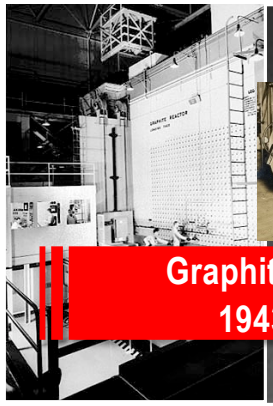
Magnetic structure determination with GSAS-II

Date: June 5, 2023
Location: ORNL, SNS. Building 8600. Room C-156.

This 1-day workshop will provide hands-on training and lectures on how to determine magnetic structures from powder and single-crystal neutron data using GSAS-II.

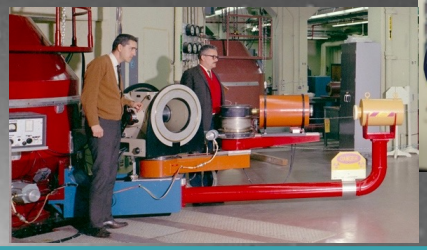
Examples from related, but weeklong, past workshops can be found here. But this year we will only use GSAS-II.

Time	Event	Presenter
8:30 – 9am	Welcome and Introductory remarks on Diffraction at ORNL	Bryan Chakoumakos
9–9:30am	Experimental aspects of Magnetic Structure Determination and Magnetic Space Groups	Stuart Calder
9:30–10:00am	A hierarchy of magnetic structures based on lattice dimensionality	Ovidiu Garlea
10:00–10:15am	*Break*	
10:15–11:05am	Introduction to GSAS-II	Brian Toby
11:05–12:00	Introduction to Magnetism in GSAS-II	Bob von Dreele
12:00–1:00pm	*Working Lunch: Diffraction instruments at SNS/HFIR*	Clarina dela Cruz
1–3pm	Hands-on Example of GSAS-II refinement of magnetic structure from Constant Wavelength Powder Diffraction Data	Keith Taddei
3-3:15pm	*Break*	
3:15-5:15pm	Hands-on Example of GSAS-II refinement of magnetic structure from TOF Powder Diffraction Data	Qiang Zhang
5:15-5:45pm	Current status of GSAS-II refinement of magnetic structure on Single Crystal Data	Yan Wu
5:45-6pm	Summary discussion. Bring your own magnetic structure data. Poster Set-up.	Everyone
6.00pm	Dinner and Poster Session in lobby of 8600	Everyone



Graphite Reactor
1943-1963

Oak Ridge Research Reactor
1958-1987



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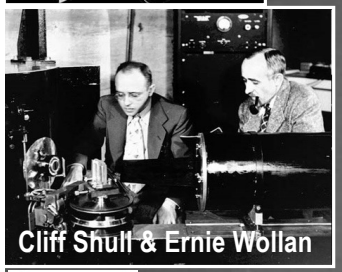
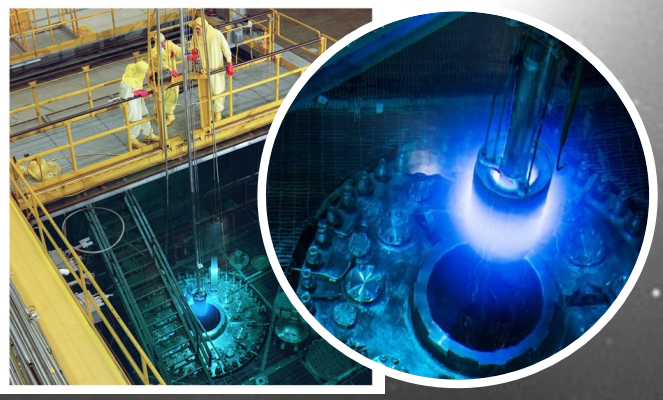


