Neutron scattering for material science and engineering

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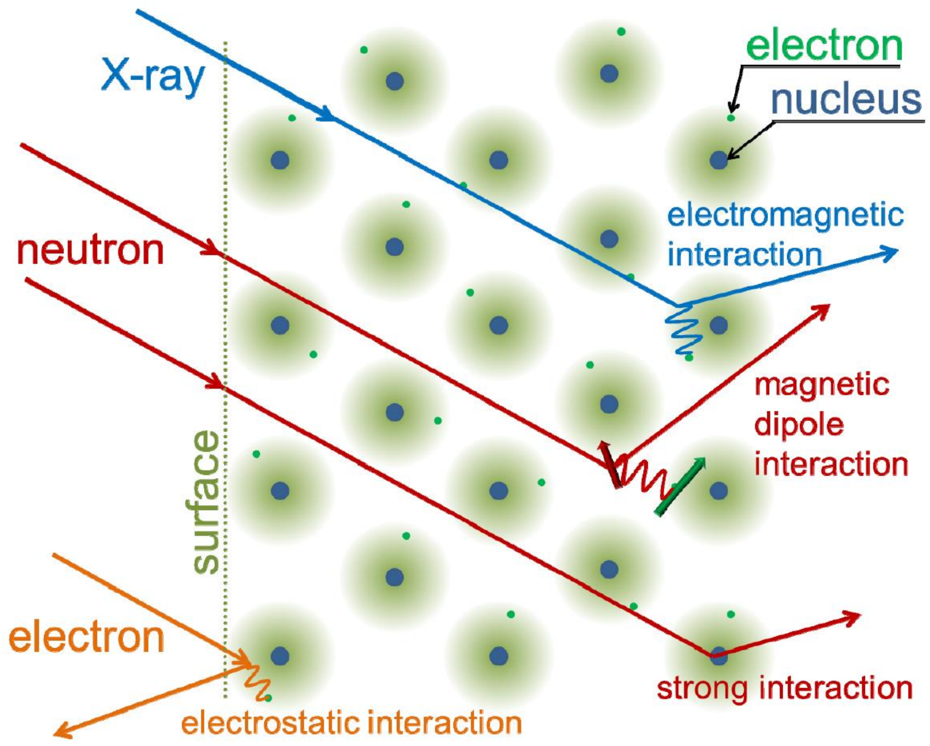
Why neutrons?

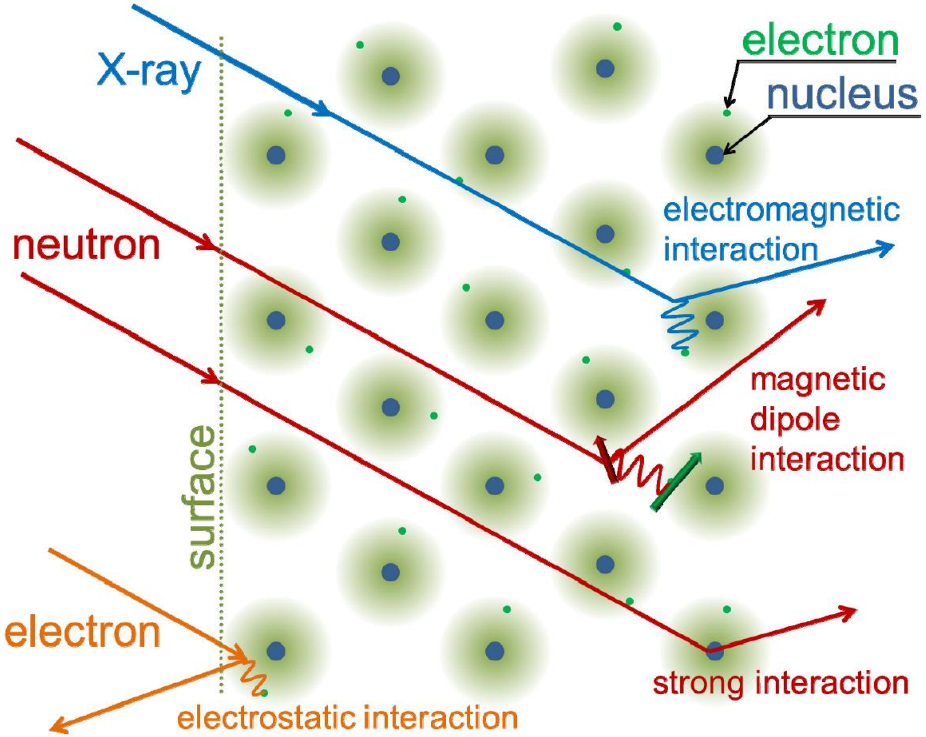
Interaction X-rays, neutrons and electrons with atoms in a 2d array

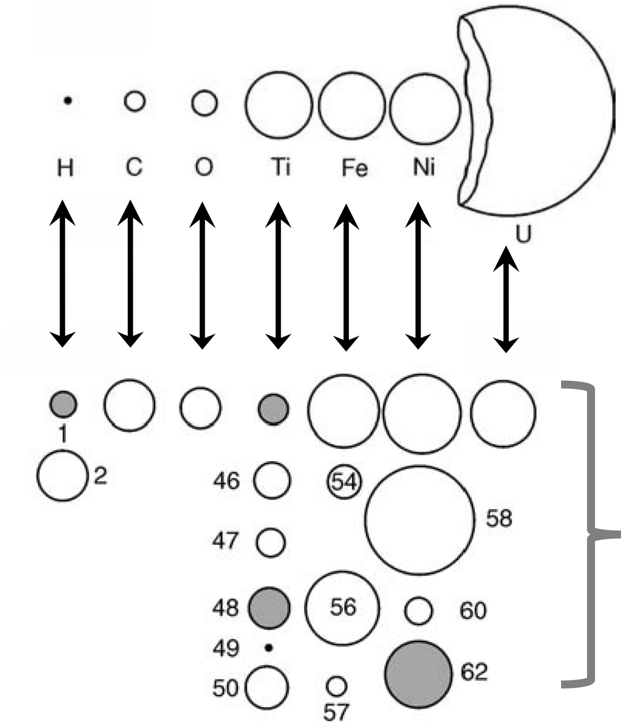


- The interaction of x-rays and electron beam with matter is, electromagnetic and electrostatic, respectively. The penetration depth is limited.

- Neutrons interact with atomic nuclei via the very short-range strong nuclear force and thus penetrates matter more deeply than either x-rays or electrons.

