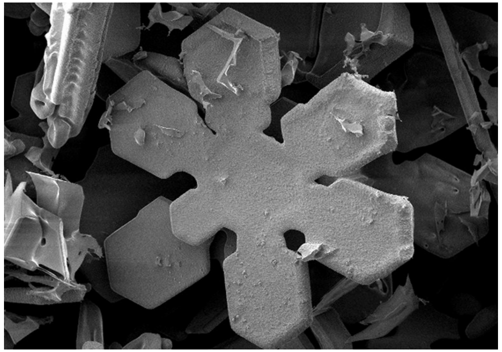


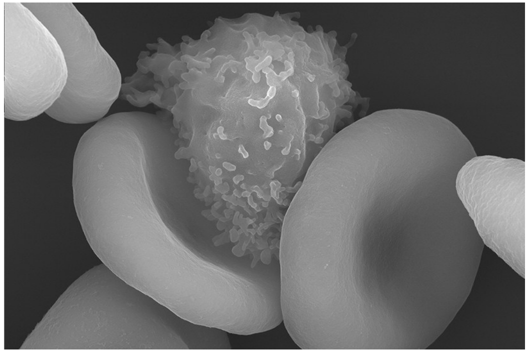
Neutron image of a coffee maker

Electrons are extremely surface sensitive

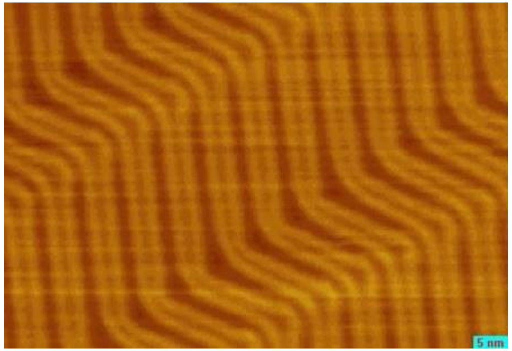


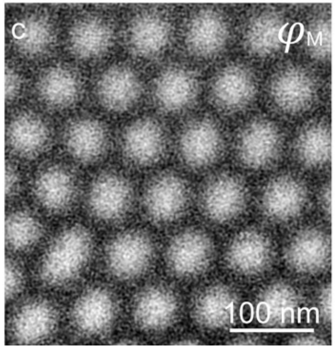
Topography *Snow* *Red blood cells*



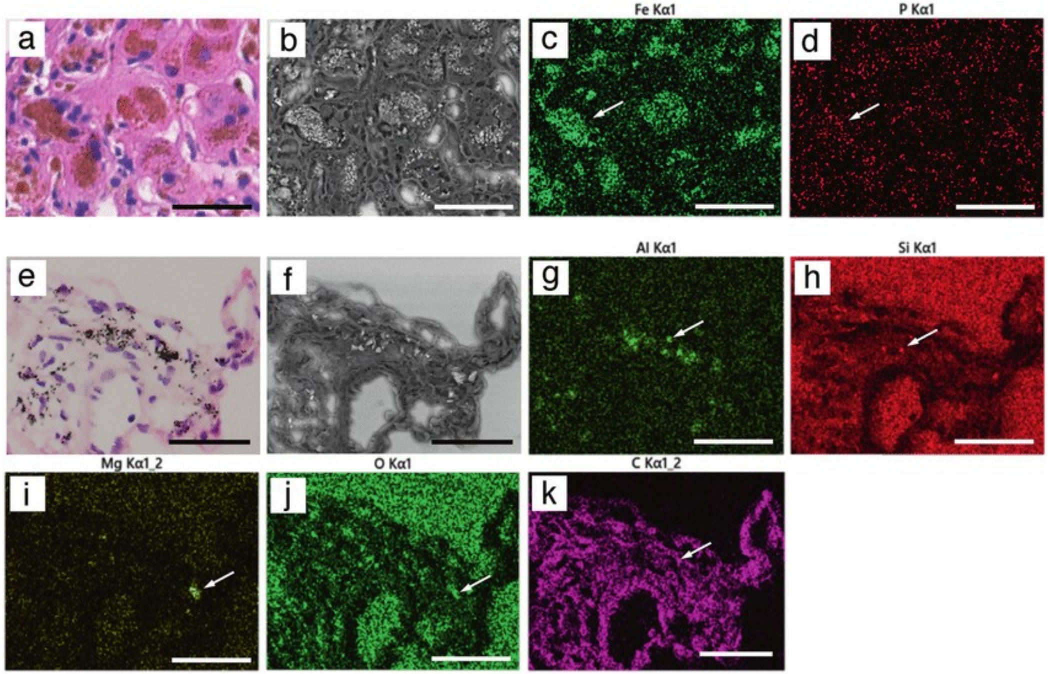


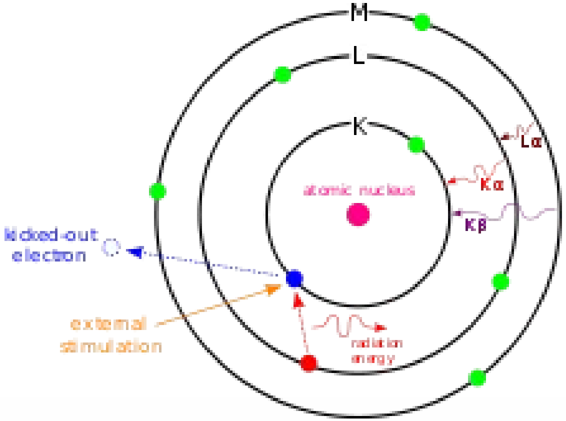
