

Experimental Aspects of Neutron Diffraction

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NCNR

University of Maryland, College Park



The Nobel Prize in Physics 1994



Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.



S Shull made use of **elastic scattering** i.e. of neutrons which change direction without losing energy when they collide with atoms.

Because of the wave nature of neutrons, a diffraction pattern can be recorded which indicates where in the sample the atoms are situated. Even the placing of light elements such as hydrogen in metallic hydrides, or hydrogen, carbon and oxygen in organic substances can be determined.

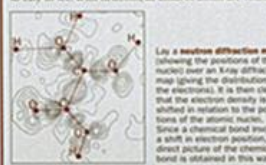
The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.



An early (1950) neutron diffractometer with flexible waveguide control here used by E.O. Wollan and C.G. Shull (standing) at Oak Ridge National Laboratory.

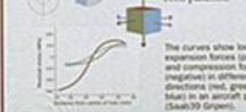
Neutrons see more than X-rays

X-rays are scattered by electrons, neutrons by atomic nuclei. With X-rays it is easier to see atoms that have many electrons. Hydrogen, for example, which has only one electron, is not so easy to see. With neutrons, all kinds of atoms are visible.



Neutrons reveal inner stresses

A hole has been punched in an important metal aircraft part. Does the part match up? Neutron diffraction can show how much the distance between the atoms has changed and hence the internal forces remaining around the hole after it has been punched.



Neutrons show what atoms remember

Of their earlier positions when they move randomly in relation to each other in liquids and solids. Even how there is in fact some local order. The atoms cannot move infinitely close to each other. Some distances are more common than others.

The time curve 1 + 0 shows the positions for liquid boron. The other curves show how the positions of the atoms change with time (1 ps = one millisecond of a millionth of a second) seen with inelastic neutron scattering. Corresponding "memory functions" can also be measured in magnets e.g. near the Curie temperature, the temperature at which magnetic order shifts to disorder.

Neutrons behave as particles and as waves

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.

Berttram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.



B Brockhouse made use of **inelastic scattering** i.e. of neutrons, which change both direction and energy when they collide with atoms. They then start or cancel atomic oscillations in crystals and record movements in liquids and metals. Neutrons can also interact with spin waves in magnets.

With his 3-axis spectrometer Brockhouse measured energies of phonons (atomic vibrations) and magnons (magnetic waves). He also studied how atomic structures in liquids change with time.

Neutrons show what atoms do

3-axis spectrometer with rotatable crystals and rotatable sample

Atoms in a crystalline sample

Neutron beam

Crystal that sorts and forwards neutrons of a certain wavelength (energy) - monochromatized neutrons

When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy (these absorb) - inelastic scattering

Crystal that sorts and forwards neutrons of a certain wavelength (energy) - monochromatized neutrons

Changes in the energy of the neutrons are first analysed in an analyser crystal...

...and the neutrons then counted in a detector.

How it started

Brockhouse and Shull made their pioneering contributions at the first nuclear reactors in the USA and Canada back in the 1940s and 1950s. It was then that the resources of the reactors became available for peacetime research.

... how it continues

Thousands of researchers are now working at the many neutron research centers throughout the world. New and very advanced neutron scattering installations have been built and more are planned in Europe, the USA and Asia. At these super-installations the researchers are studying the structure of new ceramic superconductors, molecular movements on surfaces of interest for catalytic exhaust cleaning, virus structures and the connection between the structure and the elastic properties of polymers.



KUNGL. VETENSKAPSAKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

© Information Department, Box 50006, S-104 05 Stockholm, Sweden. Tel +46-8-472 95 00, Fax +46-8-15 58 75. Editors: Bengt Balm-Björnsen, Margareta Widing-Rindt. The Royal Swedish Academy of Sciences, Author: Professor Erik S. Karlsson and Professor Carl Norberg, Department of Physics, Uppsala University, Member of the Nobel Committee for Physics. Layout and Illustrations: Kjell Lundin, Explorare AB. Printed by: Tryckindustri, 1994.

Further reading:

- D.J. Hughes *The Nuclear Reactor as a Research Instrument*, SCIENTIFIC AMERICAN, VOL. 179, AUGUST 1951, p. 23.
- H. Lengeler and J.L. Finney *The European Spallation Source*, EUROPHYSICS NEWS, VOL. 25, p. 37, 1994.
- Information about the Nobel Prize in Physics 1994 (specimens), THE ROYAL SWEDISH ACADEMY OF SCIENCES.



1932 Neutrons Discovered by Chadwick

MAY 15, 1939

PHYSICAL REVIEW

VOLUME 55

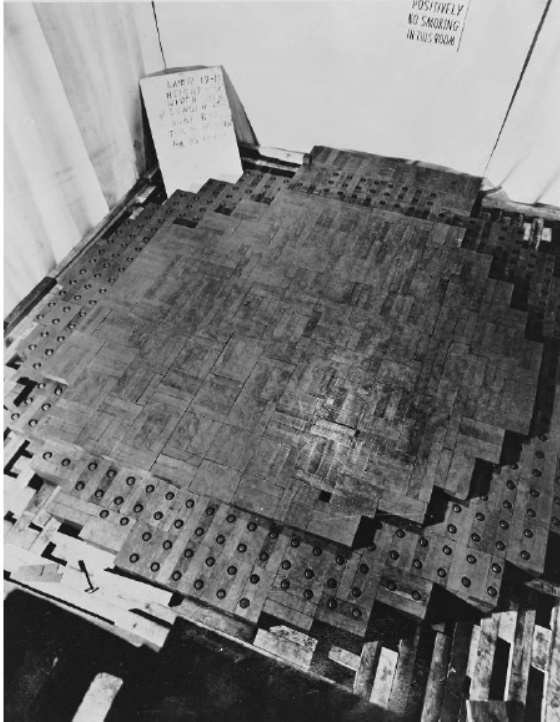
On the Magnetic Scattering of Neutrons

O. HALPERN AND M. H. JOHNSON

New York University, University Heights, New York, New York

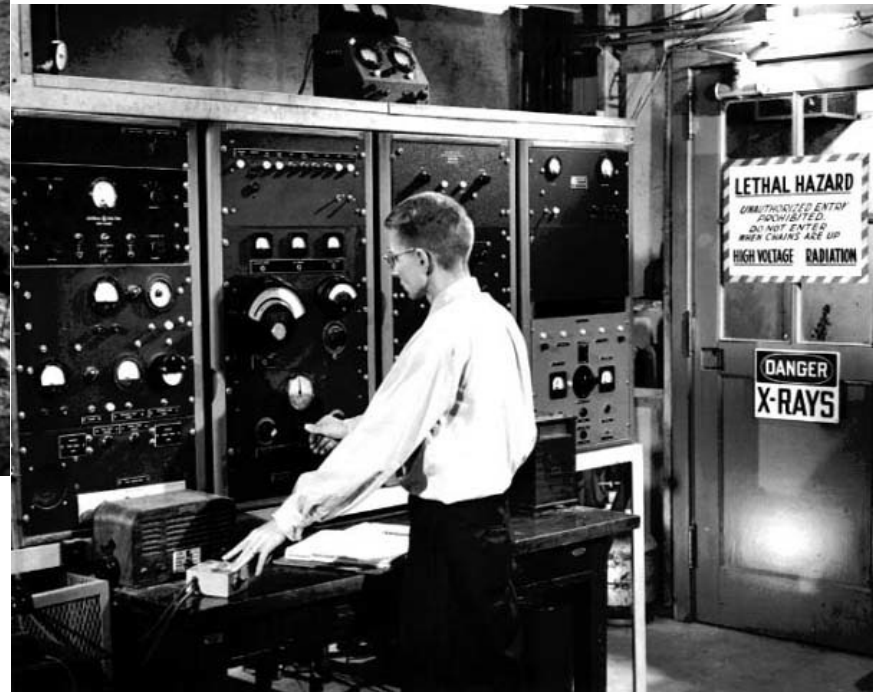
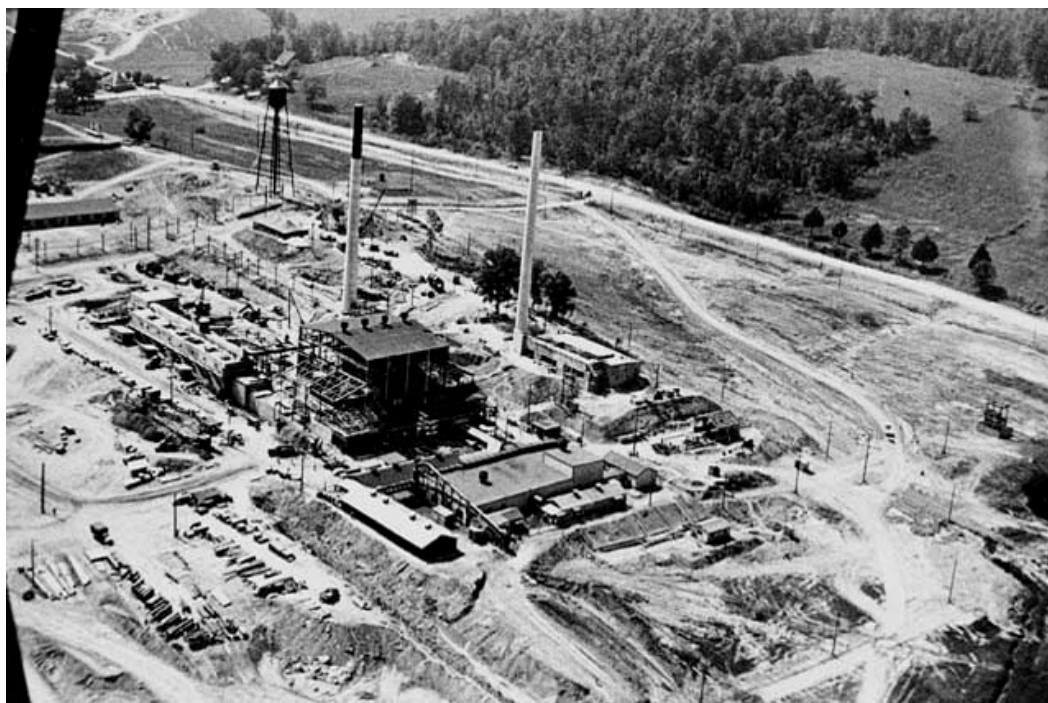
(Received December 3, 1938)

1942 Fermi's 30th pile goes critical



An Account of Oak Ridge National Laboratory's Thirteen Nuclear Reactors August 2009
<https://info.ornl.gov/sites/publications/Files/Pub20808.pdf>

ORNL Graphite Reactor 1943-1963



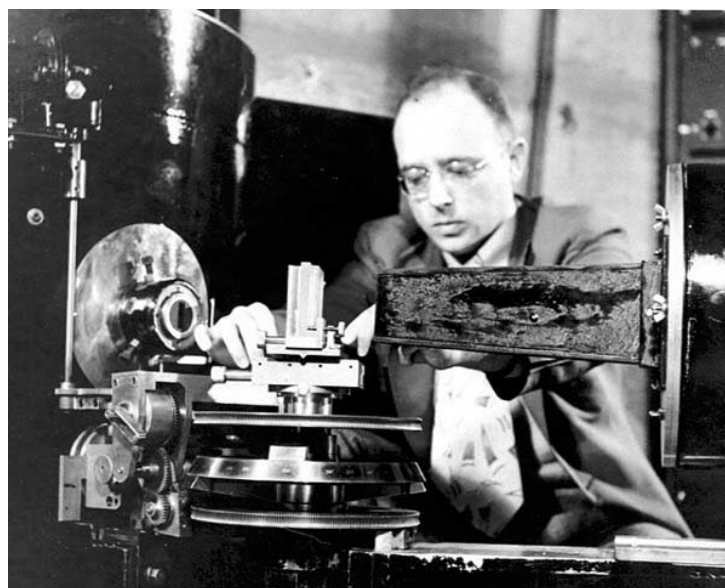
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The Diffraction of Neutrons by Crystalline Powders

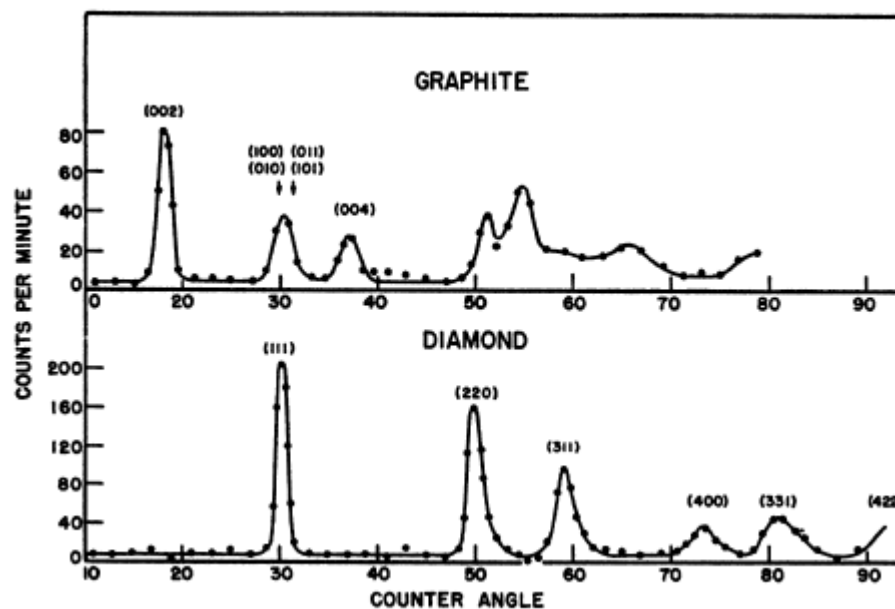
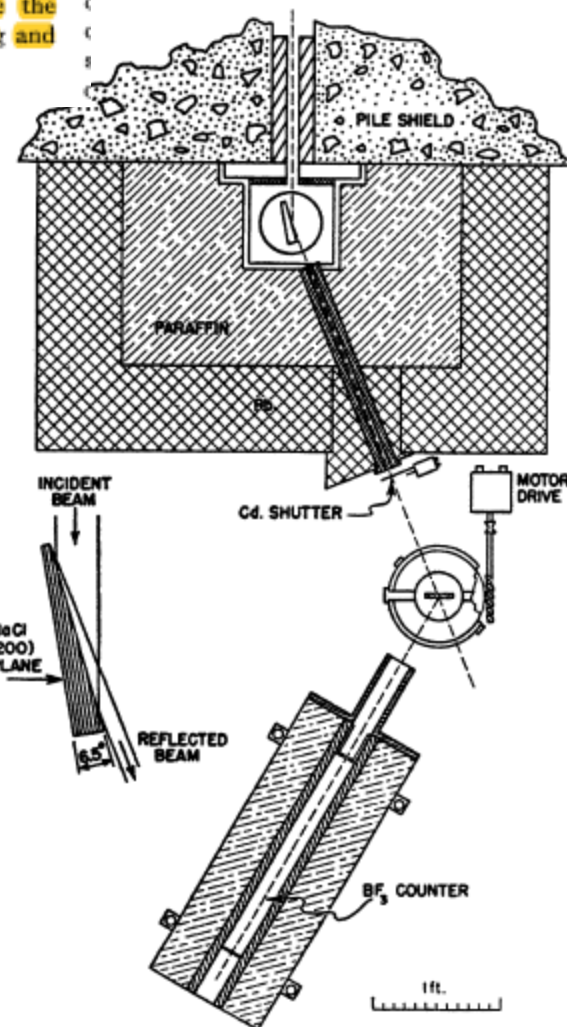
E. O. WOLLAN AND C. G. SHULL

Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received January 5, 1948)



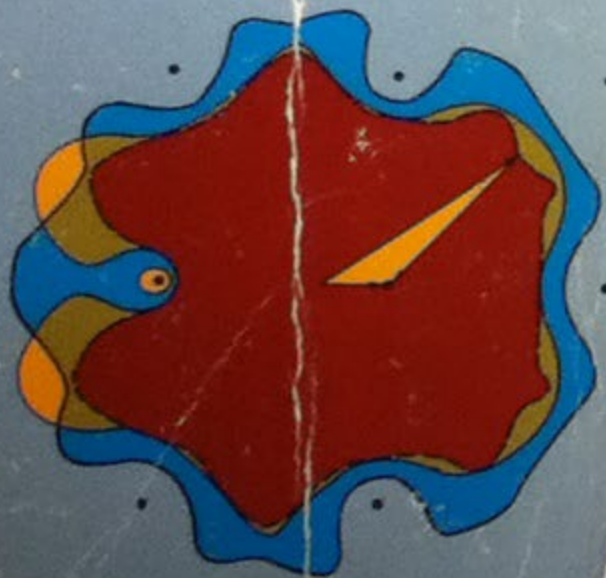
angular range. The advantage of automatic operation cannot be overestimated since the best data can be taken during the evening and night shifts.





how**stuff**works
It's good to know

INTRODUCTION TO
THE THEORY OF
THERMAL
NEUTRON
SCATTERING



G.L. Squires

Harald Ibach Hans Lüth

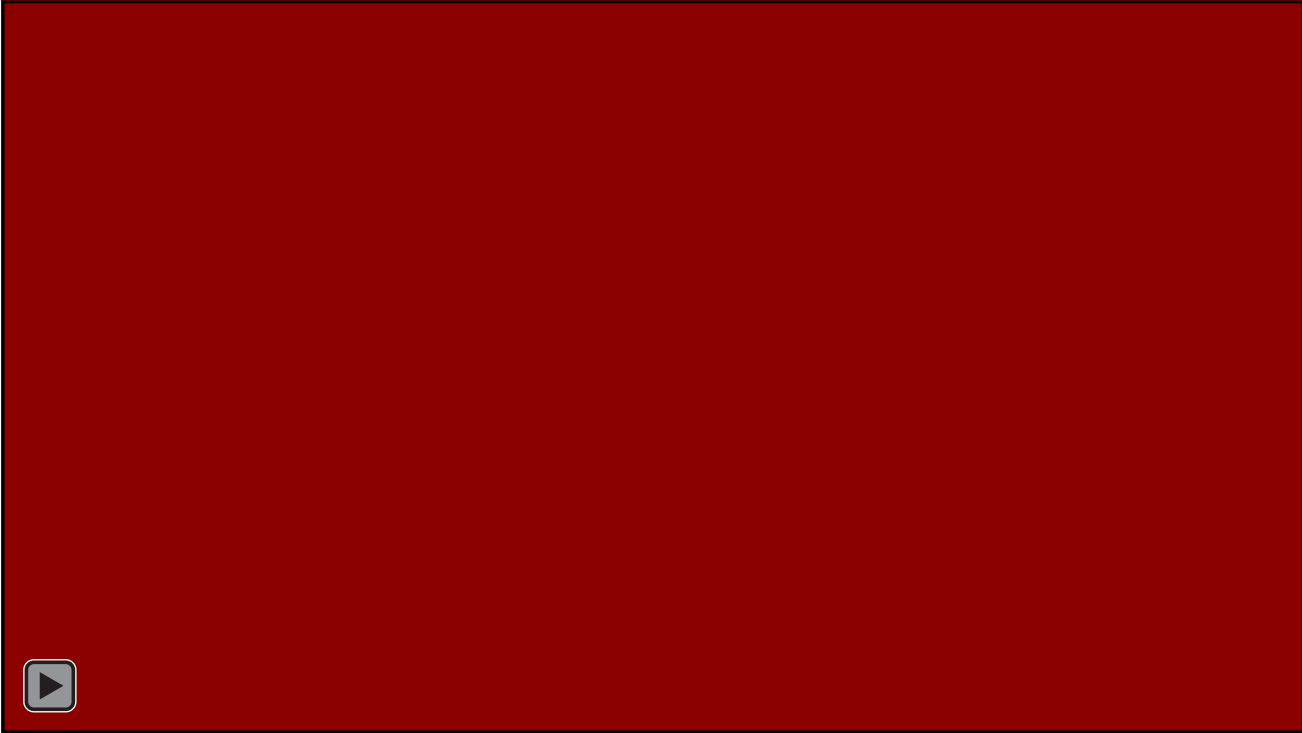
Solid-State Physics

An Introduction to Principles of Materials Science

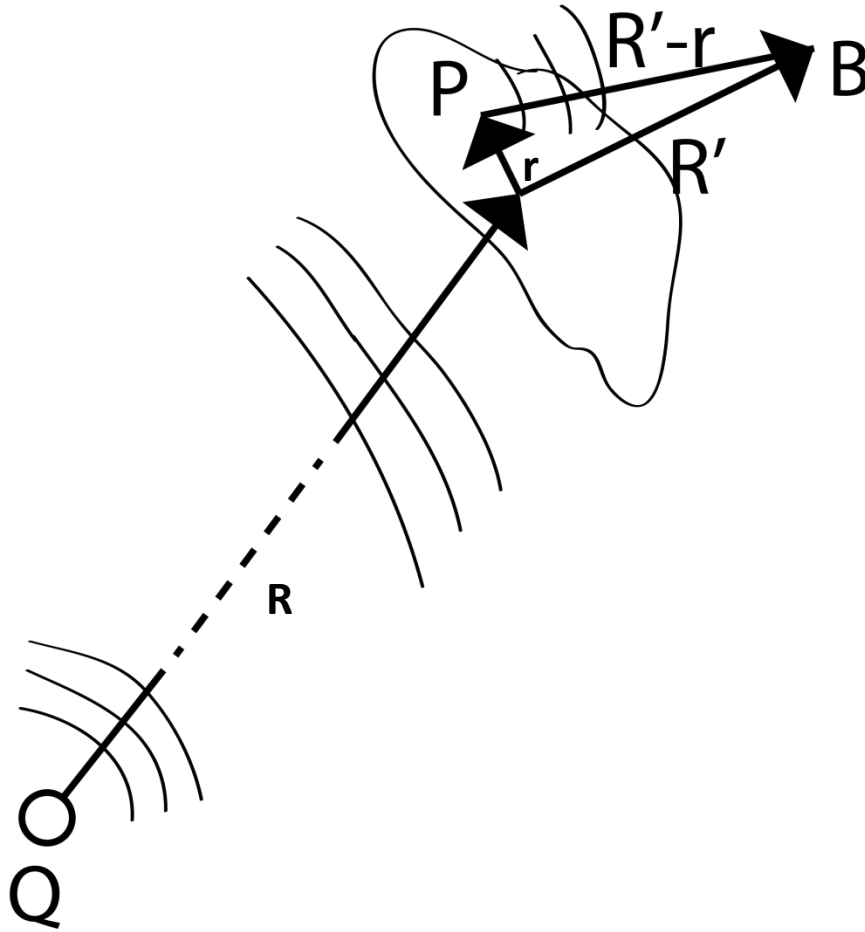
Second Edition



Springer



<http://toutestquantique.fr/en/>



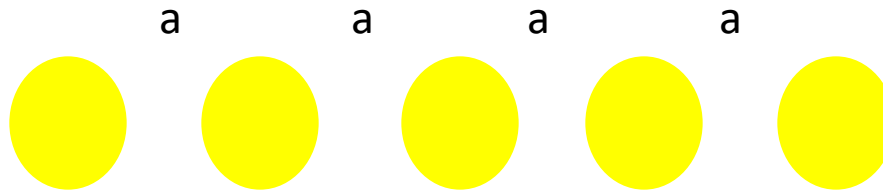
$$A_P = A_0 e^{i\vec{k}_0 \cdot (\vec{R} + \vec{r}) - i\omega_0 t}$$

$$A_B = A_P(r, t) \rho(r) \frac{e^{i\vec{k} \cdot (\vec{R}' - \vec{r})}}{|\vec{R}' - \vec{r}|}$$

$$A_B = A_P(R' \gg r, t) \rho(r) \frac{e^{i\vec{k} \cdot (\vec{R}' - \vec{r})}}{|\vec{R}'|}$$

$$I(K) \propto |A_B|^2 \propto \left| \int \rho(r) e^{i\vec{K} \cdot \vec{r}} dr \right|^2$$

Reciprocal Space



$$\rho(x) = \rho(x + na)$$

$$\rho(x) = \sum_n \rho_n e^{i(n2\pi/a)x}$$

$$\rho(\vec{r}) = \sum_n \rho_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} \quad \vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

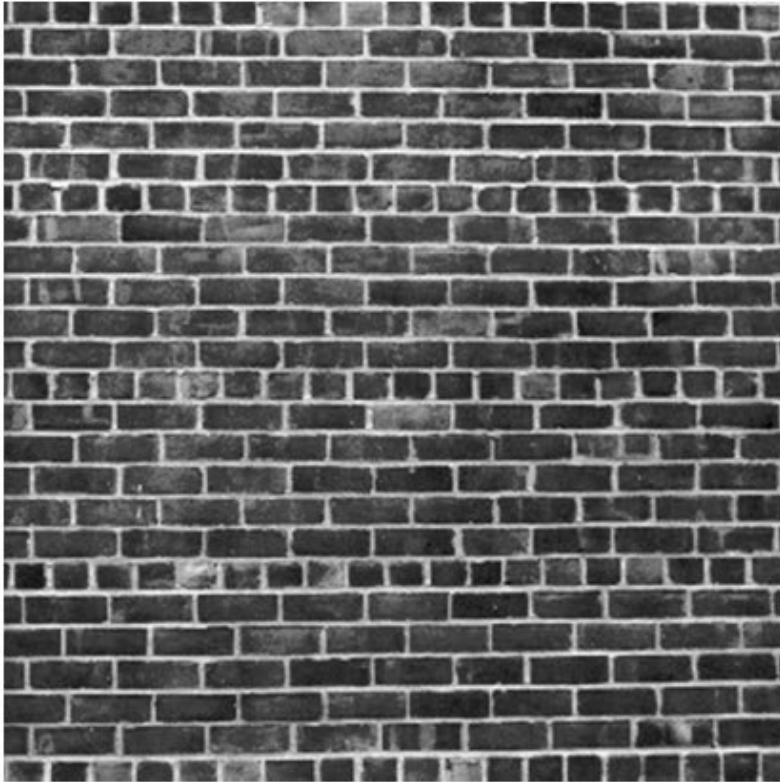
$$\vec{G} \cdot \vec{r} = 2\pi m \quad g_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$I(K) \propto |A_B|^2 \propto \left| \int \rho(r) e^{-i\vec{K} \cdot \vec{r}} dr \right|^2$$

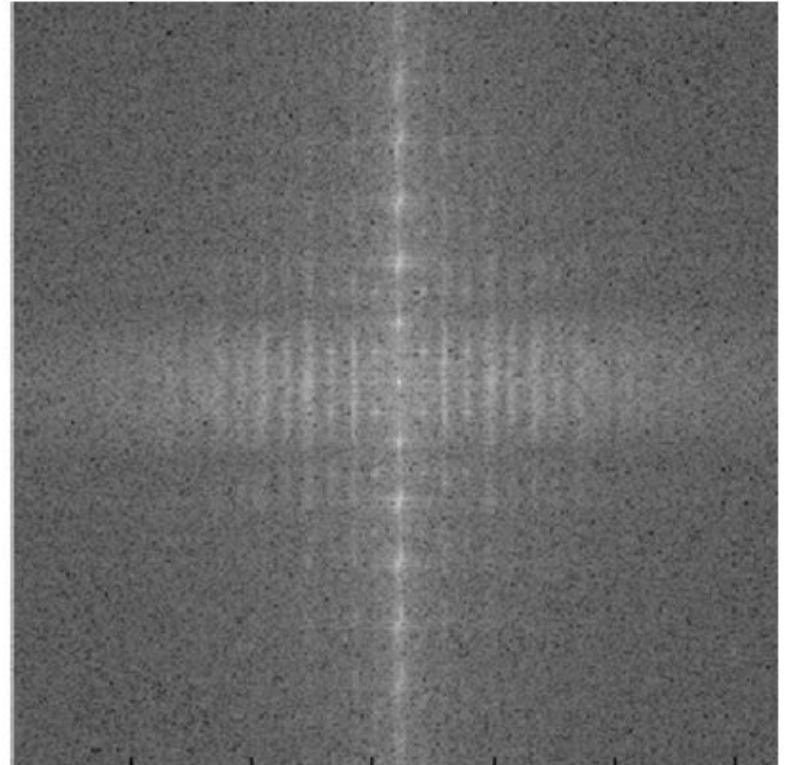


$$I(K) \propto \left| \sum_{\vec{G}} \rho_{\vec{G}}(r) \int e^{i(\vec{G}-\vec{K}) \cdot \vec{r}} dr \right|^2$$

