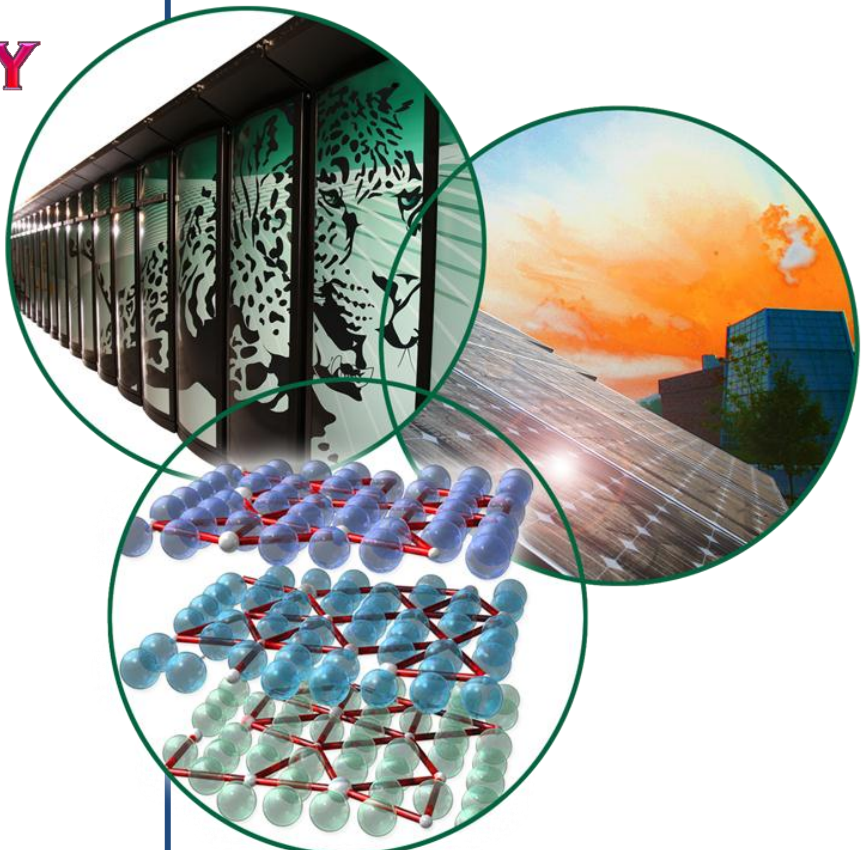
EXAMPLE 1
Study of magnetic structure of NiO by Neutron Powder Diffraction Technique



