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Magnetic Neutron Diffraction

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J. Rodriguez-Carvajal (ILL)

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What's a magnetic structure?

Why study magnetic order?

Generic description (k-vector formalism)

- Related to representation/symmetry analysis (not covered)
- Alternative to Shubnikov symmetry, which are *TABULATED* crystallographic magnetic space groups : this is however restricted to *commensurate* structures

The magnetic structure factor

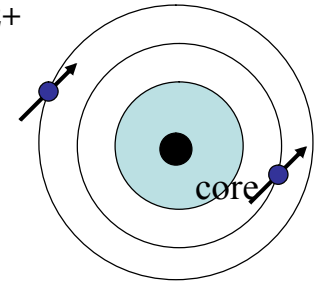
Practical aspects (Experimental choices / software, and methods for magnetic structure determination)

Note on available software:
Fullprof : General, k-vector formalism
GSAS: Contains Shubnikov symmetry, but restricted to *commensurate* structures

What's a magnetic structure?

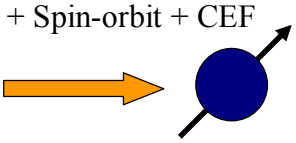
(atomic) magnetic moments (m) arise from quantum effects in atoms/ions with unpaired electrons

Ni^{2+}



« Quantum description»

Intra-atomic electron correlation
Hund's rule(maximum total S)
+ Spin-orbit + CEF



« Classical description»

$\mathbf{m} = g_J \mathbf{J}$ (**J=L+S** 4f-rare earths)

$\mathbf{m} = g_S \mathbf{S}$ (3d-transition metals)

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What's a magnetic structure?

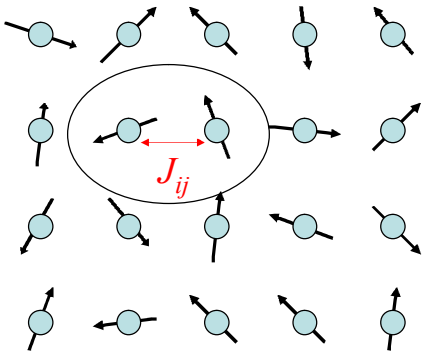
Magnet: crystal containing magnetic atoms

kT >> J_{ij},

$$E_{ij} = -J_{ij}\ \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\langle \mathbf{S}_i \rangle = 0$$

paramagnetic (disordered) state



Temperature (entropy) overcomes magnetic energy:
Entropy essentially dominated by local magnetic moment fluctuations

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What's a magnetic structure?

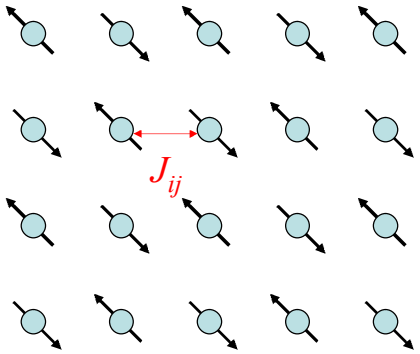
Magnet: crystal contaning magnetic atoms

$\mathbf{kT < J_{ij}}$,

$$E_{ij} = -J_{ij}\ \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\langle \mathbf{S}_i \rangle \neq 0$$

Exemple here: $J_{ij}>0$
Antiferromagnetic coupling (AF)



Magnetic energy overcomes the entropy :
⇒ Quasi-static configuration of magnetic moment with small fluctuations that are made cooperative by the magnetic exchange (spin waves excitations)

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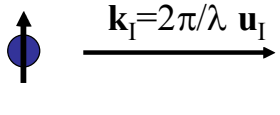
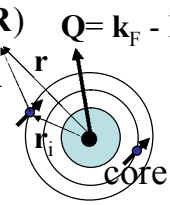
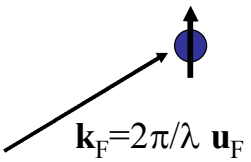
Magnetic scattering

$$\boldsymbol{\mu}_N = -\gamma\mu_N\boldsymbol{\sigma}$$



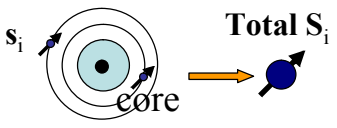




Dipolar interaction term with one electron

$$\langle \mathbf{k}_F | V_M | \mathbf{k}_I \rangle = \int e^{i\mathbf{k}_I.\mathbf{r}} \underbrace{-\gamma\mu_N\boldsymbol{\sigma}.\frac{\mu_0}{4\pi}\nabla\left(\frac{2\mu_B S\times\mathbf{R}}{R^3}\right)}_{\mathbf{B}_S(\mathbf{R})} e^{-i\mathbf{k}_F.\mathbf{r}}.d\mathbf{r}$$

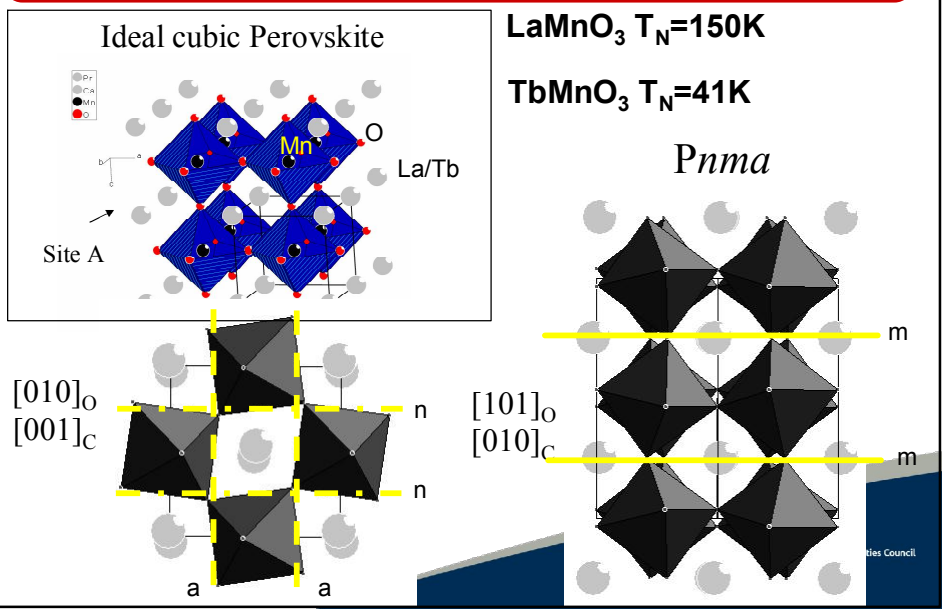
$$\langle \mathbf{k}_F | V_M | \mathbf{k}_I \rangle = 4\pi.\mathbf{Q}\times\underbrace{\left(\sum_i \exp(i\mathbf{Q}.\mathbf{r}_i).\mathbf{s}_i\right)}_{f(\mathbf{Q}).\mathbf{S}_i}\times\mathbf{Q}$$



=> vector scattering amplitude for one atom

$$\langle \mathbf{k}_F | V_M | \mathbf{k}_I \rangle = 4\pi.f(\mathbf{Q}).\mathbf{Q}\times\mathbf{S}_i\times\mathbf{Q}$$

Example: $R_{1-x}D_xMnO_3$ manganites
(R^{3+}: La, Pr… D^{2+}: Ca, Sr…)



