Part 2 extra bit: unseen complexities

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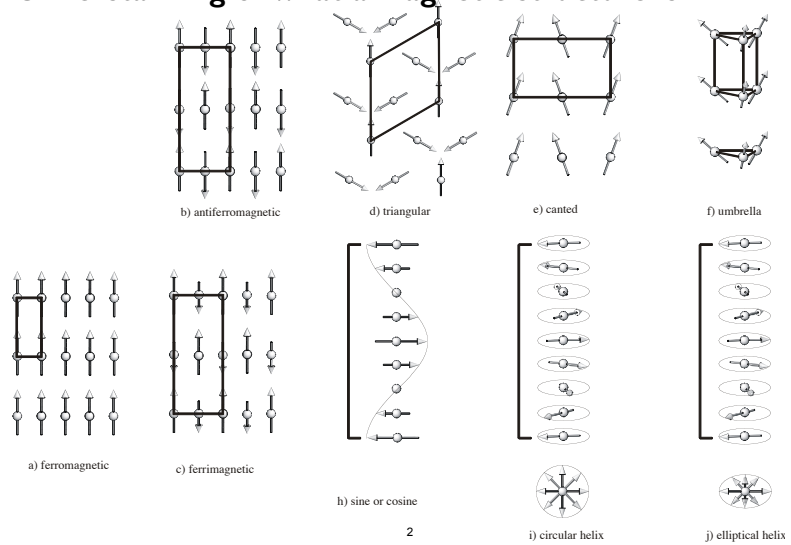
Understanding of what a magnetic structure is



But what about unseen complexities?

- Information is lost depending on the technique used
  - Go through alternative models - perhaps more than one model will fit your data. If so, think about hidden symmetries
  - Consider what you cannot see and the subtle points of a magnetic structure
  - Perhaps you need another experiment to characterise things that you cannot see and to complete the study

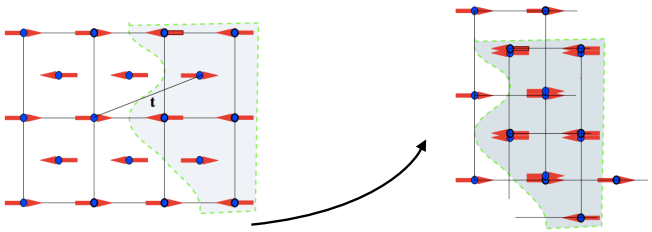
But what about unseen complexities?

- Types of domain (characterised by the types of symmetry elements lost during the magnetic ordering)

Translational domains	(translational symmetry)
Pi domains	(spin reversal)
Orientational (K, S) domains	(rotational symmetry)
Chiral domains	Centrosymmetry

Slip and translational domains

- Regions in which all the moment directions in one domain are related to another by translational symmetry
- The intensity and the polarisation scattered by the two domains are identical



Apply translation ***t***

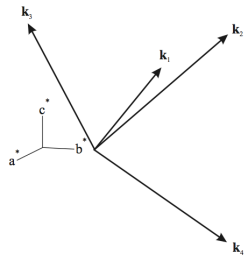
π- domains

- Regions in which all the moment directions in one domain are reversed with respect to those in the other
- Ferromagnetic domains provide a simple example
- The intensity and the polarisation scattered by the two domains are identical

k domains

- Arise if $G_k <> G_0$
  - Operating with the paramagnetic symmetry elements on ***k*** generates a set of inequivalent vectors which form the star of ***k***, e.g. $\boldsymbol{k}_1=\boldsymbol{k}_1E$, $\boldsymbol{k}_2=\boldsymbol{k}_1R_2$, $\boldsymbol{k}_3=\boldsymbol{k}_1R_3$, $\boldsymbol{k}_4=\boldsymbol{k}_1R_4$...
  - e.g. FCC lattice

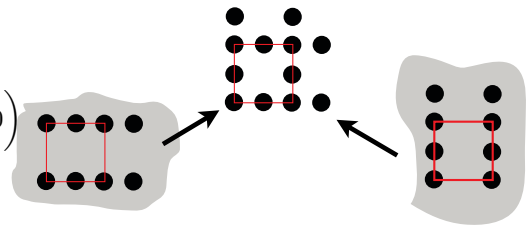
$$\vec{k}_1 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$
$$\vec{k}_2 = \left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$
$$\vec{k}_3 = \left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right)$$
$$\vec{k}_4 = \left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right)$$



k domains

- Each vector in the star generates a different configuration domain
- Each configuration domain gives a completely separate set of magnetic reflections at positions ±k from the reciprocal lattice nodes
- Each set of reflections belongs to a distinct region of the crystal, hence effectively to a single state

