Resonant and non-resonant magnetic x-ray diffraction

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Few basic information related to synchrotron radiation/X-rays

What do we get from synchrotron sources ?

From synchrotron sources we receive **very high intensity** **polarized x-rays**.

X-rays wavelength is 0.01 nm to 10 nm. (120 keV to 120 eV) **[E(keV)=12.39/λ(Å)]**

Upto few keV (2 to 3) it is called soft x-rays and above it is called hard x-rays.

How is the synchrotron radiation generated ?

Synchrotron radiation is generated by rotating a charged particle in a circular orbit at a relativistic speed. Radiation is generated in the tangential directions of the circle.

Why do we need synchrotron X-rays

To study the structure of matter through different fundamental processes like scattering, diffraction, reflectivity, absorption, fluorescence.

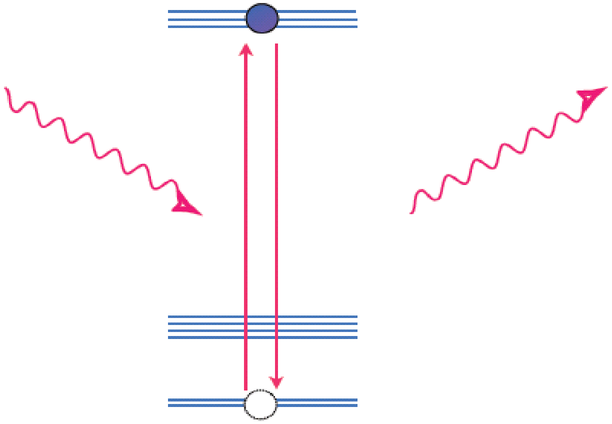
Outline

- Concept of resonant X-ray diffraction
- Resonant and non-resonant magnetic X-ray diffraction
- Experimental requirements
- Some examples
    - Multiferroic “rare earth iron borate”, $HoFe_3(BO_3)_4$
    - Chiral properties of hematite (α-Fe2O3)
    - Coexistence of Superconductivity and ferromagnetism in P-doped EuFe2As2.

Resonant x-ray diffraction

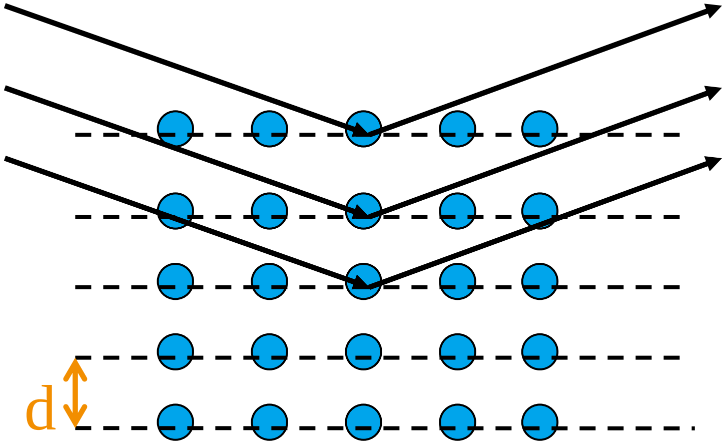
This technique combines the spectroscopy and diffraction phenomenon