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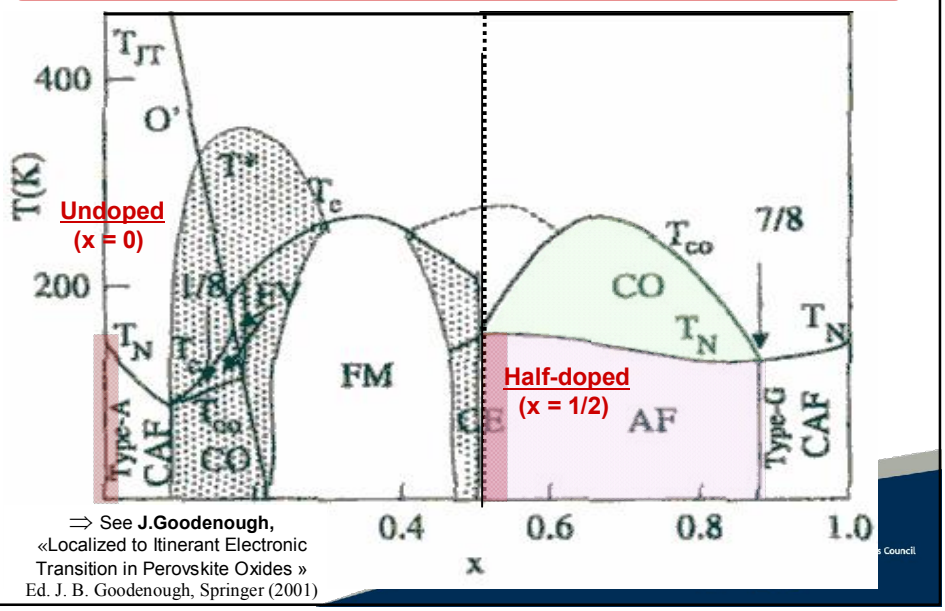

⇒ See **J.Goodenough,** «Localized to Itinerant Electronic Transition in Perovskite Oxides » Ed. J. B. Goodenough, Springer (2001)

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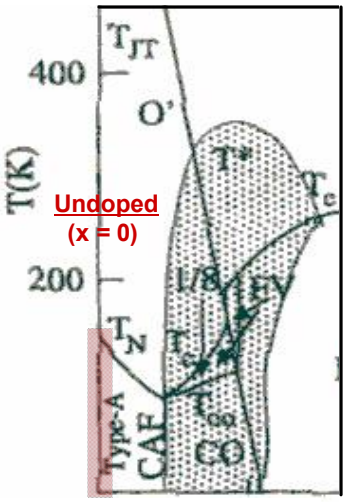

Undoped
(x = 0)

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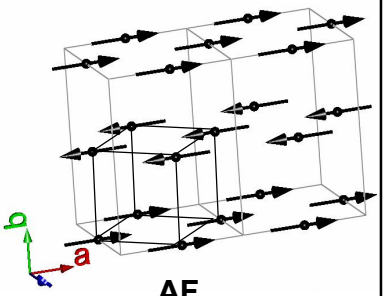
$LaMnO_3$ T_N=150K



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Commensurate structure

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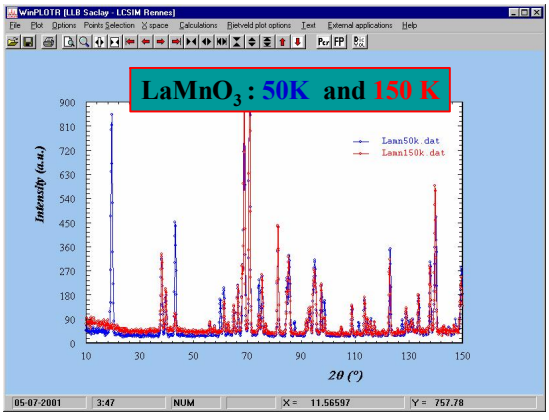

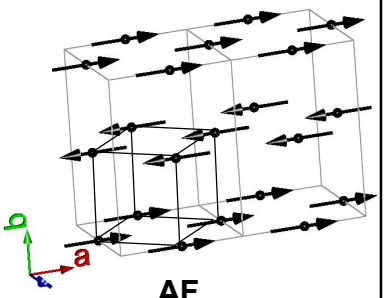

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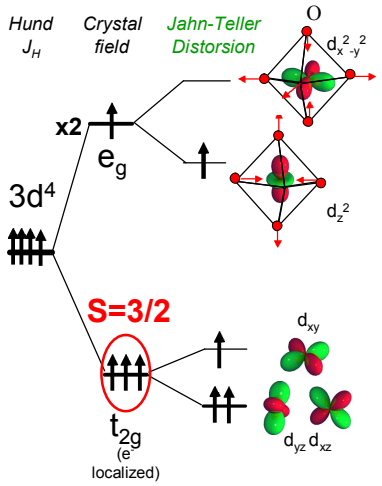
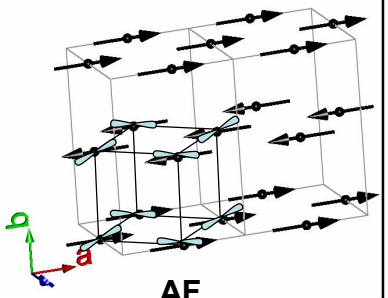
Commensurate structure

Example: $RMnO_3$ manganites

Electronic structure of Mn^{3+} (x=0)



$LaMnO_3$ T_N=150K



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Commensurate structure

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Example: $R_{1-x}D_xMnO_3$ manganites

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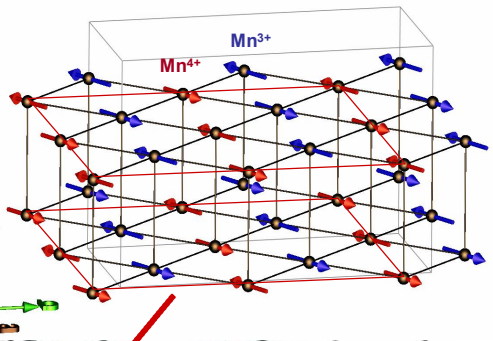

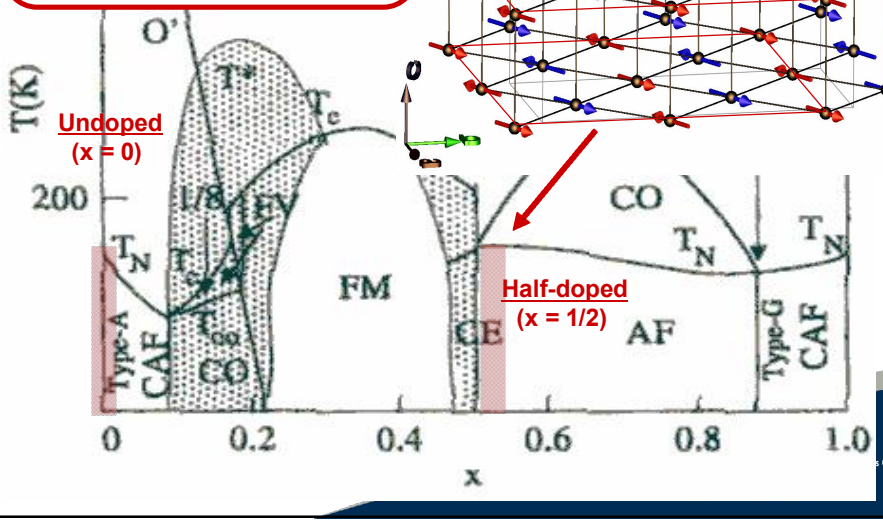

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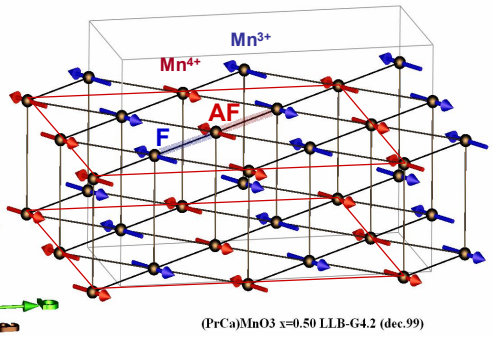