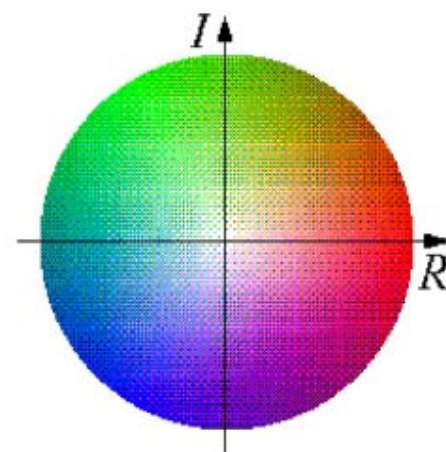
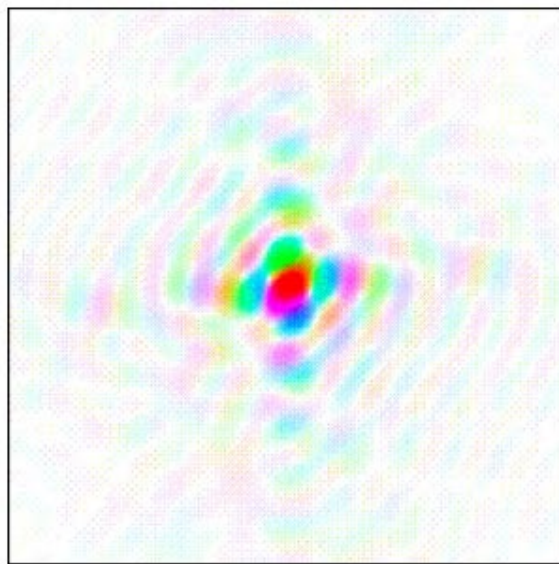
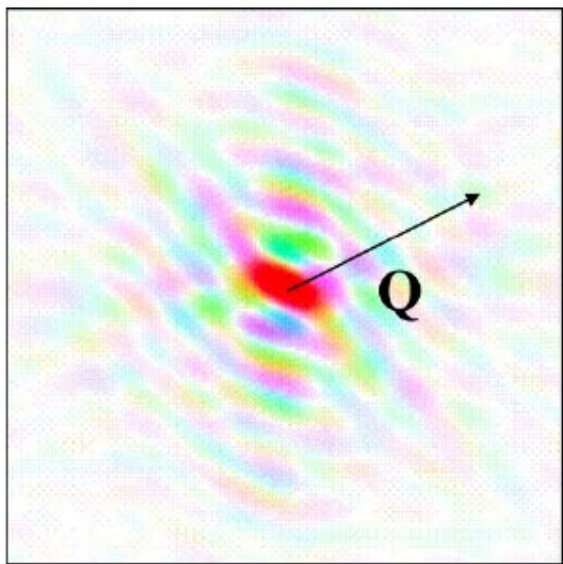
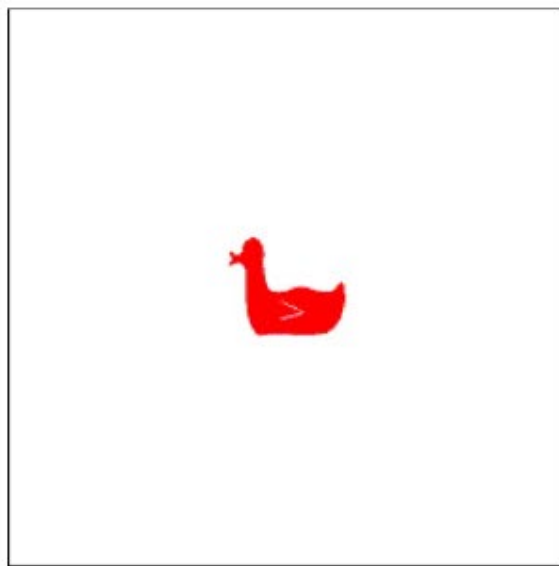
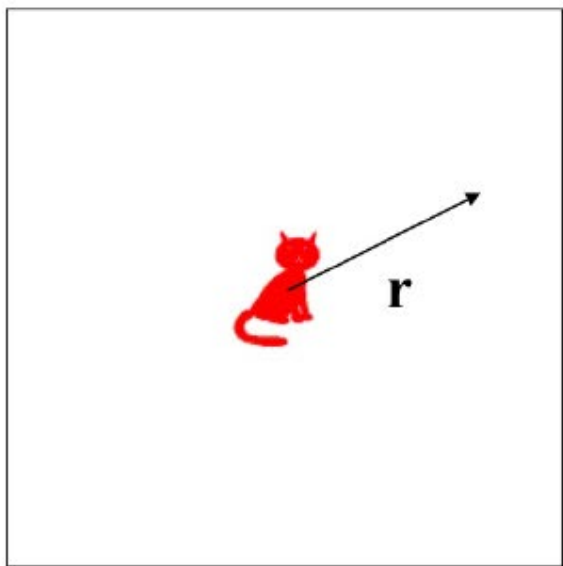
$$\int e^{i(\vec{G}-\vec{K}) \cdot \vec{r}} dr = \begin{cases} V & \text{for } \vec{G} = \vec{K} \\ \sim 0 & \text{otherwise} \end{cases} \quad \text{Laue Condition}$$

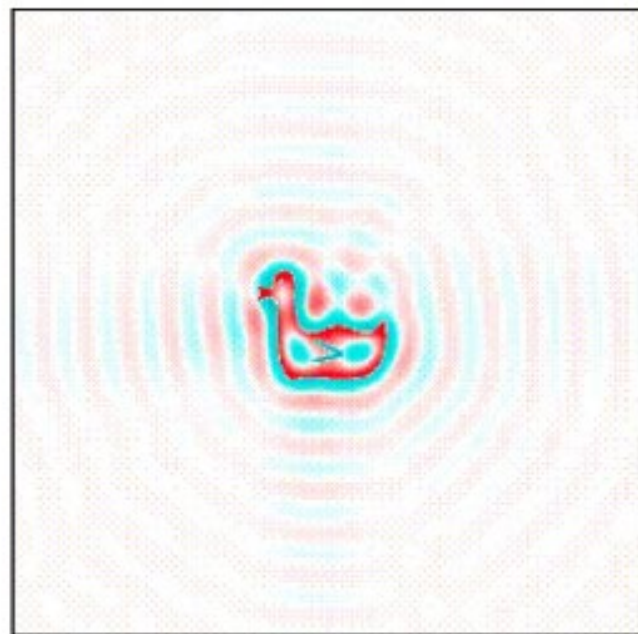
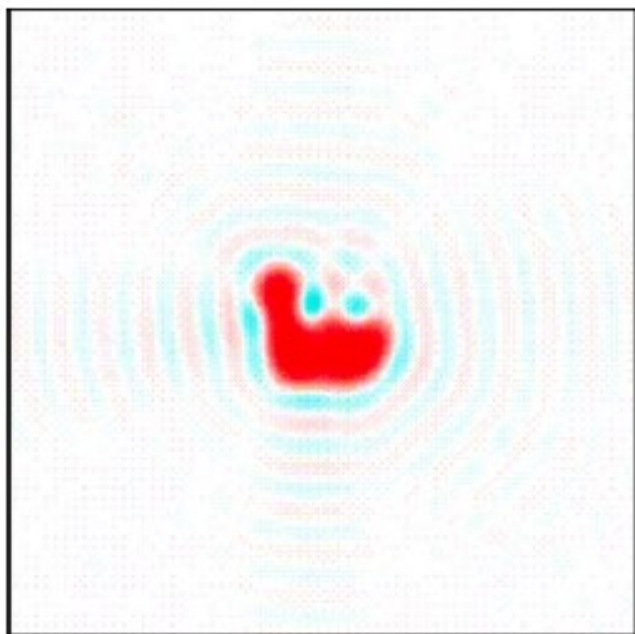
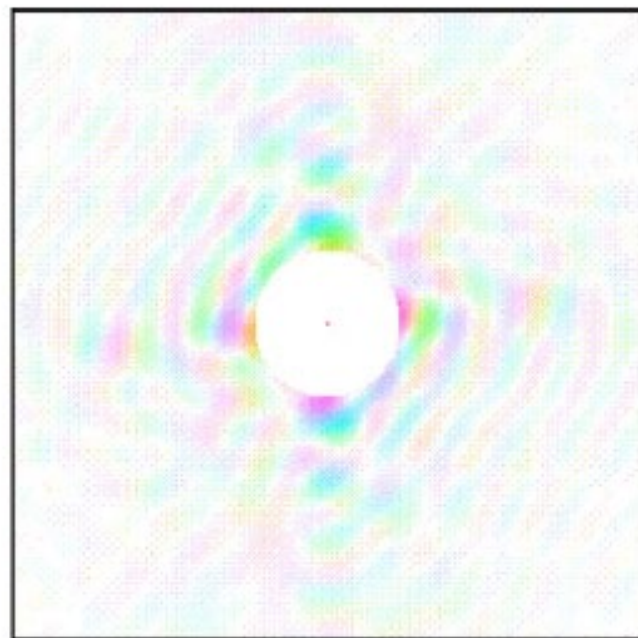
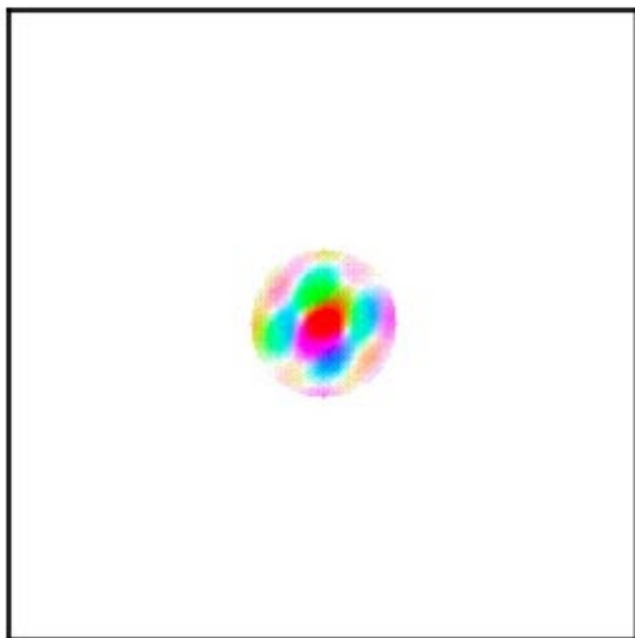


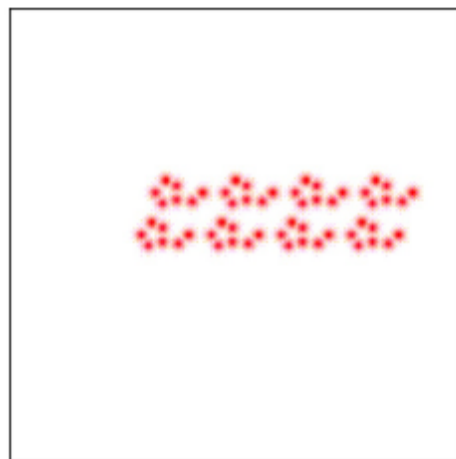
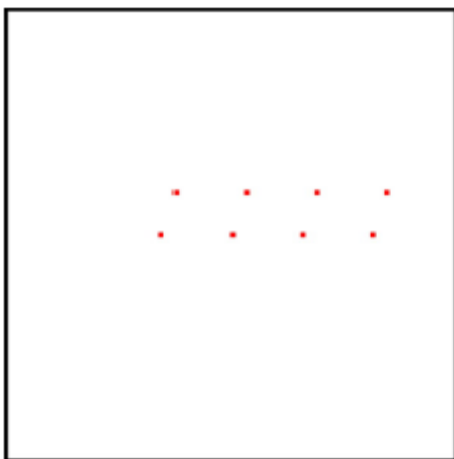
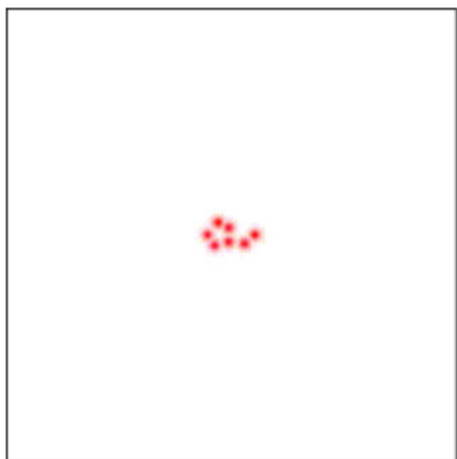
$$f(x, y)$$