Spectroscopy



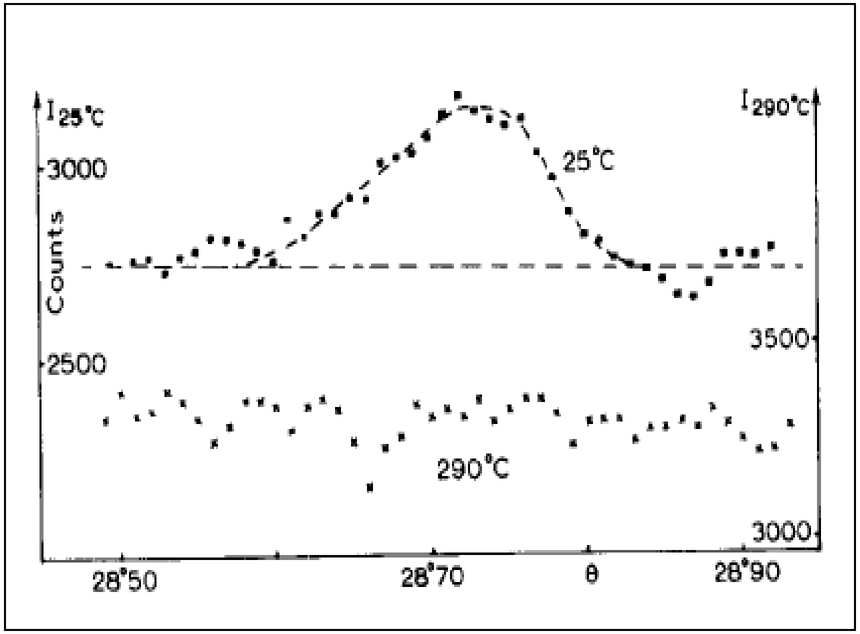
Diffraction

$\lambda = 2\, d\, \sin\theta$



Diffraction at absorption edges

Observation of first x-ray magnetic peak in NiO



(3/2 3/2 3/2) peak, 3 days counting time for each curve

Bergevin, F. de & Brunel, M. (1972) Phys. Lett. A 39, 141.
Observation of first magnetic superlattice peaks by x-ray diffraction in NiO

Why magnetic x-ray diffraction?

- Can be used for investigations of submillimeter-sized single crystals.
- Many of the technologically important RE compounds contain neutron opaque elements.
- Superior reciprocal space (Q) resolution allows more detailed study … reinvestigation of “solved” structures.
- Resonant magnetic scattering occurs at well-defined energies specific to elements of interest -- probe local magnetism.
- Orbital moment determination
- Studies of magnetic surfaces and interfaces.

Magnetic x-ray diffraction

Elastic scattering amplitude for scattering from magnetic ion:

$$\boldsymbol{f} = \boldsymbol{f}_0 + \boldsymbol{f}' + \boldsymbol{i}\boldsymbol{f}'' + \boldsymbol{f}_{mag}$$

At resonance:

$$f \approx (\boldsymbol{\epsilon}'.\boldsymbol{\epsilon})F^{(0)} - i(\boldsymbol{\epsilon}'\times\boldsymbol{\epsilon}).\boldsymbol{\mu}F^{(1)} + (\boldsymbol{\epsilon}'.\boldsymbol{\mu})(\boldsymbol{\epsilon}.\boldsymbol{\mu})F^{(2)}$$

[Hill and McMorrow, Acta Cryst. **A52**, 236 (1996).]

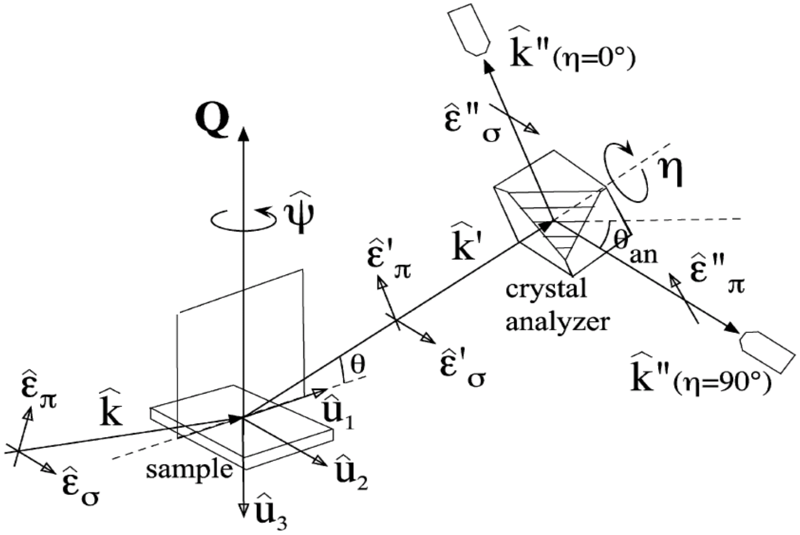
Resonant and non-resonant magnetic X-ray diffraction scheme with polarization analysis

Resonant magnetic scattering amplitude (electric dipole transitions) [Hill & McMorrow]

$$f_{E1}^{res-mag} = \begin{pmatrix} f^{\sigma\sigma'} & f^{\sigma\pi'} \\ f^{\pi\sigma'} & f^{\pi\pi'} \end{pmatrix}$$

$$= F^0 - iF^1 \begin{pmatrix} 0 & m_1 \cos\theta + m_3 \sin\theta \\ m_3 \sin\theta - m_1 \cos\theta & -m_2 \sin 2\theta \end{pmatrix}$$

$$+ F^2 \begin{pmatrix} m_2^2 & m_2(m_1 \sin\theta - m_3 \cos\theta) \\ m_2(m_1 \sin\theta + m_3 \cos\theta) & -\cos^2\theta\left(m_1^2 \tan\theta + m_3^2\right) \end{pmatrix}$$