First NPD study of $La_{1/2}Ca_{1/2}MnO_3$:

Wollan and Khoeler

Phys. Rev. **100,** 545 (1955)

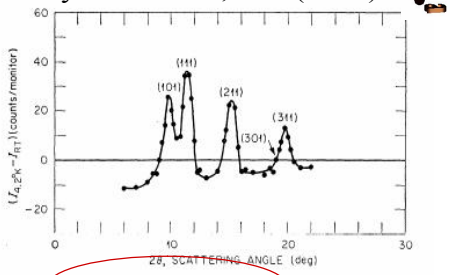
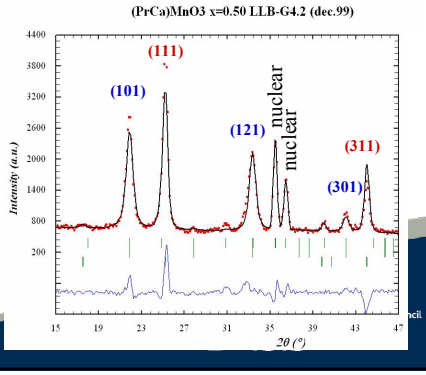


FIG. 7. Temperature difference pattern taken with Soller slits for (0.5 La—0.5 Ca)MnO_3 No. 66. *CE*-Type antiferromagnetic structure.



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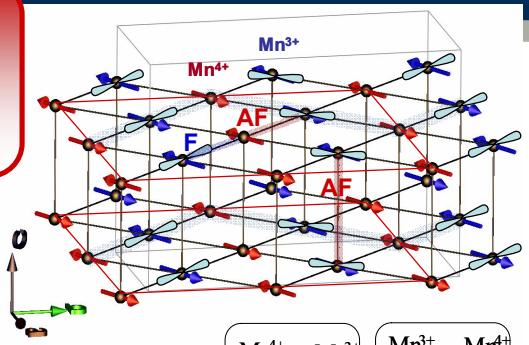
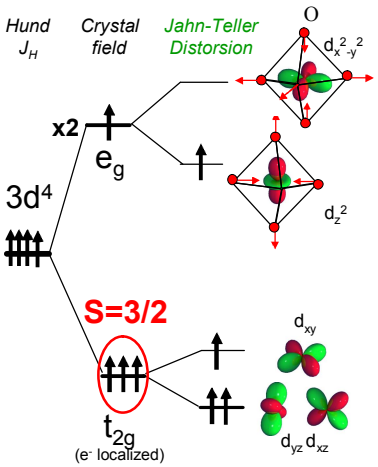
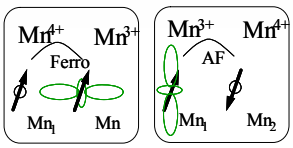


Electronic structure of Mn^{3+}

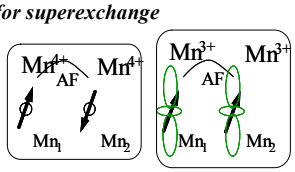


Couplings in the (a, b) plane



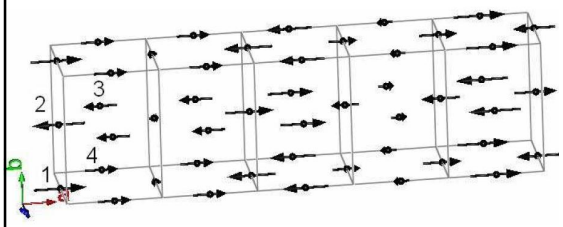
Goodenough-Kanamori-Anderson (GKA) rules for superexchange

Couplings along the c direction

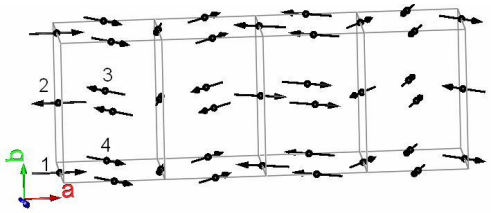


Example: $RMnO_3$ manganites

$TbMnO_3$ $T_{N2}<T<T_{N1}=41K$ Sinusoidal

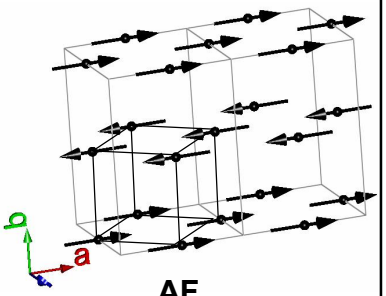


$T<T_{N2}=23K$ Cycloid



Incommensurate structures

$LaMnO_3$ $T_N=150K$



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Commensurate structure

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Why study magnetic order?

- Fundamental properties of condensed matter. Exchange interactions related to the electronic structure.
- The first (necessary) step before determining the exchange interactions (generally, with inelastic neutron scattering)

- Permanent magnet industry. Chemical substitutions controlling single ion anisotropy, strength of effective interactions, canting angles, etc: NdFeB materials, $SmCo_5$, hexaferrites, spinel ferrites.
- Spin electronics, thin films and mutilayers

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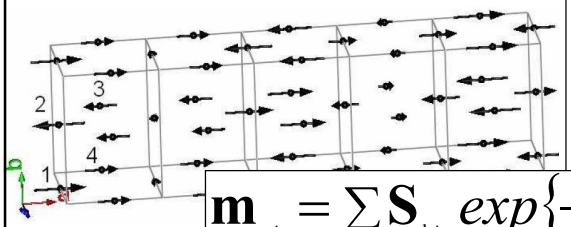
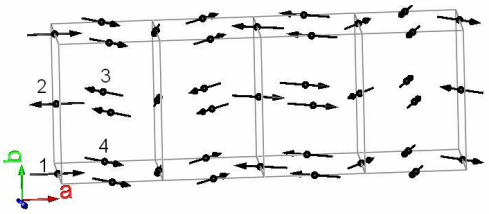


$T<T_{N2}=$

$$\mathbf{m}_{nj} = \sum_{\{k\}} \mathbf{S}_{kj} \, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$



Incommensurate structures

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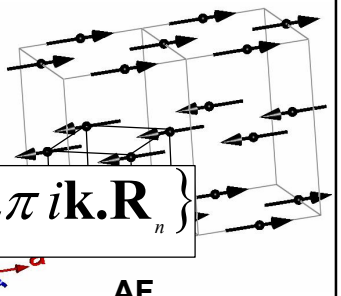