Atomic scale *Catalysis* *Nano magnets*

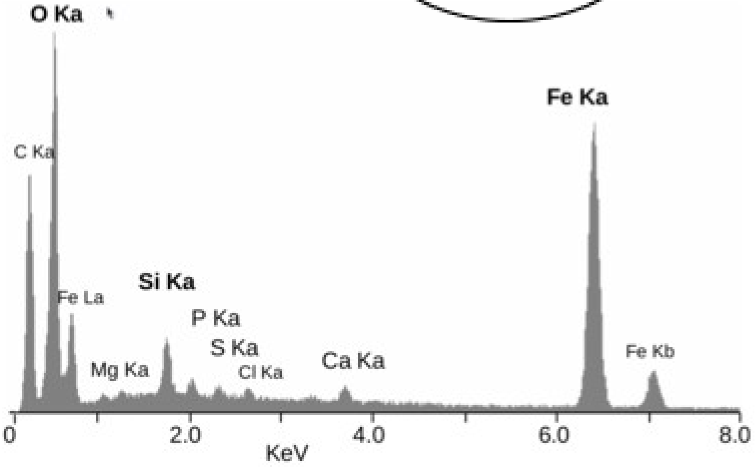




Electrons can see different elements

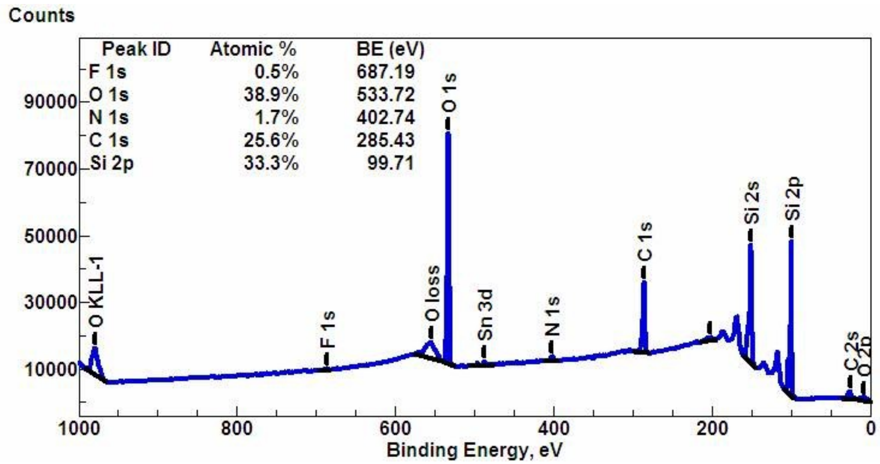




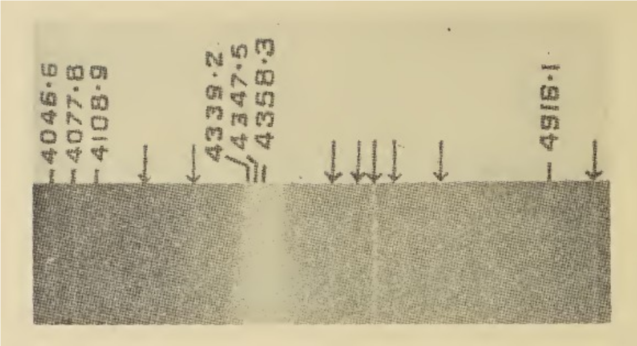


Other kinds of light scattering and spectroscopy

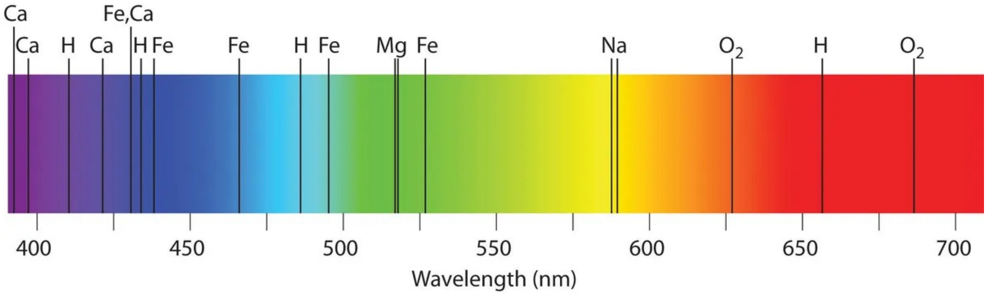
X-ray photoelectron spectroscopy



Raman scattering

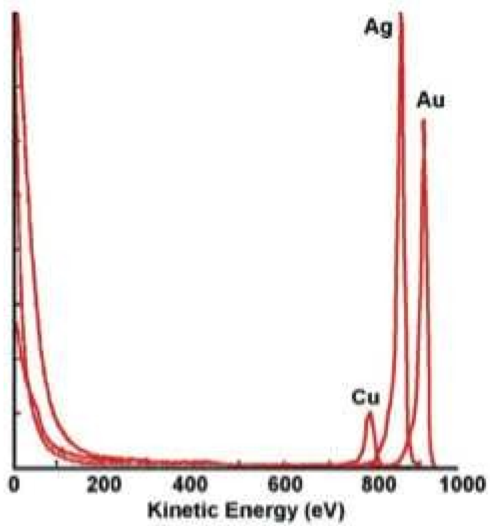