Clarina de la Cruz

ORNL Neutron Sciences

Workshop on Magnetic Structure Determination from Neutron Diffraction Data

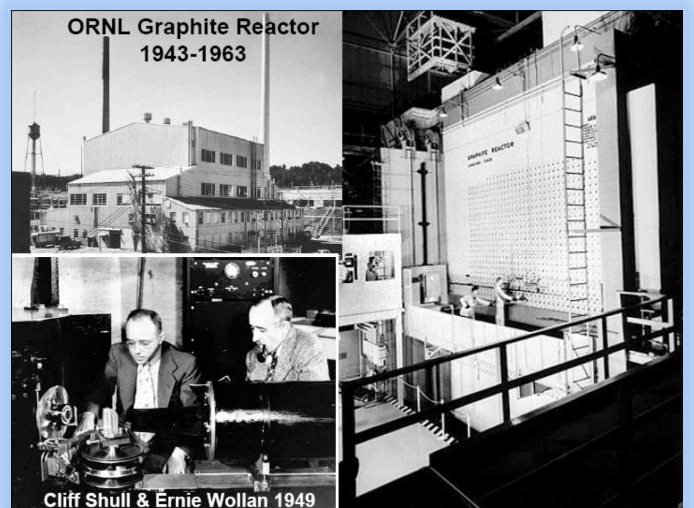
September 17, 2012

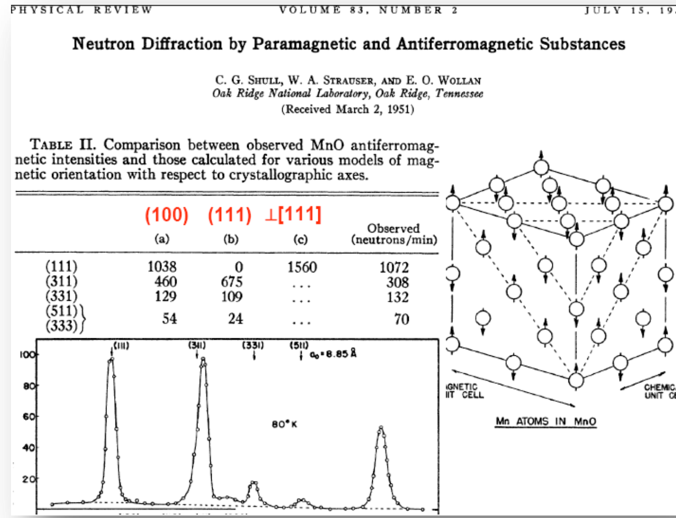
U.S. DEPARTMENT OF ENERGY

Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

❖ First neutron diffraction investigations of magnetic materials were done at Oak Ridge

Clifford G. Shull: 1994 Nobel Prize winner in Physics





PHYSICAL REVIEW VOLUME 83, NUMBER 2 JULY 15, 1951

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)

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

	(100) (a)	(111) (b)	⊥[111] (c)	Observed (neutrons/min)
(111)	1038	0	1560	1072
(311)	460	675	...	308
(331)	129	109	...	132
(511) (333)	54	24	...	70

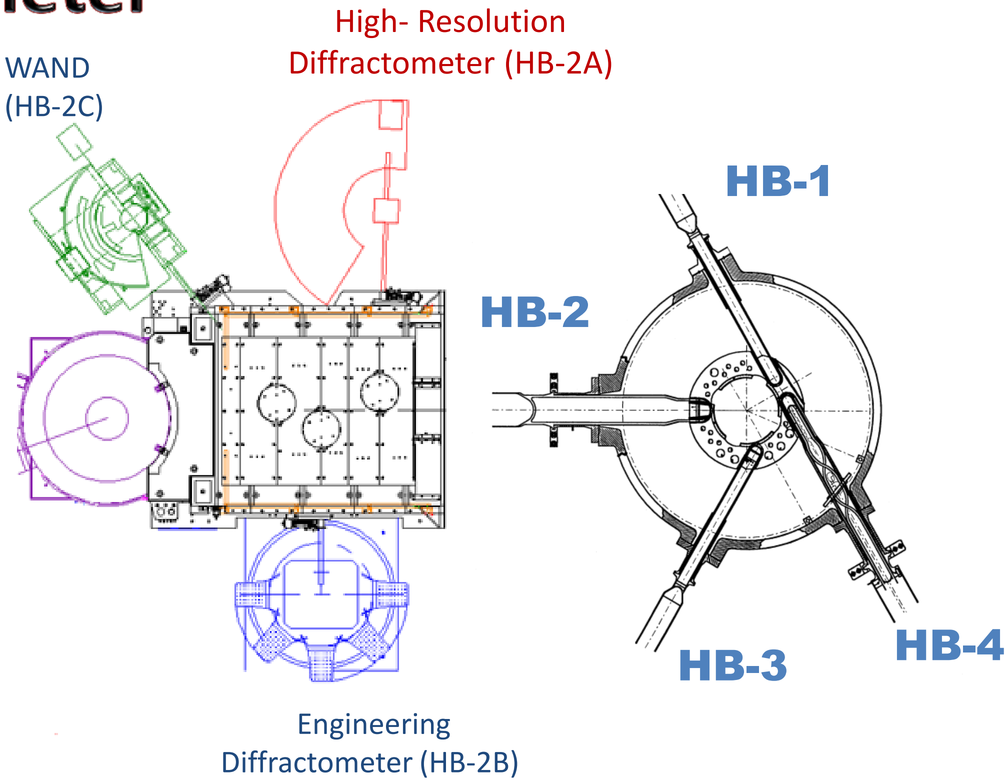
✓ The first direct evidence of antiferromagnetism was produced in determining the magnetic structure of MnO