Interaction X-rays, neutrons and electrons with atoms in a 2d array



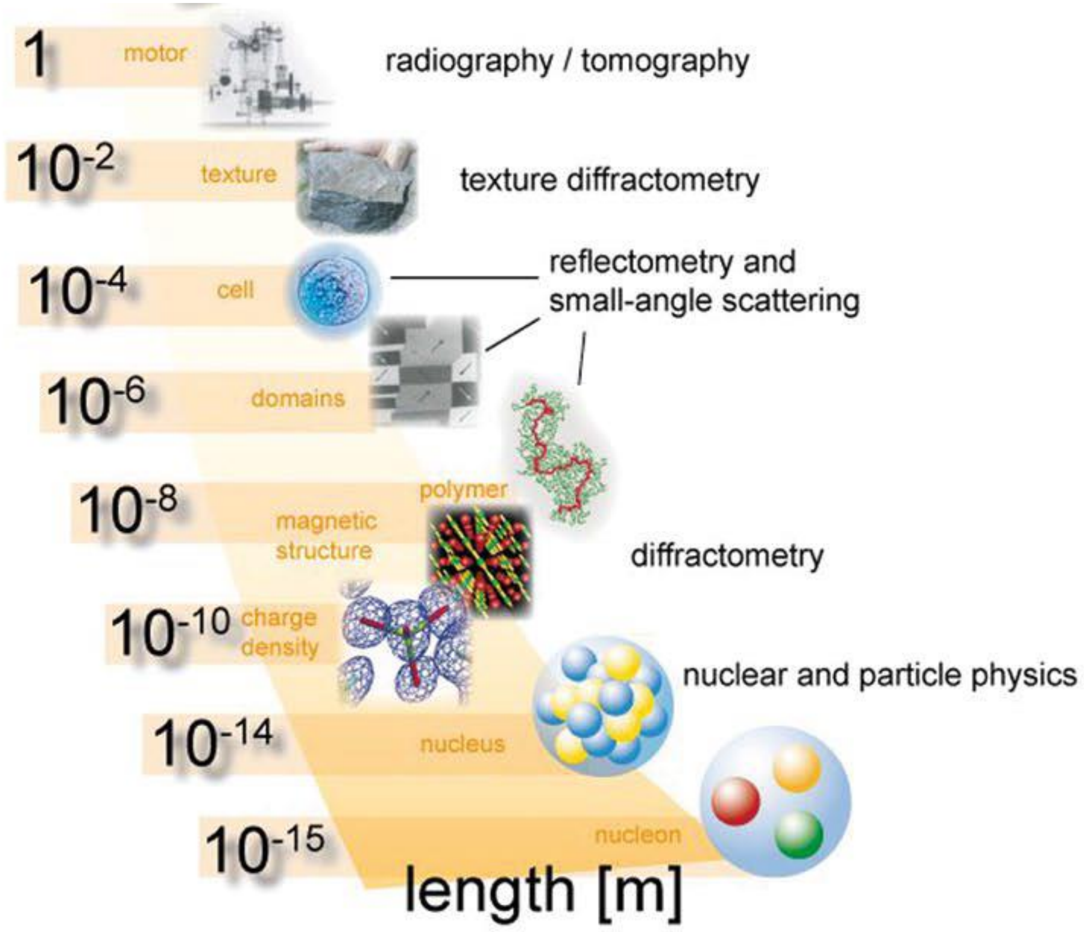


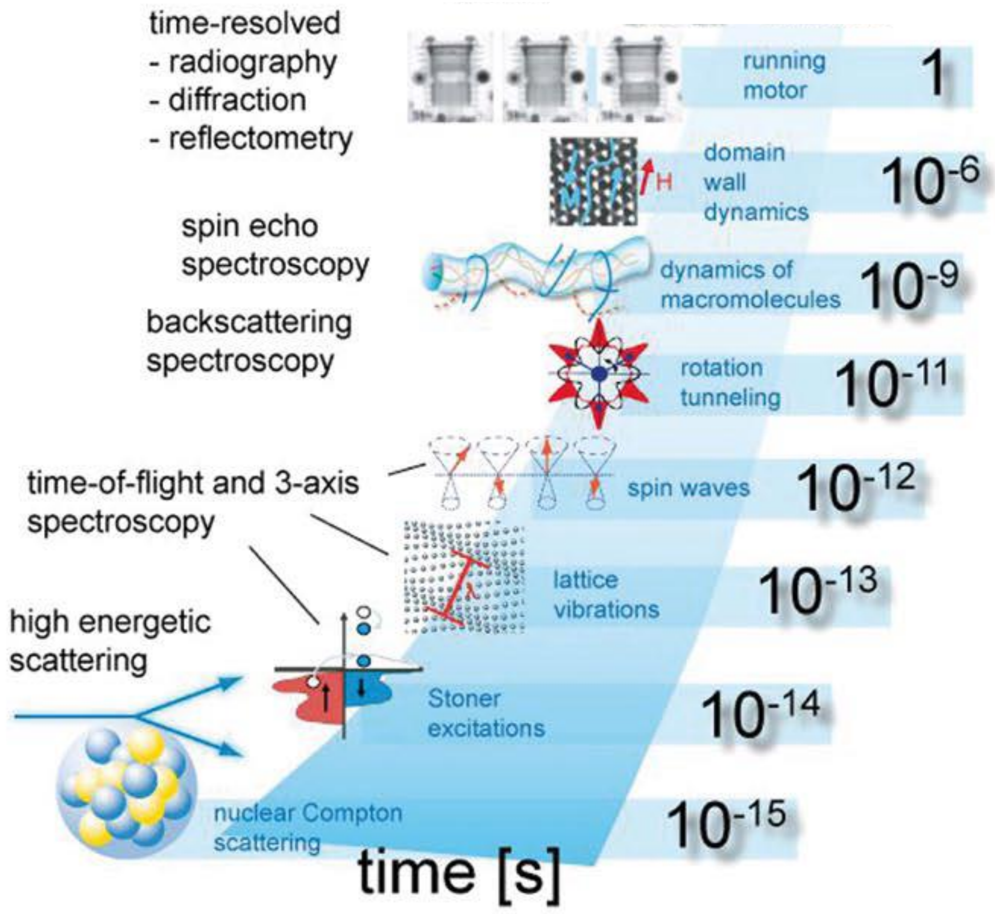
x-ray cross section:
$\propto Z^2$

Neutron cross section:
depends on interaction between the neutron and the components of the nucleus. Even isotopes of the same element can have drastically different neutron cross section!

- The interaction of x-rays and electron beam with matter is, electromagnetic and electrostatic, respectively. The penetration depth is limited.
- Neutrons interact with atomic nuclei via the very short-range strong nuclear force and thus penetrates matter more deeply than either x-rays or electrons.
- Suitable for lighter elements, distinguish neighboring elements in the periodic table, distinguish isotopes, and can probe magnetic ordering directly
- Neutrons with s=1/2 has a magnetic moment and can interact by a dipole-dipole interaction with the magnetic moment of the unpaired electron

Neutrons as probe to determine the structure and dynamics of materials





- Neutrons can be used to probe materials in the length scales of fm to a meter.
- Neutrons can also be used to probe dynamics of materials in the time scales from fs to a second.

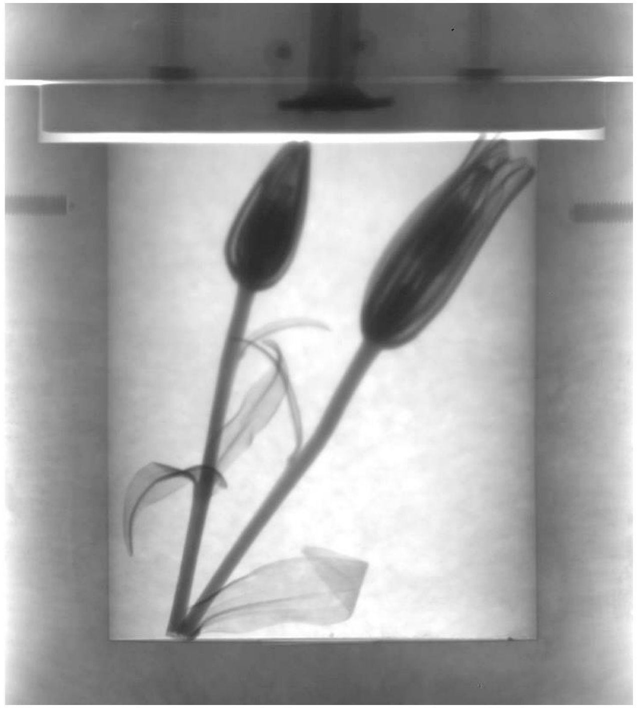
A neutron radiograph of lilies inside a thick-walled lead cylinder

Neutrons easily penetrate through few cm thick lead and show the differences between the scattering amplitudes, and therefore the absorptions by hydrogen, oxygen and heavy metal atoms.

Photographed with natural light

Top view

Neutron radiograph

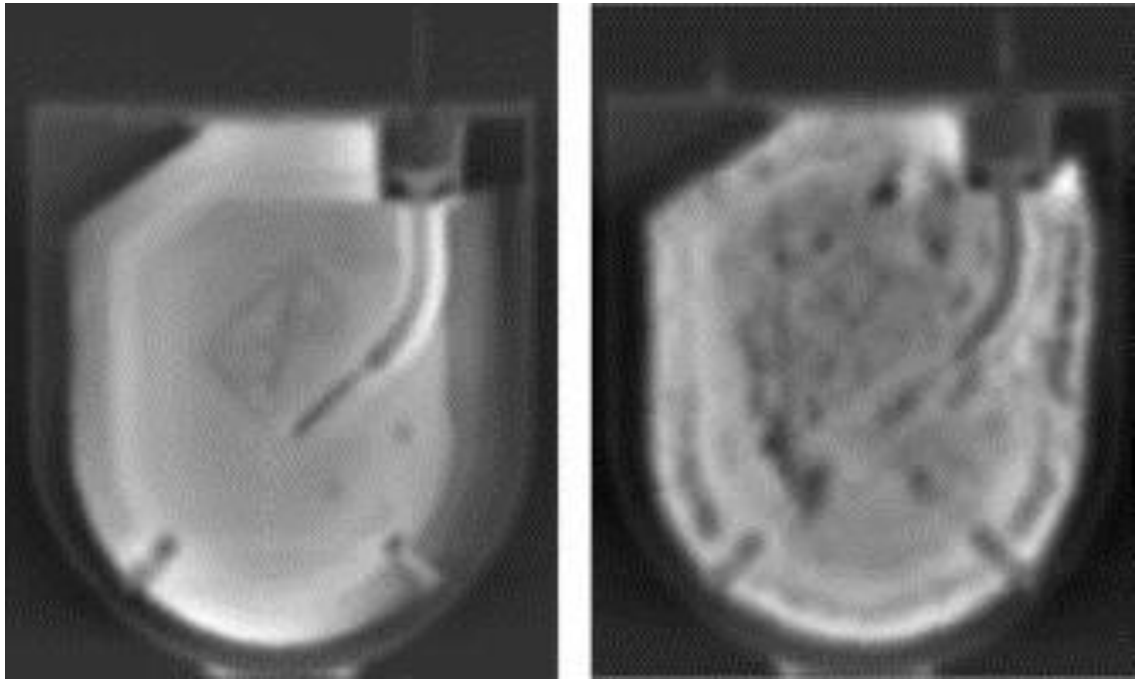


Side view

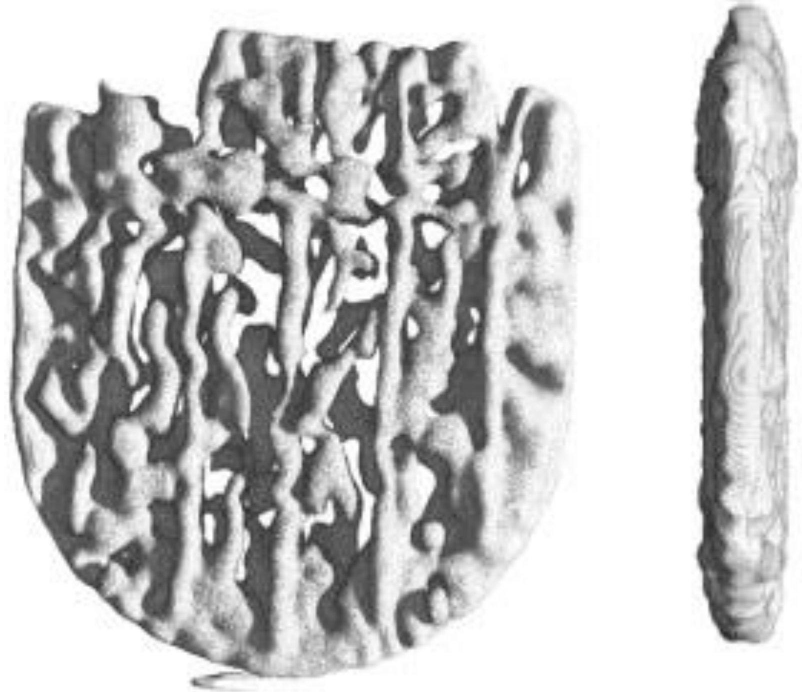
Lead is more transparent than the **lilies** for neutrons!

