


Argonne NATIONAL LABORATORY

APS
IPNS

Magnetic Powder Scattering Intensities

Magnetic structure factor theory
Magnetic scattering factor
Magnetic "extinctions" & magnetic structure

R.B. Von Dreele, IPNS/APS



THE UNIVERSITY OF CHICAGO
Office of Science
A U.S. Department of Energy Laboratory managed by The University of Chicago

Magnetic structure factor (& nuclear one, too)

Some basic assumptions:

1. Neutron beam – unpolarized
2. Polycrystalline sample – ideal random orientations (no texture)
3. Elastic scattering only – ignore inelastic magnetic scattering

→ Simplification!

→ Simplification!

Intensities = coherent nuclear scattering + coherent magnetic scattering (i.e. no cross terms)

$$d\sigma = b^2 + 2bp\lambda \cdot \mathbf{q} + p^2 q^2$$

Missing ave = 0 (λ = unit vector in neutron spin direction)

Nuclear structure factor	Magnetic structure factor
$\left \sum_n b_n \exp\{2\pi i(\mathbf{h} \cdot \mathbf{r})\} \right ^2$	$\left \sum_m \mathbf{q}_m p_m \exp\{2\pi i(\mathbf{h} \cdot \mathbf{r})\} \right ^2$
All atoms	Magnetic ions only

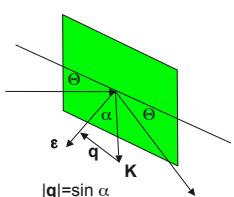
Structure factor – powders & no polarization – p's&q's? (after Bacon, 1975)

$$\mathbf{q}_m = \hat{\mathbf{a}}_h (\hat{\mathbf{a}}_h \cdot \mathbf{K}_m) - \mathbf{K}_m$$

$$p_m = \left(\frac{e^2 \gamma}{m_N c^2} \right) S_m f_m$$

$\hat{\mathbf{a}}_h$ – unit vector || \mathbf{h} – diffraction vector
 \mathbf{K}_m – unit vector || magnetic moment on atom m
 $\therefore \mathbf{q}$ small for $\mathbf{h} \parallel \mathbf{K}$ & large for $\mathbf{h} \perp \mathbf{K}$

$0.54 \times 10^{-12} \text{cm}$ – similar to b_n
 e – electron charge
 γ – neutron magnetic moment
 m_N – neutron mass
 c – speed of light



S – magnetic moment (Bohr magnetons)
 f – 1-electron magnetic form factor

Magnetic form factor - f_m

Fourier transform of unpaired e^- density:
valence e^- ; outer shell
Sharp fall off with Q (small d , etc.)

In GSAS:

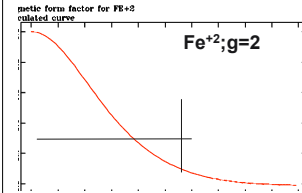
1. Tabulated by user
2. Form factor coefficients $\langle j_0 \rangle$ and $\langle j_2 \rangle$ (higher terms ignored)

$$f_m = C + \sum_{l=1}^4 A_l \exp\left(-B_l \sin^2 \Theta / \lambda^2\right) + \left(\frac{2}{g} - 1\right) \left[C + \sum_{l=1}^4 A_l \exp\left(-B_l \sin^2 \Theta / \lambda^2\right) \right] \sin^2 \Theta / \lambda^2$$

Landé g factor = 2 for 1st row transition elements:
quenched orbital contribution

In general $f_m \rightarrow 0$ for $\sin \Theta / \lambda > 0.5$; $d < 1.0$

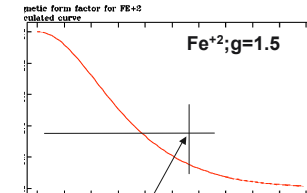
Magnetic form factors – from valence shell electrons



Orbital contribution quenched
(typical 1st row)

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

$$\mu = g\sqrt{J(J+1)} \quad \text{magnetic moment}$$



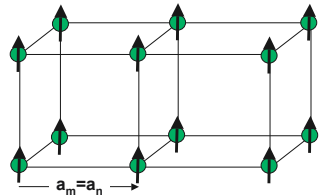
not quenched (v. slightly fatter)

$$\text{Fe}^{+2}; d^6: S=2, L=2, J=4$$

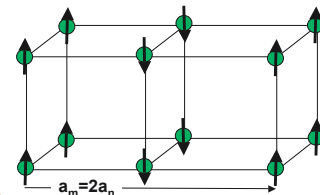
$$g=1.5; \mu_j=6.7, \mu_s=4.9$$

$$(\mu_{\text{obs}}=5.2 \text{ in FeCl}_2)$$

Magnetic structures



Ferromagnetic
No extra reflections



Antiferromagnetic
Extra reflections

Magnetic symmetry – spins & moments?