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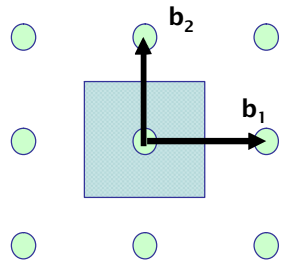
General description (k-vector formalism)

Reciprocal k-space

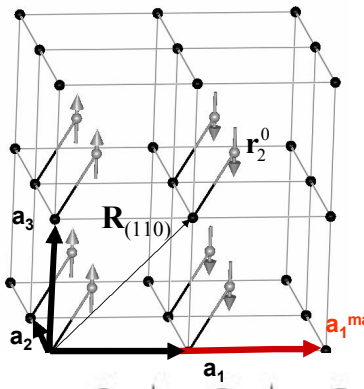


Nuclear reflections

$\mathbf{H}=h.\mathbf{b}_1+k.\ \mathbf{b}_2+l.\ \mathbf{b}_3$

$\mathbf{a}_1^{mag}=2\mathbf{a}_1 \quad \mathbf{a}_2^{mag}=\mathbf{a}_2 \quad \mathbf{a}_3^{mag}=\mathbf{a}_3$

Crystal+AF mag structure



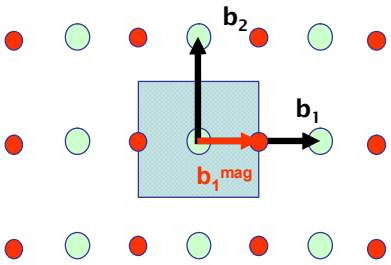
$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

$$\mathbf{r}_j^0 = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$$

$$\mathbf{r}_j^n = \mathbf{R}_n + \mathbf{r}_j^0$$

General description (k-vector formalism)

Reciprocal space



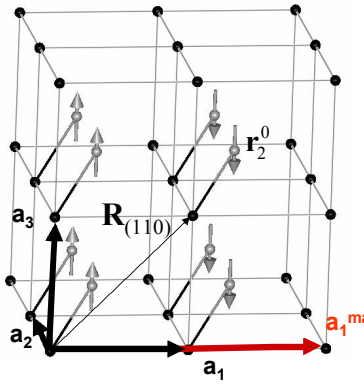
Nuclear reflections

Magnetic reflections

$\mathbf{h}=h_{mag}.\mathbf{b}_1^{mag}+k.\ \mathbf{b}_2+l.\ \mathbf{b}_3$

in fact the AF arrangement =>…
h_{mag} necessarily odd (type, 2h+1)

Crystal+AF mag structure



$\mathbf{a}_1^{mag}=2\mathbf{a}_1 \quad \mathbf{a}_2^{mag}=\mathbf{a}_2 \quad \mathbf{a}_3^{mag}=\mathbf{a}_3$

$\mathbf{b}_1^{mag}=\mathbf{b}_1/2$

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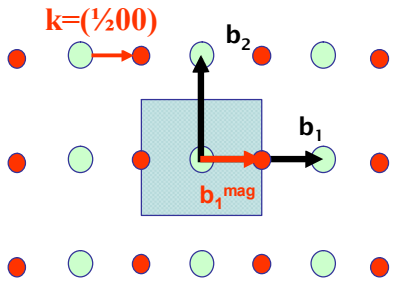
General description (k-vector formalism)

Reciprocal space



Nuclear reflections

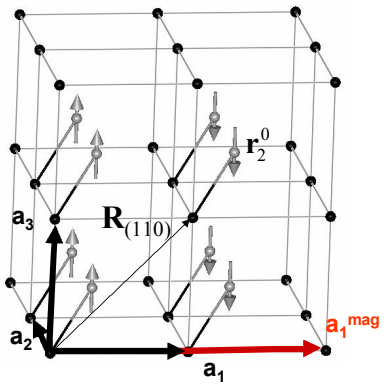
Magnetic reflections

$\mathbf{h}=(2h+1).\ \mathbf{b}_1/2+k.\ \mathbf{b}_2+l.\ \mathbf{b}_3$

$\mathbf{h}=h.\mathbf{b}_1+k.\ \mathbf{b}_2+l.\mathbf{b}_3+\mathbf{b}_1/2$

$\mathbf{h}=H+\mathbf{k}$ « Propagation vector »

Crystal+AF mag structure



$\mathbf{a}_1^{mag}=2\mathbf{a}_1$ $\mathbf{a}_2^{mag}=\mathbf{a}_2$ $\mathbf{a}_3^{mag}=\mathbf{a}_3$

$\mathbf{b}_1^{mag}=\mathbf{b}_1/2$

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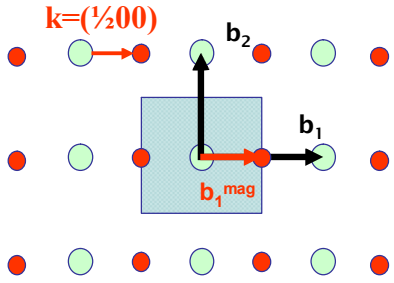
General description (k-vector formalism)

Reciprocal space



Nuclear reflections

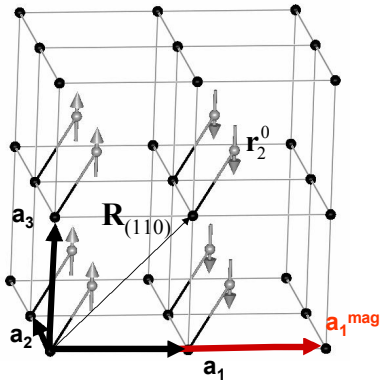
Magnetic reflections

$\mathbf{h}=(2h+1).\ \mathbf{b}_1/2+k.\ \mathbf{b}_2+l.\ \mathbf{b}_3$

$\mathbf{h}=h.\mathbf{b}_1+k.\ \mathbf{b}_2+l.\mathbf{b}_3+\mathbf{b}_1/2$

$\mathbf{h}=H+\mathbf{k}$

Crystal+AF mag structure



$$\mathbf{m}_{[n]i}=\mathbf{S}_i.\ (-1)^{n1}$$

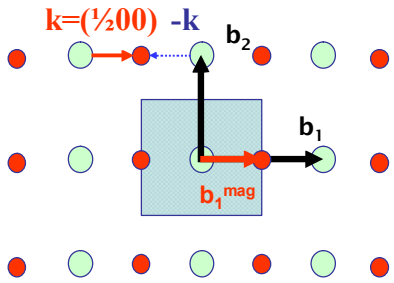
$$\mathbf{R}_n=n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3$$

$$\mathbf{m}_{nj}=\mathbf{S}_{kj}\ exp\{-2\pi i\mathbf{k}.\mathbf{R}_n\}$$

because $\mathbf{k}.\mathbf{R}_n=n_1/2$

General description (k-vector formalism)

Reciprocal space



Nuclear reflections

Magnetic reflections

h= H + **k**

Magnetic structure

$$\mathbf{m}_{nj} = \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

In our example (AF):

- k **equivalent** to –k

(2k is a reciprocal lattice vector, or k at the border of the brillouin zone)

- Only k sufficient to index all the magnetic reflections,
- And $\mathbf{S}_{kj}$ must be real