61 144.913
Pm
Promethium
[Xe] 4f^{5}6s^2
Lanthanides

High Flux Isotope Reactor
1966-present

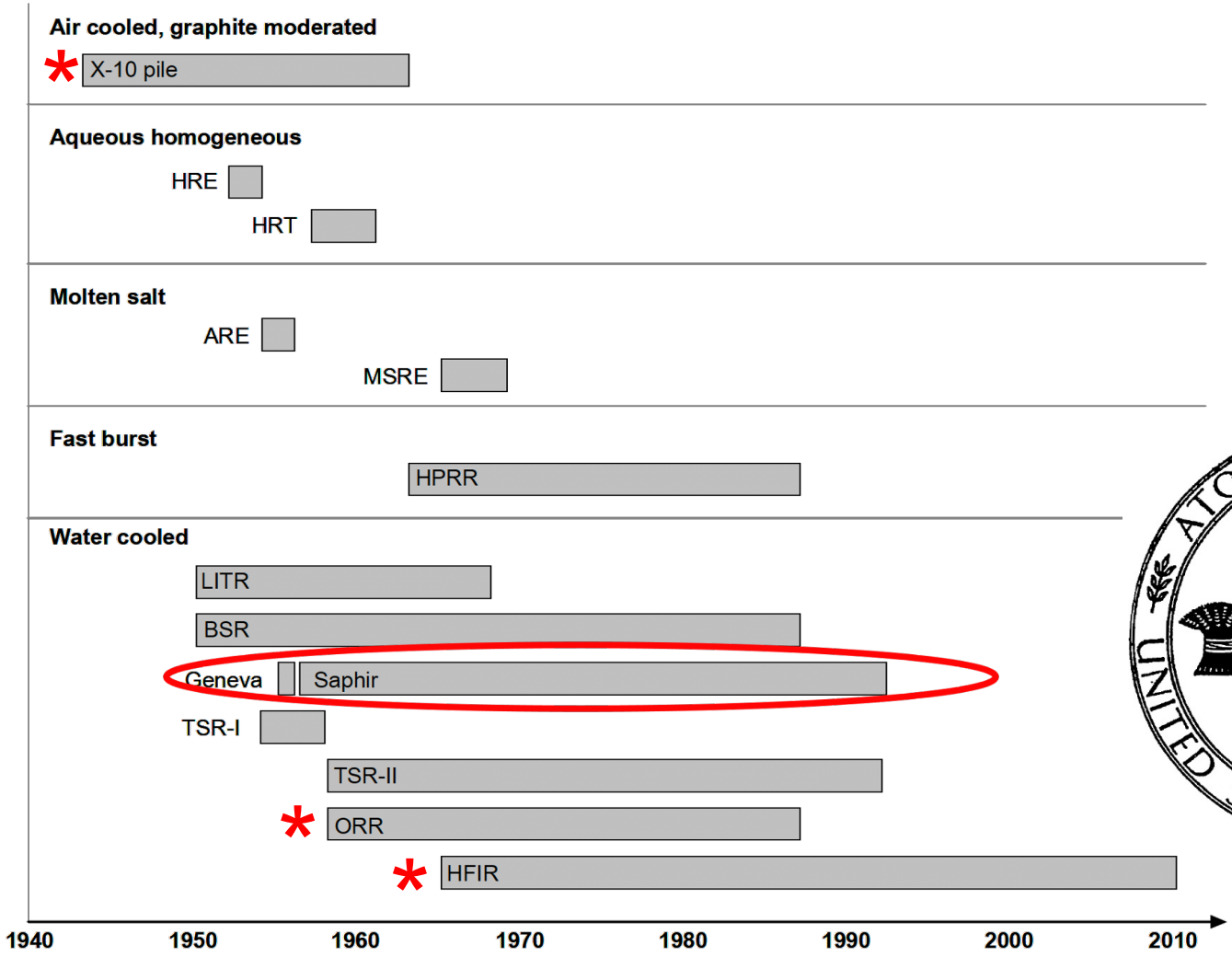
Cold Source
2007-present



Spallation
Neutron
Source
2007 -
present

Timeline of Neutron Sources* at ORNL

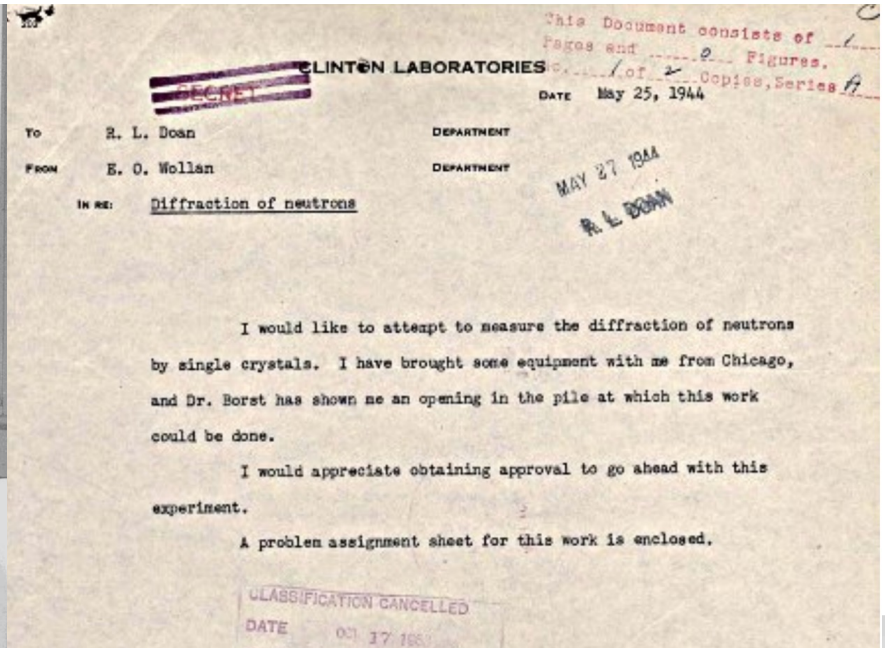
Timelines of ORNL Nuclear Reactors (from criticality to shutdown)



13 in total

Rosenthal (2010)

OAK RIDGE National Laboratory



This Document consists of 1 Pages and 2 Figures.
Copy 1 of 2 Copies, Series A

SECRET

CLINTON LABORATORIES

DATE May 25, 1944

TO R. L. Doan DEPARTMENT

FROM E. O. Wollan DEPARTMENT

IN RE: Diffraction of neutrons

MAY 27 1944
R. L. DOAN

I would like to attempt to measure the diffraction of neutrons by single crystals. I have brought some equipment with me from Chicago, and Dr. Borst has shown me an opening in the pile at which this work could be done.

I would appreciate obtaining approval to go ahead with this experiment.

A problem assignment sheet for this work is enclosed.

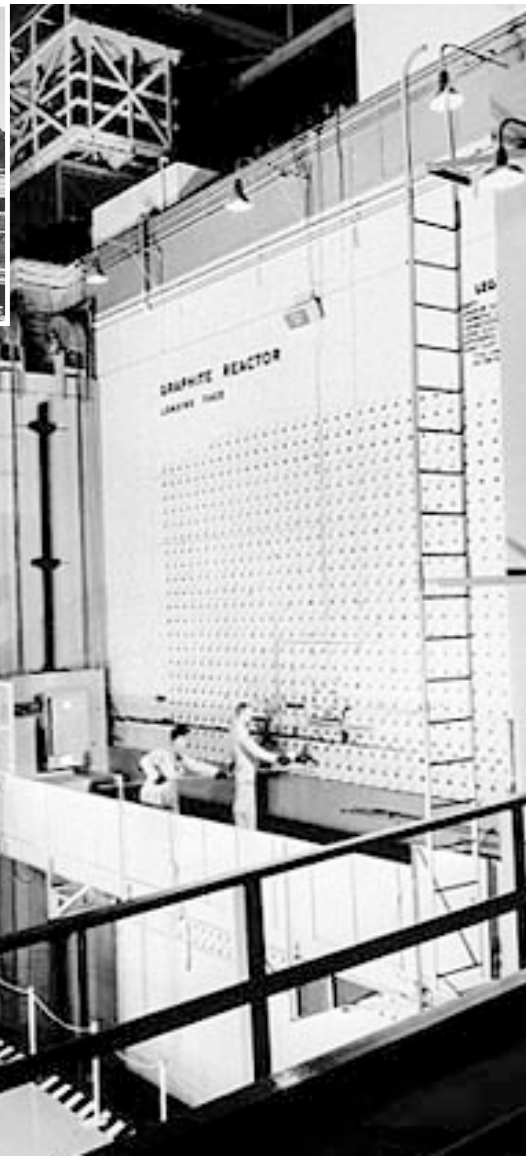
CLASSIFICATION CANCELLED
DATE OCT 17 1951

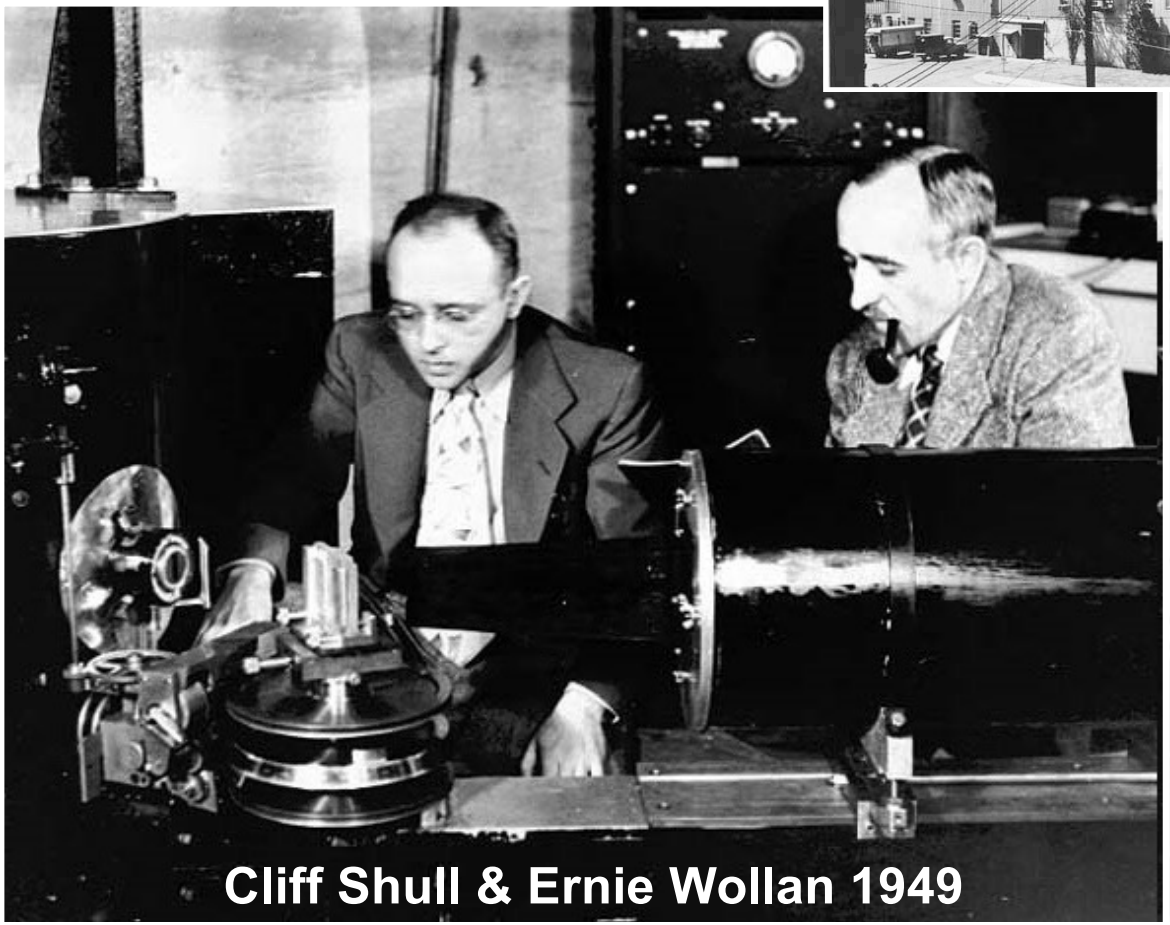
The original letter Ernest Wollan wrote in May 25, 1944 to Richard Doan, Director of Research at Clinton Laboratories, requesting approval to do neutron experiments at the X-10 pile.