Strong intensities due to resonance enhancement
Element sensitivity at absorption edges
Magnetic structure determination

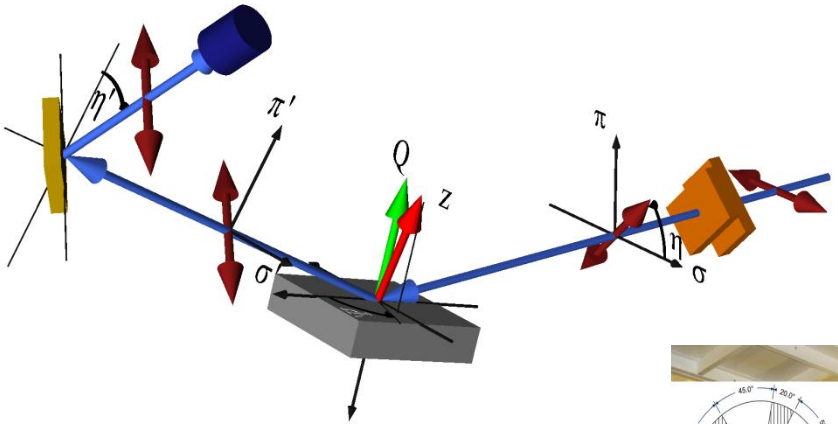
Non-resonant magnetic scattering amplitude [Blume & Gibbs]

$$f^{mag} = -i\frac{\hbar\omega}{mc^2} \begin{pmatrix} f^{\sigma\sigma'} & f^{\sigma\pi'} \\ f^{\pi\sigma'} & f^{\pi\pi'} \end{pmatrix}$$

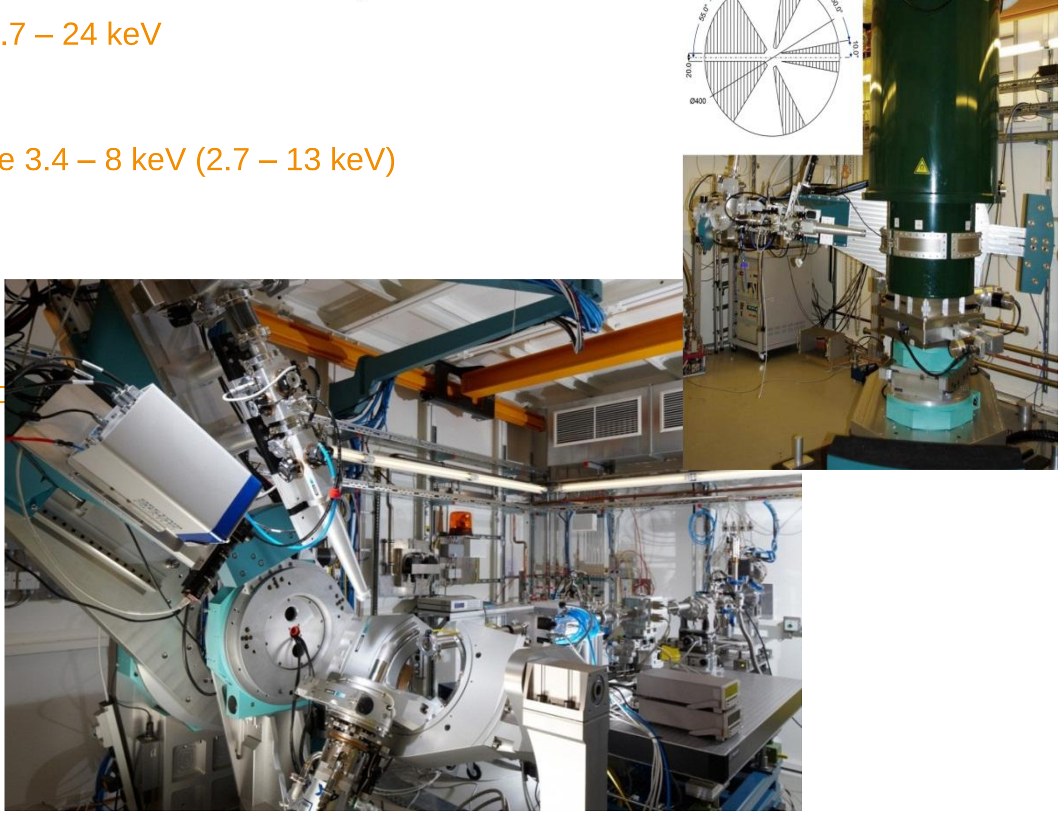
$$= -i\frac{\hbar\omega}{mc^2} \begin{pmatrix} S_2 \cos\theta & \sin\theta[\cos\theta(L_1 + S_1) + S_3 \sin\theta] \\ \sin\theta[-(L_1 + S_1)\cos\theta + S_3 \sin\theta] & \cos\theta[2L_2 \sin^2\theta + S_2] \end{pmatrix}$$