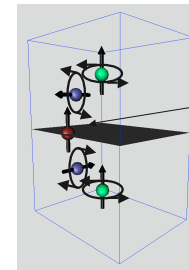
How do magnetic moments/spins transform via symmetry operations?

Operation is on spin (not moment) – physical object

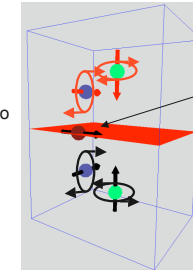
Antiooperation – spin reversal (“time reversal”)

Example; mirror – “black”

antimirror – “red”



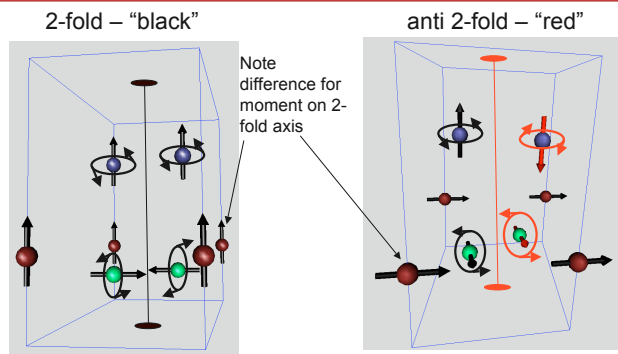
NB: moment must be perpendicular to “black” plane



NB: moment must be in “red” mirror

Result depends on orientation & position

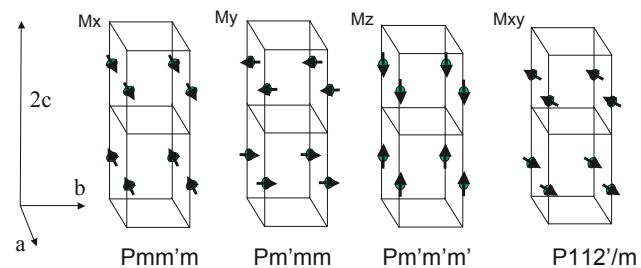
Rotations & antirotations



NB: switch “black” to “red” is NOT ferro to antiferro!!

Extinctions – moment direction $|q| = \sin \alpha$

Possible antiferromagnets (assume orthorhombic?):



(Note $\frac{1}{4}$ shift along z – to get atoms with moments in right places wrt symm operations)

Magnetic extinctions

Pmmm – no extinctions
 Pm'mm – h00 all absent
 Pmm'm – 0k0 all absent
 Pm'm'm' – h00, 0k0, & 00l all absent
 P112'/m – no extinctions
 BUT, MOMENT DIRECTION MATTERS! (remember q)
 (similar to extinctions for atoms in special positions)

NB: these rules are for magnetic atom in general position with moment pointed in a general $M_x M_y M_z$ direction.

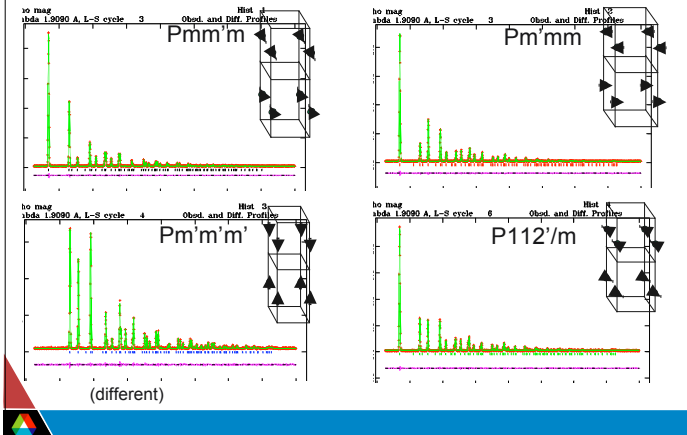
Magnetic extinctions, cont.

1st 10 nonzero magnetic reflections for antiferromagnetic cases

Pmm'm	Pm'mm	Pm'm'm'	P112'/m
001	001	---	001
011	011	011	011
101	101	101	101
111	111	111	111, -111
003	003	---	003
021	021	021	021
013	013	013	013
103	103	103	103
121	121	121	121, -121
113	113	113	113, -113

different

**Different powder patterns – all CW neutron (ILL d1a)
distinguish by intensities – only magnetic part**



So how choose magnetic symmetry/structure?

Trial & error!! (A.J. Wills – SARAH)

In GSAS – use tools

1. SPCGROUP
2. EXPEDT – magnetic operator (“black”/“red”)
3. VRSTPLOT – draw result; shows moment directions
4. Calculate pattern – check with observed data!

See tutorial....