Neutron tomography of Lithium-Iodine battery

Charged Discharged



Cross section of a tomograph: *Brighter regions indicate Li*



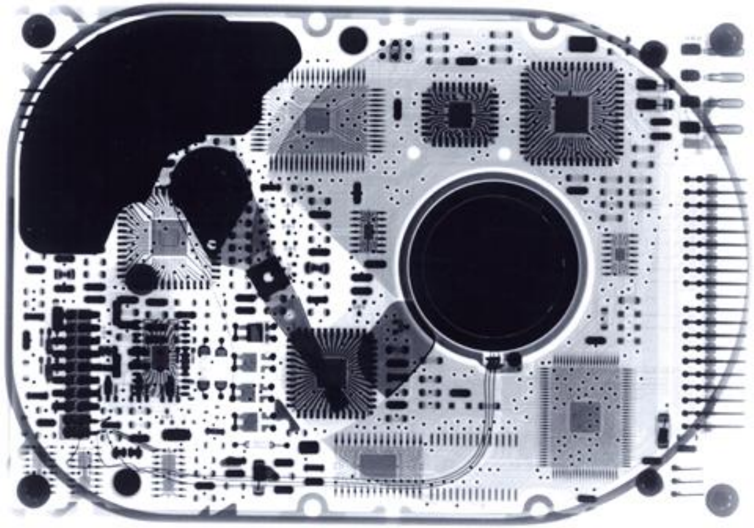
Full 3D tomograph of the battery showing he pathways of Li

Because of the high mass attenuation coefficient, the Lithium can be separated from other battery components very well, thus the Lithium distribution becomes visible

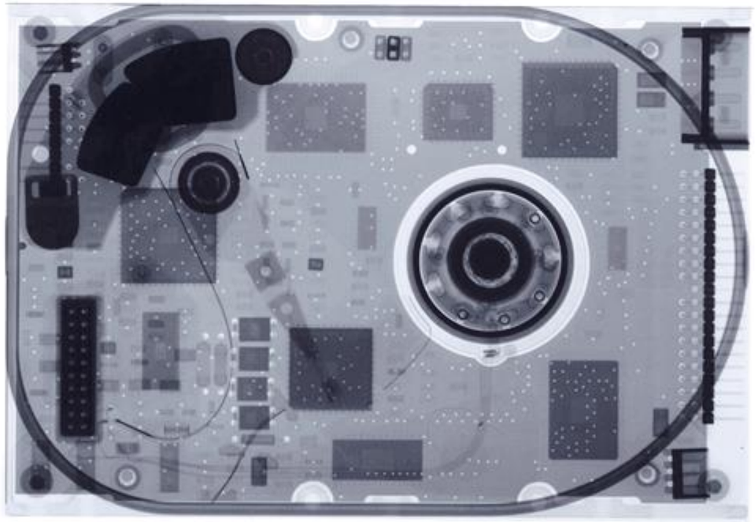
Hard drive under visible light, x-rays and neutrons

Internal hard drive under visible light

x-ray radiograph



Neutron radiograph



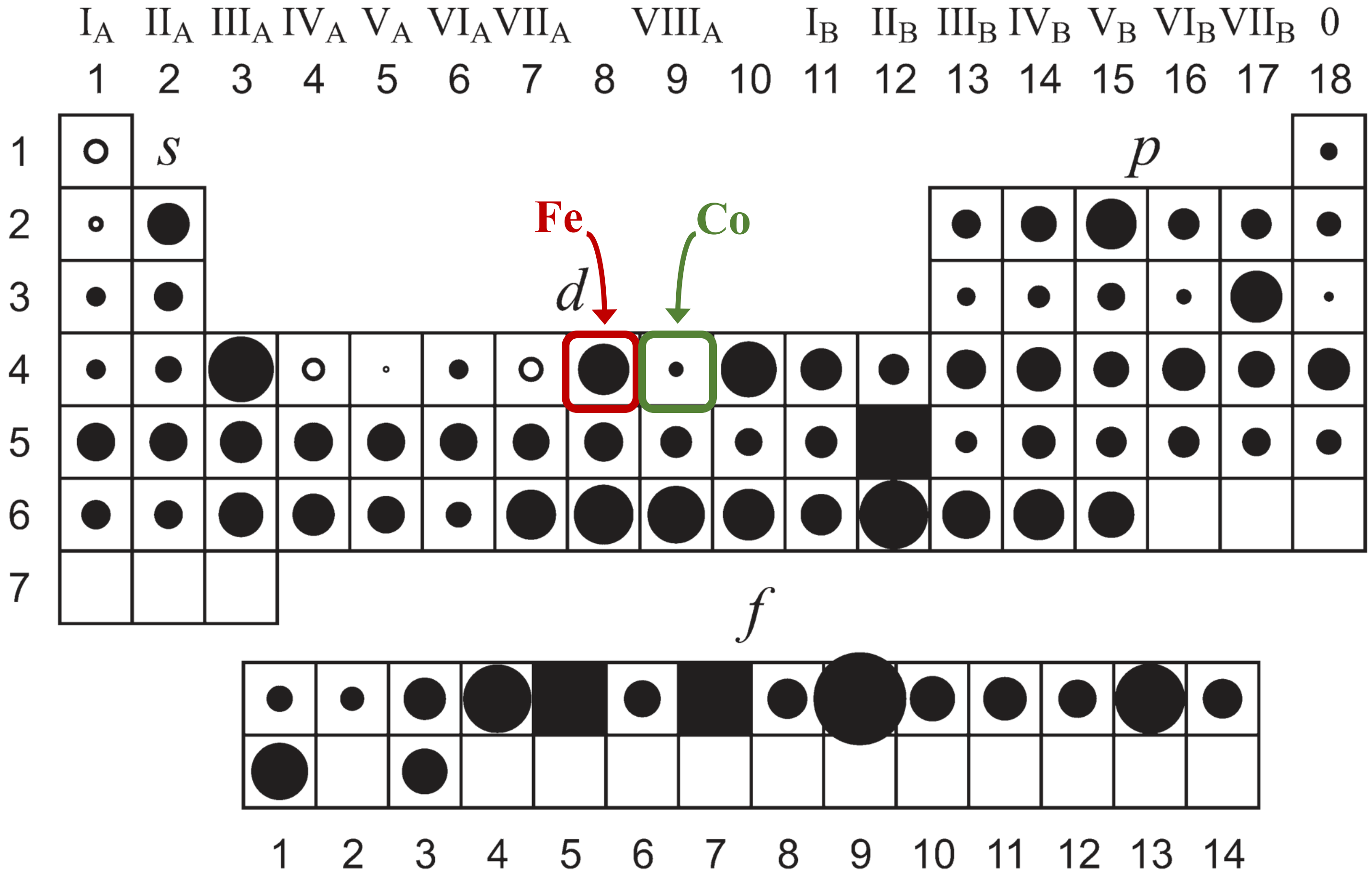
For lattice structure

Why neutrons?

Neutron scattering cross section for the neighbors Fe and Co

Neutrons can distinguish two elements with very similar atomic numbers

This is due to the fact that the neutron scattering cross section depends on the interaction with the nuclear components; the scattering cross section is very different for Fe and Co.



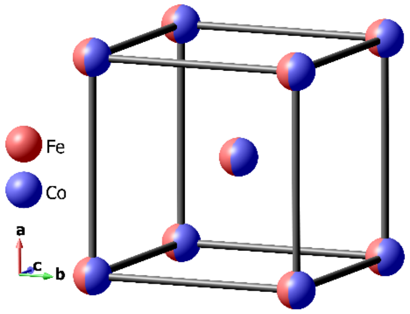
Neutron coherent scattering lengths (b) and coherent cross section (s) shown in the form of a Periodic Table of the elements in which the radius of the circle is proportional to b and the area is proportional to s.

Notice a drastically different neutron scattering cross section for Fe and Co!

Why neutrons?

Why not x-ray?

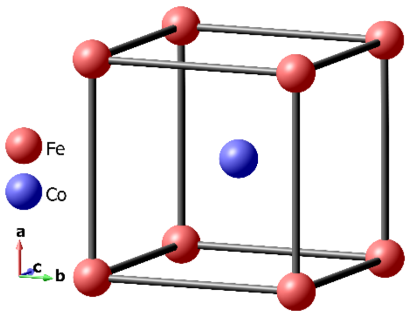
Neutron scattering cross section for the neighbors Fe and Co



Cubic crystal

$a = b = c = 2.839$ Å

$\alpha = \beta = \gamma = 90°$

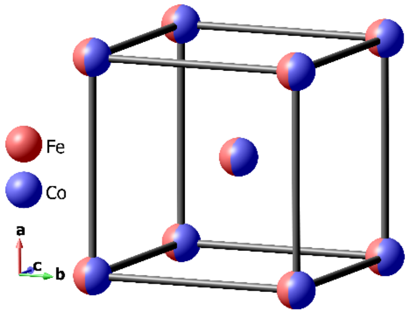


Why neutrons?

Neutron scattering cross section for the neighbors Fe and Co

Why not x-ray?

- X-ray diffraction patterns of disordered and ordered FeCo
- Since x-ray scattering lengths of Fe and Co are very similar x-rays can't identify if the systems is ordered or not.



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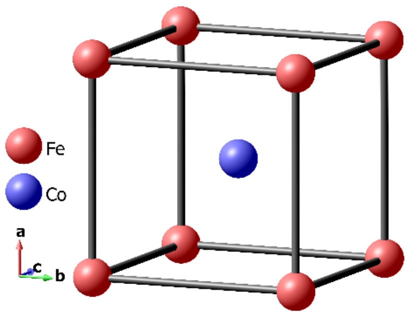

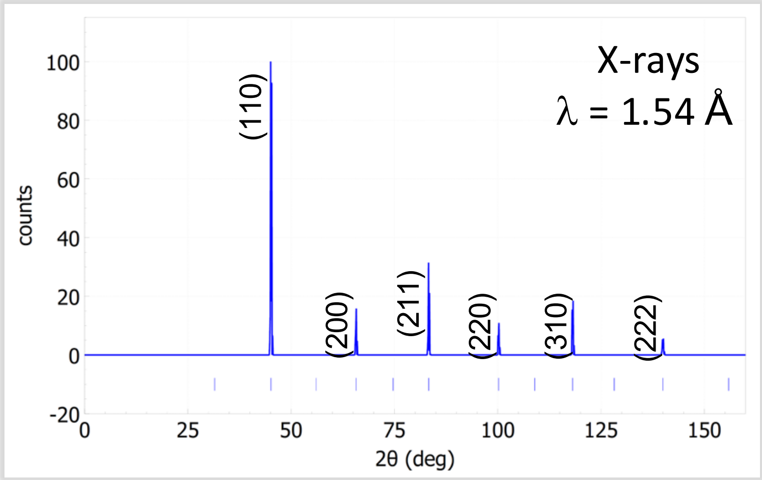

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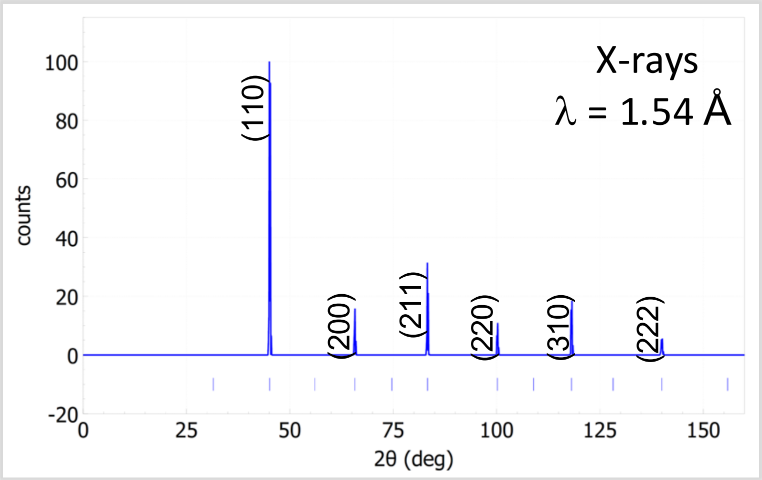

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Neutron scattering cross section for the neighbors Fe and Co

Why not x-ray?