Determination of L/S ratio
Magnetic structure determination

Resonant Scattering and diffraction experiment, at beamline P09, PETRA III



- Energy variation:
  - Large energy range: 2.7 keV – 50 keV
- Small beam focus
  - Beam size routinely (mirror): 145 x 40 μm^2
  - with Compound Refractive Lenses: ~ 50 x 4 μm^2
- Effective higher harmonic suppression
  - High harmonic suppression in full energy range 2.7 – 24 keV
- Variable x-ray polarization
  - Fully variable incident polarization in energy range 3.4 – 8 keV (2.7 – 13 keV)
  - Analysis of scattered polarization states
- Psi-diffractometer (EH1)
  - Open χ-circle → large accessible angular range
  - Quasi-simultaneous use of area and point detecto
- Heavy Load Diffractometer (EH2)
  - Horizontal 6-circle diffractometer
  - 650 kg load maximum
- Special sample environments
  - Several low temperature cryostats
  - High magnetic fields: 14T magnet, He-3 insert
  - Temperature range 300 mK < T < 800 K



J. Sync. Rad. 20, 541 (2013)

Role of magnetic structure in multiferroicity:

$P = e_3 \times Q$;

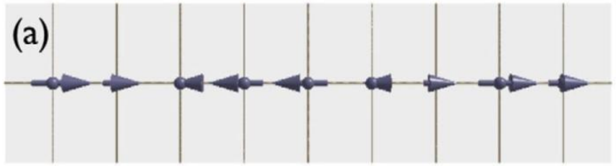
where $e_3 = S_i \times S_j$; and Q is the wave vector direction.

[M. Mostovoy, Phys. Rev. Lett. 2006, 96, 067601.]

[H. Katsura et al., Phys. Rev. Lett. 2005, 95, 057205.]