"I would like to attempt to measure the diffraction of neutrons by single crystals. I have brought some equipment with me from Chicago and Dr. Borst has shown me an opening in the pile at which this work could be done.

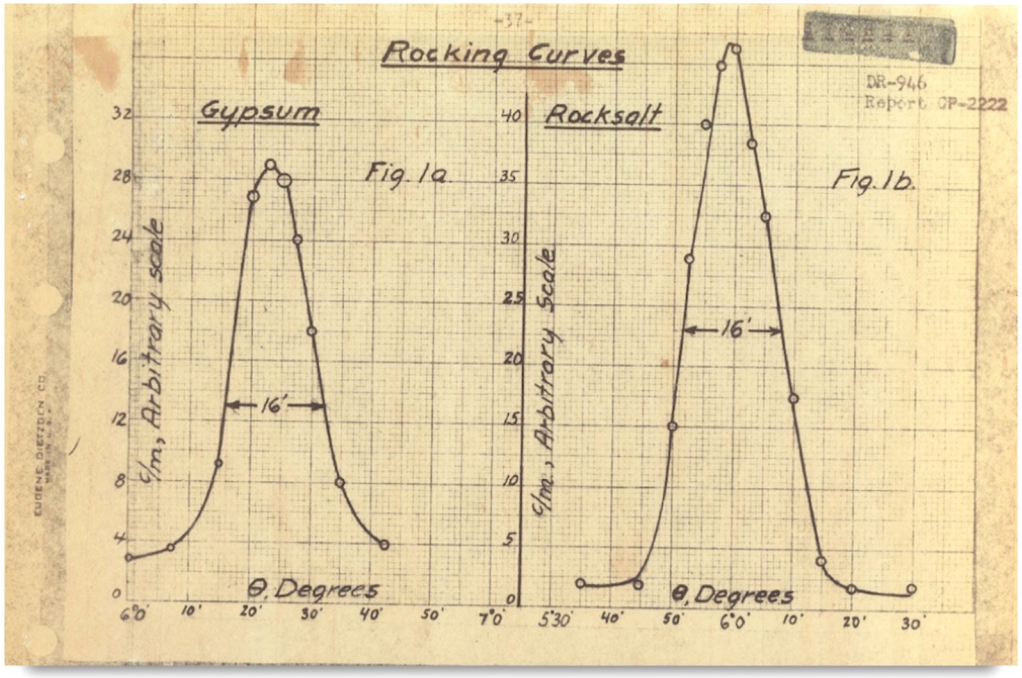
I would appreciate obtaining approval to go ahead with this experiment."

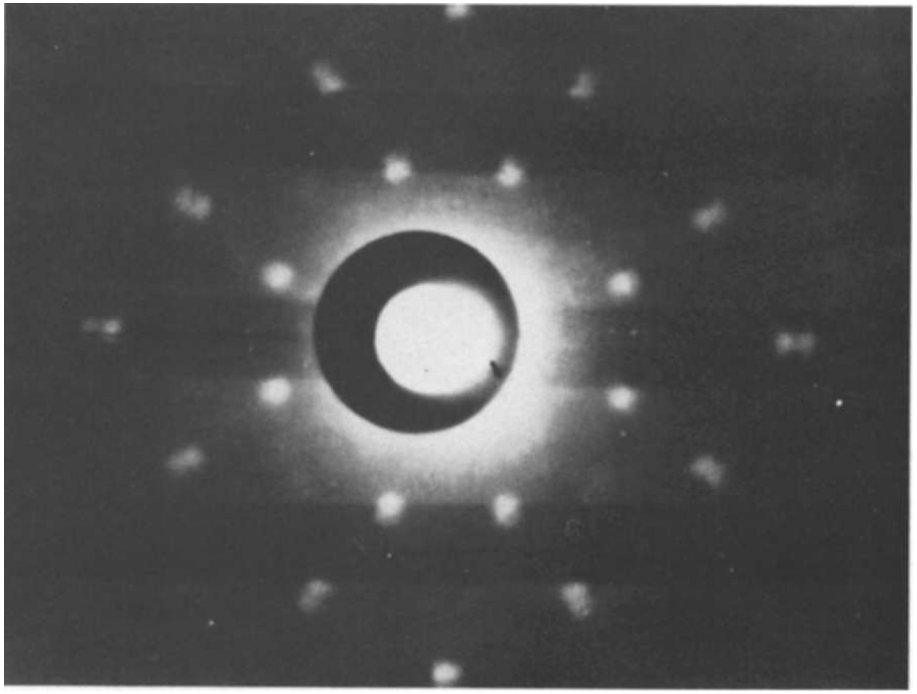
ORNL Graphite Reactor
1943-1963





Cliff Shull & Ernie Wollan 1949



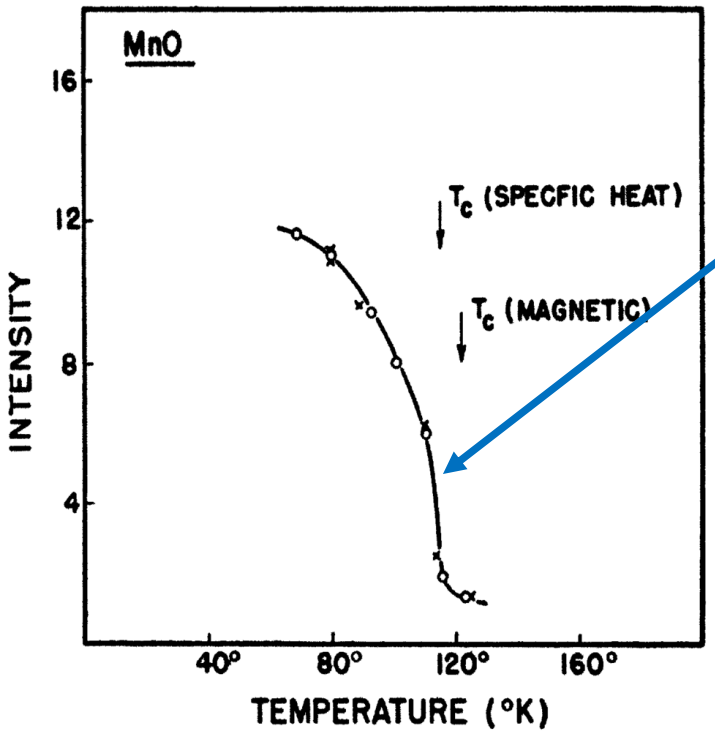


Observation of Bragg reflections via neutron diffraction by Wollan in December 1944 at the Graphite Reactor.