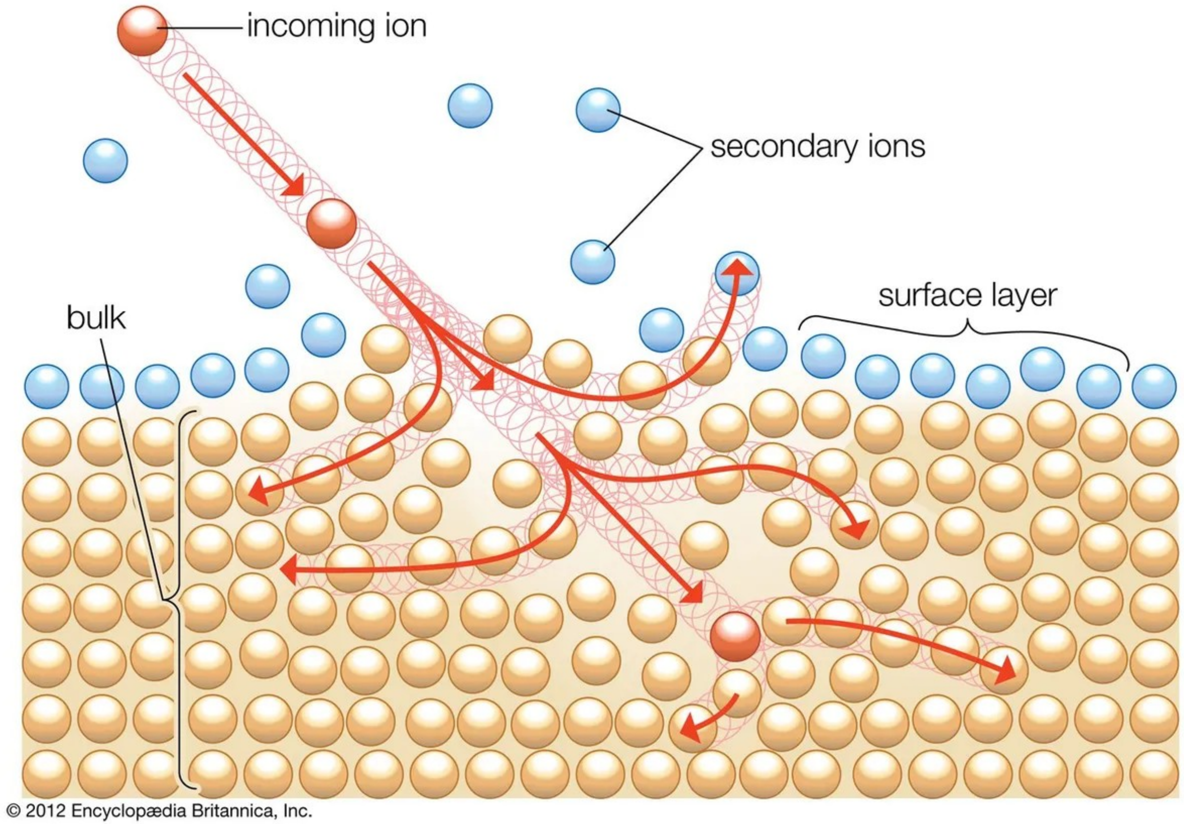
Absorption spectroscopy



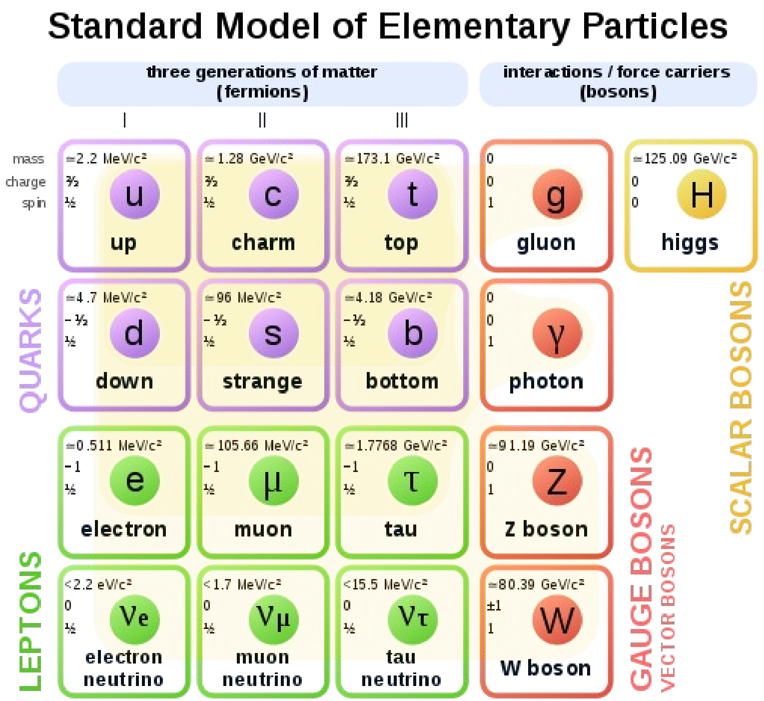
Ion spectroscopy gives information about the surface

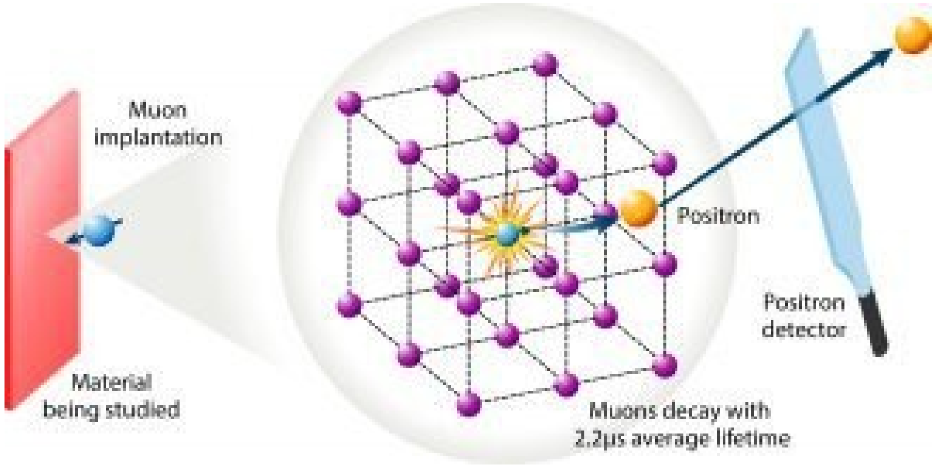
- Depth profile
- Can be destructive
- Element sensitive





Muons see local magnetism





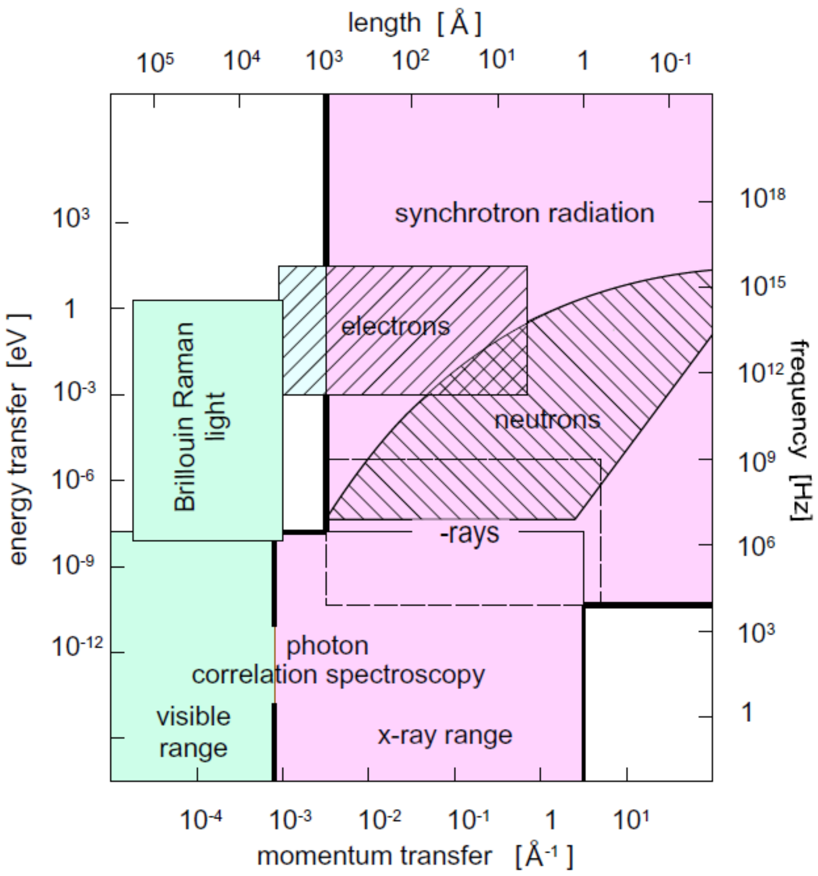
The best probe depends on what you are looking for