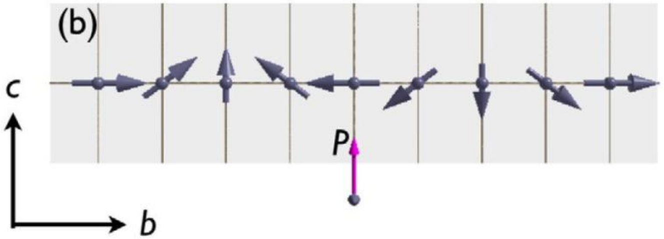
Example: $TbMnO_3$

$T_S < T < T_N$=42 K

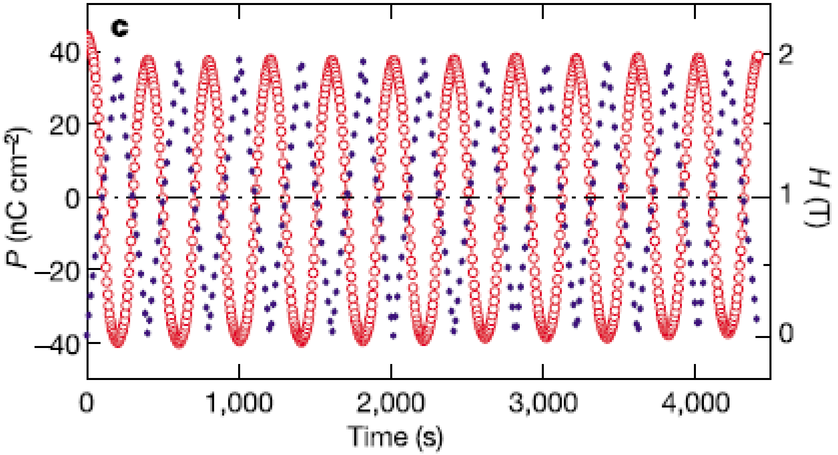


P= 0

$T < T_S$=28 K

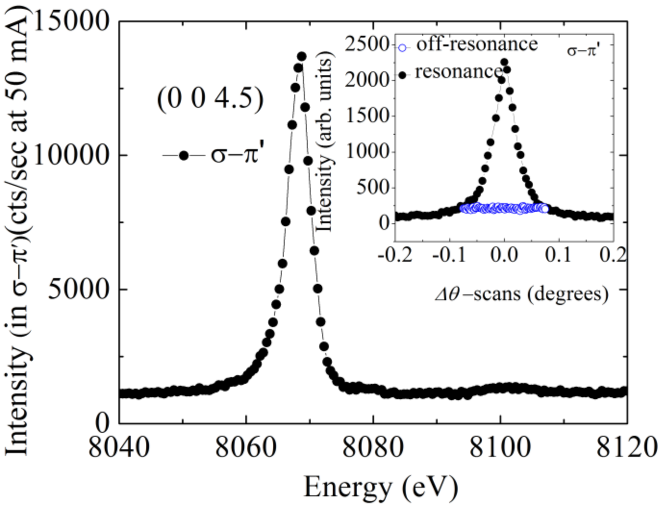


P≠ 0, P || *C*



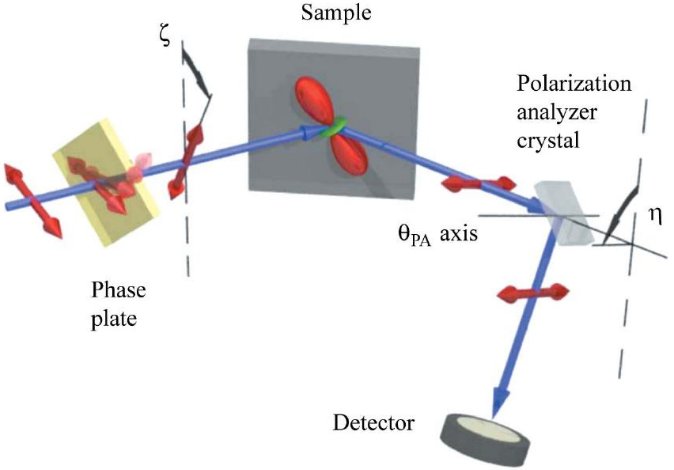
Polarization flipping by linearly varying magnetic fields from 0 to 2 T in $TbMn_2O_5$. (Nature **429**, 392 (2004)).

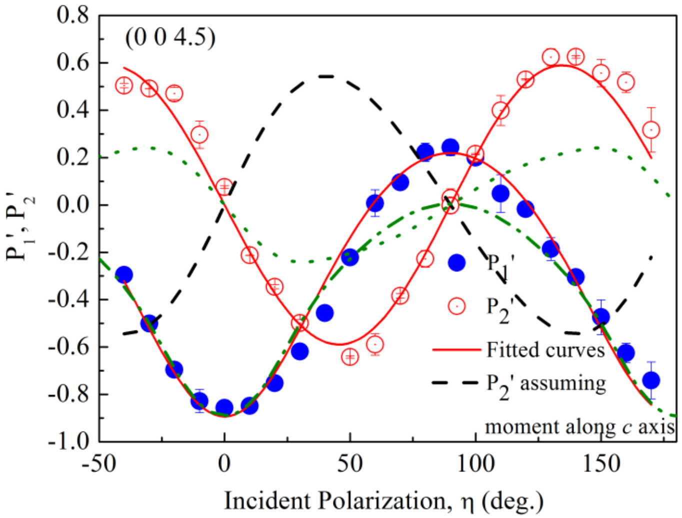
Determination of ab-plane spin spiral of Ho moments in $HoFe_3(BO_3)_4$ through Full polarization analysis at resonance at P09, PETRA III



D. K. Shukla et al. **Phys. Rev. B 86**, 224421 (2012).

Energy scan at Ho L_3 edge on (0 , 0, 9/2) at 6 K,





Fitting of Poincaré-Stokes parameter:

$$I(\eta,\eta') = \frac{P_0}{2}(1 + P_1^{'}(\eta)\cos 2\eta' + P_2^{'}(\eta)\sin 2\eta')$$

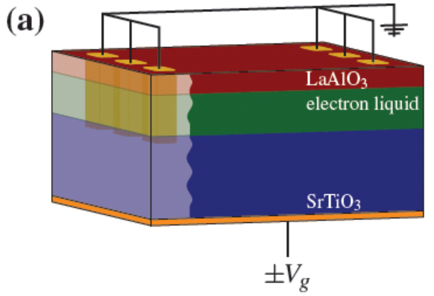
Full polarization analysis at Ho L_3 edge on (0 , 0, 9/2) at 6 K,