✓ the Néel model of ferrimagnetism was confirmed for Fe_3O_4,

✓ the first magnetic form-factor data were obtained by measuring the paramagnetic scattering by Mn compounds,

✓ the production of polarized neutrons by Bragg reflection from ferromagnets was demonstrated

HB2A Powder Diffractometer



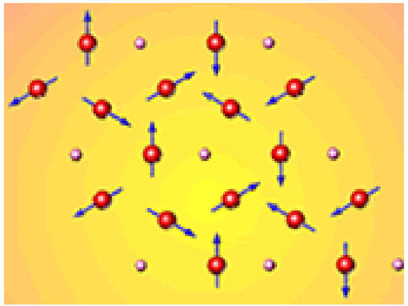
• constant-wavelength diffractometer designed to provide an optimum balance between the high flux and high resolution.

Available for user since May 2009

2010 – 2011 proposals call:
x 3 - subscription rate

Our user base in 2009-2011

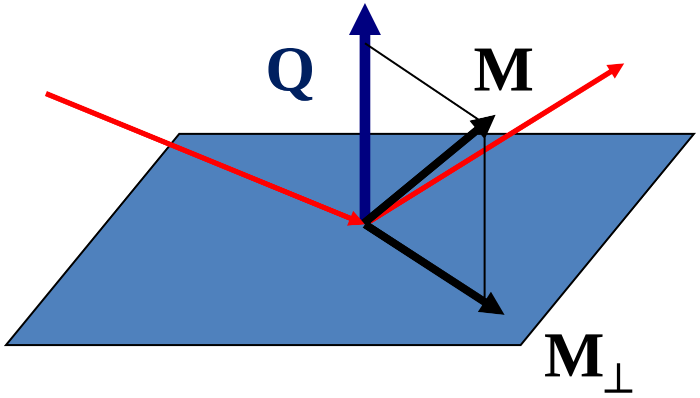
Magnetic neutron scattering



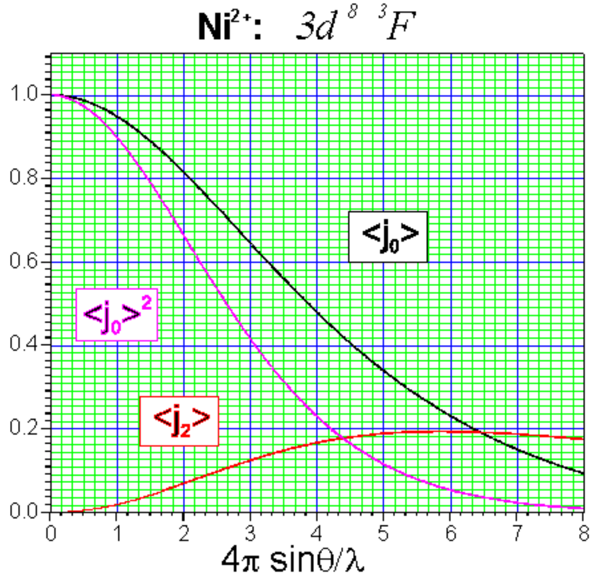
Magnetic structure factors are complex vectors

Only the perpendicular component of **M** to **Q** contributes to scattering

$$\mathbf{M}_\perp(\mathbf{Q}) = \hat{\mathbf{Q}} \times \mathbf{M}(\mathbf{Q}) \times \hat{(\mathbf{Q})}$$



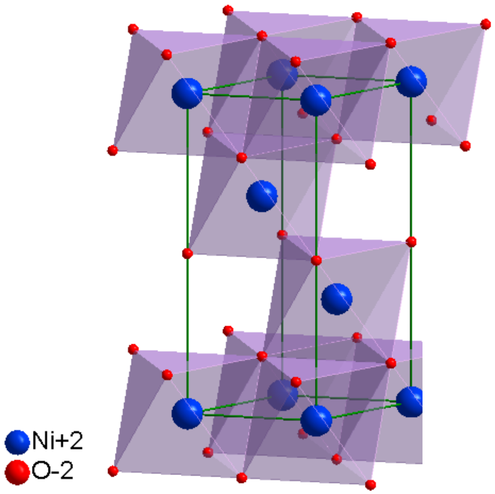
$$I_M \sim f(Q)^2\, M_\perp(Q)^2$$



$$f(Q) = \langle j_0(Q) \rangle + \left(1 - \frac{2}{g}\right) \langle j_2(Q) \rangle$$