- Energy ranges
- Characteristic sizes
- Interaction:

  Electronic

  Nuclear

  Magnetic



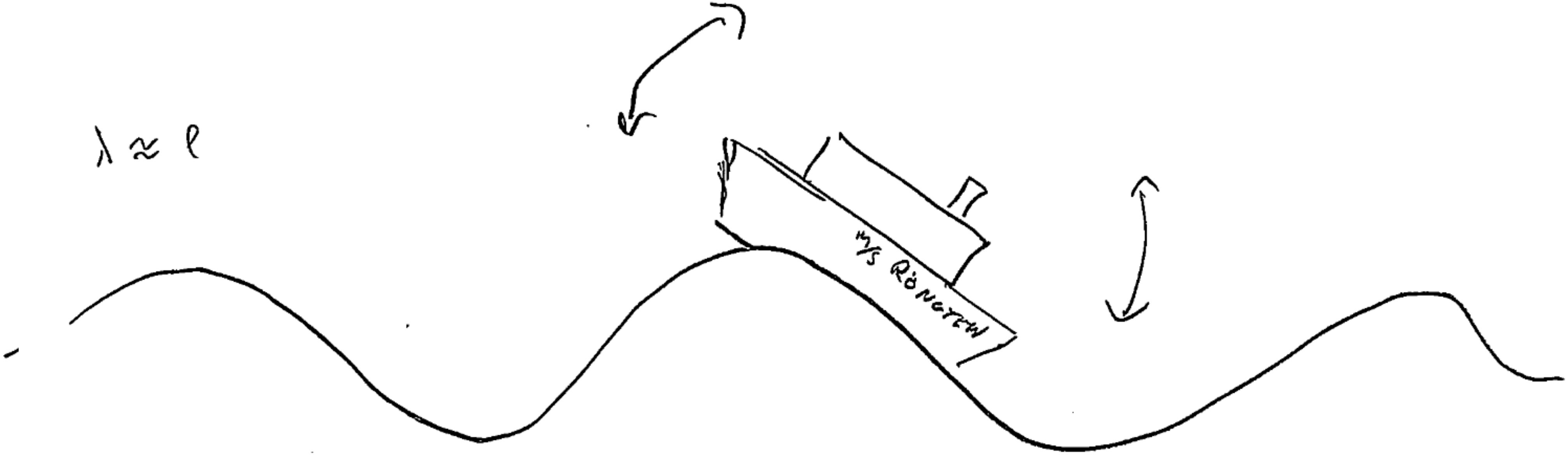
- Other things to consider:

  Sample environment

  Safety (sample and scientist)

  Cost (time and money)

The best probe depends on what you are looking for



Course format

- Mondays 13:15-17:00 in PH H3 31
- Lectures (2h/week)
  - Blackboard and slides
  - Quizzes
- Exercises (2h/week)
  - Traditional problem solving
  - Data analysis and simulations
  - Article reading and discussion
- Homework
  - Reading (textbook/notes, articles)
  - Finish exercises

- Moodle
  - Neutron notes
  - Lecture slides
  - Exercises
  - Articles
- Exam
  - Oral (date to be decided)
- Reading
  - *“Neutron Scattering – Theory, Instrumentation and Simulation”* by Kim Lefmann
  - *“Elements of Modern X-ray Physics”* by Jens Als-Nielsen and Des McMorrow

Course contents

- Neutrons (6 lectures, Ellen):
  - Basic properties, cross sections
  - Diffraction
  - Instrumentation
  - Reflectometry, SANS, imaging
  - Inelastic neutron scattering
  - Polarized neutrons

- X-rays (6 lectures, Thorsten):
  - Theory of the interaction between X-rays and matter
  - X-ray sources and instrumentation
  - X-ray absorption spectroscopy
  - X-ray emission spectroscopy and resonant inelastic X-ray scattering
  - Resonant Elastic X-ray scattering
  - Inelastic X-ray scattering

Neutrons

- *History*
- *How to make them*
- *Facilities*

Discovery of the neutron

1930
W. Bothe and H. Becker, Germany
Found a new kind of radiation

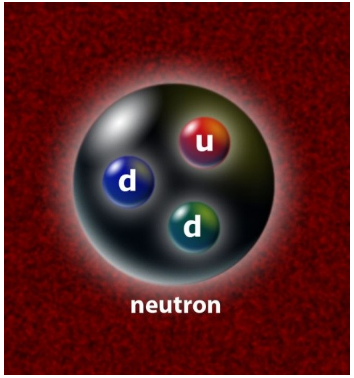
1932
I. Joliot-Curie and F. Joliot, France
Characterised the new kind of radiation

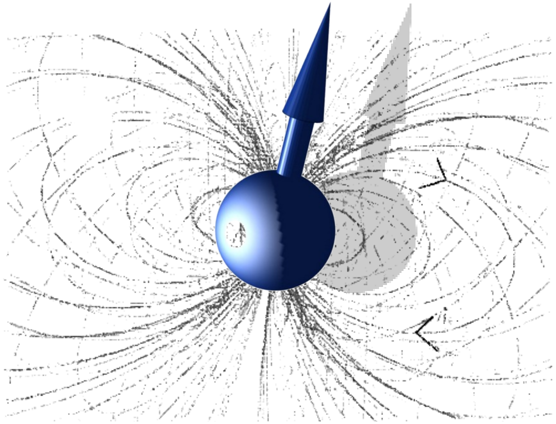
1932
J. Chadwick, England
Measured neutral particles with the same mass as the proton