$$\vec{k}_1 = \left(\frac{1}{2}, 0, 0\right)$$



$$\vec{k}_2 = \left(0, \frac{1}{2}, 0\right)$$

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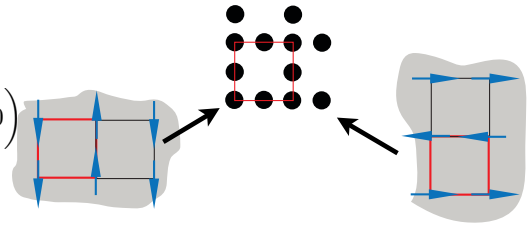
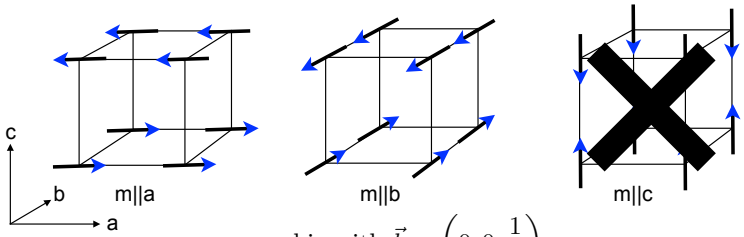


$\vec{k}_2 = \left(0, \frac{1}{2}, 0\right)$

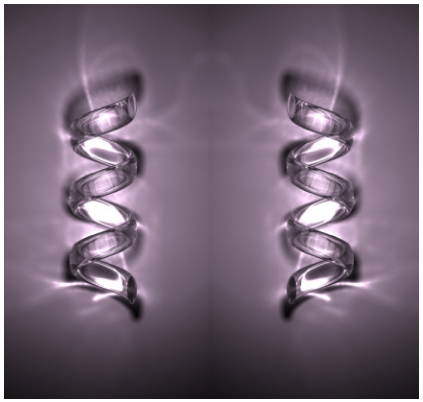
Orientational domains (S-domains)

- Occurs when the symmetry of the magnetic structure is less than that of the crystal space group
- S domains are related by the symmetry elements that are lost (***k*** does not change)
- The relationship between ***m*** and ***k*** is the same for all ***s*** domains
- Distinguish by single crystal diffraction, not powder diffraction



e.g. cubic with $\vec{k} = \left(0, 0, \frac{1}{2}\right)$

Chiral domains



- Occurs when
  - Paramagnetic space group is centrosymmetric but the magnetic structure is not
  - The magnetic moments on centrosymmetrically related sites are not parallel
  - Incommensurate structures
    - When 2***k*** is not a reciprocal lattice vector
    - In this case the two chirality domains correspond to +***k*** and -***k***.They give contributions at (hkl) ± ***k***

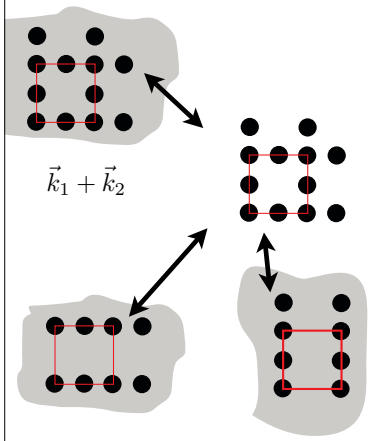
Unseen complexities

- Within the Fourier description of magnetic structures, each single domain follows

$$m_j^{\vec{k}} = \sum_{\nu,\vec{k}} C_\nu^{\vec{k}} \; \psi_\nu^{\vec{k}} \; e^{-2\pi i \vec{k}\cdot\vec{t}}$$

- In the absence of unbalancing constraints (applied magnetic or electric field, pressure, etc) these will have the same energy
- Leads to questions
  - are there S-domains
  - multi-k or k-domain?

k-domains vs multi k



$\vec{k}_1 = \left(\frac{1}{2}, 0, 0\right)$ $\vec{k}_2 = \left(0, \frac{1}{2}, 0\right)$

- Example of diffraction pattern (structure) with 2k vectors:

$$\left(\frac{1}{2}, 0, 0\right) + \left(0, \frac{1}{2}, 0\right)$$

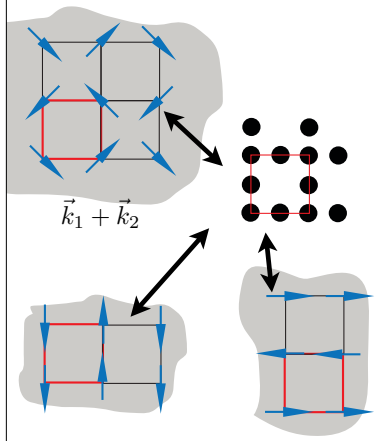
- 2k structure

  or

- 2 domains?