International Tables of Crystallography, Volume C, ed. by AJC Wilson, Kluwer Ac. Pub., 1998, p. 513

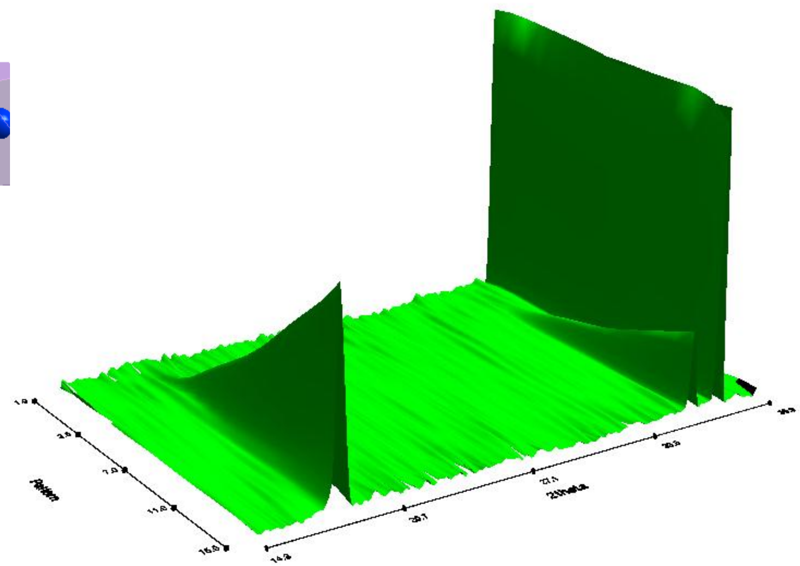
Magnetic structure of NiO

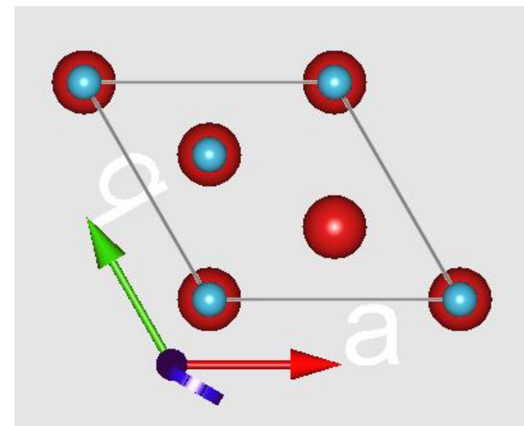


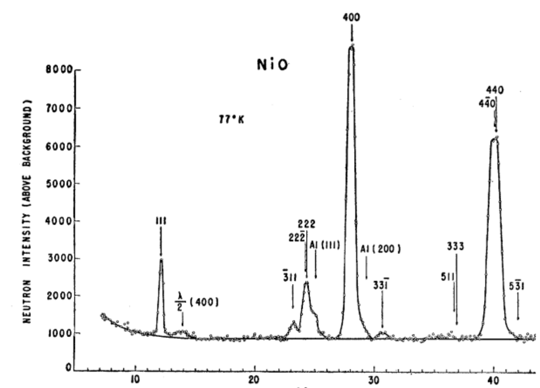
Trigonal : R-3m $(0,0,0)+ \quad (\frac{2}{3},\frac{1}{3},\frac{1}{3})+ \quad (\frac{1}{3},\frac{2}{3},\frac{2}{3})+$

a= 2.93A, c=7.23A

Ni : 3a : (0 0 0) ; O : 3b : (0 0 ½)