Physical properties of the neutron

Main characteristics:

- Neutrons are subatomic particles that have a net zero charge
- They possess a magnetic moment and are therefore sensitive to magnetic fields





Energy	Classification
0 - 5 meV	Cold
5 -100 meV	Thermal
100 meV - 1 eV	Epithermal
1 eV -100 eV	Resonant
100 eV - 100 keV	Intermediate
100 keV - 10 MeV	Fast
10 MeV - 10 GeV	Ultra-fast
>10 GeV	Relativistic

	Charge	Spin	Mass (MeV/c^2)	$\gamma/2\pi$ (kHz/G)
Electron	±e	1/2	0.511	2800
Muon	±e	1/2	105.7	13.6
Proton	+e	1/2	938.3	4.26
Neutron	**0**	**1/2**	**939.6**	**–2920**

Physical properties of the neutron

Quantum mechanical description

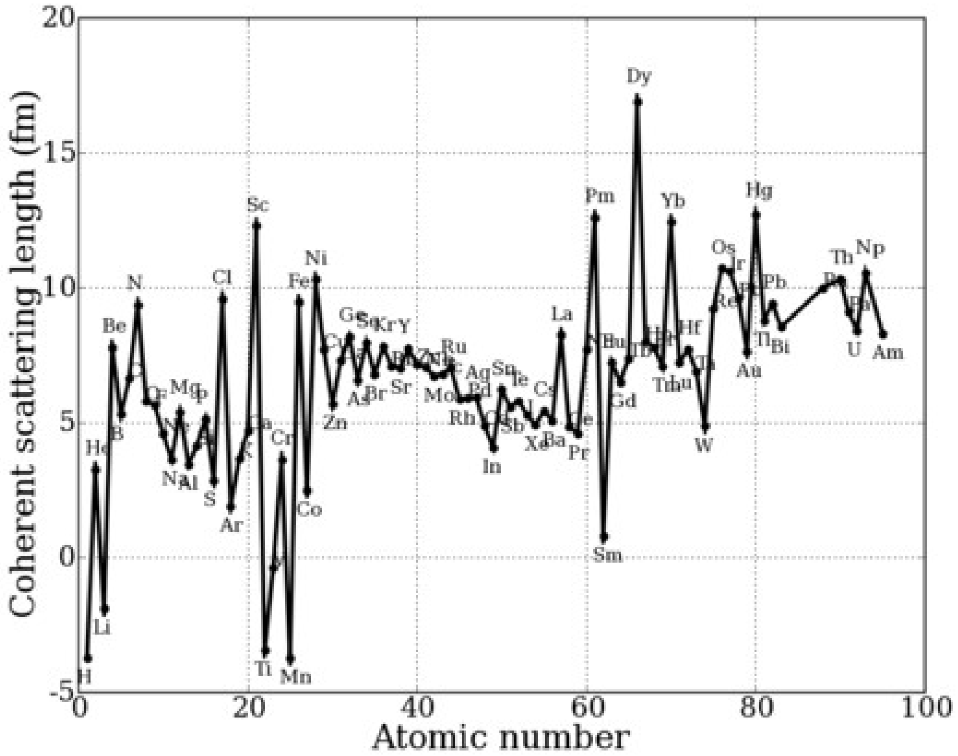
De Broglie wavelength: $p = \frac{h}{\lambda}$

Kinetic energy (non-relativistic): $E = \frac{1}{2} m v^2$

Interaction directly with the nucleus

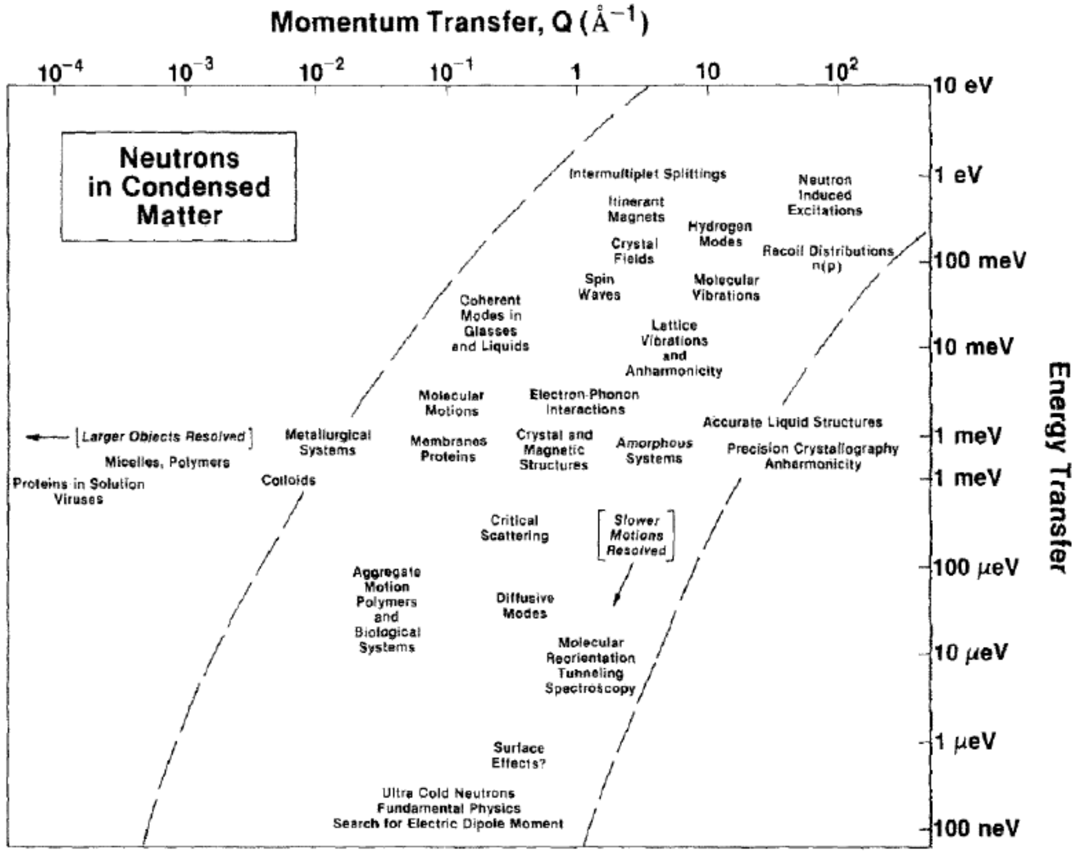
Isotope dependent interaction strength

Decays into an electron, and an anti-neutrino (decay time ~ 15 min)