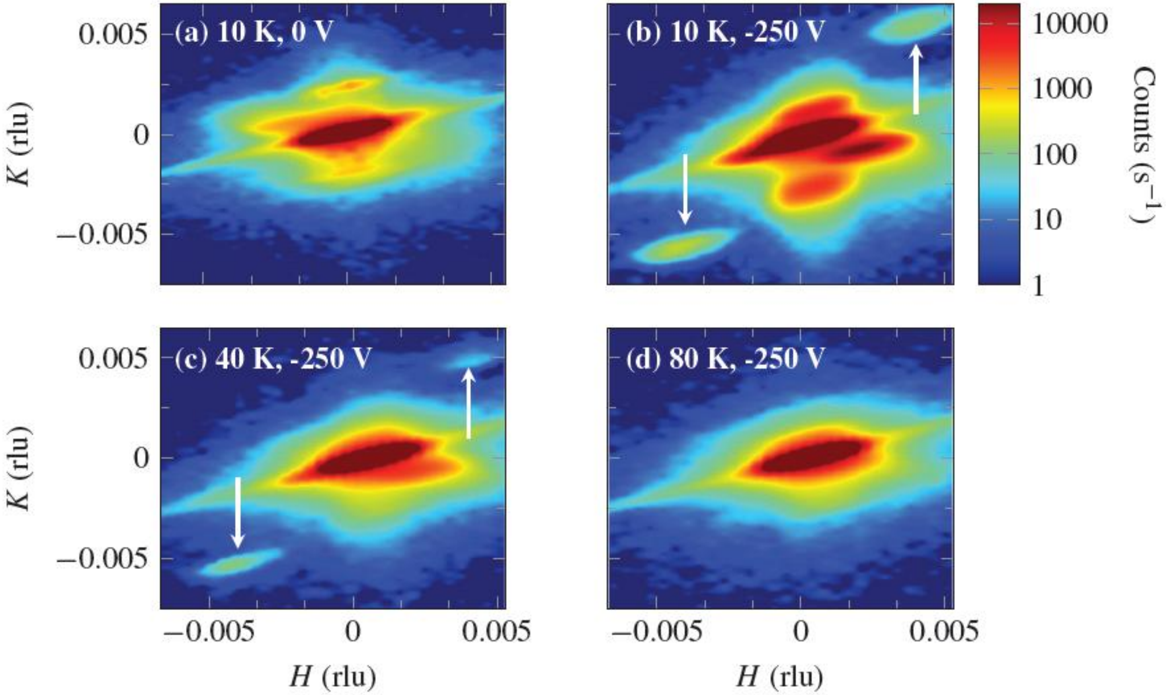
Ho moments are forming ab-plane spin spirals, making a screw-type magnetic structure.

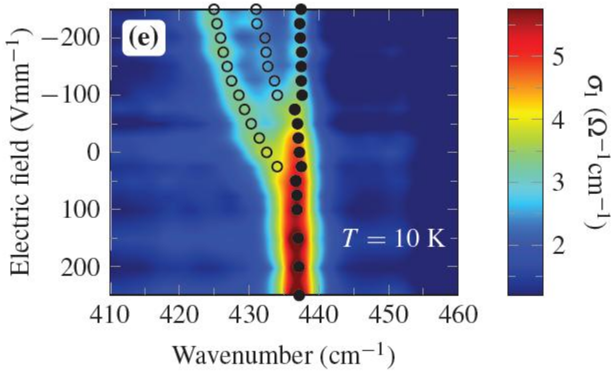
C. Mazzoli et al., PRB **76**, 195118 (2007).
M. Blume and D. Gibbs, PRB **37**, 1779 (1988).
Hill and McMorrow, Acta Cryst. **A52**, 236 (1996).

Electric field effect on the confined electrons at the $LaAlO_3/SrTiO_3$ interface