In general :

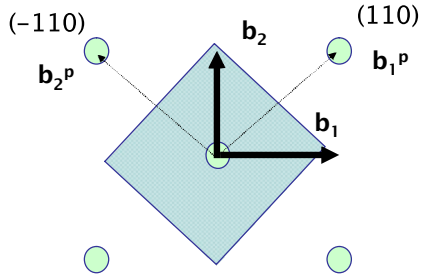
a set of {k} is needed

- And $\mathbf{S}_{kj}$ are complex vectors

$$\mathbf{m}_{nj} = \sum_{\{k\}} \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

General description (k-vector formalism)

Reciprocal space

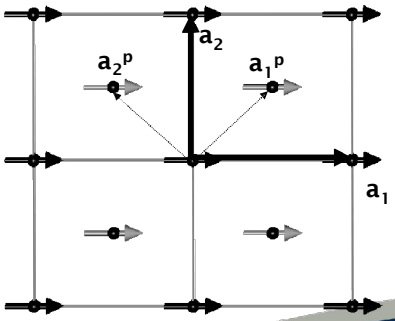


Nuclear reflections

Magnetic structure

$$\mathbf{m}_{nj} = \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

I/F-centred lattice (2D):



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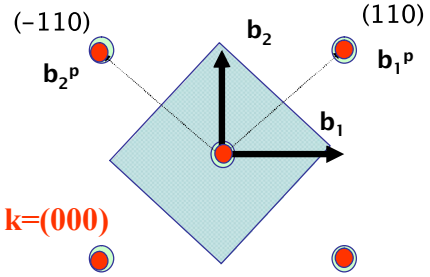
General description (k-vector formalism)

Reciprocal space



Nuclear reflections

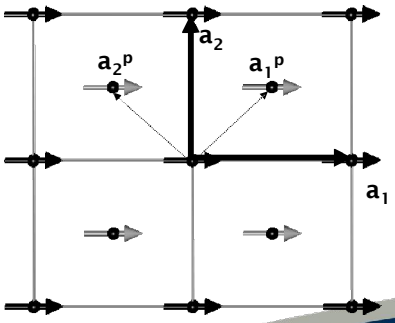
Magnetic reflections

h= H

Magnetic structure

$$\mathbf{m}_{nj} = \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

I/F-centred lattice (2D):



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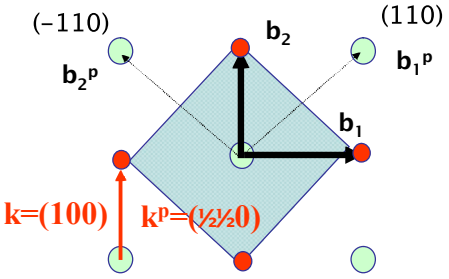
General description (k-vector formalism)

Reciprocal space



Nuclear reflections

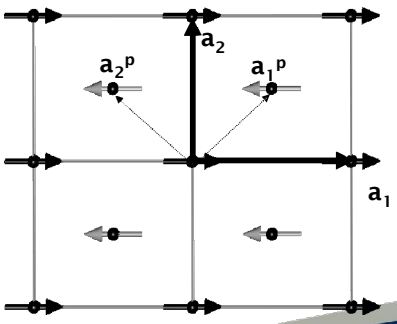
Magnetic reflections

h= H + k

Magnetic structure

$$\mathbf{m}_{nj} = \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

AF order on a centred lattice



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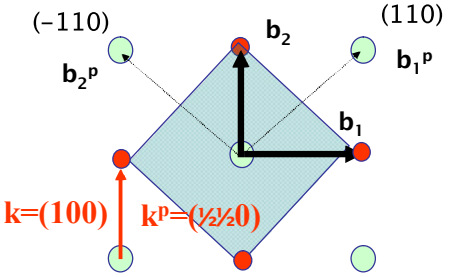
General description (k-vector formalism)

Reciprocal space



○ Nuclear reflections

● Magnetic reflections

h= H + k

Magnetic structure

$$\mathbf{m}_{nj} = \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

I-centred lattice :

- k **equivalent** to –k
  (2k is a reciprocal lattice vector)
- Because R_n contains type (½½½)… translations, k vectors, which can have integer components, have in fact non-integer components in the *primitive* cell

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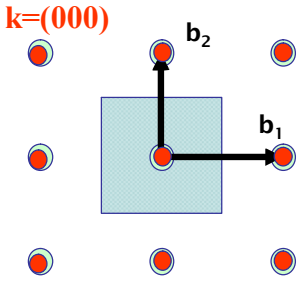
General description (k-vector formalism)

Reciprocal space

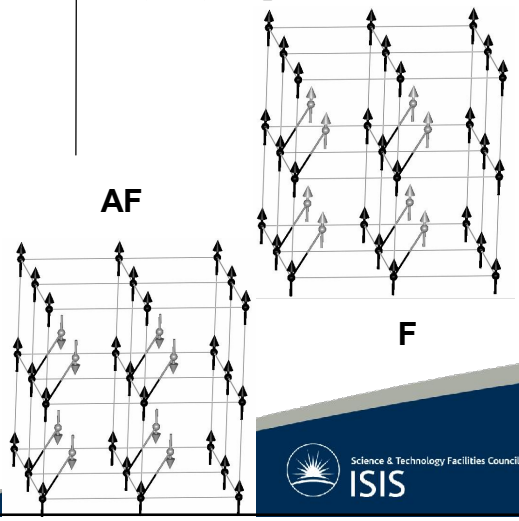


○ Nuclear reflections

● Obseved magnetic reflections

Magnetic structure

k=(000) in primitive cell:



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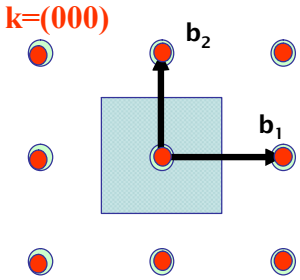
General description (k-vector formalism)

Reciprocal space



○ Nuclear reflections

● Magnetic reflections

h= H

Magnetic structure

$$\mathbf{m}_{nj} = \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

When k=(000) (primitive P):

- $\mathbf{m}_{li}=\mathbf{S}_{kj}$ whatever n:

this only means that the cell of the the magnetic structure *is the same* as that of the nuclear structure (not necessarily ferromagnetic)

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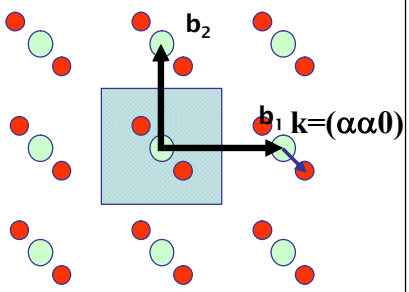
General description (k-vector formalism)

Reciprocal space



○ Nuclear reflections

● Magnetic reflections

h = **H** ± **k**

Magnetic structure

$$\mathbf{m}_{nj} = \sum_{\{k\}} \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

Especially, when {k}=k,-k: and k **NOT equivalent** to -k

- we need (k, -k) to index all the magnetic reflections,
- (k, -k) terms with complex $\mathbf{S}_{kj}$ vectors must be summed to calculate m_{lj} with the necessary condition for real $\mathbf{m}_{nj}$: $\mathbf{S}_{-kj} = \mathbf{S}_{kj}^{*}$