Vast applications in different fields of science

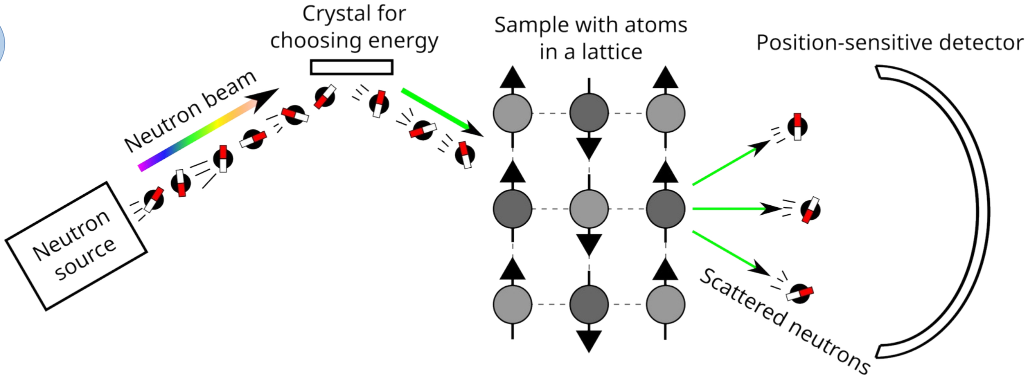
- Condensed matter
  - Magnetism, superconductivity, glasses, liquids
- Material research
  - Stress/strain, batteries
- Soft condensed matter
  - Polymers, composites
- Structural chemistry
  - Catalysis, reactions, parametric studies, molecular spectroscopy
- Geology
  - Minerals and high pressures/temperatures, hydrogen in rocks
- Life sciences
  - Membranes, proteins
- Particle physics
  - Properties of the neutron, quantum mechanics