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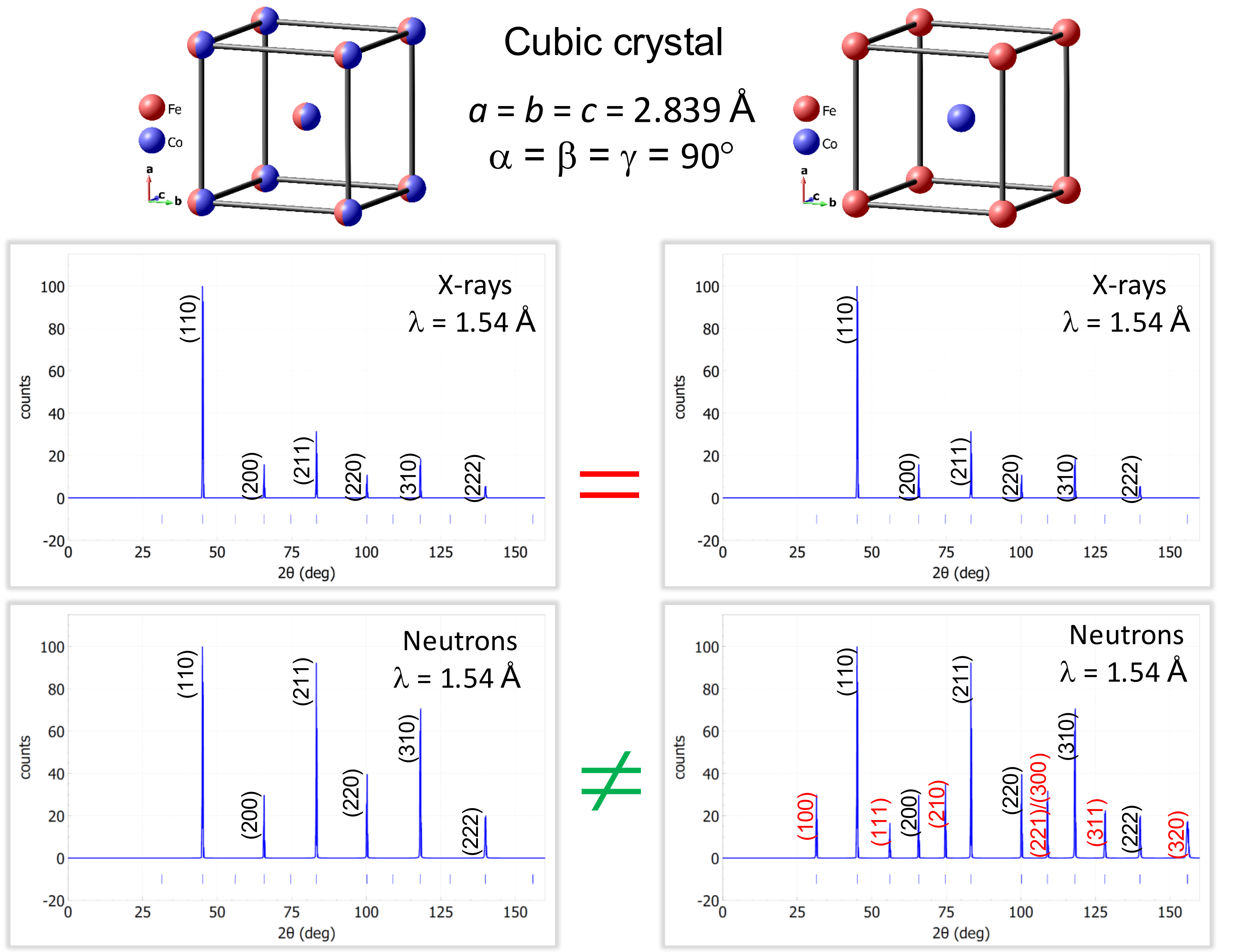
- Since the x-ray scattering lengths of Fe and Co are very similar, x-rays can't identify if the system is ordered or not.
- The neutron diffraction pattern of disordered FeCo looks similar to X-rays.
- But there are new peaks in the neutron diffraction pattern of Ordered FeCo!



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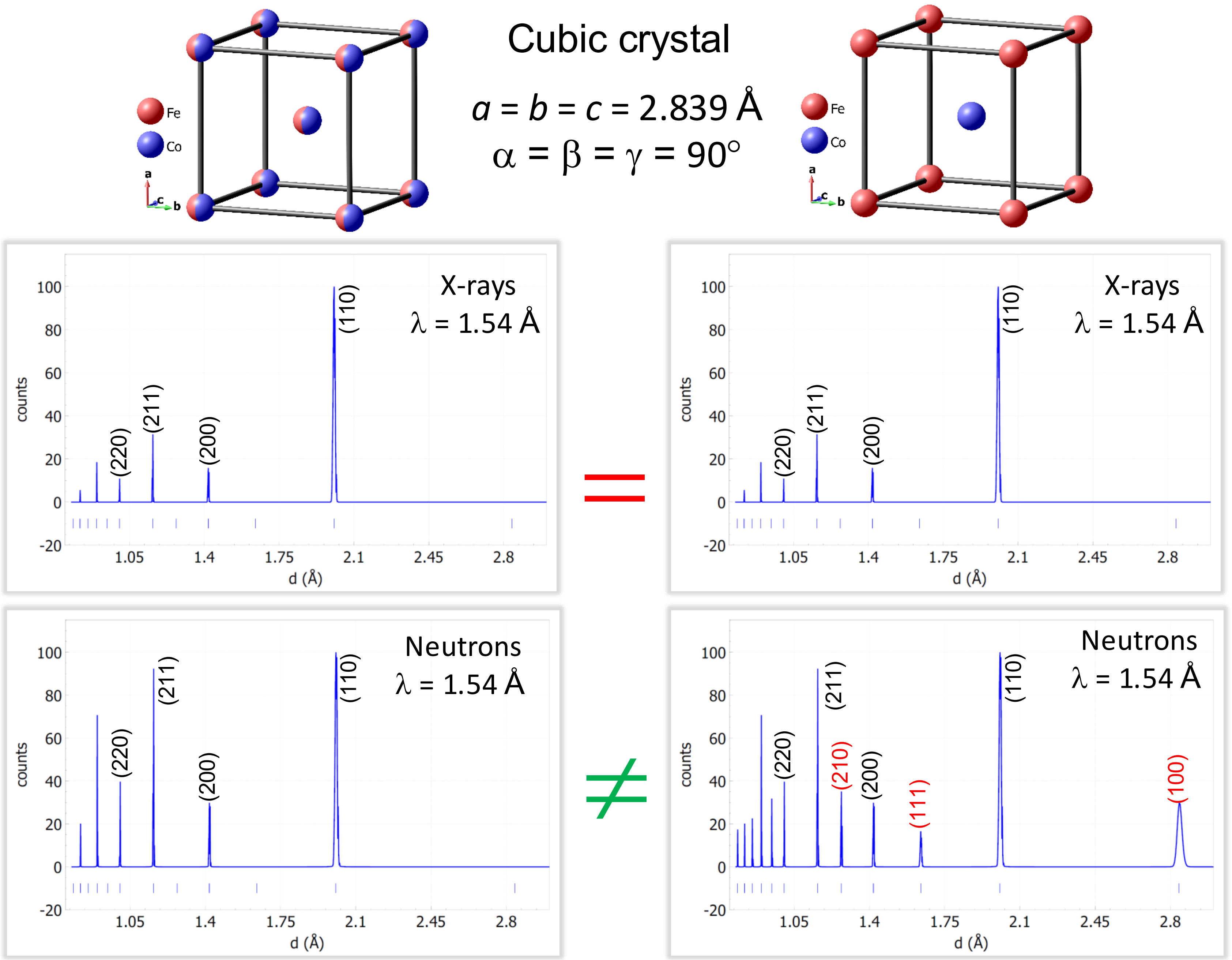
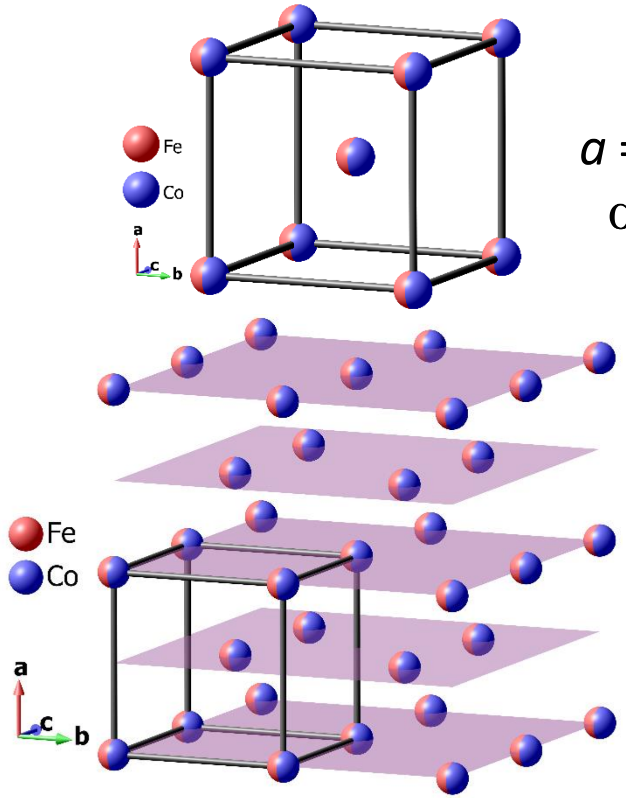


Why neutrons?