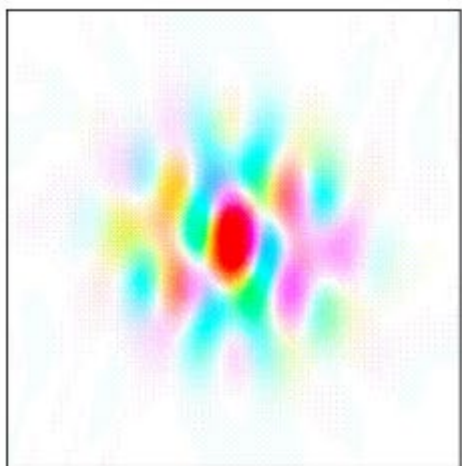


$$|F(u, v)|$$

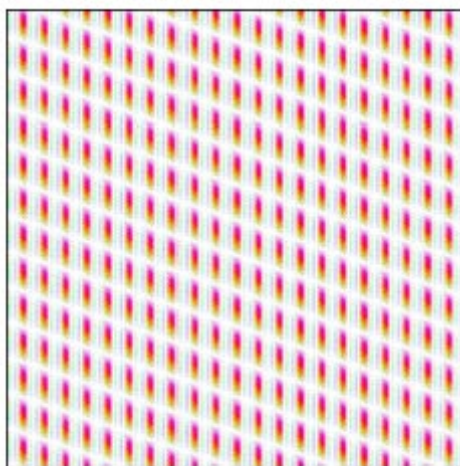




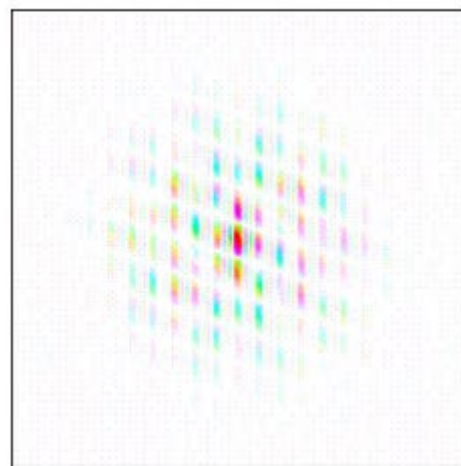


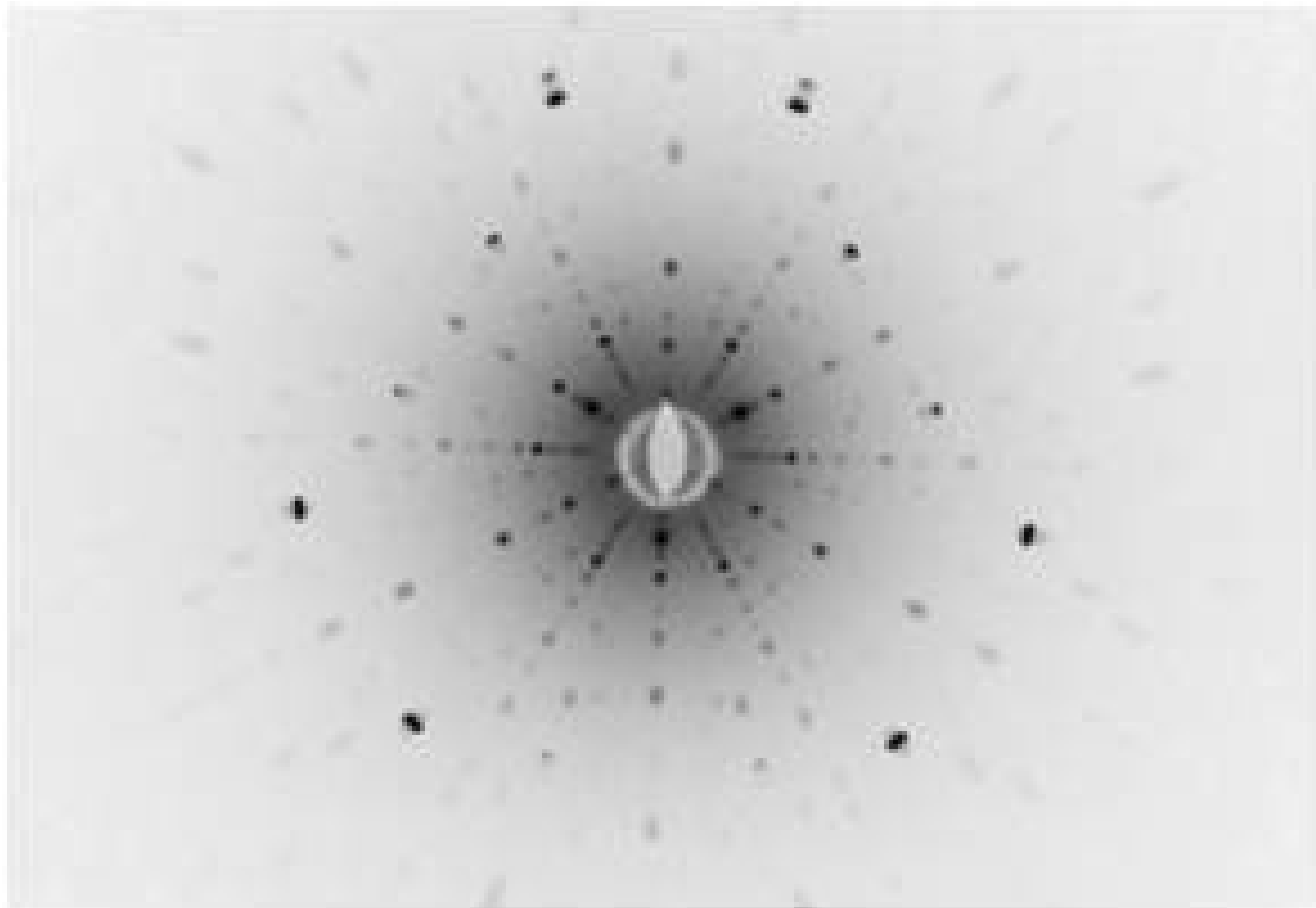


$\times$



$=$





$$I(K) \propto |A_B|^2 \propto \left| \int \rho(r) e^{-i\vec{K} \cdot \vec{r}} dr \right|^2$$

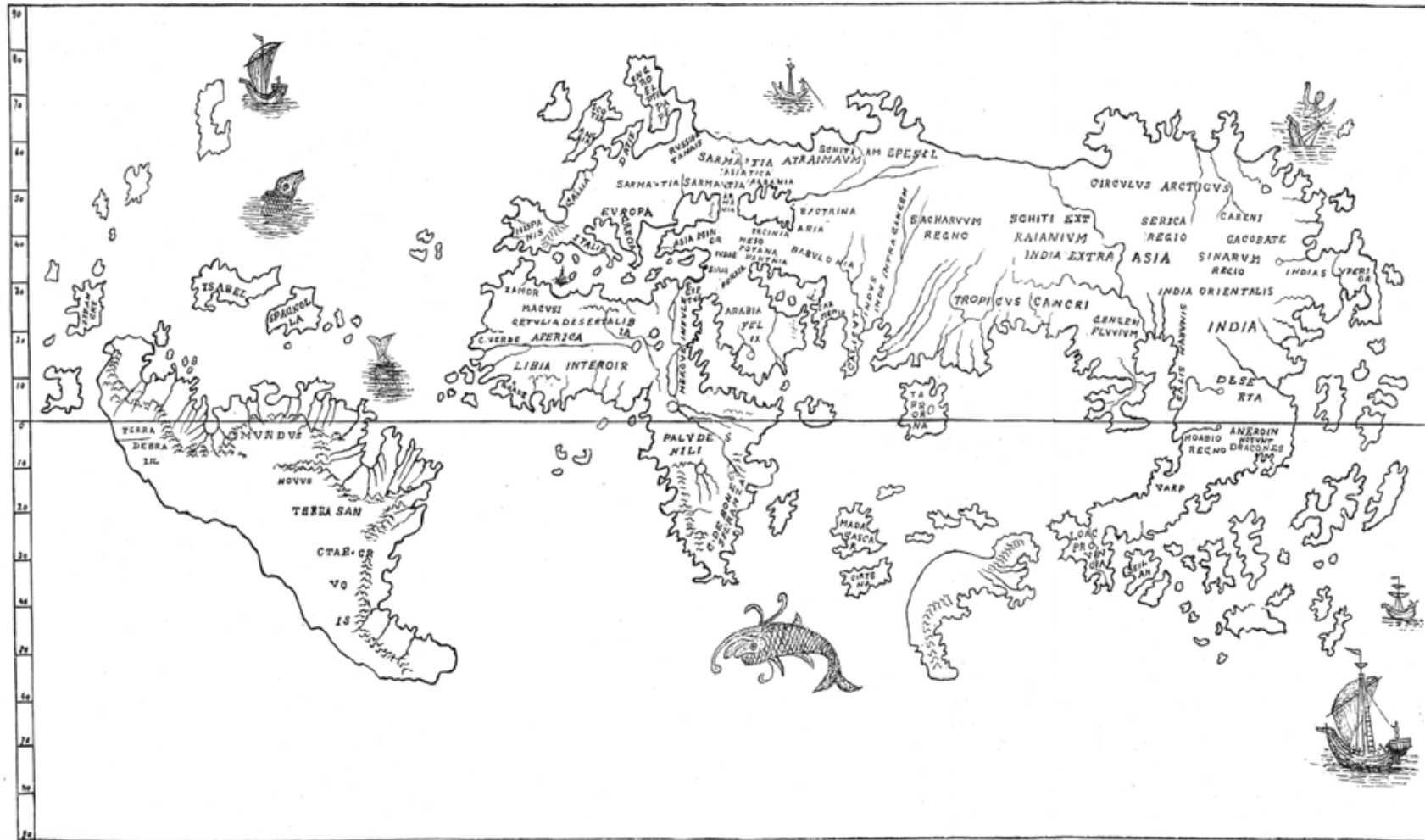


$$I(K) \propto \left| \sum_{\vec{G}} \rho_{\vec{G}}(r) \int e^{i(\vec{G}-\vec{K}) \cdot \vec{r}} dr \right|^2$$

$$\int e^{i(\vec{G}-\vec{K}) \cdot \vec{r}} dr = \begin{cases} V & \text{for } \vec{G} = \vec{K} \\ \sim 0 & \text{otherwise} \end{cases} \quad \text{Laue Condition}$$

Here there be dragons...

THE LENOX GLOBE



The Hunt-Lenox Globe, as transcribed by B.F. da Costa

$$I(K) \propto |A_B|^2 \propto \left| \int \rho(r) e^{-i\vec{K} \cdot \vec{r}} dr \right|^2$$

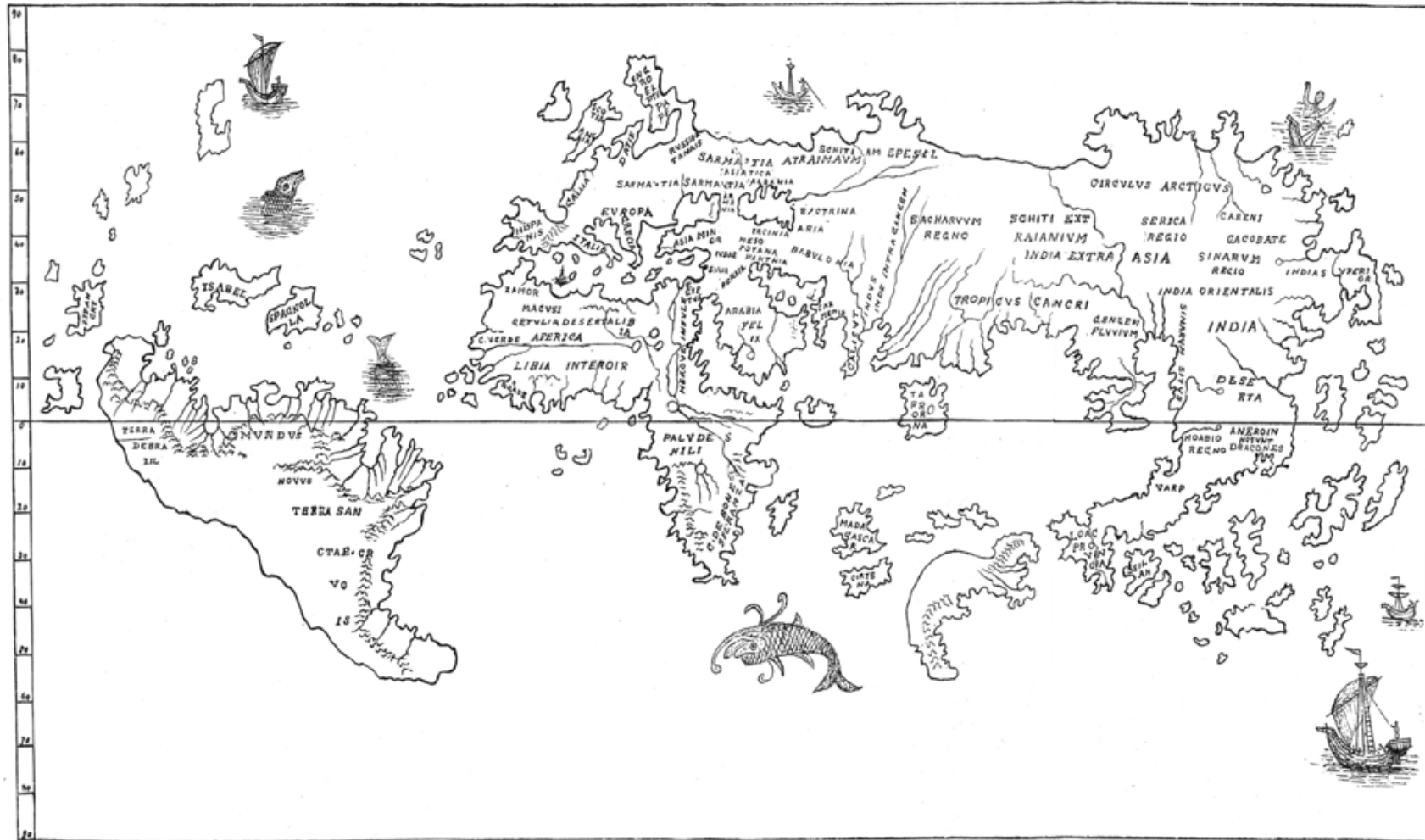


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Here there be dragons...

