Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order, nonspherical electron density

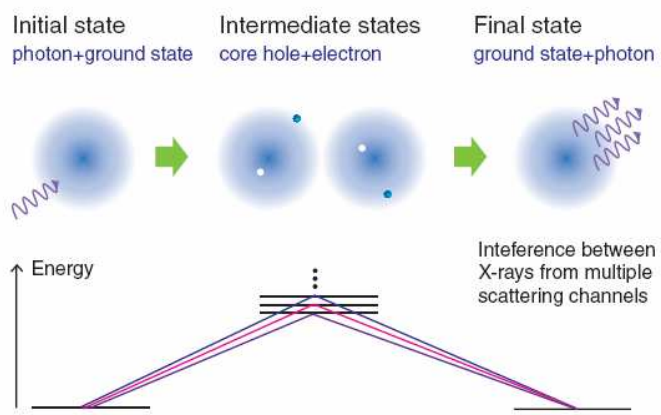
- “scanning”: domain physics

- other applications?

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)



$$M_{ng}^{i(o)}(j) = \langle \psi_n | \hat{O}^{i(o)} | \psi_g(j) \rangle \qquad \hat{O}^{i(o)} = \vec{\epsilon}^{i(o)} \cdot \vec{r}\left(1 - \tfrac{1}{2} i \vec{k}^{i(o)} \cdot \vec{r}\right)$$

$$F = \sum_j e^{i\vec{Q}\cdot\vec{R}_j}(f_{0j} + f_j' + i f_j'')$$

$$f_j(\omega) = \frac{m_e}{\hbar^2}\frac{1}{\hbar\omega}\sum_n \frac{(E_n - E_g)^3 M_{ng}^{o*}(j) M_{ng}^{i}(j)}{\hbar\omega - (E_n - E_g) - i\frac{\Gamma_n}{2}} = \Sigma_{p,q}(-)^{\bar{q}} T_q^{(p)} F_{-q}^{(p)}(j;\omega)$$

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

TABLE I. Parity and time-reversal symmetries of $F_q^{(p)}$ tensors.

Tensor	$\hat{T}$	$\hat{P}$	Multipole
$F^{(0)}(E1\text{–}E1)$	+	+	Electric charge
$F^{(1)}(E1\text{–}E1)$	–	+	Magnetic dipole
$F^{(2)}(E1\text{–}E1)$	+	+	Electric quadrupole
$F^{(1+)}(E1\text{–}E2)$	+	–	Electric dipole
$F^{(2+)}(E1\text{–}E2)$	+	–	$\vec{g}$ quadrupole
$F^{(3+)}(E1\text{–}E2)$	+	–	Electric octupole
$F^{(1-)}(E1\text{–}E2)$	–	–	Polar toroidal dipole
$F^{(2-)}(E1\text{–}E2)$	–	–	Magnetic quadrupole
$F^{(3-)}(E1\text{–}E2)$	–	–	Polar toroidal octupole
$F^{(3)}(E2\text{–}E2)$	–	+	Magnetic octupole
$F^{(4)}(E2\text{–}E2)$	+	+	Electric hexadecapole

$$M_{ng}^{i(o)}(j) = \langle \psi_n | \hat{O}^{i(o)} | \psi_g(j) \rangle \qquad \hat{O}^{i(o)} = \vec{\epsilon}^{i(o)} \cdot \vec{r}\left(1 - \tfrac{1}{2} i \vec{k}^{i(o)} \cdot \vec{r}\right)$$

$$F = \sum_j e^{i\vec{Q}\cdot\vec{R}_j}(f_{0j} + f_j' + i f_j'')$$

$$f_j(\omega) = \frac{m_e}{\hbar^2}\frac{1}{\hbar\omega}\sum_n \frac{(E_n - E_g)^3 M_{ng}^{o*}(j) M_{ng}^{i}(j)}{\hbar\omega - (E_n - E_g) - i\frac{\Gamma_n}{2}} = \Sigma_{p,q}(-)^{\bar{q}} T_q^{(p)} F_{-q}^{(p)}(j;\omega)$$

-Energy dependence

-Polarization dependence

-Azimuthal dependence

-Q-dependence

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

Spin-orbit ~ electronic correlations, ~~spin + orbit~~, $J_{effective}$ states

- spin-orbital Mott state Sr_2IrO_4 (J_{eff}=1/2), new topological states (other lattices)
- quantum spin Hall effect (Na_2IrO_3 ?)
- other exotic states (S=L=0, SL≠0, $CuIr_2S_4$?)
- relevance to quantum computing
- relevance to topological insulators