PHYSICAL REVIEW VOLUME 110, NUMBER 6 JUNE 15, 1958

Magnetic Structures of MnO, FeO, CoO, and NiO†

W. L. Roth
General Electric Research Laboratory, Schenectady, New York

Build PCR file from CIF file for PHASE 1: Nuclear Phase

1. Neutron Powder diffraction Data (2theta,intensity, standard deviation)
   HB2a, λ=1.537 Å, T=290K, 8g of powder in a vanadium tube

2. Instrument Resolution file (IRF)

3. Known Nuclear structure (CIF=crystallographic information file)

Magnetic moment of each atom: Fourier series

$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \; exp\left\{-2\pi\, i\mathbf{k}\mathbf{R}_l\right\}$$

Standard Fourier coefficients refinement:
A magnetic phase has `Jbt = +/- 1`

The magnetic symmetry is introduced together with explicit symmetry operators of the crystal structure. The refined variables are directly the components of the $\mathbf{S}_{\mathbf{k}js}$ vectors. Not all components of $\mathbf{S}_{\mathbf{k}js}$ are free (reason of the phase factors) and a relation exist between $\mathbf{S}_{\mathbf{k}j1}$ and $\mathbf{S}_{\mathbf{k}js}$

$$\mathbf{S}_{\mathbf{k}js} = M_{js}\, \mathbf{S}_{\mathbf{k}j1} exp\left\{-2\pi i \phi_{\mathbf{k}j}\right\}$$

Ni : 3a : (0 0 0), (2/3 1/3 1/3) , (1/3 2/3 2/3)

Magnetic moment of each atom: Fourier series

$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \; exp\left\{-2\pi\, i\mathbf{k}\mathbf{R}_l\right\}$$

```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   2  ==> Current R_Bragg for Pattern#  1:    18.11
!-------------------------------------------------------------------------------
magnetic
!
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ     Nvk Npr More
   1   0   0 0.0 0.0 1.0   1  -1  -1   0   0         0.000    1   7   0
!
R -1                         <--Space group symbol for hkl generation
!Nsym Cen Laue MagMat
   1   1   1   1
!
SYMM x, y, z
MSYM u,v,w,0.000
!
!Atom    Typ  Mag Vek    X       Y       Z       Biso     Occ      Rx      Ry      Rz
!      Ix      Iy      Iz     beta11  beta22  beta33   MagPh
Ni     MNI2  1   1  0.00000 0.00000 0.00000 0.30000  1.00000   1.648   0.000   0.000
                      0.00    0.00    0.00    0.00     0.00   31.00    0.00    0.00
     0.000   0.000   0.000   0.000   0.000   0.000  0.00000
      0.00    0.00    0.00    0.00    0.00    0.00     0.00
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structure. The refin

of $\mathbf{S}_{\mathbf{k}js}$ are free (rea

$$\mathbf{S}_{\mathbf{k}js} = M_{js}\, \mathbf{S}_{\mathbf{k}j1} exp\left\{-2\pi i \phi_{\mathbf{k}j}\right\}$$

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Magnetic moment of each atom: Fourier series

$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \, exp\left\{-2\pi\, i\mathbf{k}\mathbf{R}_l\right\}$$

k ?

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{2}\left(\mathbf{R}_{\mathbf{k}} + i\cancel{\mathbf{I}}_{\mathbf{k}}\right)\exp\{-2\pi i\cancel{\phi}_{\mathbf{k}}\}$$

Standard Fourier coefficients refinement:
A magnetic phase has `Jbt = +/- 1`

The magnetic symmetry is introduced together with explicit symmetry operators of the crystal structure. The refined variables are directly the components of the $\mathbf{S}_{\mathbf{k}js}$ vectors. Not all components of $\mathbf{S}_{\mathbf{k}js}$ are free (reason of the phase factors) and a relation exist between $\mathbf{S}_{\mathbf{k}j1}$ and $\mathbf{S}_{\mathbf{k}js}$

$$\mathbf{S}_{\mathbf{k}js} = M_{js}\, \mathbf{S}_{\mathbf{k}j1} exp\left\{-2\pi i\phi_{\mathbf{k}j}\right\}$$

Ni : 3a : (0 0 0), (2/3 1/3 1/3) , (1/3 2/3 2/3)

PHASE 2: AFM Magnetic Phase