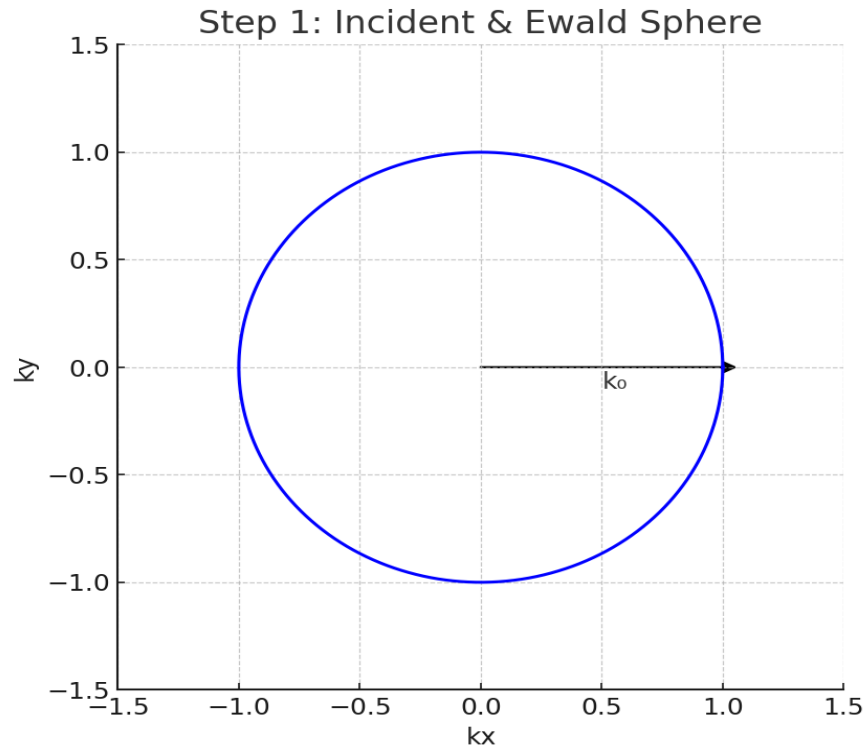
THE LENOX GLOBE



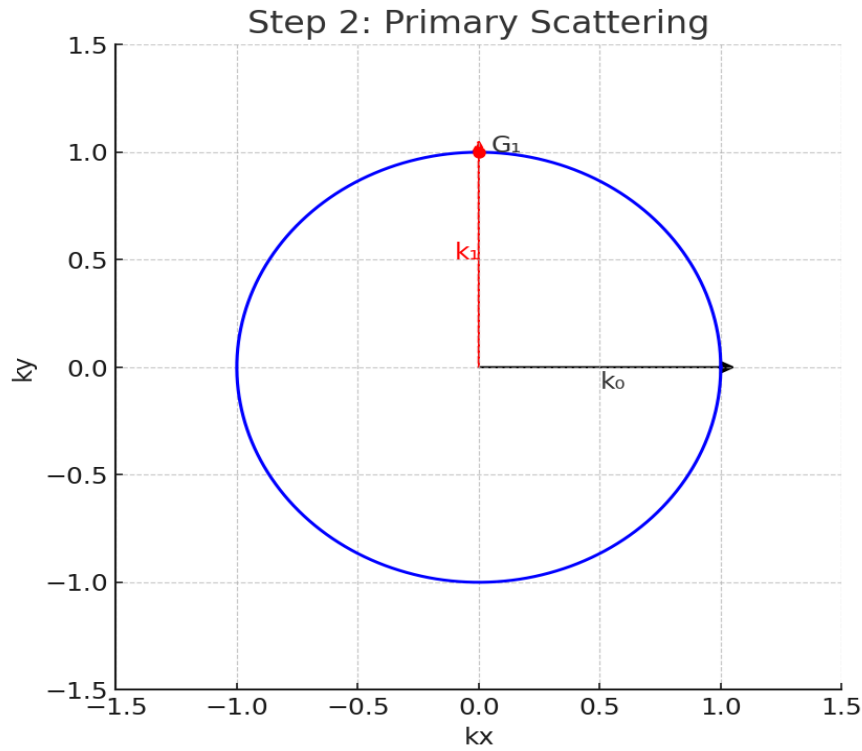
The Hunt-Lenox Globe, as transcribed by B.F. da Costa



Ewald Sphere: Single Scattering

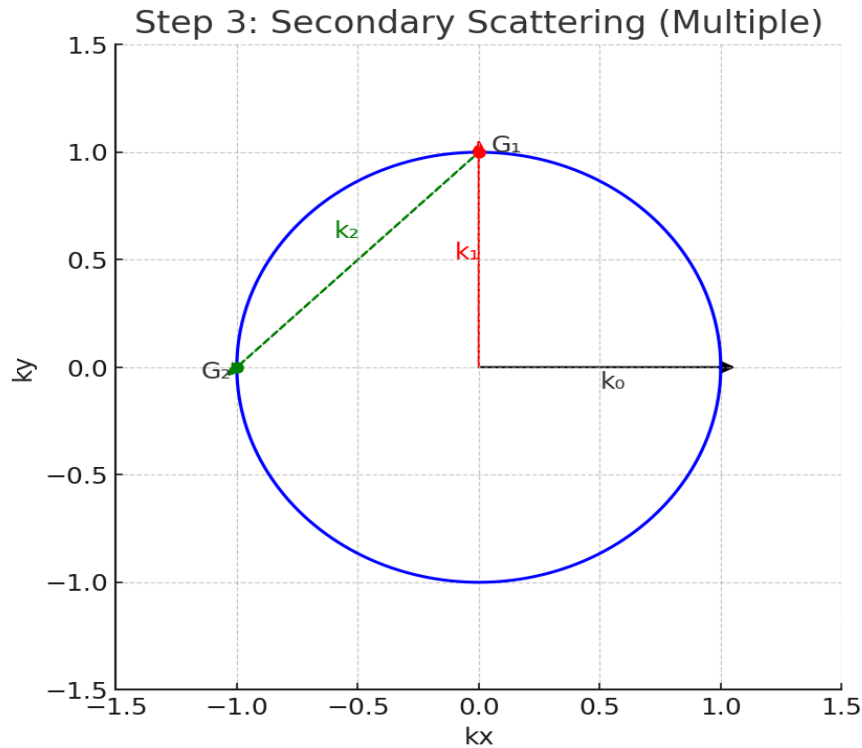


Ewald Sphere: Primary Scattering





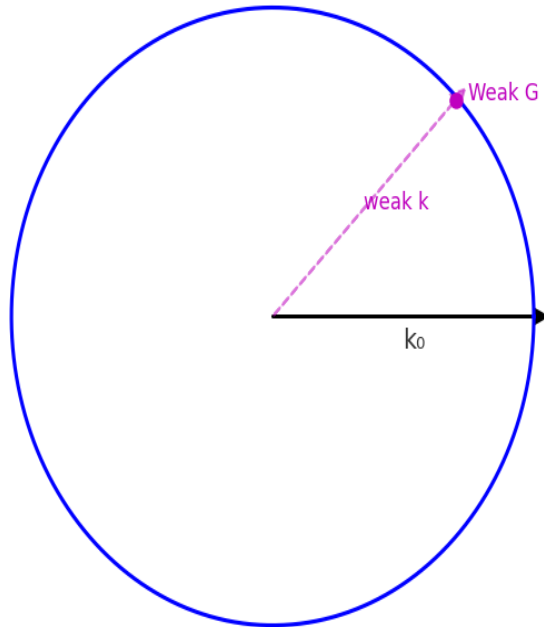
Ewald Sphere: Multiple Scattering (Secondary)



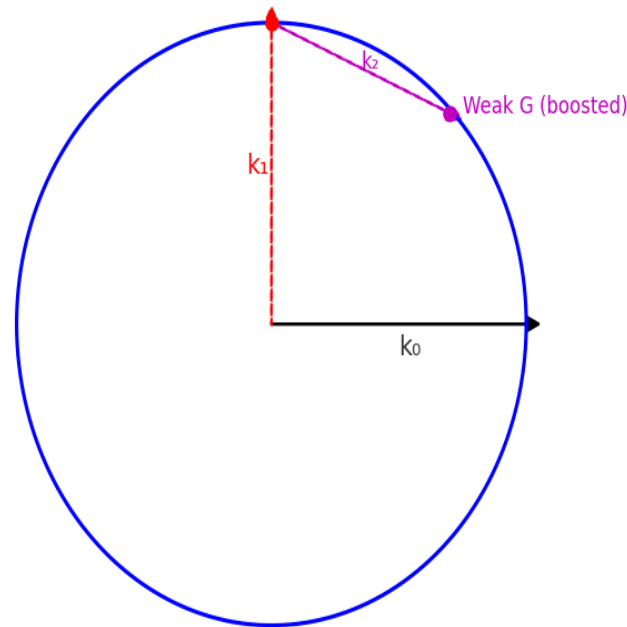


Multiple Scattering Boosting Weak Reflection

Normal Weak Reflection

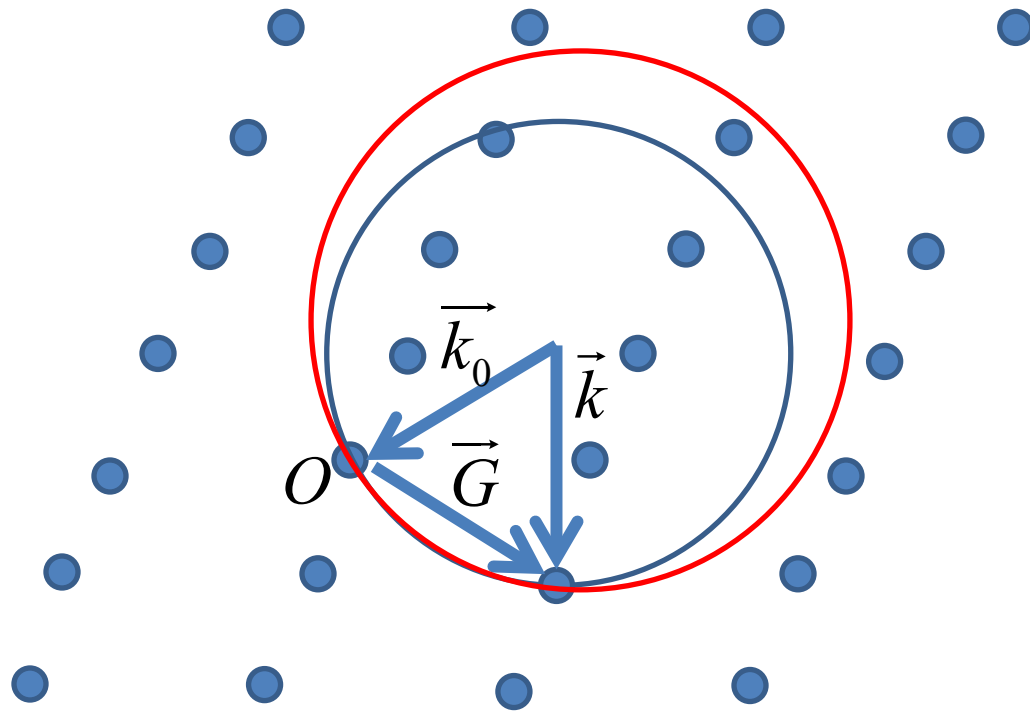


Weak Reflection Boosted by Multiple Scattering

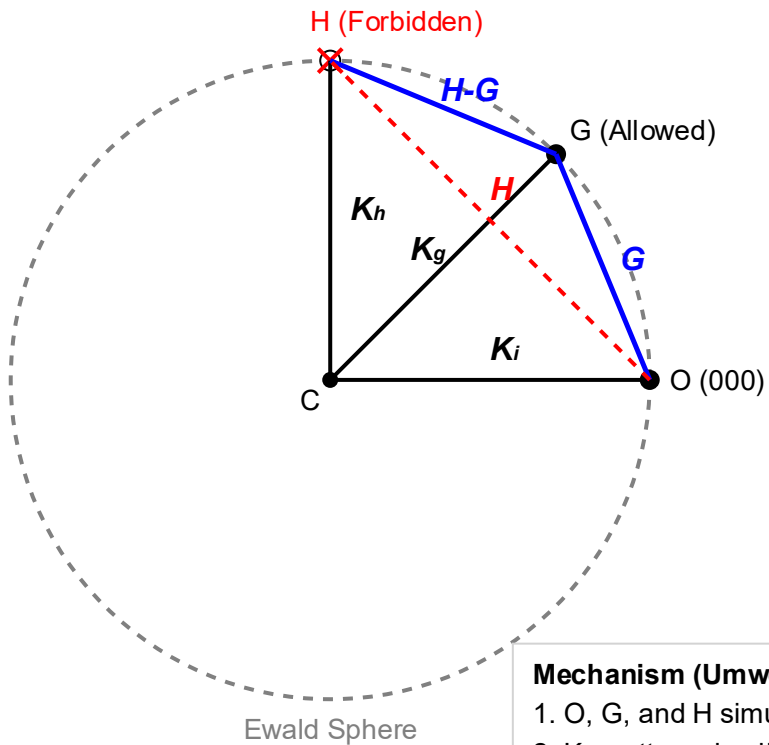




Ewald Sphere



Multiple Scattering Generating Intensity at a Forbidden Reflection



Mechanism (Umweganregung):

1. O, G, and H simultaneously lie on the Ewald sphere.
2. K_i scatters via allowed G, creating K_g .
3. K_g re-scatters via allowed H-G, creating K_h .