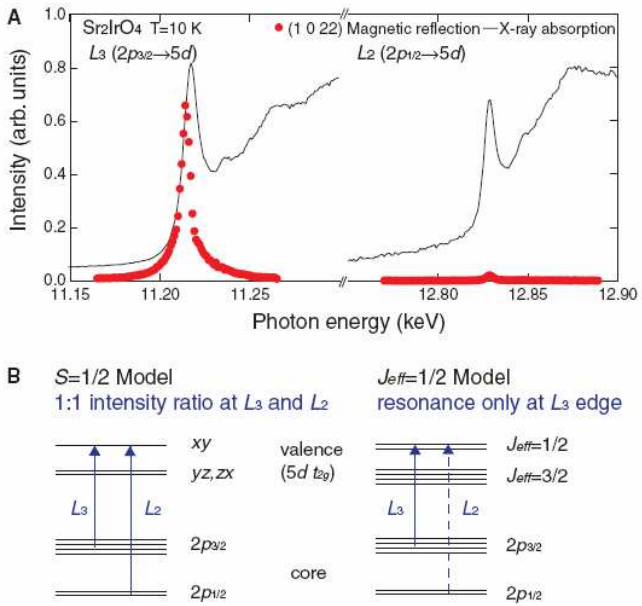
Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

Spin-orbit ~ electronic correlations, ~~spin + orbit~~, $J_{effective}$ states

- spin-orbital Mott state Sr_2IrO_4 (J_{eff}=1/2), new topological states (other lattices)



$$|J_{\rm eff} = 1/2, m_{J_{\rm eff}} = \pm 1/2\rangle$$
$$= \frac{1}{\sqrt{3}}(|xy,\mp\sigma\rangle \mp |yz,\pm\sigma\rangle + i|zx,\pm\sigma\rangle)$$

B.J. Kim et al., Science 323, 1329 (2009)

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

New states of matter, exotic electronic states

Q: other stuff where spin-orbit matters

- multiferroics
- magnetic recording media (Co:Pt, $Fe_{48}Pt_{52}$)

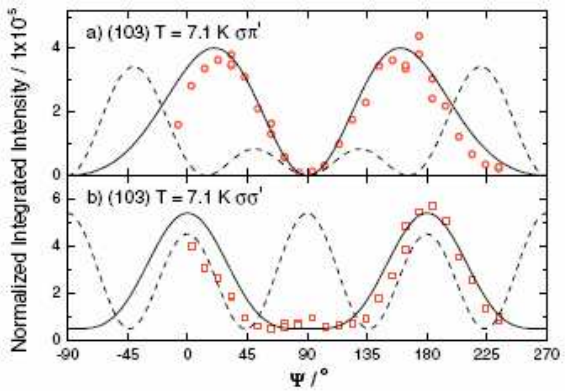
Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

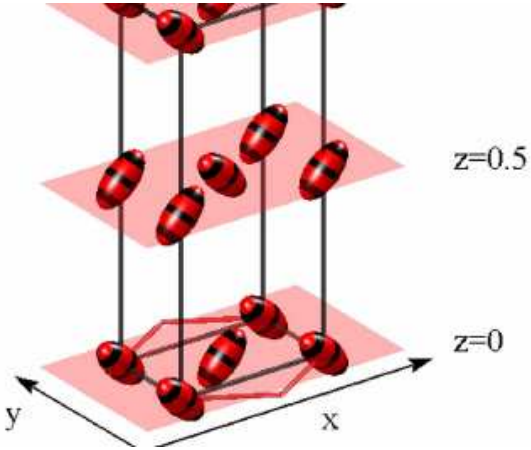
-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

- “hidden” order parameters in heavy fermion systems

Anti-ferro-quadrupolar order in UPd_3, Walker et al., PRL 97, 137203 (2006)





Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

-“hidden” order parameters (77 refs: $U(Ru,Rh)_2Si_2$ mostly, but others too)

-multipolar orders are common (NpO_2 octupolar order and hidden parameter, etc)

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

- ruthenates – current issues?