Neighboring Element Discrimination: *Ordered and disordered FeCo*

- Since Fe and Co have very different neutron scattering lengths, the scattering from adjacent layers in ordered FeCo is not equivalent!
- A new order emerges with a different interplanar spacing, resulting in new peaks!

Neutrons can distinguish two elements with very similar atomic numbers



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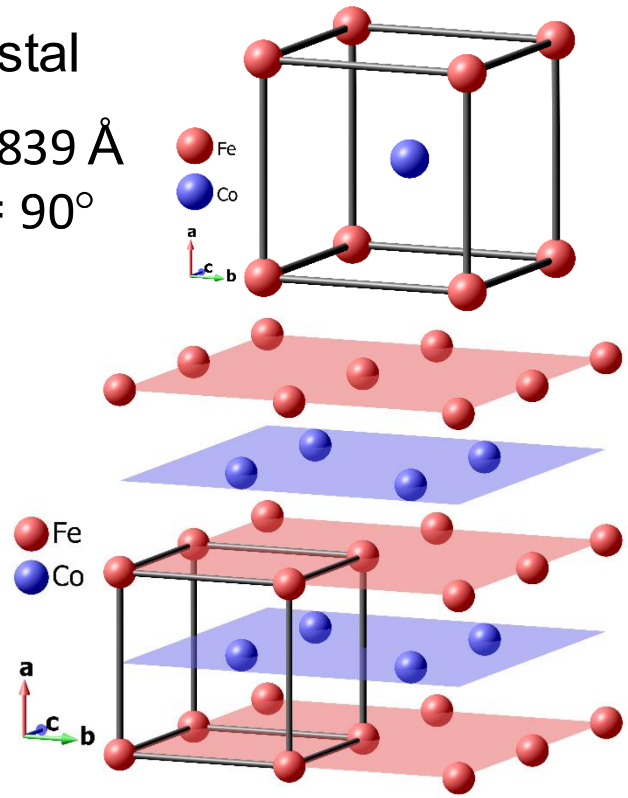

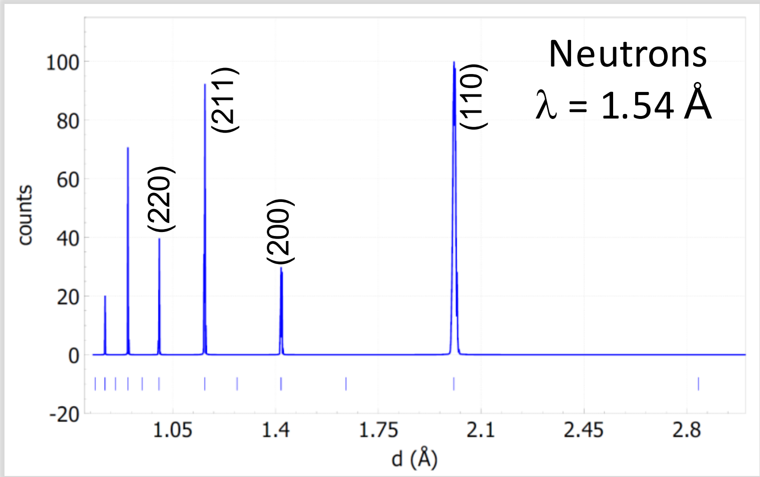

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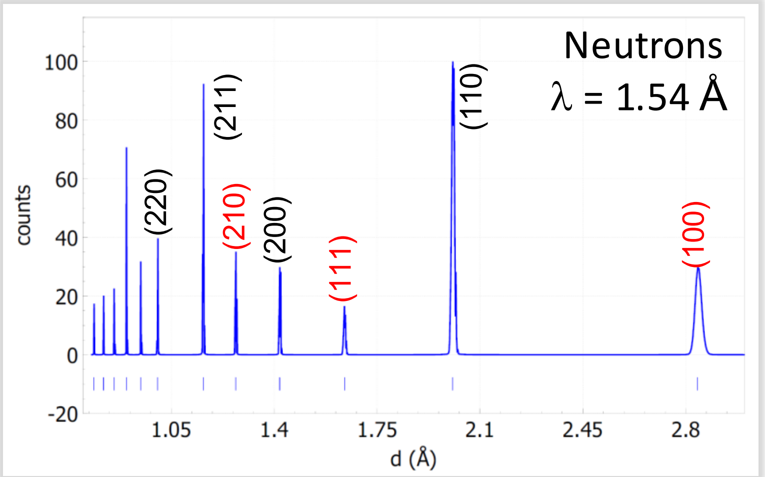


For magnetic structure

Why neutrons?

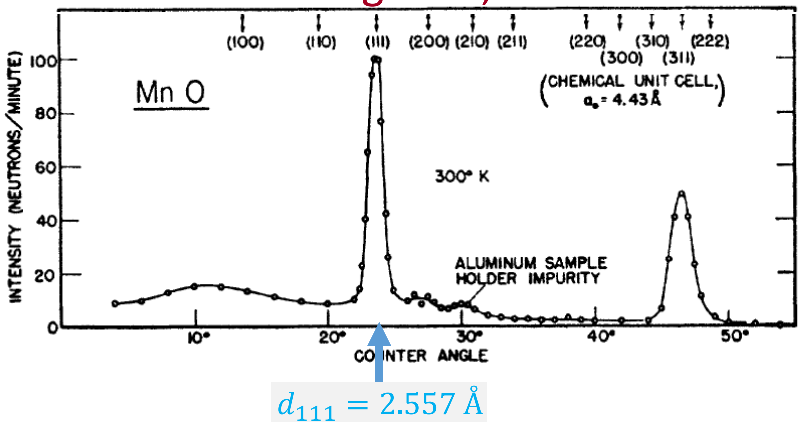
Spin ½ particles with magnetic moment

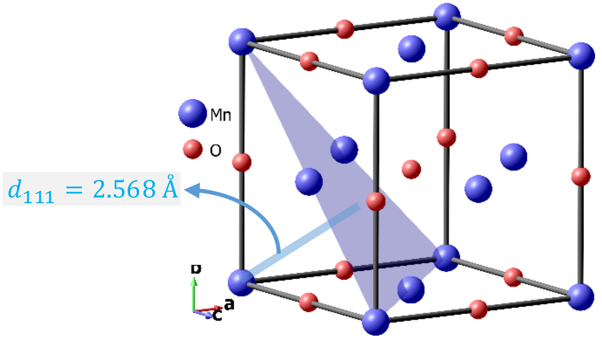
- Interact with magnetic moments of the elements in the sample being probed
- Directly probes microscopic magnetic order, in addition to lattice structure.
- The magnetic scattering length is comparable to the nuclear scattering length. So the magnetic and nuclear signals have comparable strengths.

Detection of Antiferromagnetism in MnO

Crystal unit cell: $a = b = c \approx 4.43$ Å

Paramagnetic, 300 K





C. G. Shull & J. S. Smart, Phys. Rev. **76** (1949) 1256

Why neutrons?

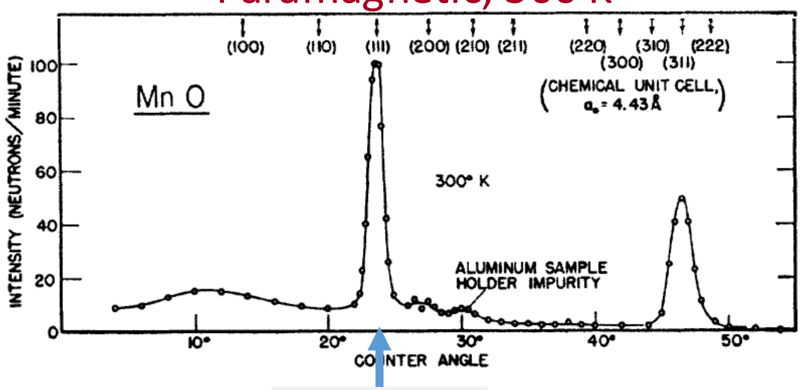
Detection of Antiferromagnetism in MnO

Neutrons can distinguish two elements with very similar atomic numbers

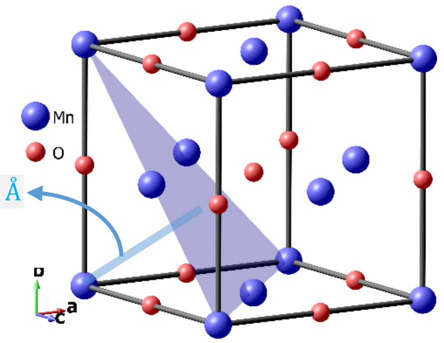
- Just like in the earlier case, due to the alignment of the magnetic spins of Mn^{2+}, a new ordering has emerged.
- Adjacent (111) planes have spins aligned in opposite directions.
- So the ordering is antiferromagnetic in nature.
- Notice that repeating the lattice unit cell can not repeat the magnet unit as well, since the spins at each corner have opposite sign!