x

k-domains vs multi k



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- Example of diffraction pattern (structure) with 2k vectors:

$$\left(\frac{1}{2}, 0, 0\right) + \left(0, \frac{1}{2}, 0\right)$$

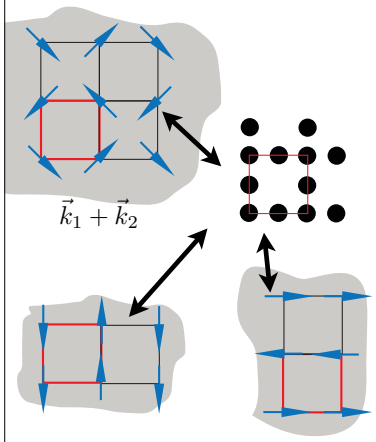
  – Both will contribute to the same reflections

  – Cannot distinguish by simple diffraction

    - 2k structure
    - 2 k-domains

13

k-domains vs multi k



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- External constraint, e.g.

  – Applied magnetic field

  – Pressure

  - Leads to

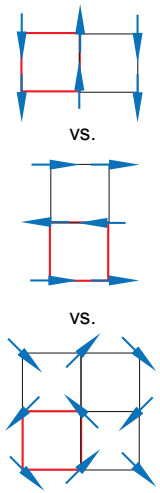
    – Unbalancing domains

    – Domain repopulation

- Multi-k and k domains structures, S-domain structures respond differently

14

Diffraction- Single crystal and powder



- Powder diffraction

  – (diffraction pattern projected onto a line)

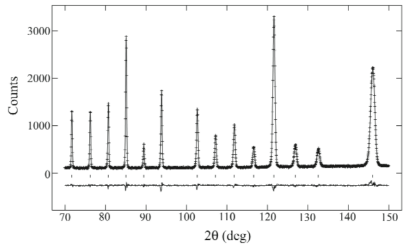
  – Cannot even see k-domains/multi-k

  – But you can always consider the possibilities and effects such as single-ion anisotropy...

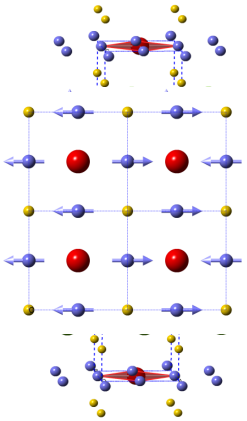
- Single crystal diffraction

  - Possible to apply constraint to differentiate k domains from multi-k

  - explore S-domains



$La_2O_2Fe_2OSe_2$ - Representational Analysis



- Related to the iron-based superconductors, but has magnetic order
- Want to understand drives and the competition between magnetic order and superconductivity
- Antiferromagnetic order below ~ 90 K
- $\boldsymbol{k}_1$=(½, 0 ½) and $\boldsymbol{k}_2$=(0 ½ ½) with respect to the crystallographic space group I4/mmm
  - In 1-k structure, 2 orbits. Need : Γ_2 (m||a) on Fe1 and Γ_3 (m||a) on the Fe2 site. Collinear
  - 2 k structure, just Γ_3 from Fe2 and **think about why it is 2-k**

D.G. Free and J.S.O. Evans Phys. Rev. B **81**, 214433 2010, E. McCabe, C. Stock, E.F. Rodriguez et al., Phys. Rev. B 89, 100402 (2014)

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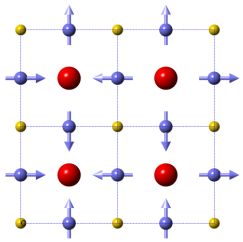

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  - 2 k structure, just Γ_3 from Fe2 and **think about why it is 2-k**
    - **Care. Both components have the same energy. Not possible to make 2-k structure with 2nd order terms**
    - **Need Ising anisotropy with higher order anisotropic exchange terms**

D.G. Free and J.S.O. Evans Phys. Rev. B **81**, 214433 2010, E. McCabe, C. Stock, E.F. Rodriguez et al., Phys. Rev. B 89, 100402 (2014)

So, what are magnetic symmetries?

Parts of the puzzle and a language to frame its possibilities:

- Space group G_0
- k-vector, $\boldsymbol{k}$ and its space group, $G_{\boldsymbol{k}}$
- IRs, Γ and associated basis vectors, ψ
- Isotropy vector, η and associated subgroup, G_η
- Magnetic space group, MSG - a convenient classification of magnetic symmetry; not always the same as IR / basis vector symmetry
- Magnetic point group, MPG - a convenient underused classification
- *Combine symmetry types with Landau theory to make phase diagram*
- *Is one of the classifications preferable?* ***The answer depends on what one wants to use a classification for***

Magnetic (space groups) *or* representation theory - *Just a question of priorities and needs?*

- Subtle physical properties will come from a subtle electronic properties and subtle couplings. Expect a subtle magnetic structure
- The wolf in sheep clothing