The first neutron Laue diffraction pattern of NaCl measured by Wollan, Shull, and Marney in 1947 at the Graphite Reactor.

Detection of Antiferromagnetism by Neutron Diffraction*

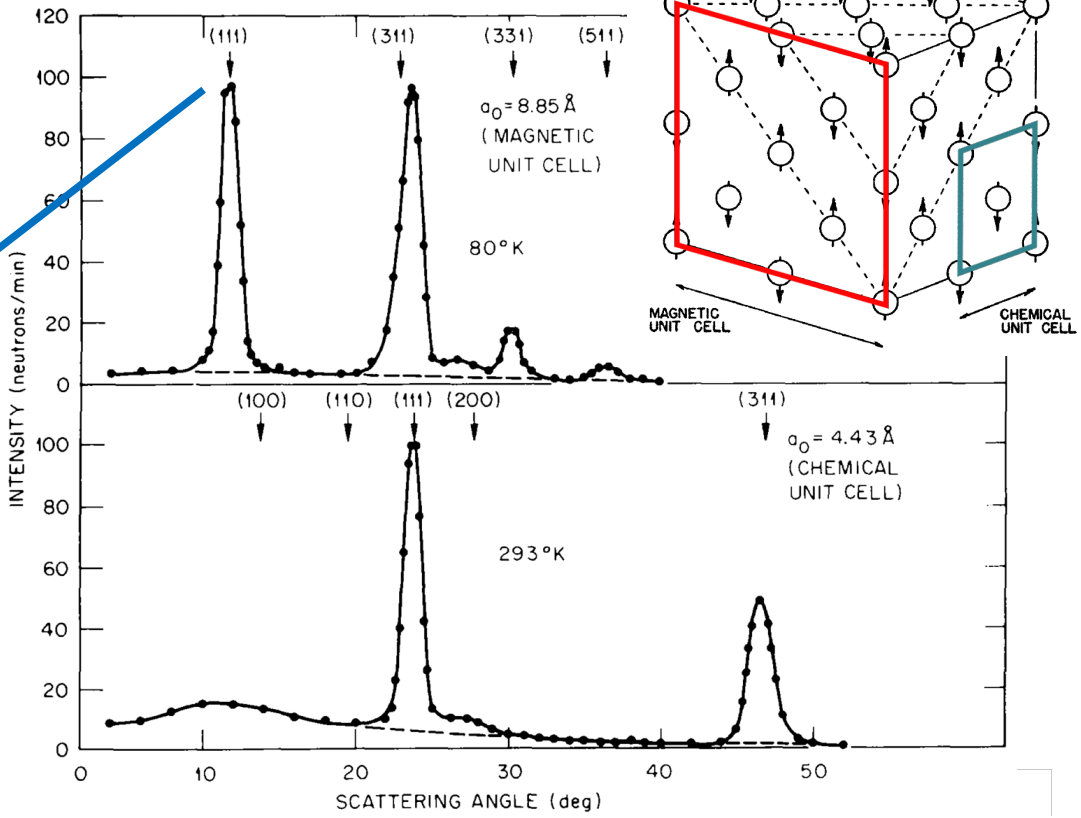
C. G. Shull
Oak Ridge National Laboratory, Oak Ridge, Tennessee
AND
J. Samuel Smart
Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland
August 29, 1949
***Physical Review* 76 (1949) 1256**



Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

C. G. Shull, W. A. Strauser, and E. O. Wollan
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received March 2, 1951)
***Physical Review 83* (1951) 1256**

MnO



OAK RIDGE National Laboratory

PHYSICAL REVIEW VOLUME 100, NUMBER 2 OCTOBER 15, 1955

Neutron Diffraction Study of the Magnetic Properties of the Series of Perovskite-Type Compounds $[(1-x)\mathrm{La}, x\mathrm{Ca}]\mathrm{MnO}_3$†

E. O. Wollan and W. C. Koehler
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received May 9, 1955)

In Web of Science Core Collection

2,329
Citations

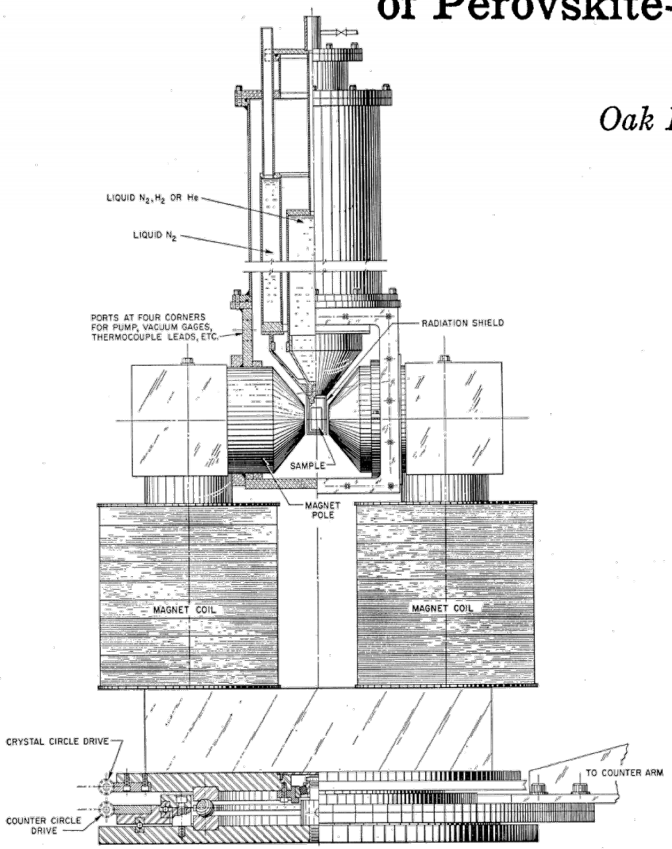
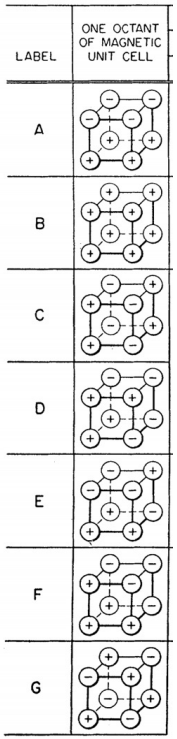
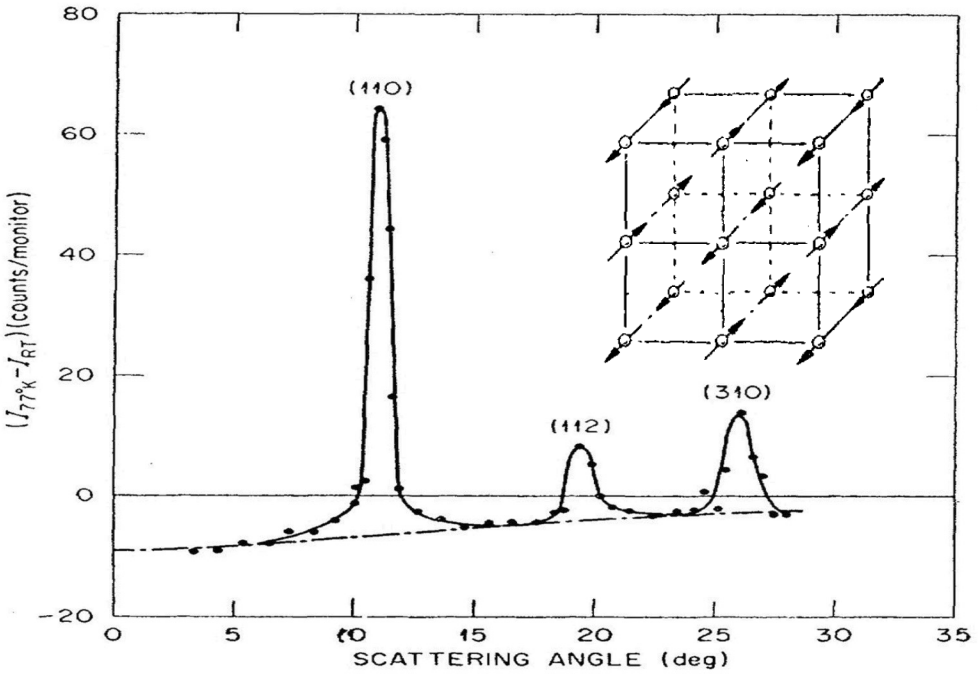


FIG. 1. Neutron spectrometer with cryostat and magnet.