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

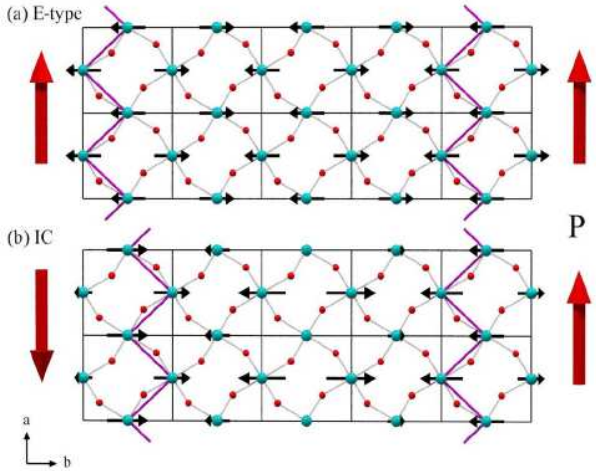
-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

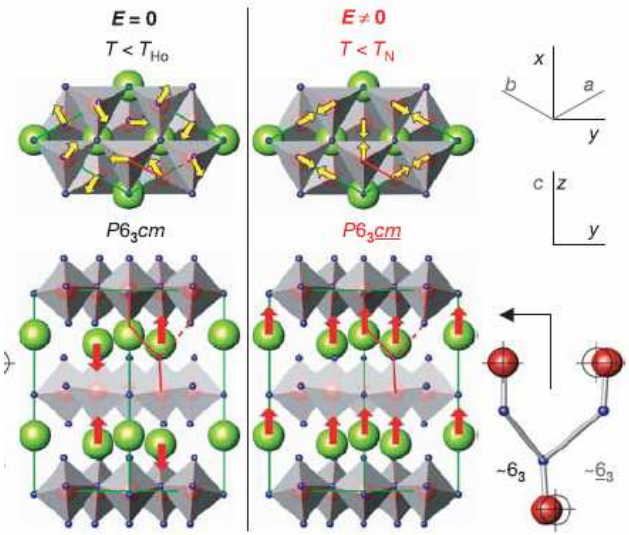
Lanthanides

arguably, many systems with magnetic order

-novel multiferroics (element selectivity important)



$HoMnO_3$



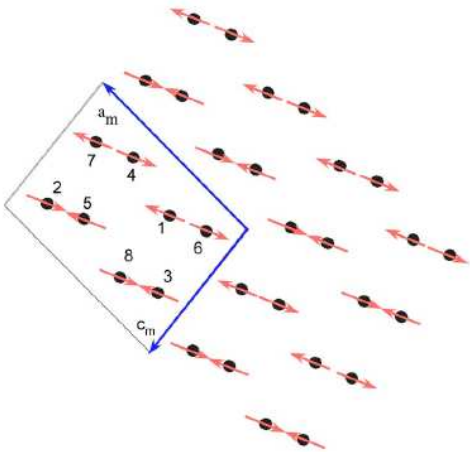
Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

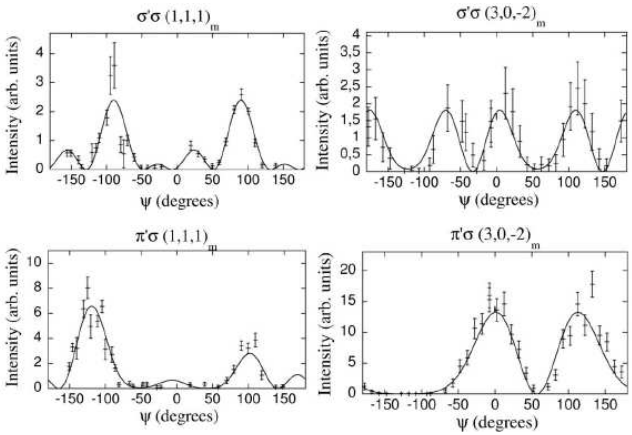
-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

- charge and orbital order in a large number of relevant materials: manganites, vanadites, ferrites, etc

- modern analysis methods of local crystal structure (eg. in manganites), and of the electronic state (multipole orders)





Octupole and anapole order on the V ions in V_2O_3: reassessment of the origin of the magnetic order and of the nature of the Mott state.