M. Roessle et al. **Phys. Rev. Lett. 110,** 136805 (2013)

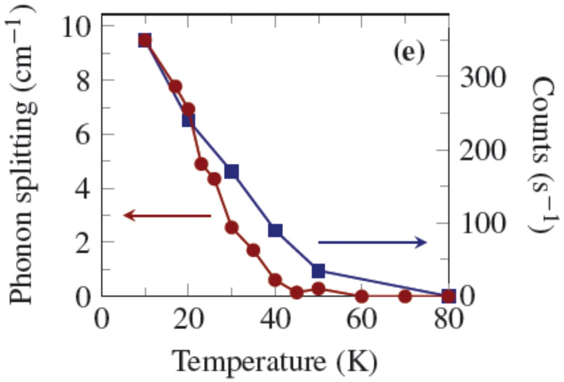






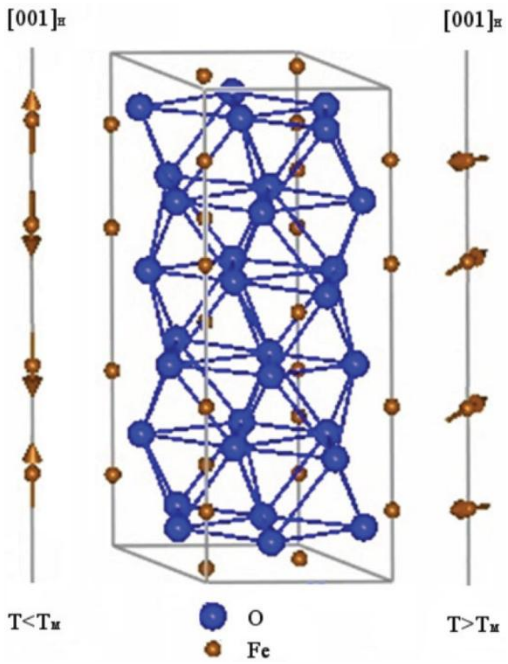
- → field induced polar layer in $SrTiO_3$
- → localization of electrons for negative gate voltage

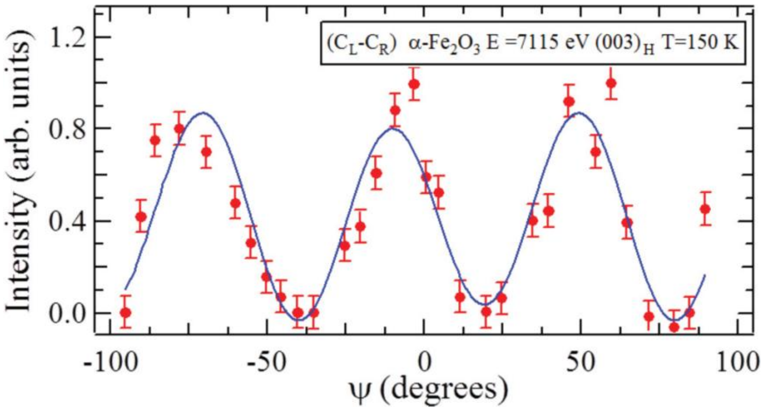
- → satellite peaks with 60 nm period develop parallel to the LAO/STO interface



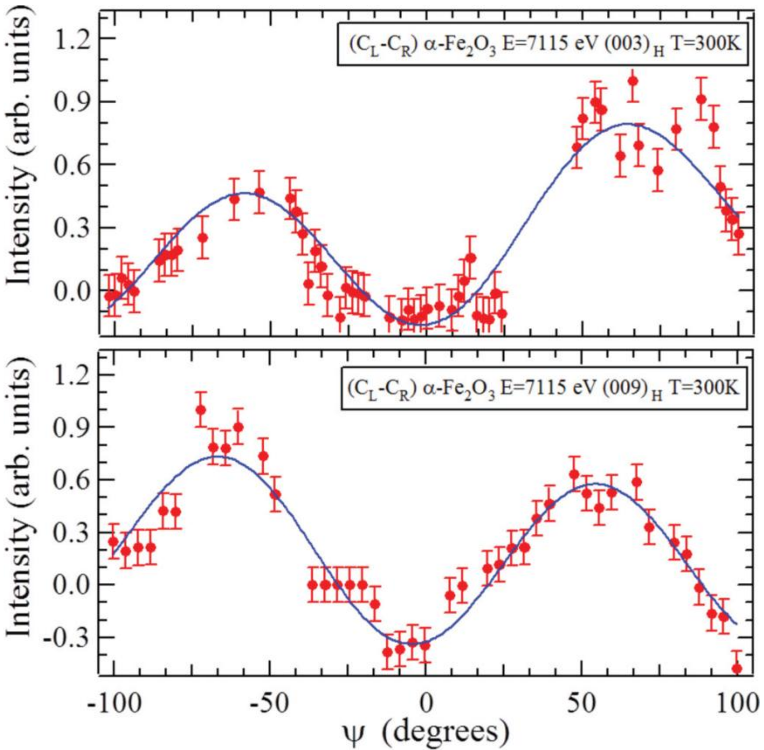
Chiral proerties of α-Fe_2O_3, investigated using cricularly polarized X-rays