OAK RIDGE National Laboratory

Clifford Shull – selected honors and awards received

Nobel Prize in Physics, 1994

Gregori Aminoff Prize, 1993

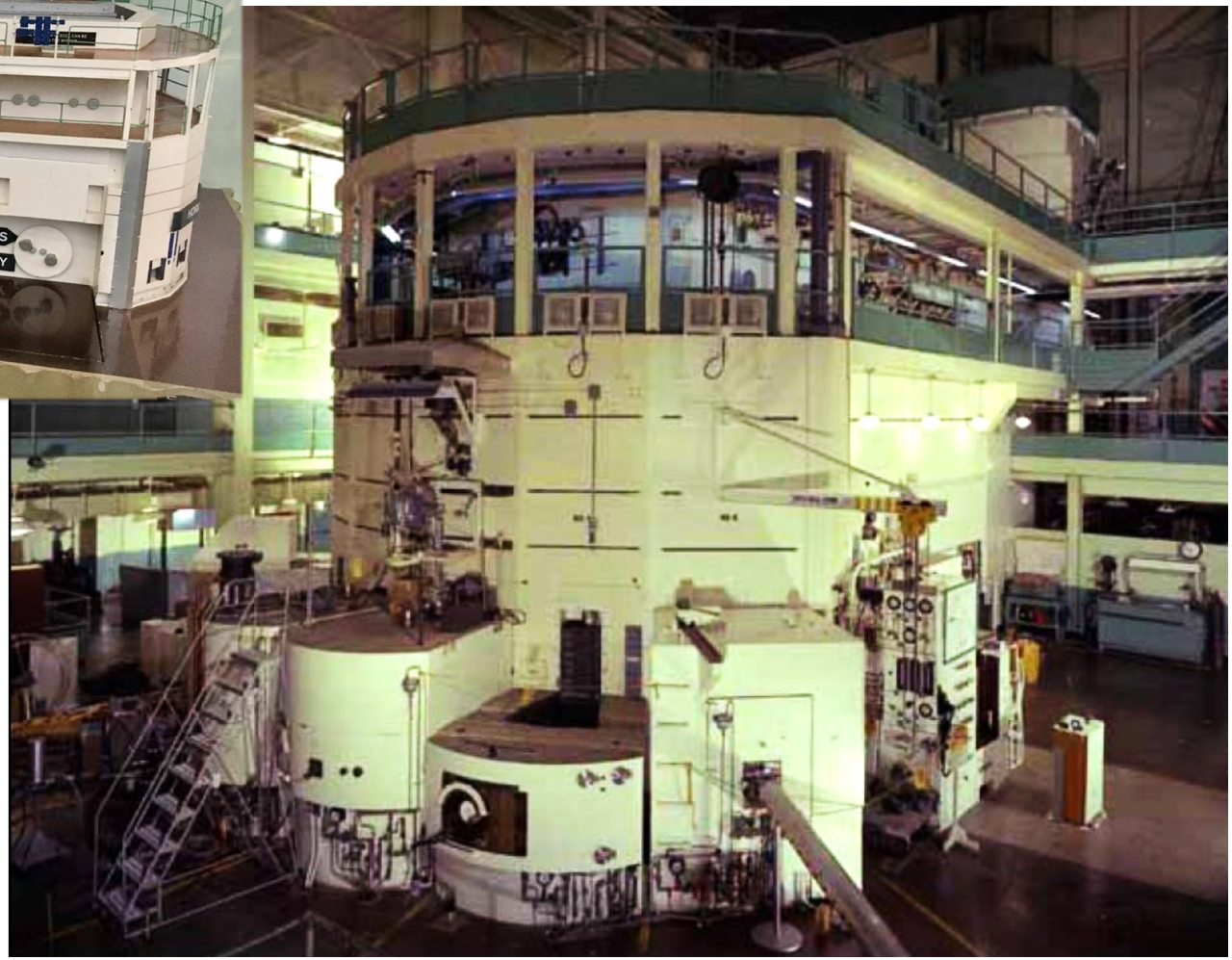
Elected to the National Academy of Sciences, 1975

Oliver E. Buckley Condensed Matter Physics Prize, 1956

Steve Spooner Herb Mook

Ralph Moon Mike Wilkinson

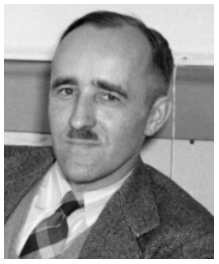
For the development and application of neutron diffraction methods for studies of atomic and magnetic structures of solids

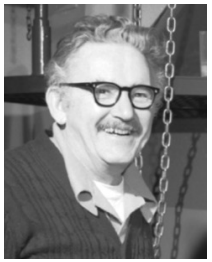


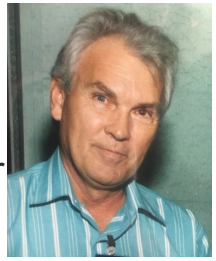
Oak Ridge Research Reactor (ORR) 1958-1987 20 MW

OAK RIDGE National Laboratory

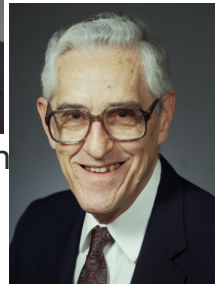
ORR HB-3 Magnetism diffractometer, designed so that both the strength and direction of the magnetic field could be varied.