Crystal unit cell: $a = b = c \approx 4.43$ Å

Paramagnetic, 300 K



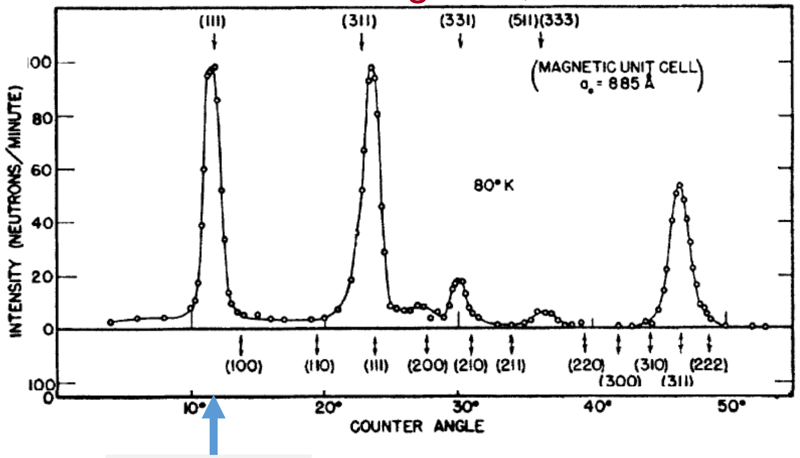
$d_{111} = 2.557$ Å



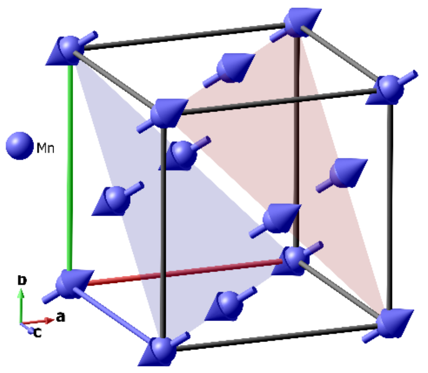
$d_{111} = 2.568$ Å

Magnetic unit cell: $a = b = c \approx 8.885$ Å

Antiferromagnetic, 80 K



$d_{???} = 5.136$ Å



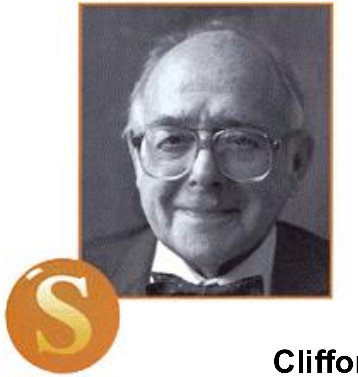
C. G. Shull & J. S. Smart, Phys. Rev. **76** (1949) 1256

Why neutrons?

Detection of Antiferromagnetism in MnO

Neutrons can distinguish two elements with very similar atomic numbers

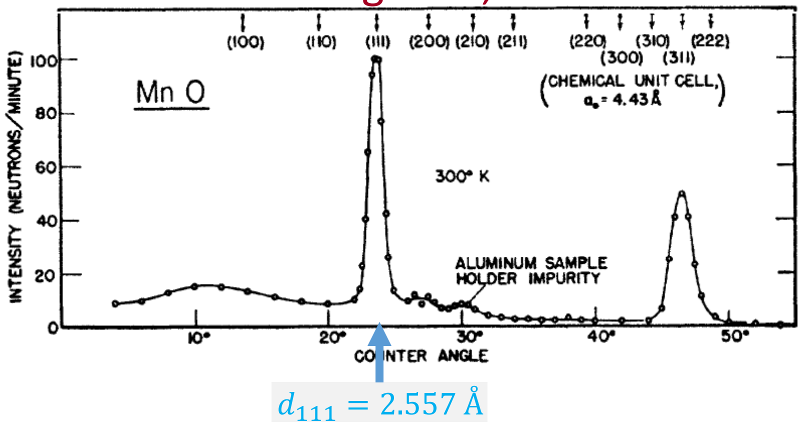
- We need a larger unit cell to obtain repeating magnetic order.
- The magnetic unit cell is twice as big as crystallographic unit cell, along all three crystallographic directions!

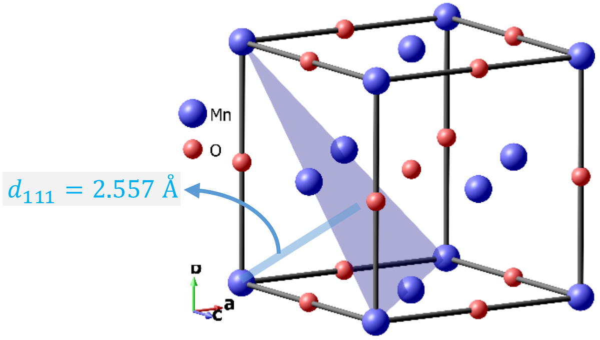


Clifford G. Shull
MIT, Cambridge, Massachusetts, USA

Crystal unit cell: $a = b = c \approx 4.43$ Å

Paramagnetic, 300 K





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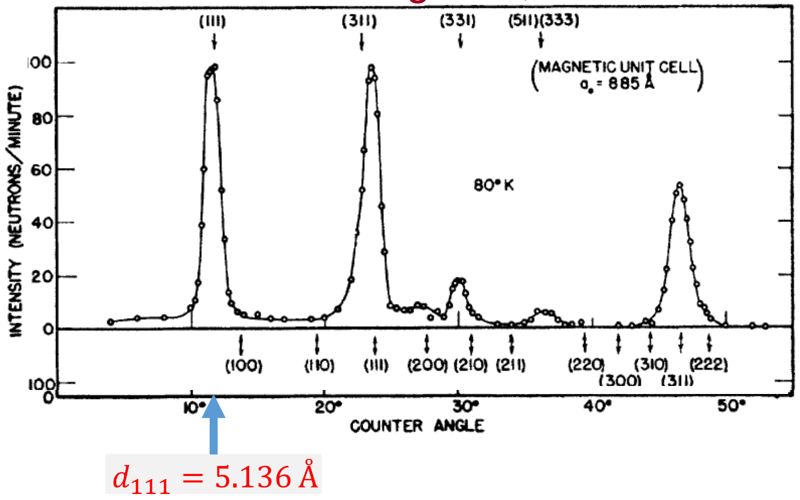
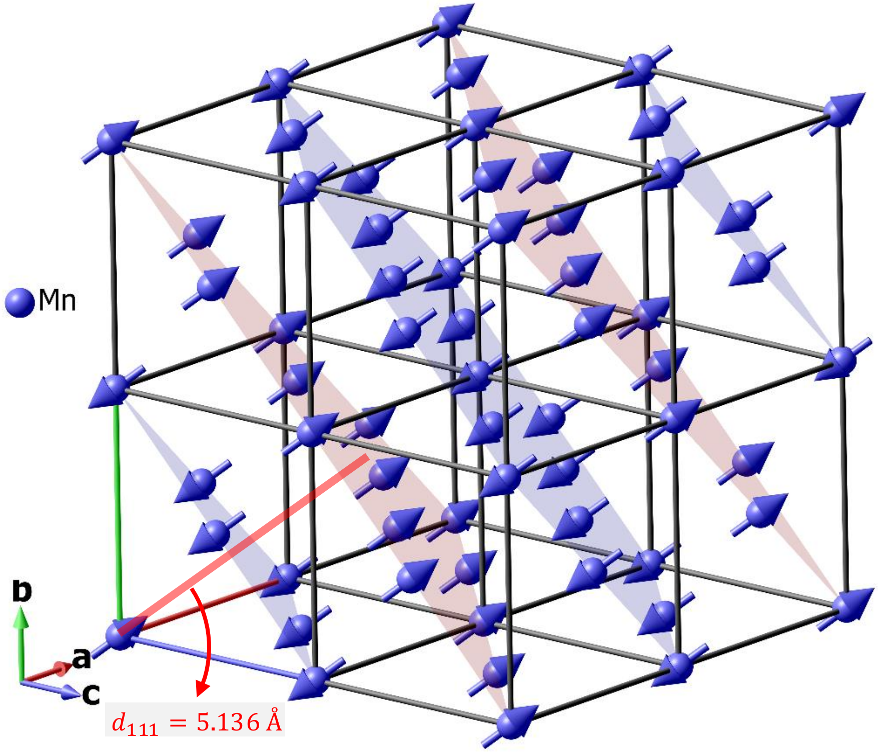
Antiferromagnetic, 80 K





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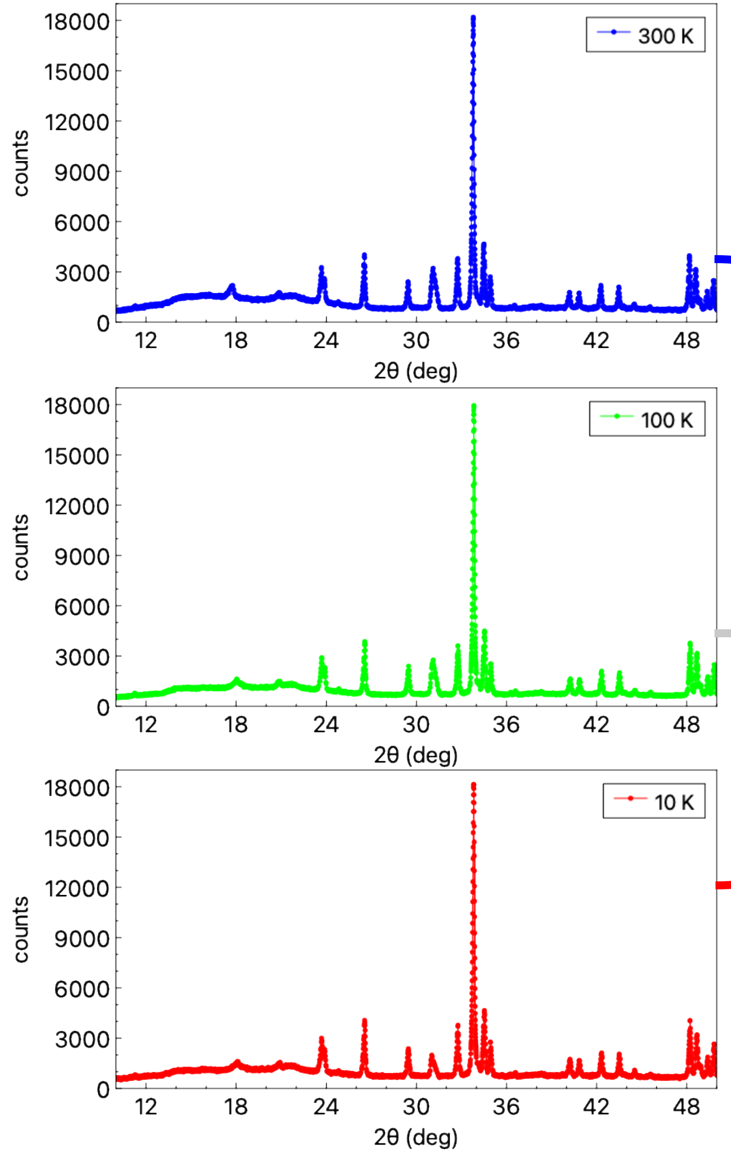
Magnetic order in $HoCrO_3$