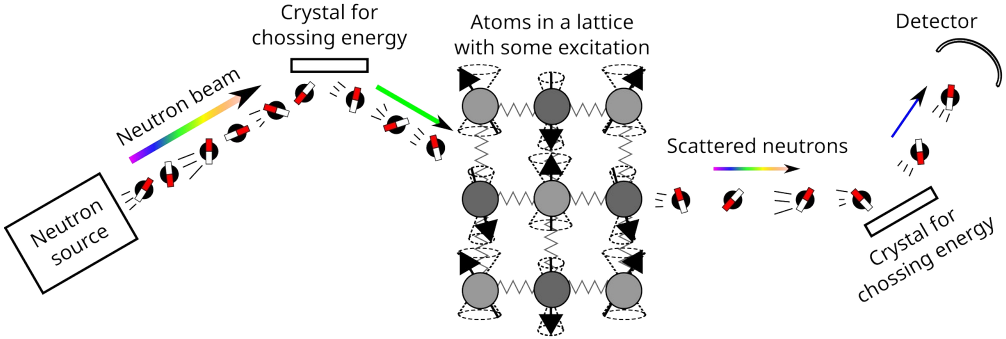


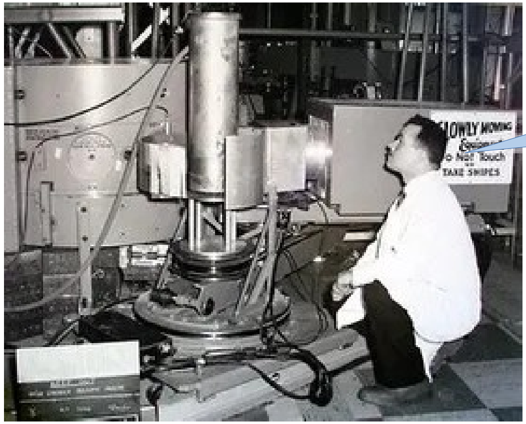
Nobel prize in physics in 1994

Neutrons show where atoms are

C. Shull





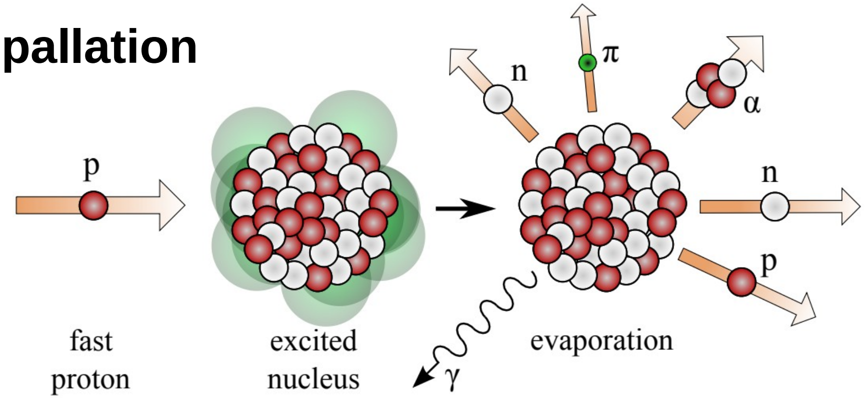


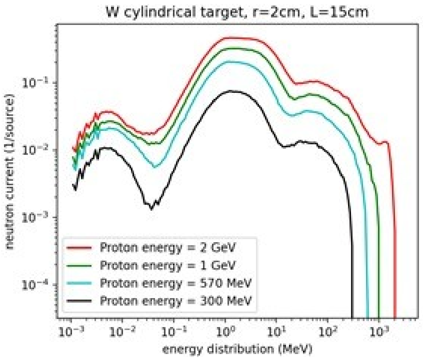
Neutrons show what atoms do

B. N. Brockhouse

Neutrons are generated in either a ***spallation*** process or by ***fission***

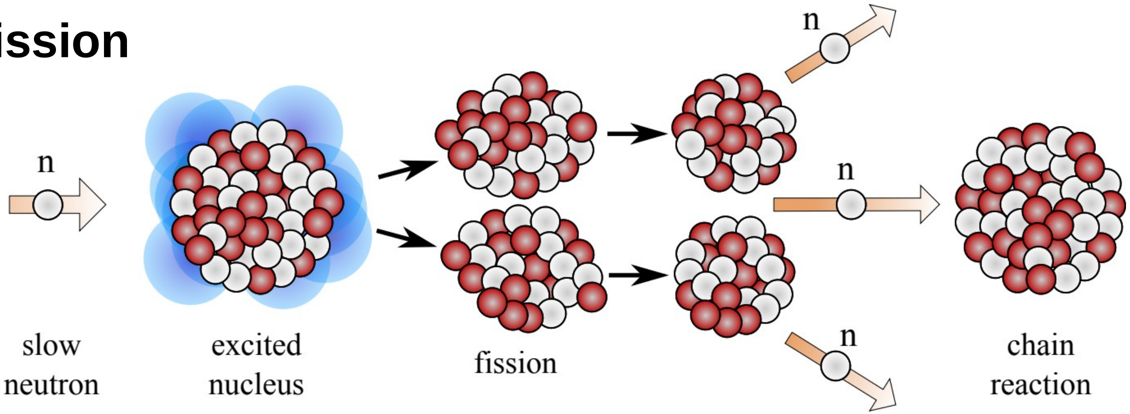
Spallation



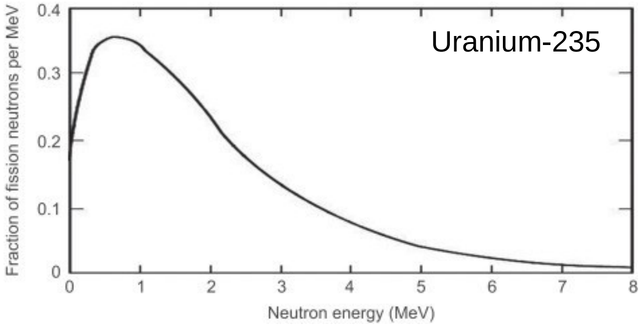


Spallation:
Energies up to MeV range

Fission



Fission:
Energies peak in MeV range

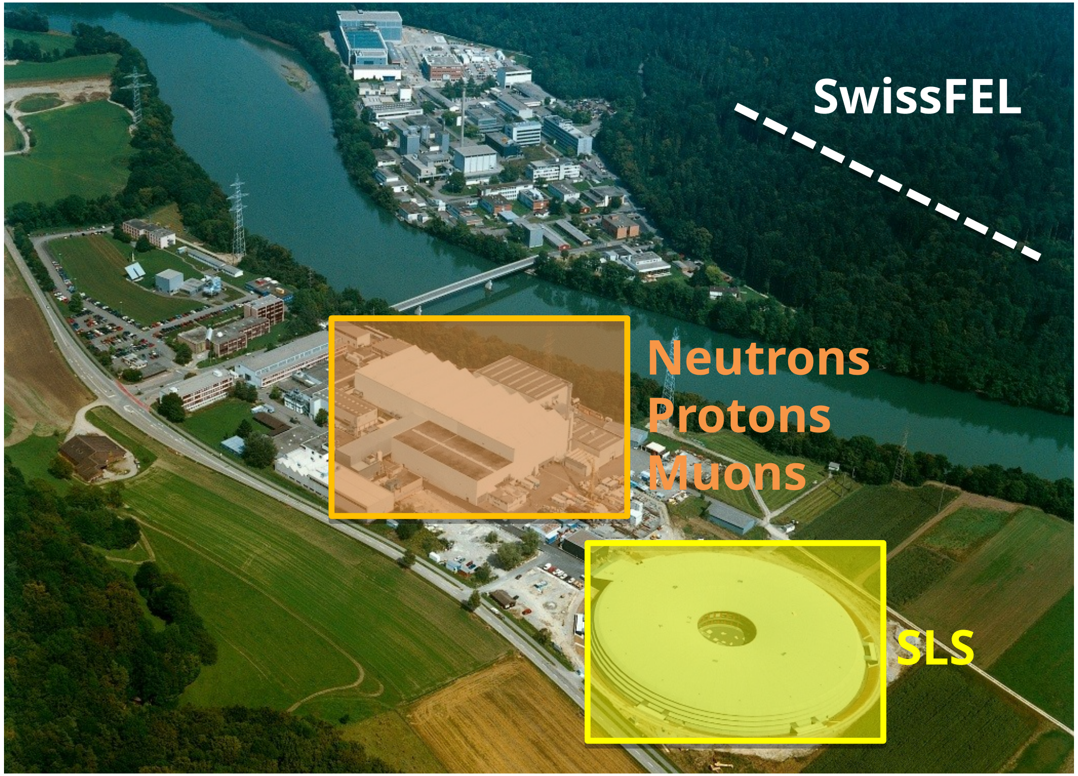


In either case the neutrons produced need to be slowed down

Neutron facilities around the world

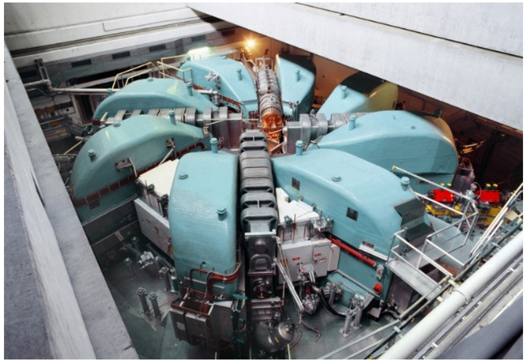
The Swiss Spallation Source at the Paul Scherrer Institute

- 50 MHz source, i.e. continuous
- Lower energy spallation source – comparable to medium flux reactor
- Flexible operation, e.g. 6 days a week, or 50 days
- Switch accelerator off, source switches off instantly
- Hour long thunderstorm – shutdown to protect accelerator?