Result: $H = G + (H-G)$

The Renninger effect – an example and its implication

J. C. Speakman

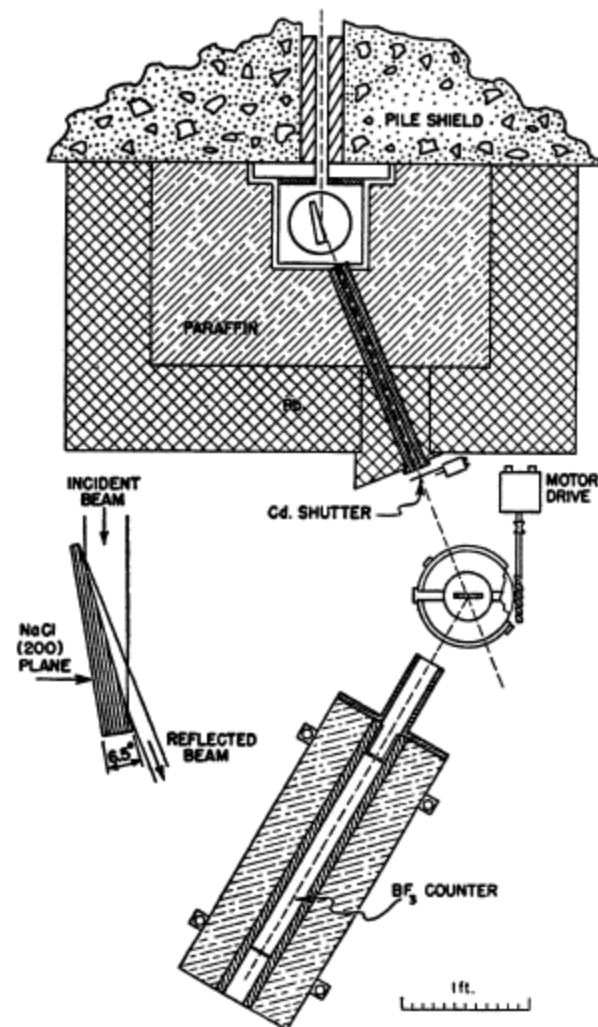
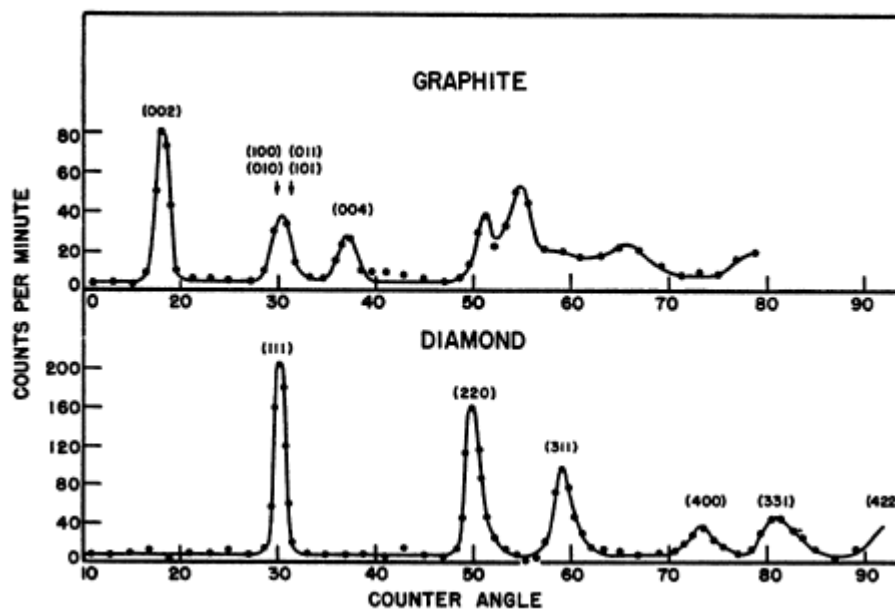
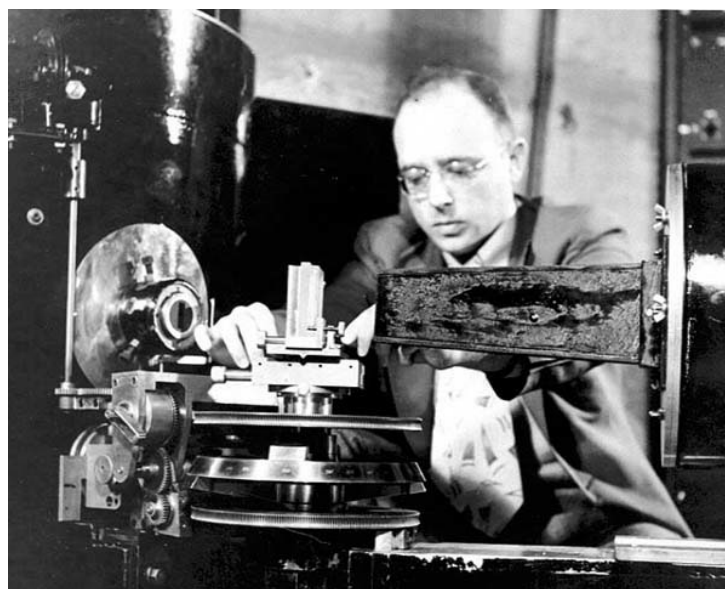
<https://doi.org/10.1107/S0365110X65001275>

The Diffraction of Neutrons by Crystalline Powders

E. O. WOLLAN AND C. G. SHULL

Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received January 5, 1948)





So...

- See scattering where reciprocal lattice point lies on Ewald Sphere
- But, whither magnetism???

1932, Néel predicts Antiferromagnetic order

Detection of Antiferromagnetism by Neutron Diffraction*

C. G. SHULL

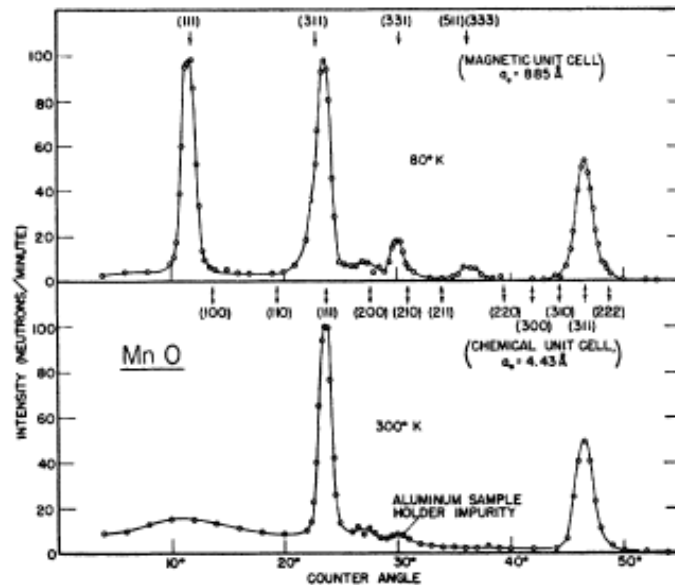
Oak Ridge National Laboratory, Oak Ridge, Tennessee

AND

J. SAMUEL SMART

Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland

August 29, 1949

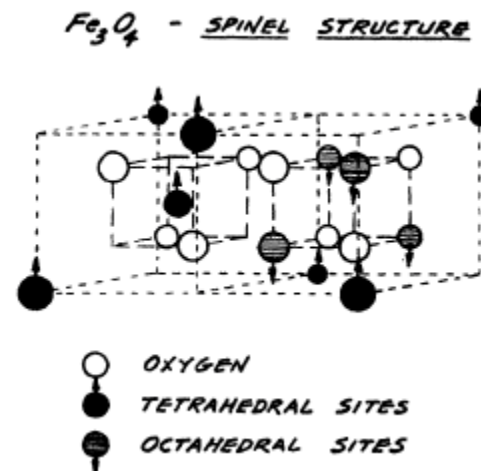


Magnetic Structure of Magnetite and Its Use in Studying the Neutron Magnetic Interaction

C. G. SHULL, E. O. WOLLAN, AND W. A. STRAUSSER

Oak Ridge National Laboratory, Oak Ridge, Tennessee

December 8, 1950





how**stuff**works
It's good to know

$$F(q) = \sum_i f_i e^{iq \cdot r_i}$$

$$I \propto |F|^2$$

sensitive to component of moment $\perp Q$



orthorhombic cell

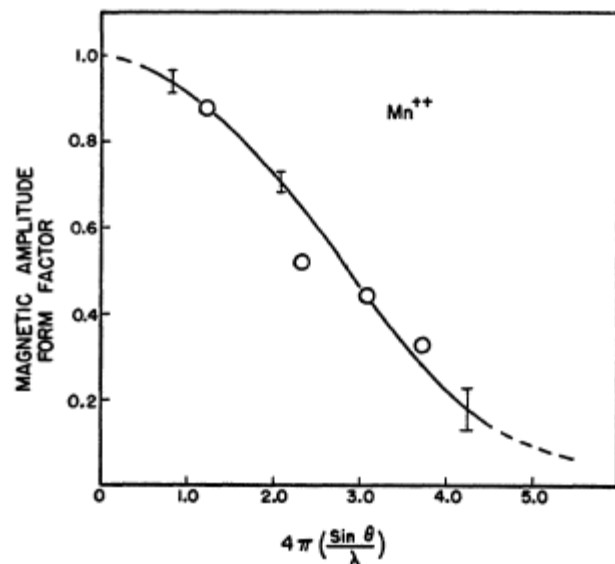
00L reflections?

H00 reflections

K00 ?

Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

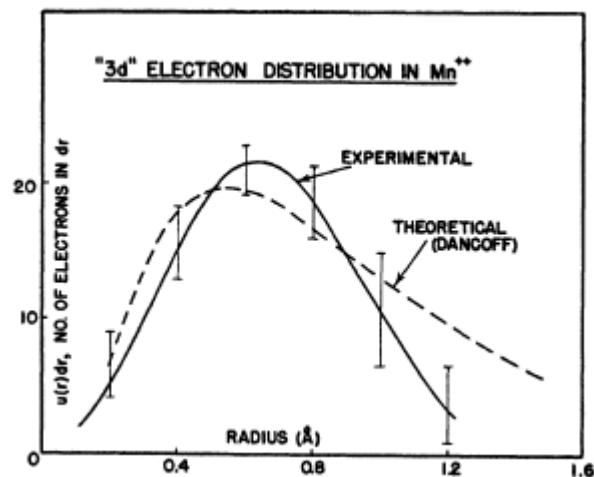
C. G. SHULL, W. A. STRAUSSER, AND E. O. WOLLAN
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received March 2, 1951)



$$d\sigma_m = \frac{2}{3} S(S+1) (e^2 \gamma / mc^2) f^2 d\Omega,$$



$$u(r) = (2r/\pi) \int_0^\infty k f(k) \sin kr dk$$



On the Magnetic Scattering of Neutrons

The direct experimental evidence of the neutron, obtained so far, indicates its mass and the range of forces within which it interacts with other heavy particles. The angular moments of nuclei make it practically sure that it has an angular momentum $\frac{1}{2}\hbar/2\pi$. Furthermore there are good theoretical reasons to believe that it should have a magnetic moment of the same order of magnitude as the measured moment of the proton but having the opposite direction with respect to the angular momentum; these conclusions are partly based on Fermi's theory of the β -decay, partly on the known magnetic moment of the deuteron. Since the Stern-Gerlach method may meet considerable difficulties when applied to neutron beams, we want to propose a different way of obtaining information about the magnetic moment of the neutron which seems considerably simpler and promising in several other respects.

Consider an atom (or molecule) which in its ground state has a total magnetic moment $\mathbf{u}$ caused by the spin or the orbital motion of the atomic electrons. The magnetic field around and within the atom can in any case be described by an average dipole density distribution $\mathbf{u}g(\mathbf{r})$ with $\int g(\mathbf{r})d\tau=1$. It will scatter neutrons on account of two reasons:

- (1) Because of the interaction of the neutron with the atomic nucleus (or nuclei);
- (2) Because of the inhomogeneous magnetic field in its surrounding acting on the magnetic moment of the neutron.

The reduction factor for the radiation of the nucleus as a whole depends on the adopted nuclear model and cannot easily be calculated. But it seems plausible that the total effect will be essentially the same as for two particles.

F. BLOCH

Stanford University,

G. GAMOW

George Washington University,
July 9, 1936

On the Magnetic Scattering of Neutrons

J. S. SCHWINGER

Columbia University, New York, N. Y.

(Received January 11, 1937)

The scattering of slow neutrons by atoms is considered, assuming that, in addition to the ordinary nuclear forces, there is a magnetic interaction between the neutron and the atomic electrons. It is found that the neutrons scattered from an unpolarized beam will be partially polarized in virtue of this magnetic interaction. Since the scattered intensity depends not only upon the intensity, but also upon the spin density of the incident beam, the polarization thus produced can manifest itself by a second scattering. An expression is derived for the neutron intensity after double scattering from magnetized iron plates. Under

optimum conditions, it is found that the scattered intensity with parallel orientation of magnetizations is 15 times that with antiparallel orientation. The partial polarization of the scattered neutrons indicates that the undeviated neutron beam will also have a nonvanishing spin density. Expressions are derived for the intensity and spin density of a neutron beam after traversing a certain thickness of magnetized iron. These results are used in the discussion of three types of experiments for producing and detecting a polarized beam of neutrons.

Magnetic Interaction between Neutrons and Electrons*

H. EKSTEIN

Armour Research Foundation, Chicago, Illinois

(Received July 11, 1949)

The phenomenological interaction operator between neutrons and electrons is usually assumed to be $-\mu\mathbf{s}\cdot\mathbf{B}$. ($\mu\mathbf{s}$ magnetic moment of the neutron, $\mathbf{B}$ magnetic field of the electrons.) Bloch has pointed out that other operators are possible. It is shown that the class of operators considered by Bloch is equivalent with the form $-\mu\mathbf{s}\cdot(\mathbf{H}+4\pi C\mathbf{M})$ where $\mathbf{M}$ is the spin momentum density of the electrons, $\mathbf{H}=\mathbf{B}-4\pi\mathbf{M}$ and C is an indeterminate constant. Diffraction by ferromagnetic crystals and magnetic double refraction are calculated for this interaction. Present experimental evidence excludes the value $C=0$. Experimental methods for measuring C are discussed.