Incommensurate structures

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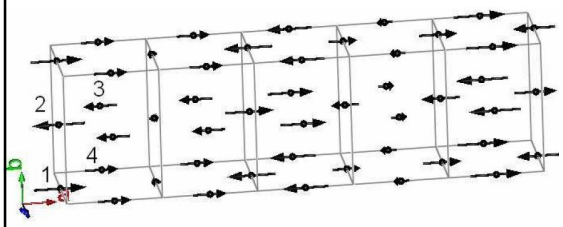
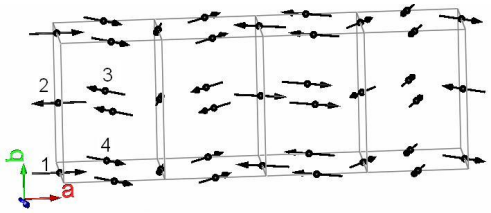
General description : Application

$TbMnO_3$ $T_{N2}<T<T_{N1}=41K$ Sinusoidal

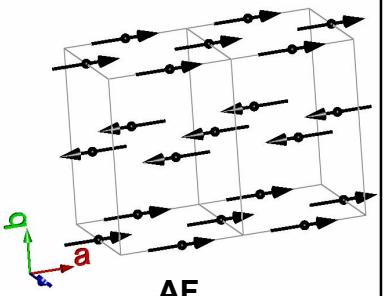


$T<T_{N2}=23K$ Cycloid



Incommensurate structures

$LaMnO_3$ $T_N=150K$



AF

Commensurate structure

Science & Technology Facilities Council ISIS

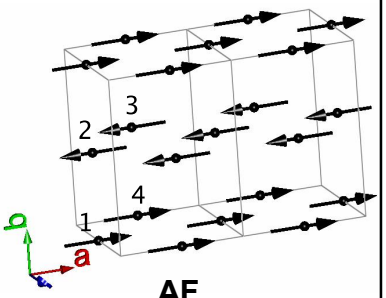
General description : Application

$$\mathbf{m}_{nj} = \sum_{\{k\}} \mathbf{S}_{kj} \, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

k=(000) $\quad \mathbf{m}_{li}=\mathbf{S}_{kj}$

$\mathbf{S}_{k1}= -\mathbf{S}_{k2}= -\mathbf{S}_{k3}= \mathbf{S}_{k4}$,
all reals vectors

$LaMnO_3$ $T_N=150K$



AF

Commensurate AF structure

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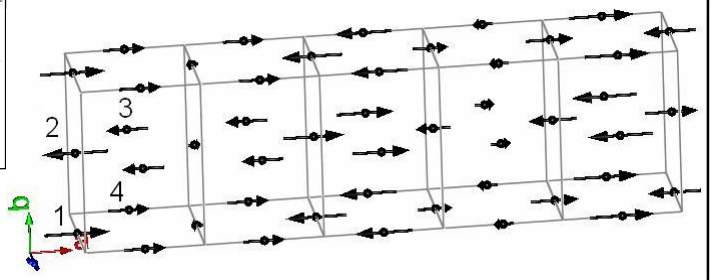
General description : Application

$TbMnO_3$ T_N<41K k=(0.28 0 0)

$$\mathbf{m}_{li} = \mathbf{S}_i^{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}_l} + \mathbf{S}_i^{-\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_l}$$
$$\mathbf{S}_i^{-\mathbf{k}} = \mathbf{S}_i^{*\mathbf{k}}$$



$$S_j^{\mathbf{k}} = 1/2(\mathbf{A}_j + i.\mathbf{B}_j)e^{-i\phi}$$

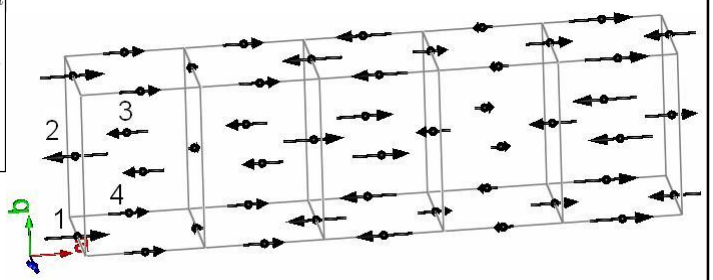
$$\mathbf{S_{jl}} = \mathbf{A_j}\cos(\mathbf{k}\cdot\mathbf{R_l} + \phi_j) + \mathbf{B_j}\sin(\mathbf{k}\cdot\mathbf{R_l} + \phi_j)$$

ISIS

General description : Application

$TbMnO_3$ T_N<41K k=(0.28 0 0)

$$\mathbf{m}_{li} = \mathbf{S}_i^{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}_l} + \mathbf{S}_i^{-\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_l}$$
$$\mathbf{S}_i^{-\mathbf{k}} = \mathbf{S}_i^{*\mathbf{k}}$$



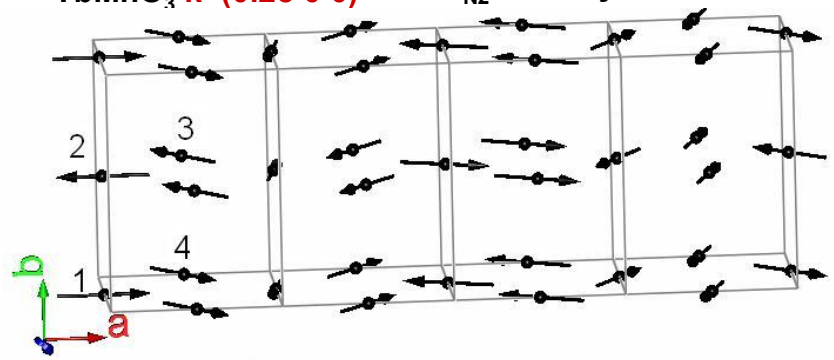
$$S_j^{\mathbf{k}} = 1/2(\mathbf{A}_j + i.\mathbf{B}_j)e^{-i\phi}$$

$\mathbf{B_j}$=0

$$\mathbf{S}_1^{\mathbf{k}} = (C_1, 0, 0)$$
$$\mathbf{S}_2^{\mathbf{k}} = (-C_1, 0, 0) \quad \phi$$
$$\mathbf{S}_3^{\mathbf{k}} = (-C_1 e^{-2i\pi.\mathbf{k}_x/2}, 0, 0)$$
$$\mathbf{S}_4^{\mathbf{k}} = (C_1 e^{-2i\pi.\mathbf{k}_x/2}, 0, 0)$$

General description : Application

$TbMnO_3$ k=(0.28 0 0) $T<T_{N2}$=23K Cycloid



$$S_j^{\mathbf{k}} = 1/2(\mathbf{A}_j + i.\mathbf{B}_j)e^{-i\phi}$$

$$\mathbf{B}_j \perp \mathbf{A}_j$$

$$\begin{aligned}
\mathbf{S}_1^{\mathbf{k}} &= 1/2(u, 0, i.v) \\
\mathbf{S}_2^{\mathbf{k}} &= 1/2(-u, 0, -i.v) \\
\mathbf{S}_3^{\mathbf{k}} &= 1/2.e^{-2i\pi.\mathbf{k}_x/2}(-u, 0, i.v) \\
\mathbf{S}_4^{\mathbf{k}} &= 1/2.e^{-2i\pi.\mathbf{k}_x/2}(u, 0, -i.v)
\end{aligned}$$

ϕ

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What's a magnetic structure?