A. Rodrıguez-Fernandez et al. **Phys. Rev. B 88,** 094437 (2013)





Phase-I

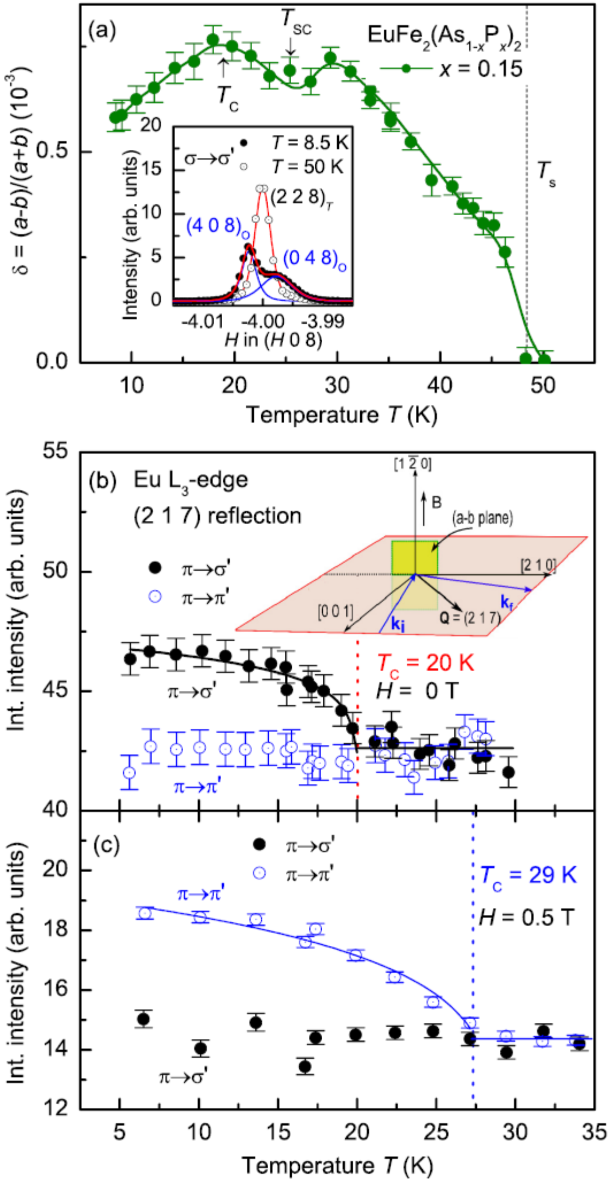


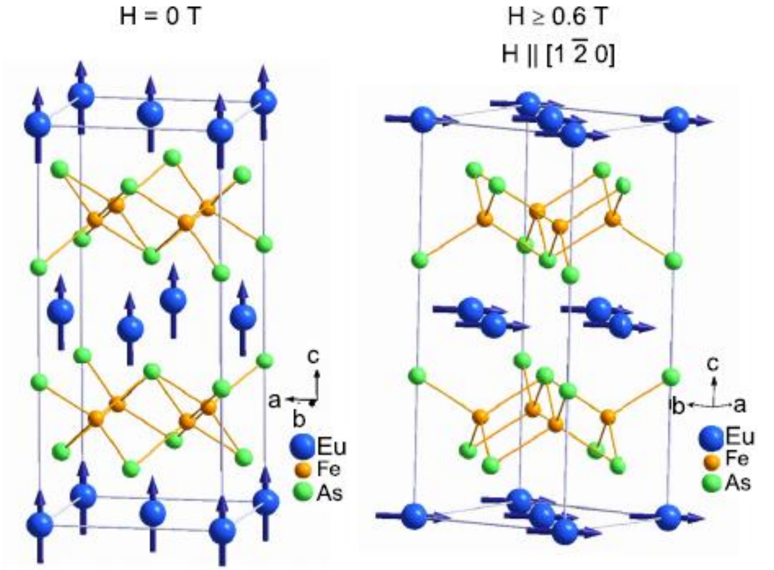
Phase-II

- → circular polarized incident x-rays tuned near the iron *K edge* was used.
- → Magnetoelectric multipoles, fully characterize the high-temperature canted phase.
- → Orbital angular momentum accompanies the collinear motif, and it is absent in the canted motif.

Coexistence of Superconductivity and ferromagnetism in P-doped EuFe2As2

Nandi et. al., **Phys. Rev. B 89,** 014512 **(2014)**





- The long-range ferromagnetic order of the Eu2+ moments aligned primarily along the c axis coexists with the bulk superconductivity at zero field.

- Under an applied magnetic field, superconductivity still coexists with the ferromagnetic Eu2+ moments, which are polarized along the field direction.

- A spontaneous vortex state is proposed for the coexistence of superconductivity and ferromagnetism in EuFe2(As0.*85P0.15)2.*

Thank you all for your kind attention.