Neutron Scattering and Polarization by Ferromagnetic Materials

C. G. SHULL, E. O. WOLLAN, AND W. C. KOEHLER
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received August 20, 1951)

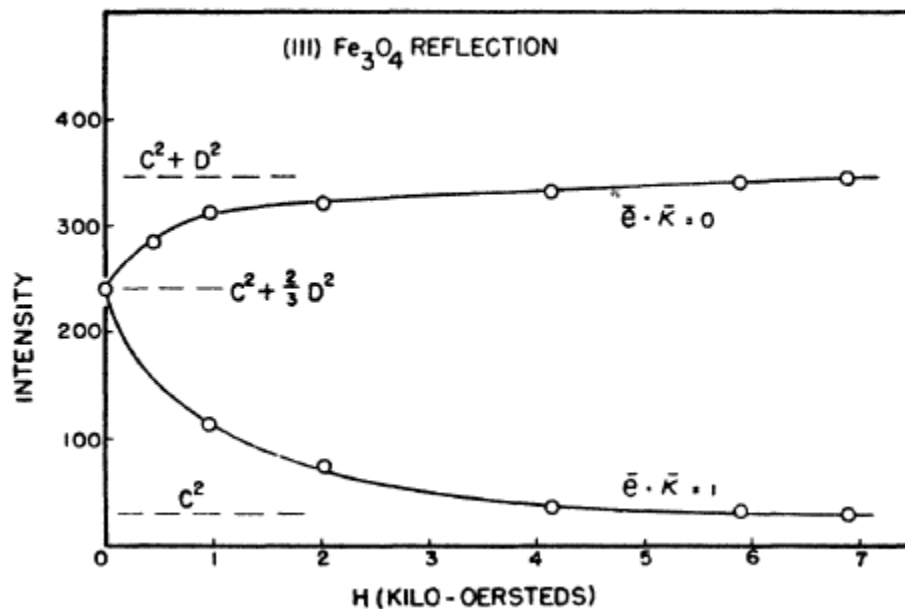
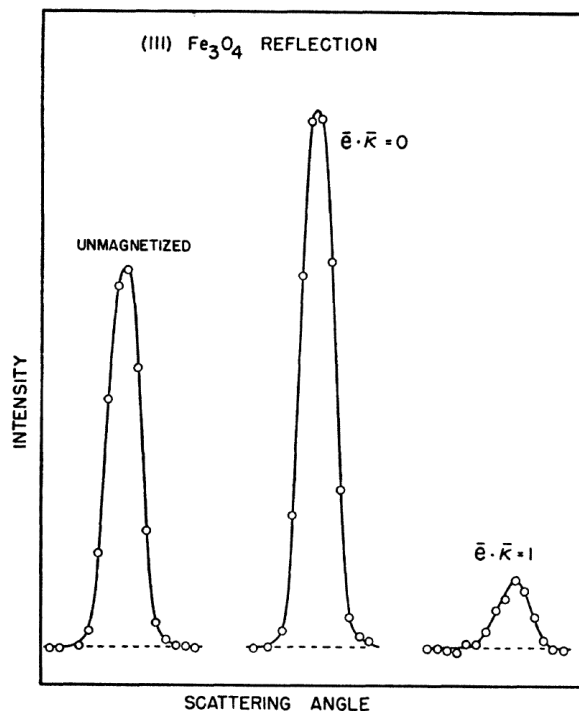
$$F^2 = C^2 + 2CD\mathbf{q} \cdot \boldsymbol{\kappa} + D^2q^2$$

$$\mathbf{q} = \mathbf{e}(\mathbf{e} \cdot \boldsymbol{\kappa}) - \boldsymbol{\kappa} \quad \text{and} \quad q^2 = 1 - (\mathbf{e} \cdot \boldsymbol{\kappa})^2$$

$$D = (e^2/mc^2)\gamma Sf = 0.539 \times 10^{-12} Sf \text{ cm}$$

where $\mathbf{e}$ is the unit scattering vector and $\boldsymbol{\kappa}$ a unit vector parallel to the magnetic moment vector of the magnetic ion. The magnetic scattering amplitude D is given by

$$\mathbf{q}_0 = \mathbf{e}(\mathbf{e} \cdot \boldsymbol{\kappa})$$



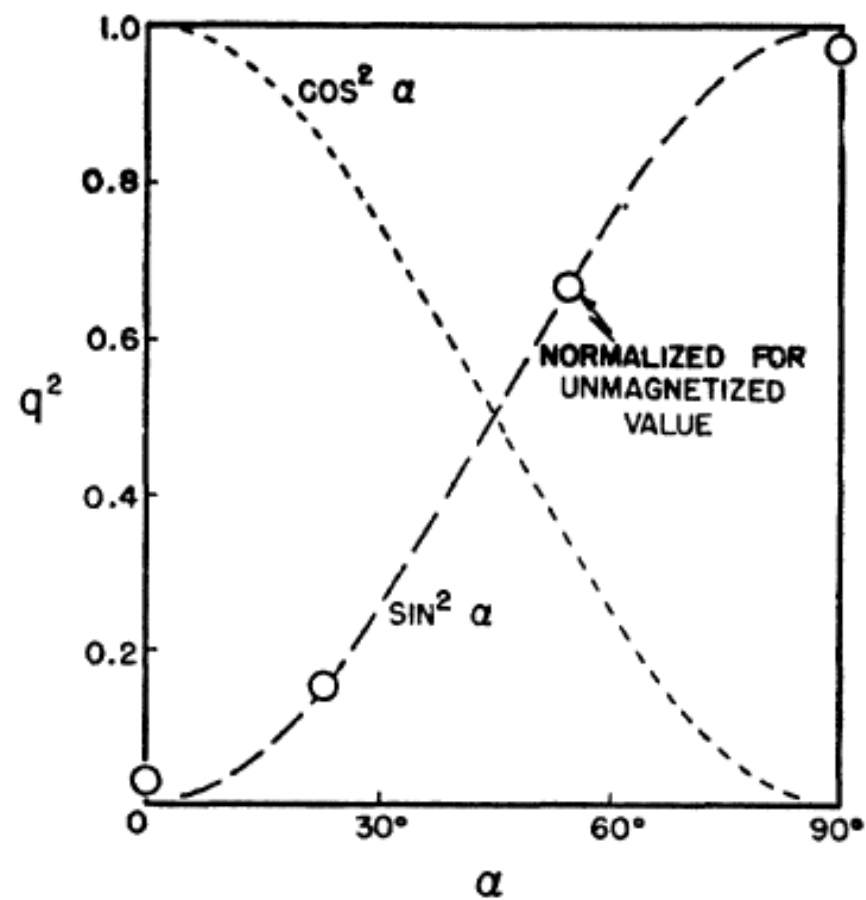


FIG. 10. Variation of q^2 with the angle α between the and scattering vectors.

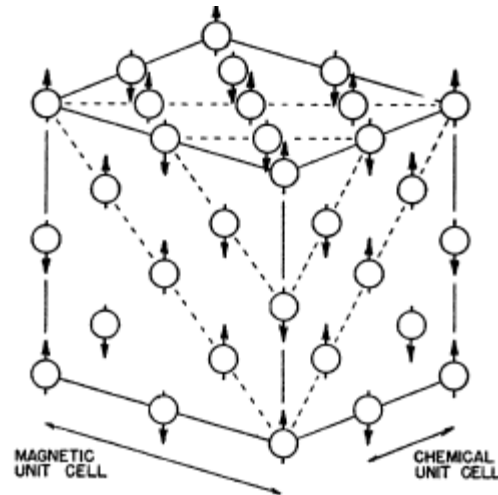
(a) The magnetic moments are aligned along arbitrary $[100]$ directions, in other words, along the cube axes, as illustrated in Fig. 5. For this case it can be shown that q^2 (average) = $\frac{2}{3}$ for each of the four observed magnetic reflections in MnO.

(b) The magnetic moments are aligned perpendicular to the ferromagnetic (111) sheets. For this case, q^2 vanishes for the (111) reflection and becomes $32/33$ for the (311) and $32/57$ for the (331) reflections.

(c) The magnetic moments are aligned arbitrarily in the ferromagnetic (111) sheets. Here q^2 should be 1 for the (111) reflection and various odd values for the other reflections, depending upon the assignment of moment orientation within the sheet.

TABLE II. Comparison between observed MnO antiferromagnetic intensities and those calculated for various models of magnetic orientation with respect to crystallographic axes.

	Calculated for various oriented models			Observed (neutrons/min)
	(a)	(b)	(c)	
(111)	1038	0	1560	1072
(311)	460	675	...	308
(331)	129	109	...	132
(511) (333)}	54	24	...	70

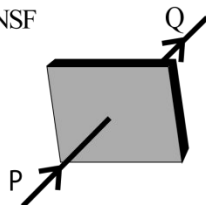


Neutron Scattering and Polarization by Ferromagnetic Materials

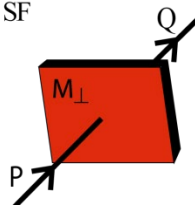
C. G. SHULL, E. O. WOLLAN, AND W. C. KOEHLER
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received August 20, 1951)

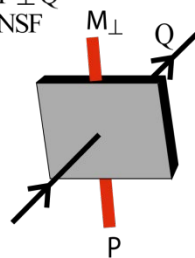
(a) $P \parallel Q$
NSF



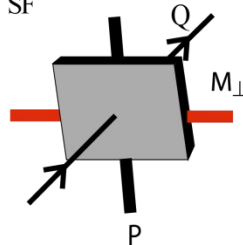
(b) $P \parallel Q$
SF



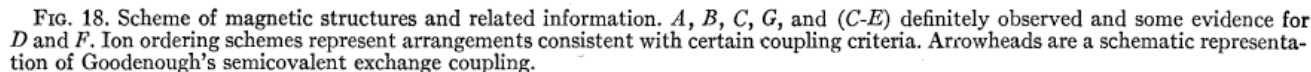
(c) $P \perp Q$
NSF



(d) $P \perp Q$
SF



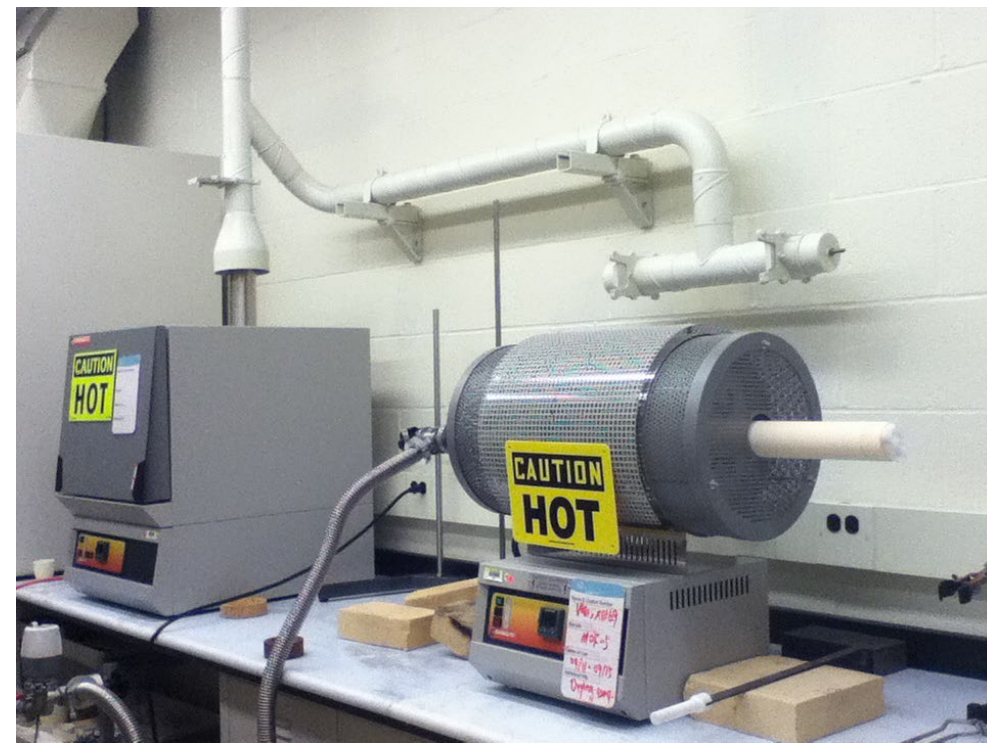
E. O. WOLLAN AND W. C. KOEHLER
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received May 9, 1955)



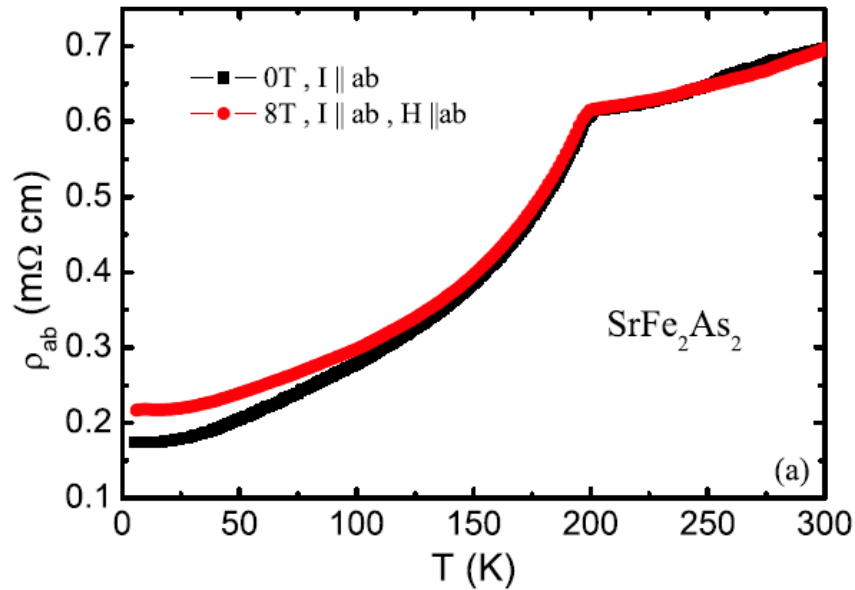
Intermission



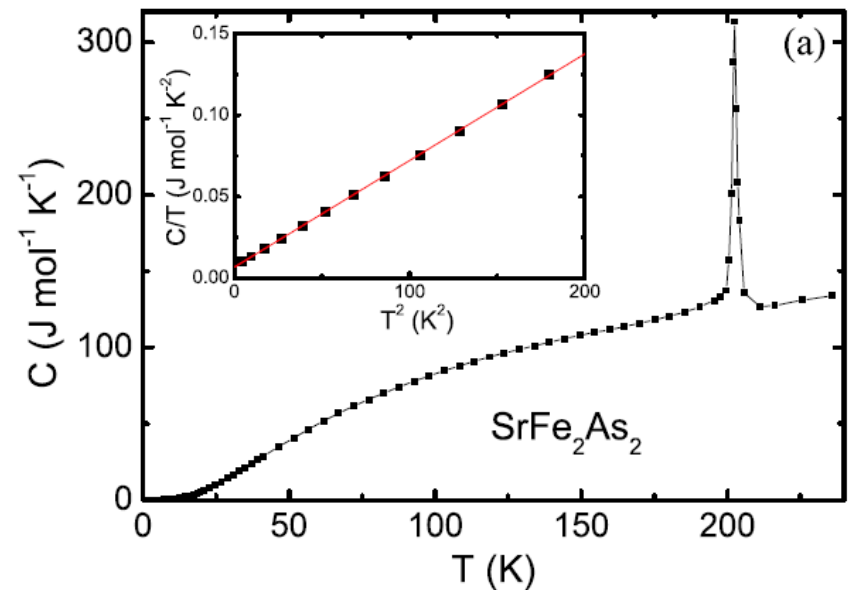
How it starts?