Why study magnetic order?

Generic description (k-vector formalism)

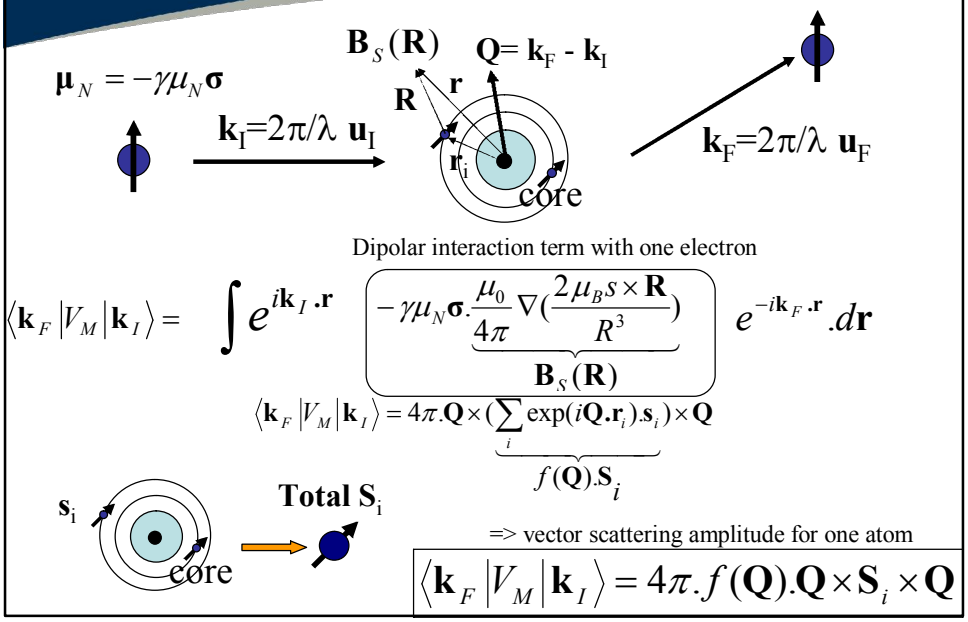
- Related to representation/symmetry analysis (not covered)
- Alternative to Shubnikov symmetry, which are *TABULATED* crystallographic magnetic space groups : this is however restricted to *commensurate* structures

The magnetic structure factor

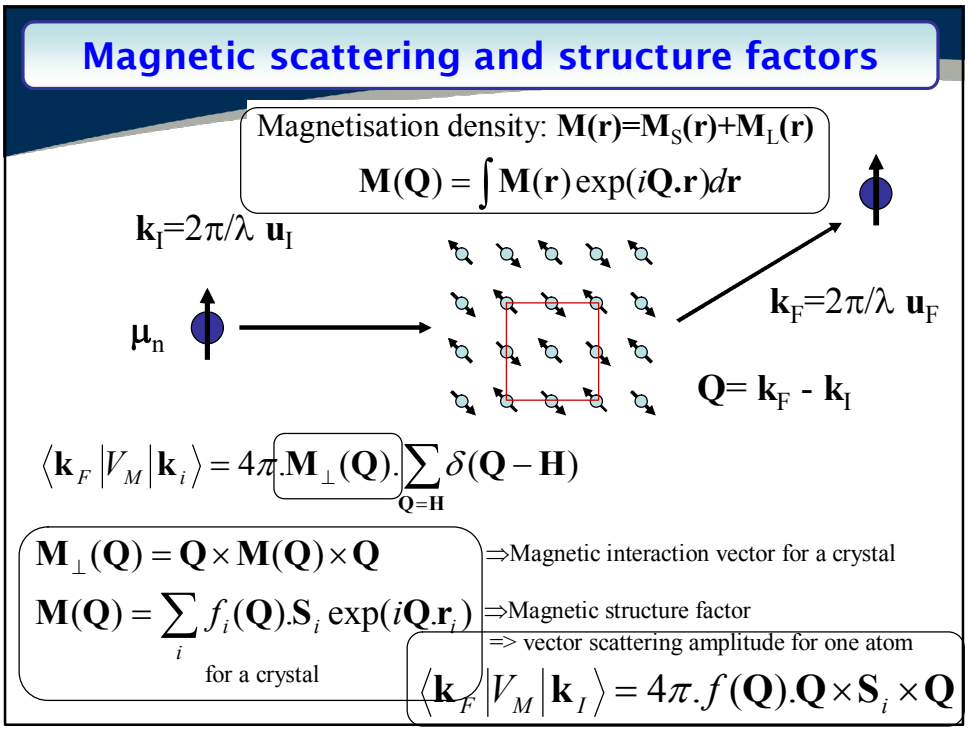
Practical aspects (Experimental choices / software, and methods for magnetic structure determination)

Note on available software:
Fullprof : General, k-vector formalism
GSAS: Contains Shubnikov symmetry, but restricted to *commensurate* structures

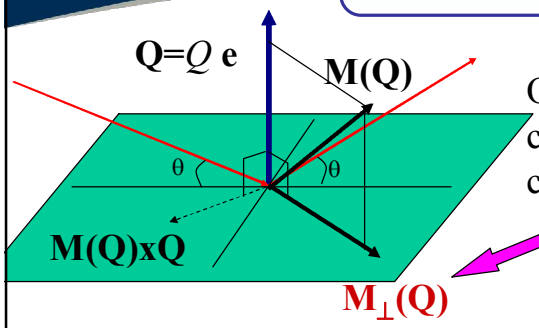
Magnetic scattering and structure factors



Magnetic scattering and structure factors



Magnetic scattering and structure factors



Only the perpendicular component of **M** to **Q**=2π**h** contributes to scattering

$$\mathbf{M}_\perp(\mathbf{Q}) = \mathbf{Q}\times\mathbf{M}(\mathbf{Q})\times\mathbf{Q}$$ ⇒Magnetic interaction vector for a crystal

$$\mathbf{M}(\mathbf{Q}) = \sum_i f_i(\mathbf{Q}).\mathbf{S}_i \exp(i\mathbf{Q}.\mathbf{r}_i)$$ ⇒Magnetic structure factor

for a crystal

=> vector scattering amplitude for one atom

$$\langle \mathbf{k}_F | V_M | \mathbf{k}_I \rangle = 4\pi . f(\mathbf{Q}).\mathbf{Q}\times\mathbf{S}_i\times\mathbf{Q}$$

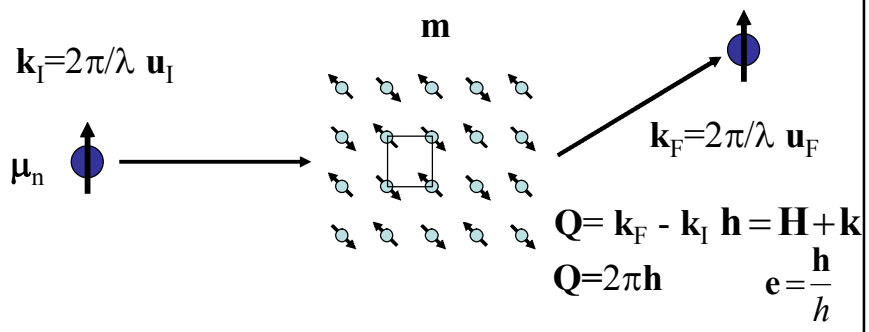
Magnetic scattering and structure factors