Example material of today's hands-on workshop

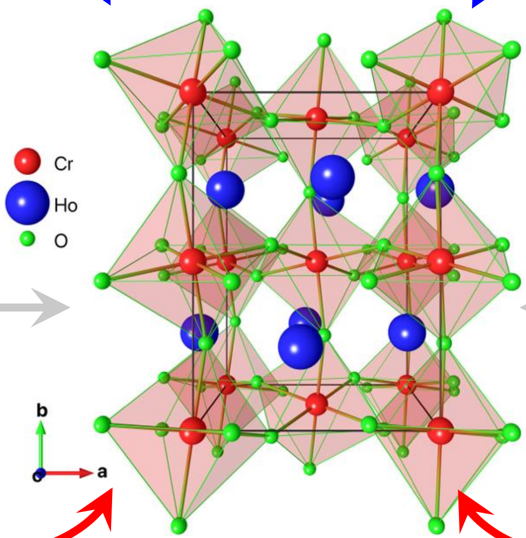
X-ray vs. Neutron powder diffraction

X-ray powder diffraction



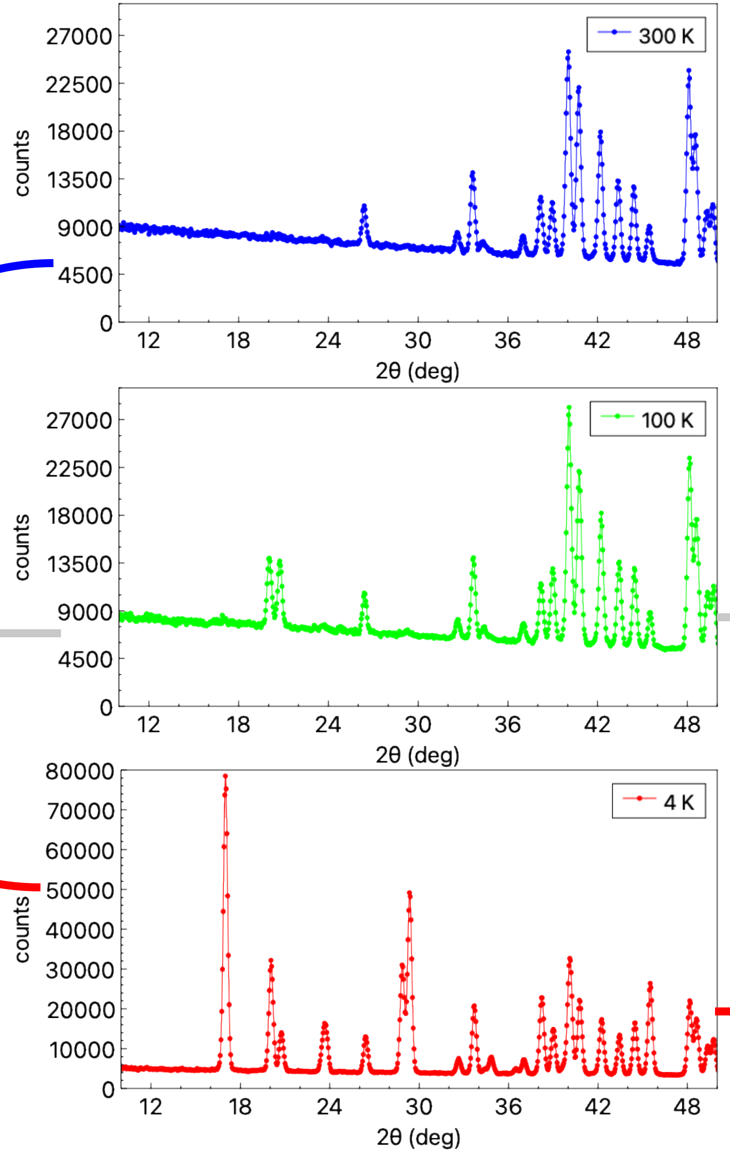
$HoCrO_3$

Orthorhombic space group:
Pnma (*Pbnm*) #62



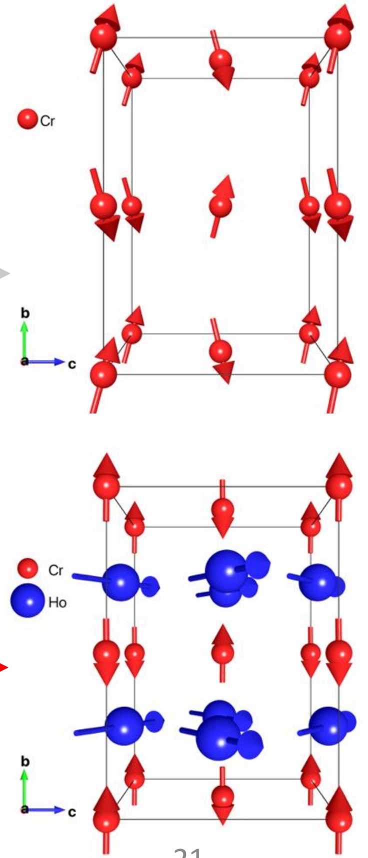
Atom	x	y	z
Cr (4a)	0.0000	0.0000	0.0000
Ho(4c)	0.43449	0.25000	0.00670
O1(4c)	0.53340	0.25000	0.58885
O2(8d)	0.19680	0.05420	0.30450

Neutron powder diffraction



X-ray diffraction:
Lattice structure

Neutron diffraction:
Lattice + Magnetic



Hyperfine and crystal field effects in $HoCrO_3$

Specific heat of $HoCrO_3$ shows:

1. **Anomaly centered around ~0.3 K:**

   Nuclear hyperfine Schottky peak due to hyperfine splitting of ^{165}Ho nuclei with I=7/2

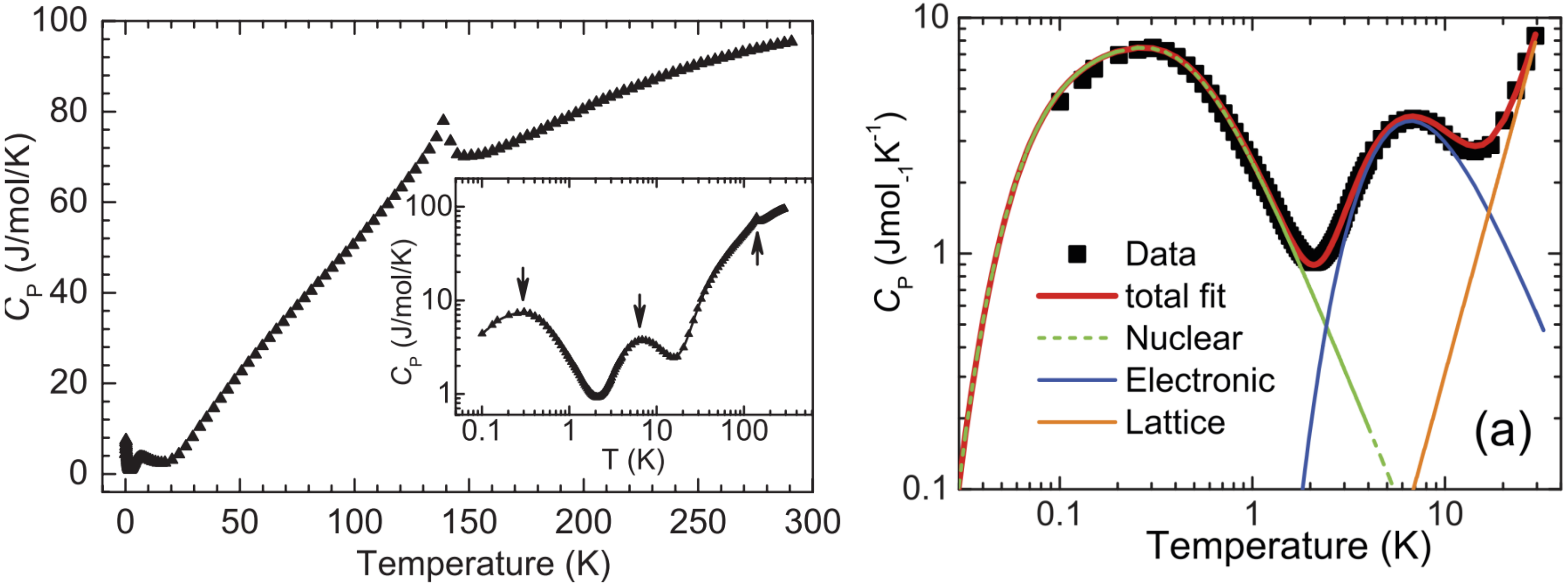
2. **Anomaly centered around ~7 K:**

   Electronic Schottky (crystal field) contribution from thermal depopulation of the $^5I_8$ ground state multiplet of Ho^{3+}

3. **Onset of magnetic ordering around** T_N = 142 K.