Ernie Wollan

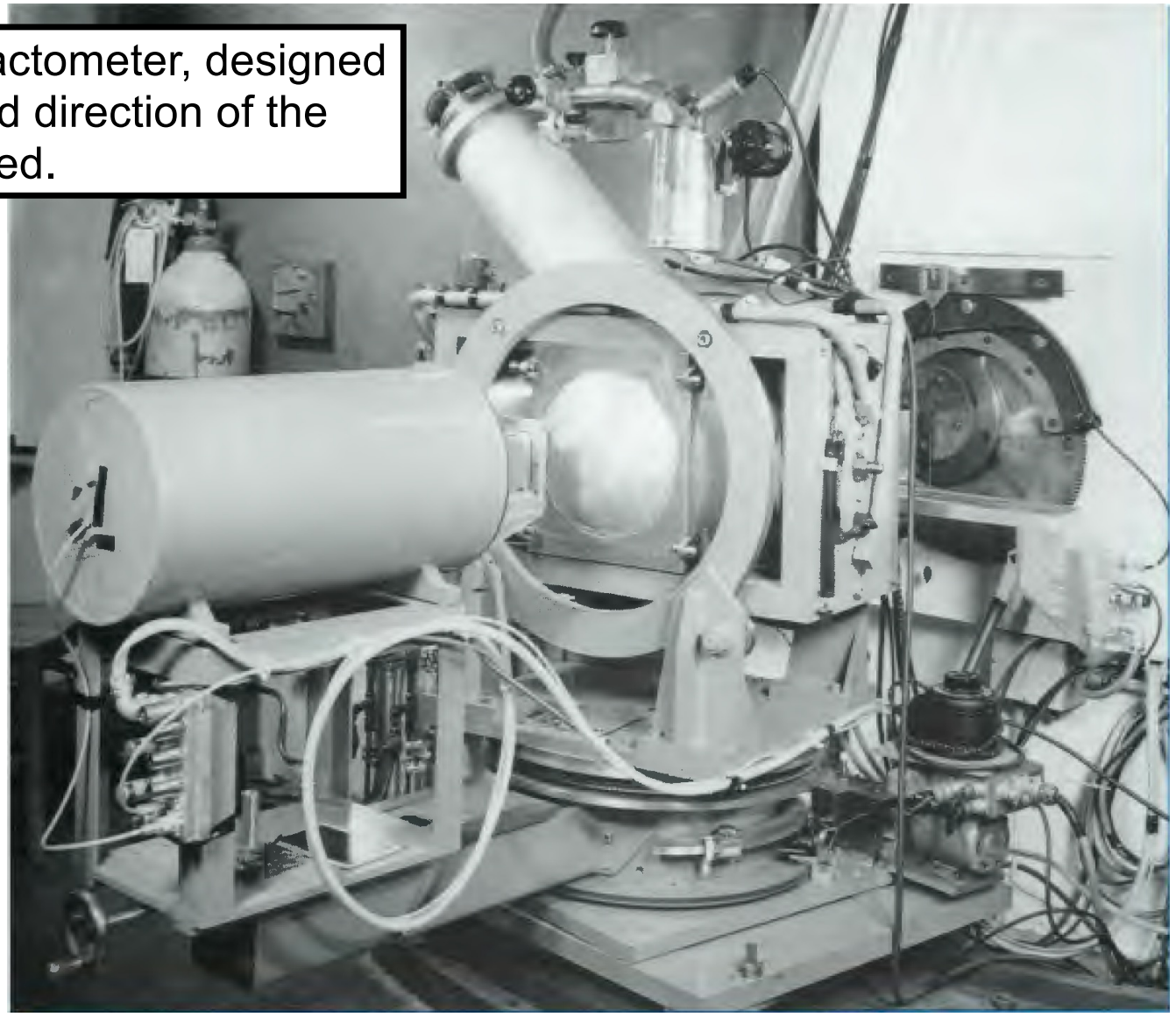

Wally Koehler


Joe Cable


Mike Wilkinson


Ralph Moon


Ray Child



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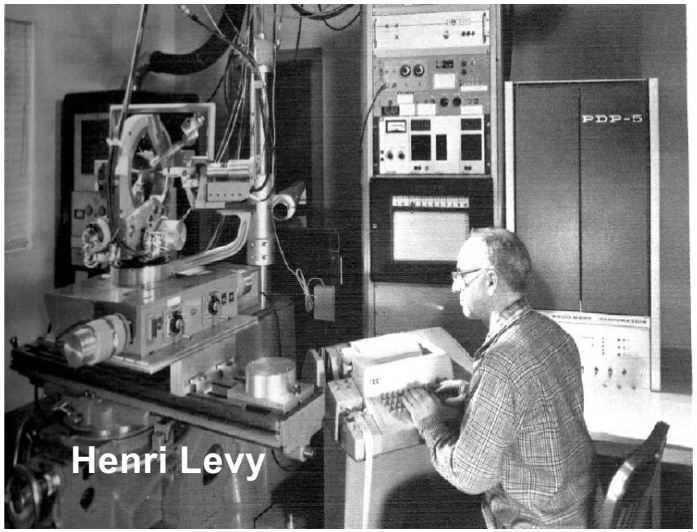
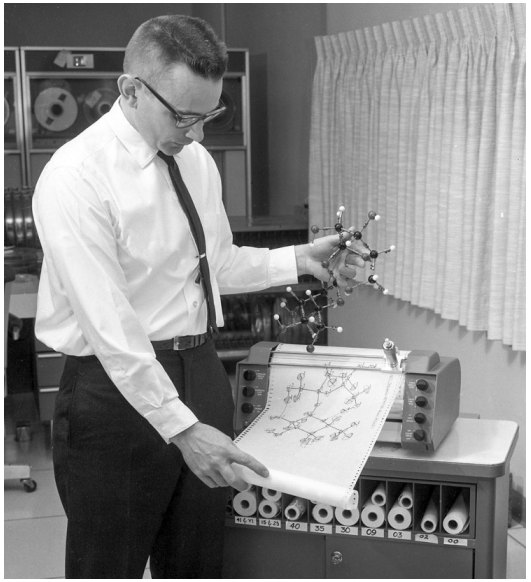
ORNL Early history in crystallography

Bill Busing, Hal Smith, Pete Peterson, Henri Levy, automatic three-circle neutron diffractometer 1961

automated X-ray diffractometers, 1960's





Carroll Johnson, ORTEP thermal ellipsoid plotting program for crystal structure drawings 1965

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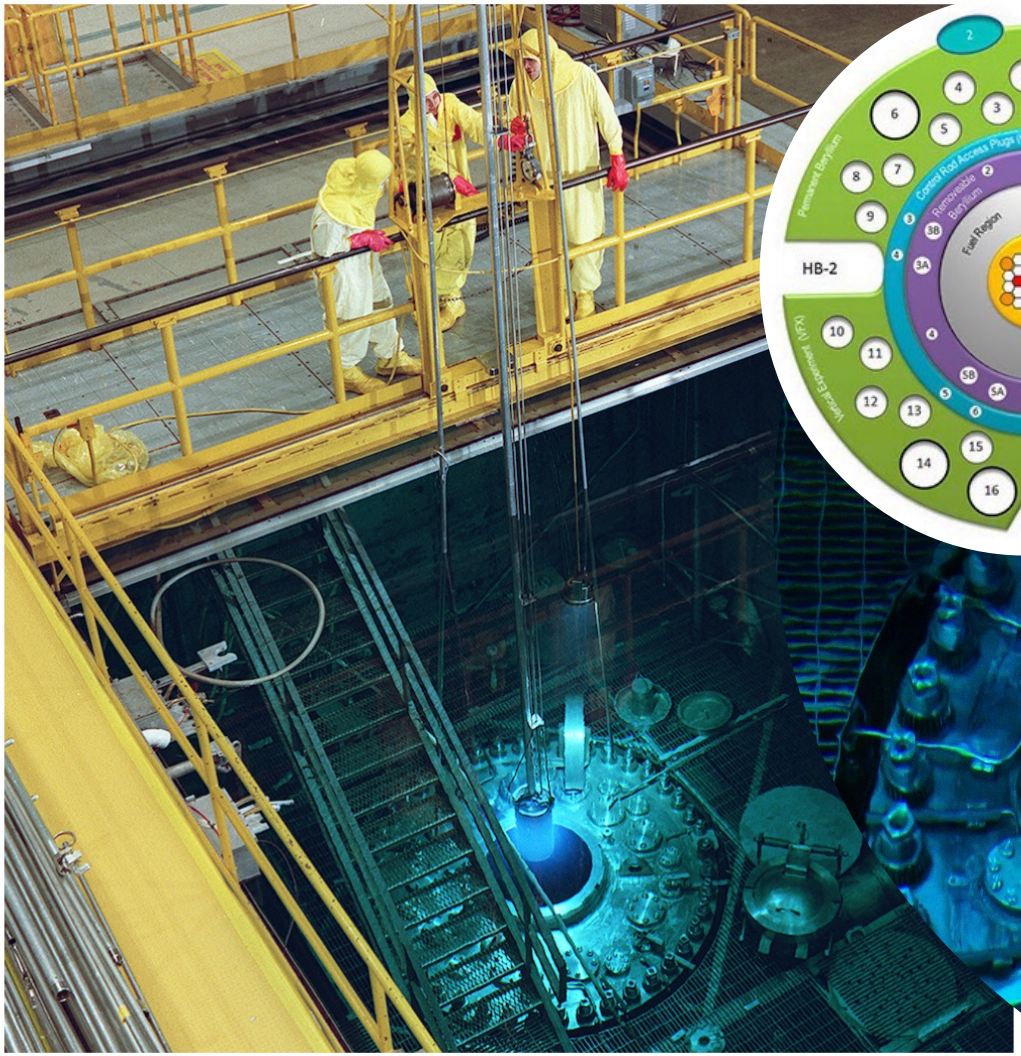
HIGH FLUX ISOTOPE REACTOR (1965 – present)