Lovesey et al, PRB 75, 014409 (2007)

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order (nonspherical electron density)

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

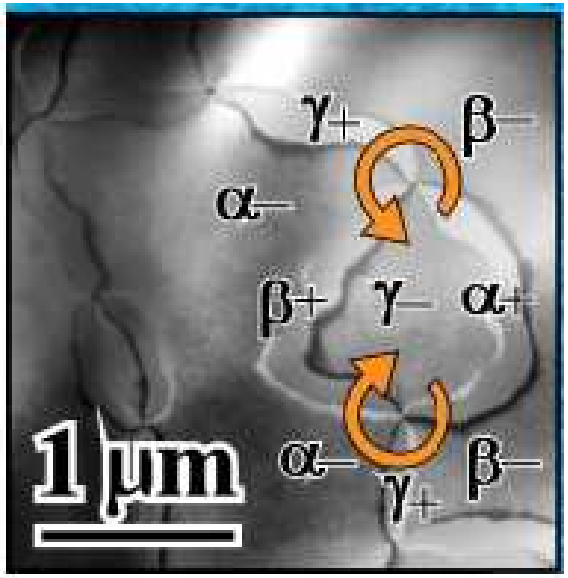
- materials with induced order on non-magnetic ions, as in UGa_3 and UAs

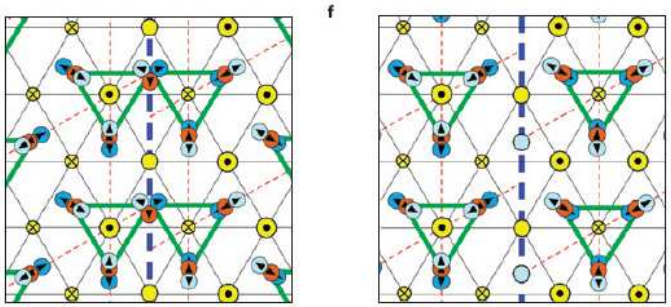
Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

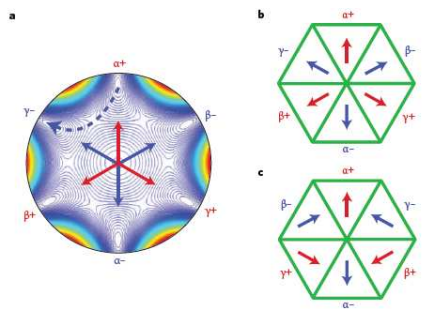
- “scanning”: domain physics

Domains in multiferroics (enough signal ?)

h-$YMnO_3$





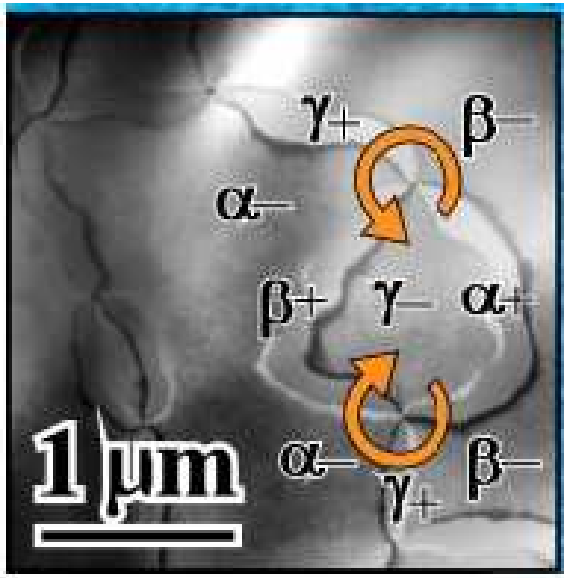


Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

- “scanning”: domain physics

Domains in multiferroics (enough signal ?)