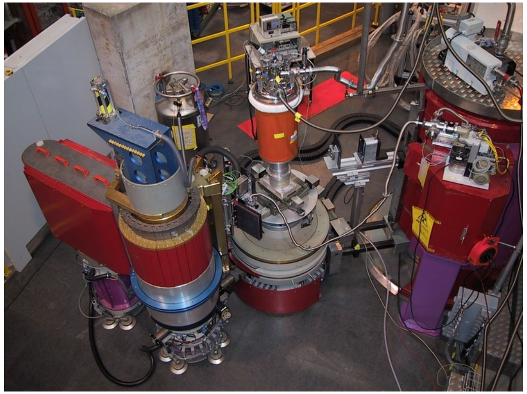


A closer look at the Swiss neutron source

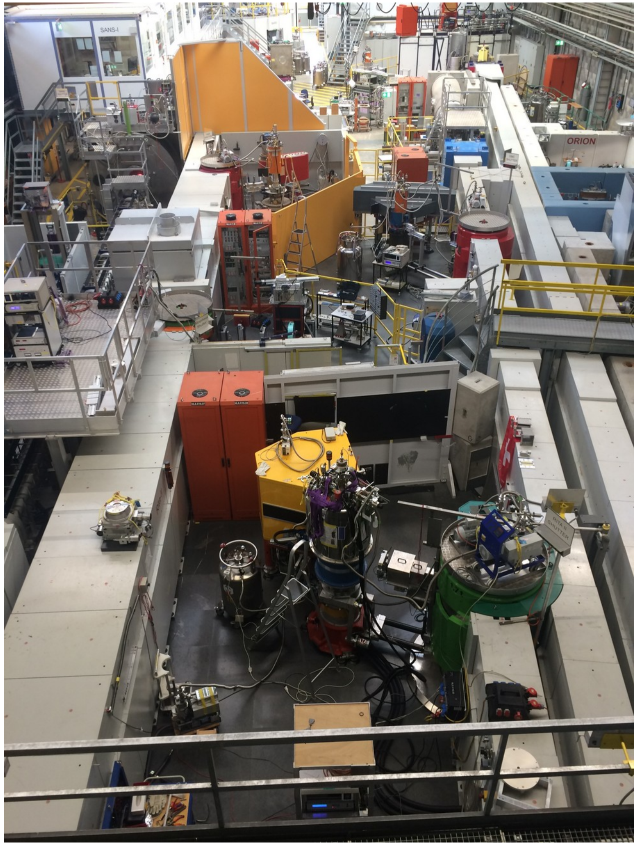
Cyclotron



Neutron instrument



Guide hall



Visit to the Paul Scherrer Institute

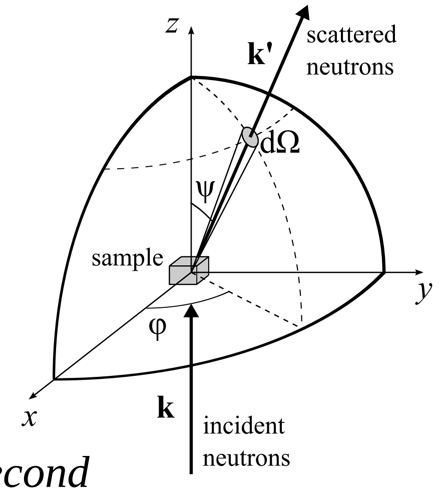
Theory of neutron scattering

Neutron scattering cross sections

Flux: $$\Psi = \frac{number\ of\ neutrons\ hitting\ a\ surface\ per\ second}{surface\ area\ perpendicular\ the\ beam}$$

Cross section: $$\sigma = \frac{number\ of\ scattered\ neutrons\ per\ second}{\Psi}$$

Differential cross section: $$\frac{d\sigma}{d\Omega} = \frac{1}{\Psi} \frac{number\ of\ scattered\ neutrons \in d\Omega\ per\ second}{d\Omega}$$



Partial differential cross section:

$$\frac{d^2\sigma}{d\Omega\, dE_f} = \frac{1}{\Psi} \frac{number\ of\ scattered\ neturons \in d\Omega \wedge with\ energies \in the\ interval\ [E_f, E_f + dE_f]\ per\ second}{d\Omega\, dE_f}$$

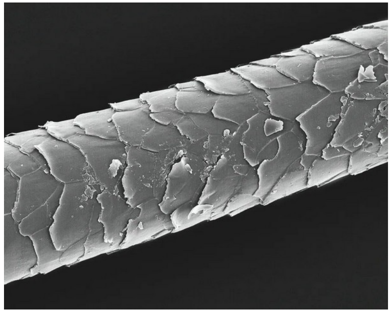
Neutron scattering is an unlikely event

Unit: 1 barn = 10^{-24} cm^2

Surface of France = 643 801 km^2 ~$10^6 km^2$

1 barn corresponds to hitting a $100 \times 100\ \mu m^2$ spot in France

Luckily we have 10^{23} atoms



Neutron scattering and absorption processes

Absorption cross section:

$$\sigma_{\mathrm{a}} = \sigma_{\mathrm{a,\,th}} \frac{v_{\mathrm{th}}}{v} = \sigma_{\mathrm{a,\,th}} \frac{\lambda}{\lambda_{\mathrm{th}}}$$

Coherent scattering:

Collective behavior, interference

Incoherent scattering:

No structural information

Z	Nucleus	b (10^{-15} m)	σ_{inc} (10^{-28} m^2)	$\sigma_{\mathrm{a,th}}$ (10^{-28} m^2)
1	^{1}H	-3.742	80.27	0.3326
1	^{2}D	6.674	2.05	0.000519
2	^{3}He	5.74	1.532	5333
2	^{4}He	3.26	0	0
3	Li	-1.90	0.92	70.5
4	Be	7.79	0.0018	0.0076
5	B	5.30	1.70	767
6	C	6.6484	0.001	0.00350
7	N	9.36	0.50	1.90
8	O	5.805	0	0.00019
9	F	5.654	0.0008	0.0096
10	Ne	4.566	0.008	0.039
11	Na	3.63	1.62	0.530
12	Mg	5.375	0.08	0.063
13	Al	3.449	0.0082	0.231
14	Si	4.1507	0.004	0.171
15	P	5.13	0.005	0.172
16	S	2.847	0.007	0.53
17	Cl	9.5792	5.3	33.5
18	Ar	1.909	0.225	0.675
19	K	3.67	0.27	2.1
20	Ca	4.70	0.05	0.43
21	Sc	12.1	4.5	27.5
22	Ti	-3.37	2.87	6.09
23	V	-0.443	5.08	5.08
24	Cr	3.635	1.83	3.05
25	Mn	-3.750	0.40	13.3
26	Fe	9.45	0.40	2.56
27	Co	2.49	4.8	37.18
28	Ni	10.3	5.2	4.49
29	Cu	7.718	0.55	3.78
30	Zn	5.68	0.077	1.11
32	Ge	8.185	0.18	2.20
48	Cd	4.83	3.46	2520

On to the blackboard…