PHYSICAL REVIEW VOLUME 181, NUMBER 2 10 MAY 1969

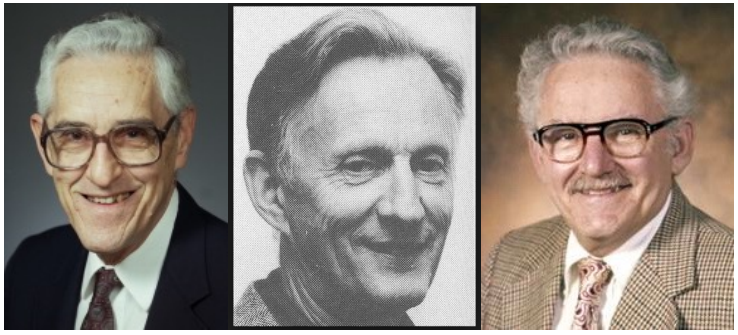
Polarization Analysis of Thermal-Neutron Scattering*

R. M. MOON, T. RISTE,† AND W. C. KOEHLER
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830
(Received 30 December 1968)

567
Times Cited

A triple-axis neutron spectrometer with polarization-sensitive crystals on both the first and third axes is described. The calculation of polarized-neutron scattering cross sections is presented in a form particularly suited to apply to this instrument. Experimental results on nuclear incoherent scattering, paramagnetic scattering, Bragg scattering, and spin-wave scattering are presented to illustrate the possible applications of neutron-polarization analysis.

"This technique permits the accurate separation of magnetic scattering from nuclear scattering, and it is used in neutron centers worldwide to study many classes of materials."



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Detection of Antiferromagnetism by Neutron Diffraction*

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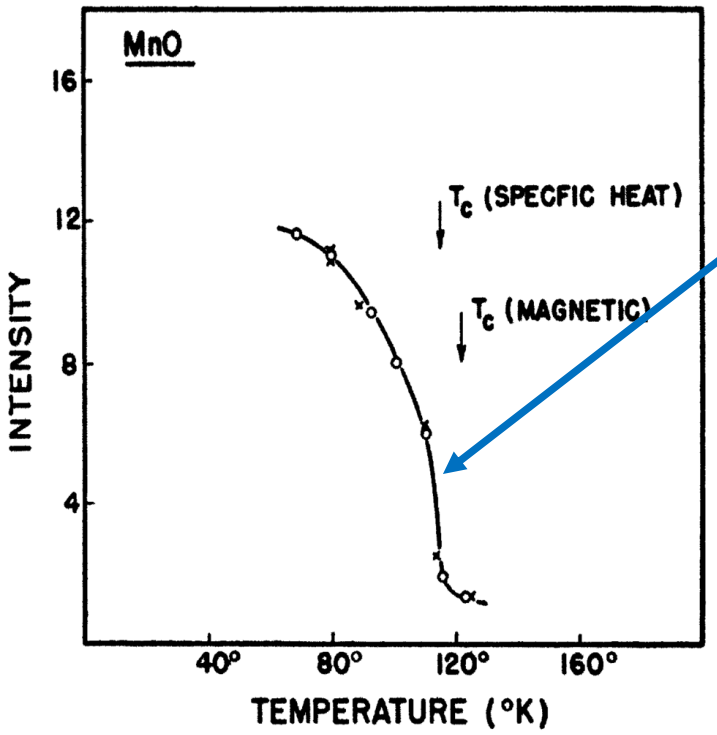

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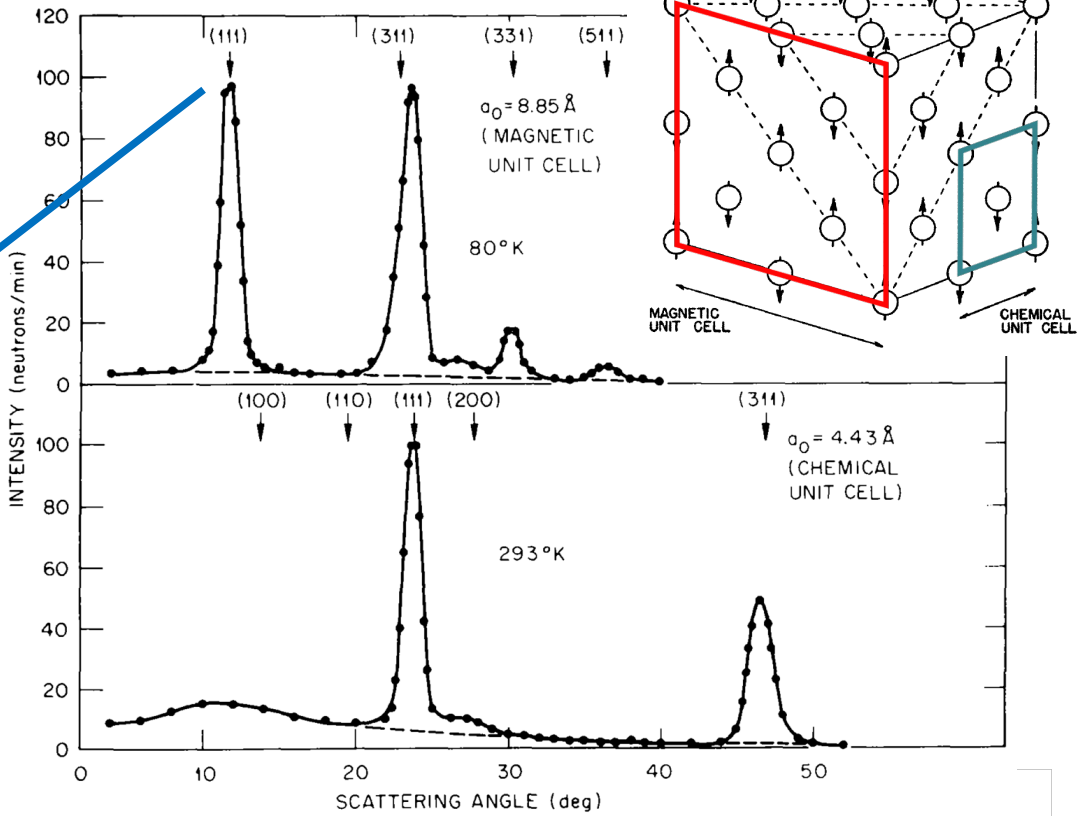