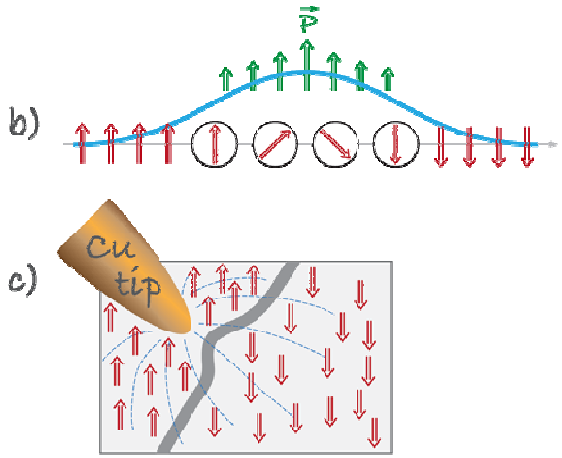
h-$YMnO_3$



-vortex interactions

-graph theory

-control of domain walls



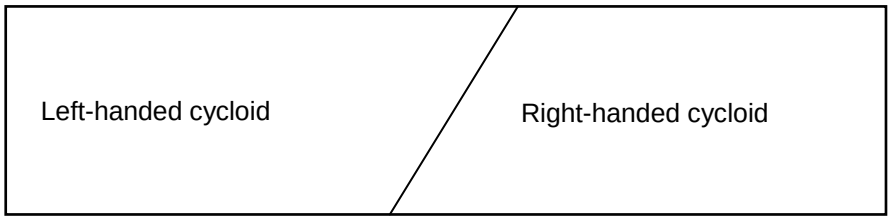
Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

- “scanning”: domain physics

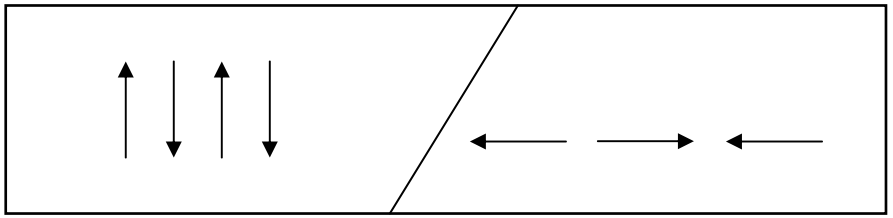
Domains in multiferroics (enough signal ?)

$TbMnO_3$

$BiFeO_3$



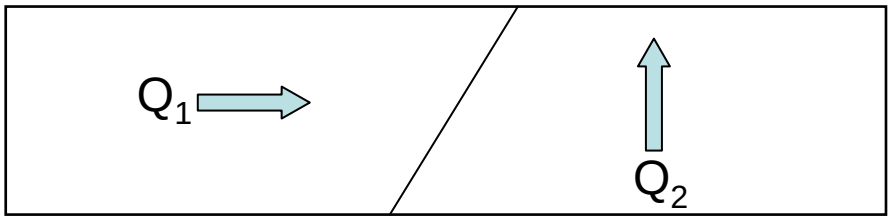
Circular dichroism



Linear dichroism

$CoCr_2O_4$

$Ba_2CoGe_2O_7$



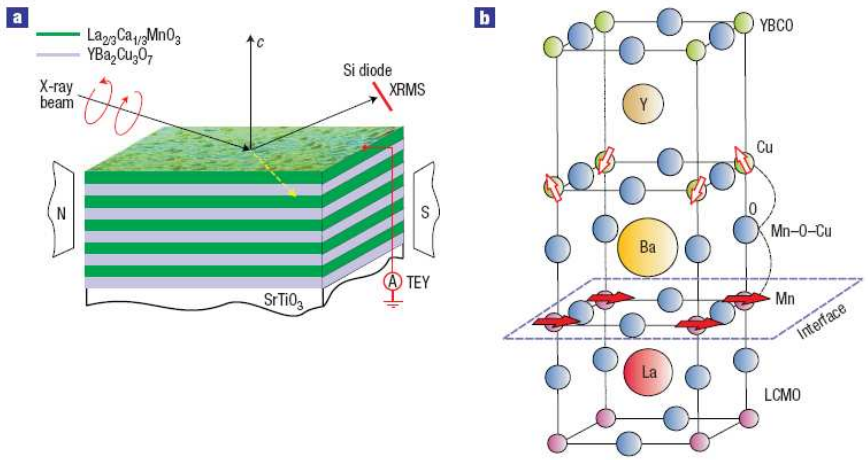
Multiple Q

Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

- other applications?

“traditional” magnetic layered systems?

oxide superlattices – can anything be done?



Resonant X-ray Scattering: Magnets and Strongly-Correlated Systems

-“traditional”: magnetic order, multipolar order, nonspherical electron density

- “scanning”: domain physics

- other applications?

Edges: 3d K, 4d L, 5d L, 4f L, 5f M (2.5 – 15 keV)

Polarization control of the incoming beam; Polarization analysis

Microbeam and scanning capability