C. M. N. Kumar, *et al.*, JPCM **28** (2016)

Specific heat of $HoCrO_3$ in the temperature range 100 mk – 295 K



From specific heat data fitting:

Hyperfine splitting energy:
~ 22.5(2) μeV

First three crystal field levels:
1.379(5) meV, 10.37(4) meV, 15.49(9) meV

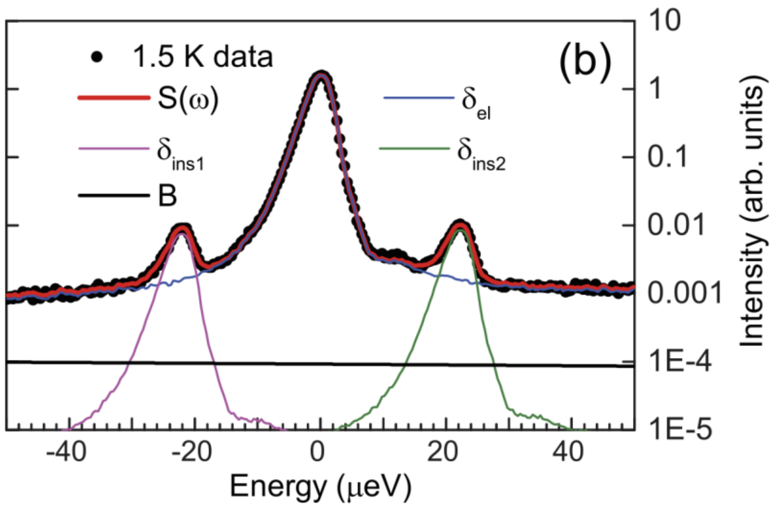
Inelastic neutron scattering measurements should be able directly resolve these energy levels

Hyperfine and crystal field effects in $HoCrO_3$

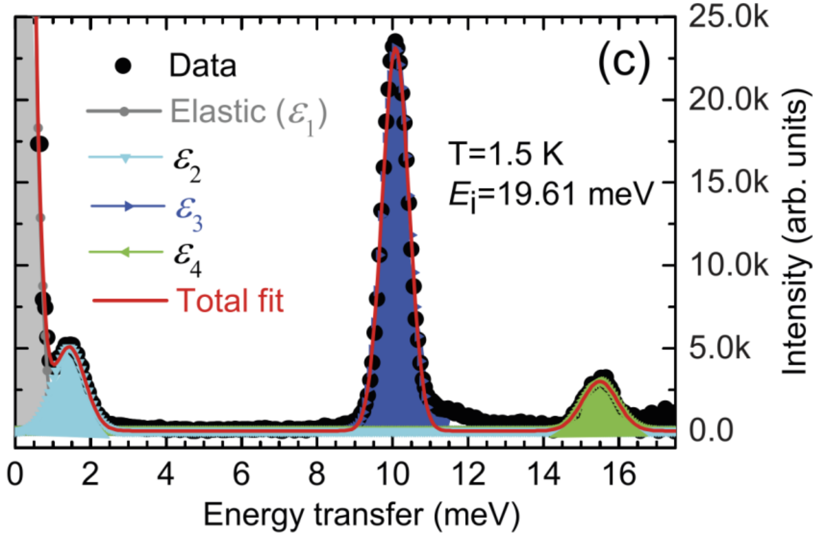
Inelastic neutron scattering measurements directly reveal:

- Hyperfine splitting energy level
- Multiple crystal field levels.

Neutron inelastic scattering in two different energy ranges



Hyperfine levels



Crystal field levels

From specific heat data fitting:

Hyperfine splitting energy:
~ 22.5(2) μeV

First three crystal field levels:
1.379(5) meV, 10.37(4) meV, 15.49(9) meV

Directly observed from inelastic neutron scattering:

Hyperfine splitting energy:
~ 22.18(4) μeV

First three crystal field levels:
1.45(6) meV, 10.07(4) meV, 15.49(2) meV

C. M. N. Kumar, *et al.*, JPCM **28** (2016)

Fantastic neutrons and where to find them!

Operational Neutron Facilities with User Programs (2025)

Europe

- **ILL – Institut Laue–Langevin (France):** https://www.ill.eu
- PSI – SINQ (Switzerland): https://www.psi.ch
- ISIS Neutron and Muon Source (UK): https://www.isis.stfc.ac.uk
- BNC – Budapest Neutron Centre (Hungary): https://www.bnc.hu
- MLZ / FRM-II (Germany): https://www.mlz-garching.de
- ESS – European Spallation Source (Sweden) (First users in 2027?): https://europeanspallationsource.se

North America

- NIST Center for Neutron Research (USA): https://www.nist.gov/ncnr
- ORNL – SNS & HFIR (USA): https://neutrons.ornl.gov

Asia

- J-PARC MLF (Japan): https://mlfinfo.jp
- JRR-3 (Japan): https://jrr3.jaea.go.jp
- CARR – China Advanced Research Reactor (China): https://english.ciae.ac.cn
- CSNS – China Spallation Neutron Source (China): https://csns.ihep.ac.cn

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- PSI – SINQ (Switzerland): https://www.psi.ch
- ISIS Neutron and Muon Source (UK): https://www.isis.stfc.ac.uk
- BNC – Budapest Neutron Centre (Hungary): https://www.bnc.hu
- MLZ / FRM-II (Germany): https://www.mlz-garching.de
- ESS – European Spallation Source (Sweden) (First users in 2027?): https://europeanspallationsource.se

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Asia

- J-PARC MLF (Japan): https://mlfinfo.jp
- JRR-3 (Japan): https://jrr3.jaea.go.jp
- CARR – China Advanced Research Reactor (China): https://english.ciae.ac.cn
- CSNS – China Spallation Neutron Source (China): https://csns.ihep.ac.cn

Founder countries:
France
Germany
United Kingdom

Scientific partners:
Austria
Belgium
The Czech Republic
Denmark
Italy
Poland
Slovakia
Spain
Sweden
Switzerland

NEUTRONS FOR SOCIETY

Travel and accommodation expenses are covered for up to 2 users per accepted proposal

Before planning a neutron scattering experiment: Essential facts

- Neutron scattering ≠ lab technique → only at large-scale facilities
- Beamtime is peer-reviewed, and competition is high
- Two proposal calls/year at most facilities
- Proposal quality decides if and how much beamtime you get
- Success rate around 50%, depending on instrument demand
- Timeline from submission → experiment: 2–9 months, so prepare early

The scientific excellence: The heart of your proposal

The proposal should contain a 2-3-page statement of research. Most facilities have specific guidelines on the proposal format, and even proposal templates are available. Prepare the proposal according to the facility guidelines while addressing the following points.

1. Fundamental Research Questions

- ✓ Why is this research scientifically interesting?
- ✓ What gap in knowledge does it address?
- ✓ What are the expected outcomes?

2. Justification for Neutron Scattering

- ✓ Why is this neutrons specifically required?
- ✓ What unique insights do neutrons provide?
- ✓ Why not use alternative techniques?

3. Instrument Selection

- ✓ Why is this particular instrument?
- ✓ What are the capabilities and limitations (if any)?
- ✓ How does it match your experimental needs?

4. Experimental Design and Planning

- ✓ Realistic beam time calculation
- ✓ Clear methodology and data collection strategy?
- ✓ Sample characterization and preparation details?

4. Literature and content

- ✓ Cite relevant literature supporting your approach
- ✓ Acknowledge previous work in the field
- ✓ Explain how your work advances the field

The success rate of a proposal depends on several aspects, and even good proposals get rejected. Try a different facility or try the same facility again, addressing any issues raised by the reviewers.

Before submission of a beam time proposal: consider this

Contact an Instrument Scientist to discuss your research

- Technical guidance and feasibility assessment
- Choosing the right instrument
- Sample requirements (form, size, mass, sample-environment compatibility)
- Estimating experiment time
- Logistics: scheduling, transport, storage
- Proposal preparation tips
- Support for data analysis and publication

Impactful applications of neutron science

Energy Storage and Materials Science: The Battery Revolution

The global shift to sustainable energy and electric mobility demands better batteries. Neutron scattering provides unique atomic-level insights that drive the development of next-generation energy storage materials.

Technique	Application in Energy Storage	Key Insight Provided by Neutrons
Neutron Diffraction (ND)	Lithium-ion and Sodium-ion batteries	**Locating Light Ions**: Precisely maps the position and diffusion pathways of light ions (Li^+, Na^+) within electrode materials, which is nearly impossible with X-rays.
Small-Angle Neutron Scattering (SANS)	Solid-State Electrolytes and Electrodes	**Microstructure Analysis**: Characterizes the size, shape, and distribution of nanoparticles, pores, and interfaces in solid-state electrolytes and composite electrodes, which dictate performance and safety.
In-Operando Studies	All Battery Types	**Real-Time Monitoring**: Allows scientists to monitor structural changes, phase transitions, and lithium-ion flow while the battery is charging and discharging, providing crucial structure-performance relationships.

Probing Biomolecular Mechanisms for Drug Design with Neutrons

Neutron crystallography reveals hydrogen positions and molecular dynamics, offering insights into enzyme function that are essential for modern drug discovery.

Technique	Application in Structural Biology	Key Insight Provided by Neutrons
Neutron Crystallography	Enzymes and Proteins	**Proton Location**: Directly locates hydrogen atoms and their transfer pathways, which are essential for understanding enzyme catalysis, drug binding, and the mechanisms of antibiotic resistance.
Quasi-Elastic Neutron Scattering (QENS)	Cell Membranes and Hydration	**Molecular Dynamics**: Measures the dynamics of water molecules and lipids in cell membranes, providing insight into how proteins fold and interact with their environment.
Small-Angle Neutron Scattering (SANS)	Macromolecular Complexes	**Contrast Variation**: Uses deuterium labeling to selectively "hide" or "highlight" specific components (e.g., a protein, a lipid, or a drug molecule) within a large complex to determine its overall shape and assembly.

Impactful applications of neutron science

Engineering and Industrial Applications: Quality Control and Stress Analysis

Neutrons' deep penetration enables non-destructive testing and quality control of large or complex industrial components, making them a powerful tool for engineering applications.

Technique	Application in Engineering	Key Insight Provided by Neutrons
Neutron Diffraction	Aerospace and Automotive Components	**Residual Stress Mapping**: Measures internal stresses (residual stress) deep within welds, engine parts, and structural components without cutting them. This is critical for predicting component lifetime and preventing catastrophic failure.
Neutron Imaging (Radiography & Tomography)	Fuel Cells, Heritage Objects, and Industrial Parts	**Non-Destructive Visualization**: Creates high-resolution 3D images of the interior of opaque objects. It is particularly effective for visualizing the flow of water in operating fuel cells or the distribution of lubricants in engines.
Prompt Gamma Activation Analysis (PGAA)	Quality Control and Forensics	**Elemental Composition**: Provides highly accurate, non-destructive elemental analysis of bulk samples, used in quality control for materials and in forensic science.

Conclusion: The future is Neutron-Powered

Why Neutrons?

- **Foundational probe** for breakthroughs in energy, biology, and engineering
- **Unrivaled sensitivity** to light elements, isotopes, and magnetism
- **Non-destructive,** deeply penetrating, ideal for in-operando and real-world conditions

The Modern Neutron Landscape

- **Brighter sources:** Next-generation facilities (e.g., ESS) → faster, higher-resolution science
- **Advanced instruments:** Real-time in-situ and in-operando capabilities
- **Computational power:** AI-enhanced modelling and sophisticated data analysis

Neutrons remain irreplaceable for understanding matter.

Join the neutron community and drive your next research breakthrough!