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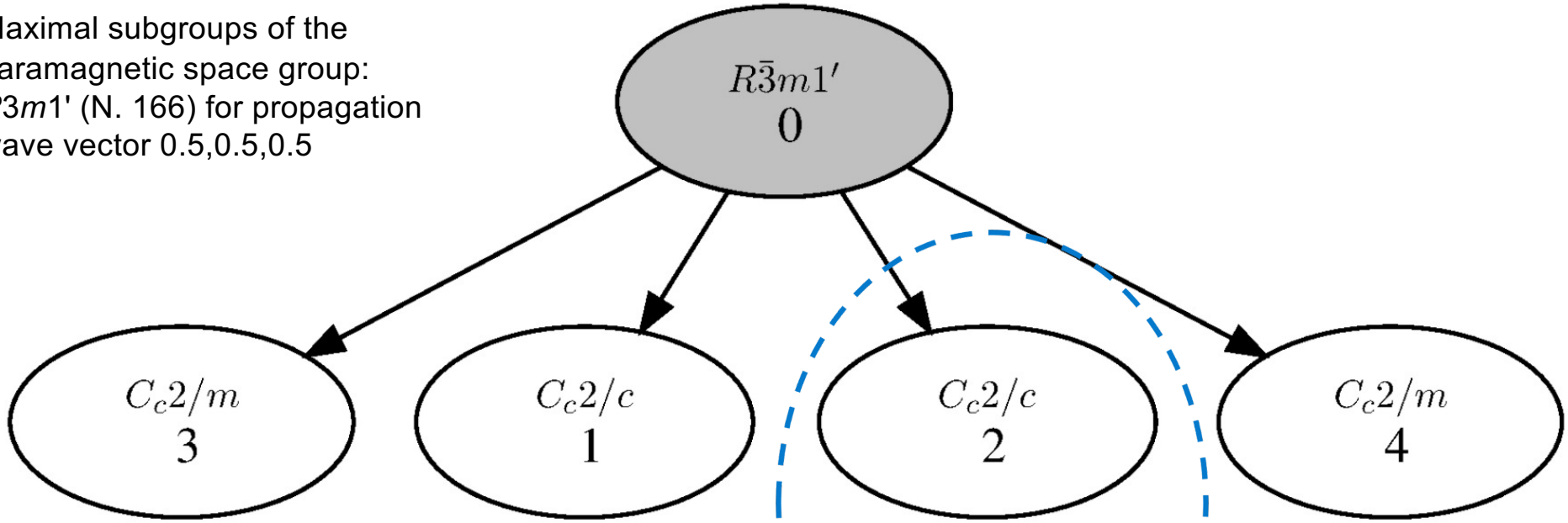
MnO rhombohedrally distorts at the magnetic transition. This was known even by Shull et al.

Maximal subgroups of the paramagnetic space group: *R*3*m*1' (N. 166) for propagation wave vector 0.5,0.5,0.5



Mn1 (0,0,0) (M_x,M_x,0)
Mn2 (1/3,1/6,1/6) (M_x,M_x,0)

Mn1 (0,0,0) (0,0,0)
Mn2 (1/3,1/6,1/6) (M_x,-M_x,M_z)

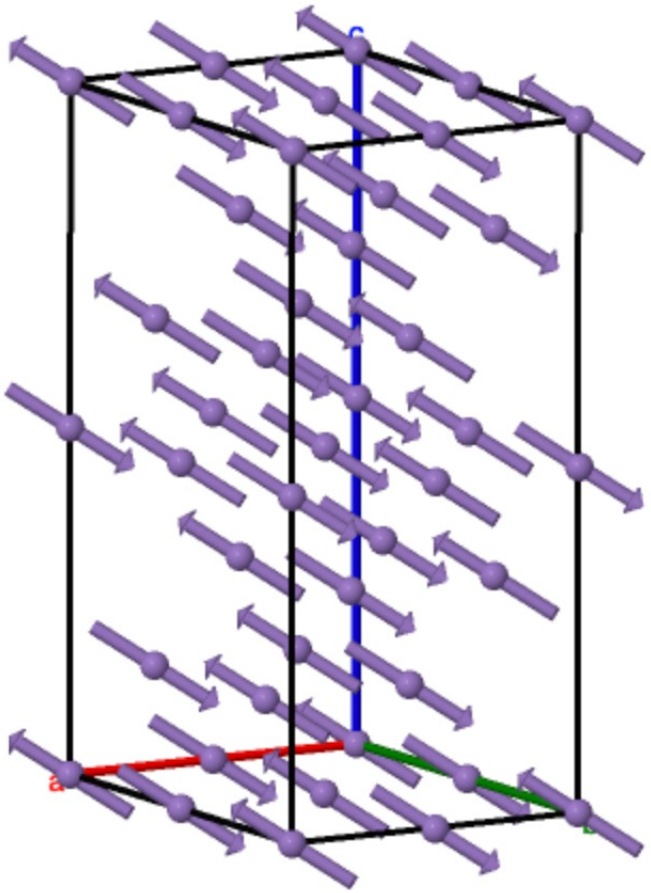
Mn1 (0,0,0) (M_x,M_x,M_z)
Mn2 (1/3,1/6,1/6) (M_x,M_x,M_z)

Mn1 (0,0,0) (M_x,M_x,0)
Mn2 (1/3,1/6,1/6) (0,0,0)

OAK RIDGE National Laboratory

MnO

C_c2/c



Mn1 (0,0,0) (M_x,M_x,M_z)
Mn2 (1/3,1/6,1/6) (M_x,M_x,M_z)

The magnetic structure of MnO continues to be studied.

Goodwin et al. (2006) determined by reverse Monte Carlo approach that the Mn moments point in the <1,1,-2> directions.

Paddison et al. (2018) studied the paramagnetic state using a combination of single-crystal neutron scattering and reverse Monte Carlo refinements.

Various Speakers

- Branton Campbell (BYU)
- Juan Rodriguez-Carvajal (ILL)
- Juan Manuel Perez Mato (Universidad del Pais Vasco)
- Andrew Wills (UCL)
- Brian Toby (Argonne National Laboratory)
- Václav Petříček (Czech Academy of Sciences)
- Margarida Henriques (Czech Academy of Sciences)
- Efrain Rodriguez (University of Maryland)
- William Ratcliff (NIST)
- Stuart Calder (ORNL)
- Ovi Garlea (ORNL)
- Huibo Cao (ORNL)
- Clarina Dela Cruz (ORNL)
- Qiang Zhang (ORNL)
- Keith Taddei (ORNL)

Overview
Agenda
Tutorial Examples
Presentations
Software
Past Workshops
Travel and lodging information
Speakers

Administrative Support
Keosha Anderson
andersonkj@ornl.gov
865-241-5176

About the School

The school will provide hands-on training and lectures on how to determine magnetic structures from powder and single-crystal neutron data. The techniques and theory of representational analysis and magnetic space groups will be introduced by leading experts and demonstrated in a series of hands-on examples.

The format will follow past workshops. But this year it is back to in-person student attendance!

Lectures and hands-on tutorial sessions will be presented in a hybrid mixture of in-person and virtual. These will cover:

1. Symmetry analysis using representation theory and the SARAh program and ISOTROPY Suite
2. Magnetic space groups using the Bilbao Crystallographic Server
3. Refinement strategies using the FullProf Suite, GSAS-II and Jana
4. Magnetic structure determination from powder and single-crystal data

The school is intended for graduate students, postdocs, and research scientists who have a working knowledge of crystallographic refinement and will benefit from incorporating the techniques of magnetic structure determination from neutron diffraction into their research.

Past Workshops

- 2020 School
- 2019 School
- 2016 School
- 2014 School
- 2012 School

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Magnetic structure determination with GSAS-II

Date: June 5, 2023
Location: ORNL, SNS. Building 8600. Room C-156.

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5:45-6pm	Summary discussion. Bring your own magnetic structure data. Poster Set-up.	Everyone
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