Bulk Data Comes In

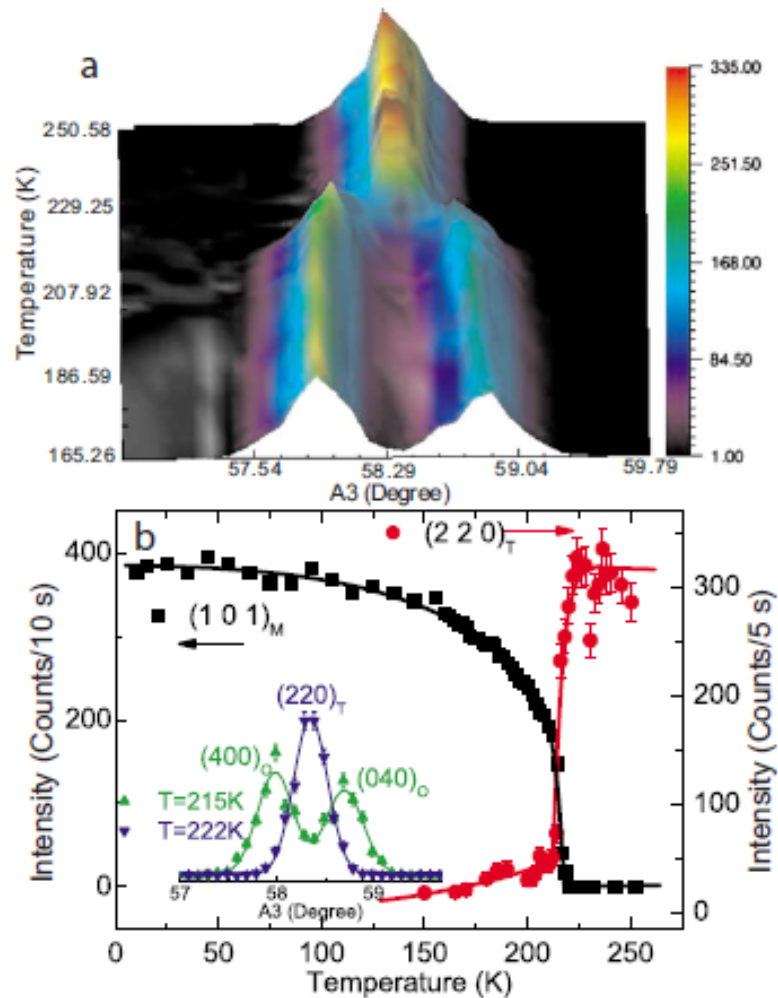


Physical Review B **78**, 22514 (2008)



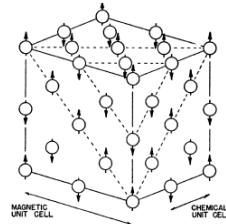


Neutrons to the Rescue



Physical Review B **78**, 140504 (2008)

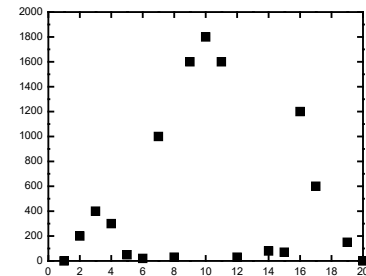
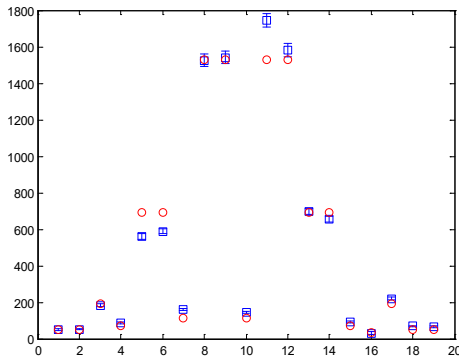
Guess and Check (Refinement)



Update model

Predict Intensities from model

Compare predicted intensities to data



Choices

Goodness of Fit

$$\chi^2 = \sum_1^n w_i (y_i - y_{ci}(\alpha))^2 \qquad w_i = \frac{1}{\sigma_i^2}$$

or

$$R_{wp} = 100 \left(\frac{\sum_1^n w_i (y_i - y_{ci}(\alpha))^2}{\sum_1^n w_i (y_i)^2} \right)^{\frac{1}{2}}$$

Optimization Approaches

Simulated Annealing

Marquardt-Levenberg

Genetic Algorithm

Markov Chain Monte Carlo



How I proceed

- Think about the problem
- Powder diffraction
- Think some more
- Try Representational Analysis (or Group theory)
- Single crystal diffraction
- Think a lot!!!
- Polarized diffraction
- Spherical polarimetry
- Think some more...

Y_{Mn}₂O₅

PRL 96, 097601 (2006)

PHYSICAL REVIEW LETTERS

week ending
10 MARCH 2006

Ferroelectricity Induced by Acentric Spin-Density Waves in Y_{Mn}₂O₅

L. C. Chapon,¹ P. G. Radaelli,^{1,2} G. R. Blake,^{1,3} S. Park,⁴ and S.-W. Cheong⁴

Powder

Journal of the Physical Society of Japan
Vol. 76, No. 7, July, 2007, 074706
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Spiral Spin Structure in the Commensurate Magnetic Phase of Multiferroic RMn₂O₅

Hiroyuki KIMURA*, Satoru KOBAYASHI¹, Yoshikazu FUKUDA, Toshihiro OSAWA,
Youichi KAMADA, Yukio NODA, Isao KAGOMIYA², and Kay KOHN³

x_{tal}

PHYSICAL REVIEW B 78, 245115 (2008)

Spiral spin structures and origin of the magnetoelectric coupling in Y_{Mn}₂O₅

J.-H. Kim,¹ S.-H. Lee,^{1,*} S. I. Park,² M. Kenzelmann,³ A. B. Harris,⁴ J. Schefer,³ J.-H. Chung,⁵ C. F. Majkrzak,⁶
M. Takeda,⁷ S. Wakimoto,⁷ S. Y. Park,⁸ S.-W. Cheong,⁸ M. Matsuda,⁷ H. Kimura,⁹ Y. Noda,⁹ and K. Kakurai⁷

X_{tal}+spherical polarimetry

PHYSICAL REVIEW B 79, 020404(R) (2009)

Incommensurate magnetic structure of Y_{Mn}₂O₅: A stringent test of the multiferroic mechanism

P. G. Radaelli,^{1,2} C. Vecchini,^{1,3} L. C. Chapon,¹ P. J. Brown,⁴ S. Park,⁵ and S.-W. Cheong⁵

X_{tal}+more representation analysis

Powder Diffraction

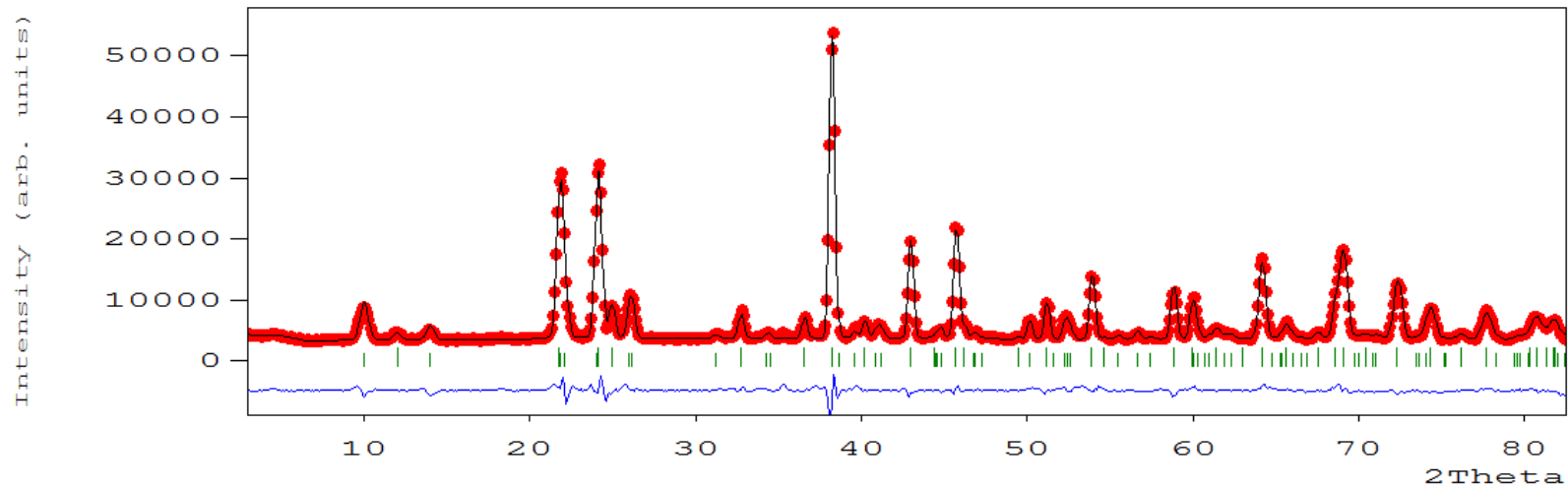
Advantages

- You get the big picture
- Can get the propagation vector
- Avoids the muss and fuss of extinction
- It's often Good Enough™

Disadvantages

- Can be hard to truly index k — is it $[3\ 4\ 0]$ or $[0\ 0\ 5]$?
- You average over all symmetry equivalent k at any particular Bragg angle
- You lose information in the powder averaging
- No domain info
- No multi- k info
- Can be very hard to determine phase

Cycle: 2 Chi2: 18.2 dy.dat



Single Crystal Diffraction

Advantages

- Can fully determine $\mathbf{k}$
- Can investigate domain populations
- Can apply probes (magnetic field, E-field, pressure, etc.) along a particular direction to see effect on magnetic ordering

Disadvantages

- Extinction
- Absorption depends on shape
- Reciprocal space is large...
- Crystal growth is hard...

TOOLS OF THE TRADE

FOR MAGNETIC NEUTRON SCATTERING



Version Control for Powder Refinement

Using **TortoiseGit** to track your **FullProf** (.pcr) refinements

Why? Every fit iteration changes your **.pcr**. Git snapshots each step so you can compare R-factors, roll back a diverged model, and share the exact input that produced a plot.

1 Create the repo

Put your **.pcr**, **.dat**, **.hkl**, **.cif** in one project folder.
Right-click folder → **Git Create repository here**.

2 First commit

Right-click → **Git Commit** → **"master"**.
Stage the input files;
write "Initial model" and commit.

3 Refine & re-commit

Run FullProf, tweak parameters. After each good cycle, Commit with a message: "Released B-iso".

4 Compare & revert

Right-click → TortoiseGit → Show Log to diff .pcr versions & Rp/Rwp. Revert to any earlier snapshot.

Key menu commands (right-click any file/folder)

Git Commit snapshot • **Show Log** history/diff • **Revert** undo edits • **Create Branch** try a model • **Push** backup to remote

Tip: Commit the **.pcr** inputs — not the large **.prf/.out** outputs. Add a **.gitignore** so your repo stays small and diffs stay readable.

Seeing What Changed

Use **WinMerge** to diff two **.pcr** files side-by-side — pair it with TortoiseGit as your visual diff tool

Why? .pcr files are dense text. WinMerge highlights every line that moved — a released parameter, a new phase, a changed background — so you can **see exactly what you did** between two refinement cycles.

A. Compare two files directly

- Select **model_v1.pcr** and **model_v2.pcr**
- Right-click → **WinMerge**
- Or drag both onto the WinMerge window

B. Wire it into TortoiseGit

TortoiseGit → **Settings** → **Diff Viewer**

Set external diff to:

WinMergeU.exe /e /u /wl %base %mine

Now **Show Log** → **Compare** opens

each committed .pcr version in WinMerge.

WinMerge — model_v1.pcr ↔ model_v2.pcr

v1 (before)	v2 (after)
!Nph Dum las ...	!Nph Dum las ...
Bkg 145.2 -22.1	Bkg 145.2 -22.1
a 5.4021	a 5.4038
Biso 0.50 0.00	Biso 0.63 21.00
!	Occ 0.98 41.00
U 0.021 0.00	U 0.021 0.00
Rp 8.41 Rwp 11.2	Rp 6.02 Rwp 8.1

Tip: Yellow = changed value, green = new line. Watch **Rwp** drop as you release parameters — the diff tells you which change earned it.

Ask the Manual, Don't Scroll It

Use **Google NotebookLM** to ask questions of the **FullProf manual** while reading **dyc.pcr**

Why? NotebookLM (Google's AI research notebook) answers **only from the sources you upload** — and cites the page. No hallucinated keywords: every answer links back to the FullProf PDF.

1

Create a notebook & add sources

Go to notebooklm.google.com. Click New → Add sources. Upload the FullProf manual PDF, the .pcr manual, and the release-notes / What's New file.

2

Ask in plain English

"In dyc.pcr, what does $J_{bt} = 10$ mean for the nuclear phase?" • "How is the propagation vector $k=(0,0,0.165)$ entered for the magnetic phase?"

3

Follow the citations

Each answer shows numbered citations — click to jump to the exact manual page. Save good answers as Notes; generate an Audio Overview.

FullProf Notebook · 3 sources

FullProf_Manual.pdf

Release_notes.txt

dyc.pcr

In dyc.pcr, what does $J_{bt} = 10$ mean for phase 1, and how is the propagation vector for the magnetic phase set?

Phase 1 uses **$J_{bt} = 10$** → a magnetic phase described by real spherical components (Rx,Ry,Rz) [1].

The magnetic phase 2 lists its k-vector under Propagation vectors: **$k = (0, 0, 0.1651)$** [2].

Sources: [1] Manual §Jbt codes [2] dyc.pcr

Tip: Upload **dyc.pcr** alongside the manual — answers are grounded **only** in your sources, so click each citation to confirm against the real page.

Questions?