For non-polarised neutrons

$$I_{\mathbf{h}} = \mathbf{M}_{\perp\mathbf{h}} \cdot \mathbf{M}^*_{\perp\mathbf{h}} + N_{\mathbf{h}} N^*_{\mathbf{h}}$$

	Magnetic Phase:	***Nuclear Phase:***
Scattering vector	$\mathbf{h} = \mathbf{H} \pm \mathbf{k}$	$\mathbf{h}=\mathbf{H}$
Structural model	**Arrangement of the moments** $\mathbf{m}_{li} = \sum_{\{\mathbf{k}\}} \mathbf{S}^{\mathbf{i}}_{\mathbf{k}} exp\{-2\pi i \mathbf{k}\mathbf{R}_l\}$	**Atomic positions** $\mathbf{r}^0_{li} = \mathbf{R}_l + \mathbf{r}_i$
Structure Factor/ Intensity	$\mathbf{M}(\mathbf{h}) = p\sum_{j=1}^{n} f_j(\mathbf{h})\,\mathbf{S}^j_k \; exp\{2\pi i \mathbf{h}\mathbf{r}_j\}$ $\mathbf{M}_{\perp\mathbf{h}}$=**M(h)**-**e** (**e**·**M(h)**) with $\mathbf{e} = \frac{\mathbf{h}}{h}$ $I_{\mathbf{h}} = \mathbf{M}_{\perp\mathbf{h}} \cdot \mathbf{M}^*_{\perp\mathbf{h}}$	$F(\mathbf{H}) = \sum_{j=1}^{n} b_j exp\{2\pi i \mathbf{H}\mathbf{r}_j\}$ $I^{\text{nuc}}_{\mathbf{H}} = F(\mathbf{H}) \cdot F^*(\mathbf{H})$

Magnetic structure factor:
Summary of working formulas



$\mathbf{Q}= \mathbf{k}_F - \mathbf{k}_I \quad \mathbf{h}=\mathbf{H}+\mathbf{k}$

$\mathbf{Q}=2\pi\mathbf{h} \qquad \mathbf{e}=\frac{\mathbf{h}}{h}$

$$\mathbf{M}_{\perp\mathbf{h}} = \mathbf{e}\times\mathbf{M}(\mathbf{h})\times\mathbf{e} = \mathbf{M}(\mathbf{h}) - \mathbf{e}\,(\mathbf{e}\cdot\mathbf{M}(\mathbf{h}))$$

$$\mathbf{M}(\mathbf{h}) = p\sum_{j=1}^{n} f_j(\mathrm{h})\,\mathbf{S}_k^j \; exp\left\{2\pi i\mathbf{h}.\mathbf{r}_j\right\}$$

$$I_{\mathrm{h}} = \mathrm{M}_{\perp\mathrm{h}} \cdot \mathrm{M}^*_{\perp\mathrm{h}}$$

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What's a magnetic structure?
Why study magnetic order?

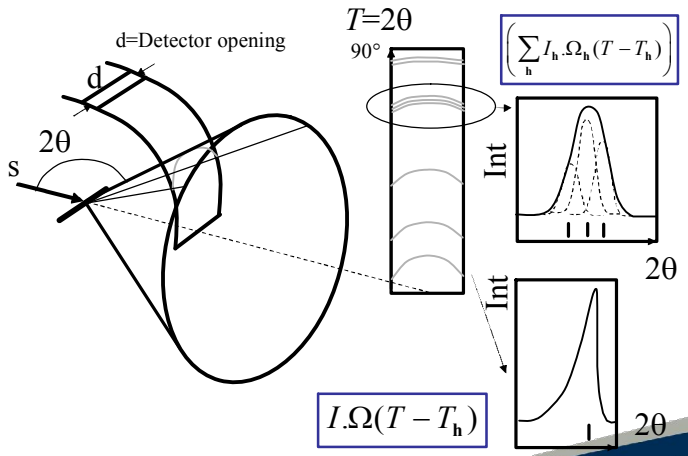
Generic description (k-vector formalism)
- Related to representation/symmetry analysis (not covered)
- Alternative to Shubnikov symmetry, which are *TABULATED* crystallographic magnetic space groups : this is however restricted to *commensurate* structures

The magnetic structure factor

Practical aspects (Experimental choices / software, and methods for magnetic structure determination)
Note on available software:
Fullprof : General, k-vector formalism
GSAS: Contains Shubnikov symmetry, but restricted to *commensurate* structures

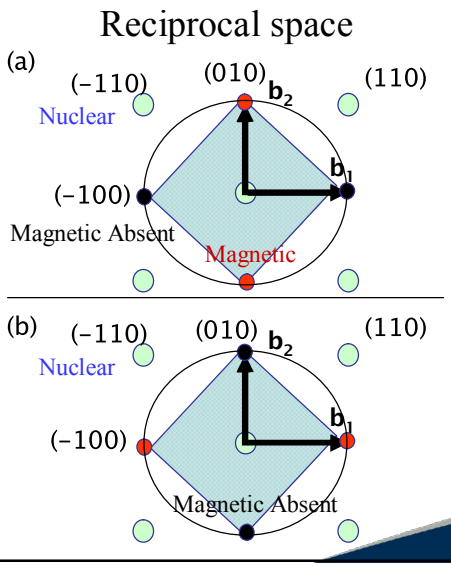
Practical aspects

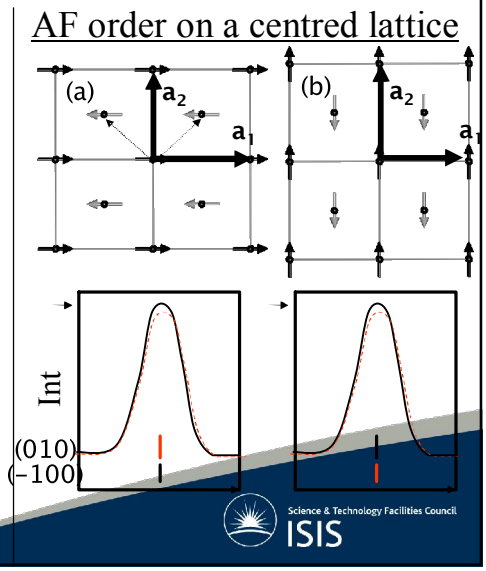
Powder diffraction: beneficiate from the power of the rieteveld technique, but problem of accidental overlap…



Practical aspects

Powder diffraction: problem of accidental overlap…





From simple to complex cases…

$$\mathbf{m}_{nj} = \sum_{\{k\}} \mathbf{S}_{kj}\, exp\{-2\pi i \mathbf{k}.\mathbf{R}_n\}$$

$$S_j^{\mathbf{k}} = 1/2(\mathbf{A}_j + i.\mathbf{B}_j)e^{-i\phi}$$

$$\mathbf{B}_j \perp \mathbf{A}_j \text{ and } A=B$$

$$\mathbf{k} = (0.0386(5),\ 0,\ 0.4229(6))$$

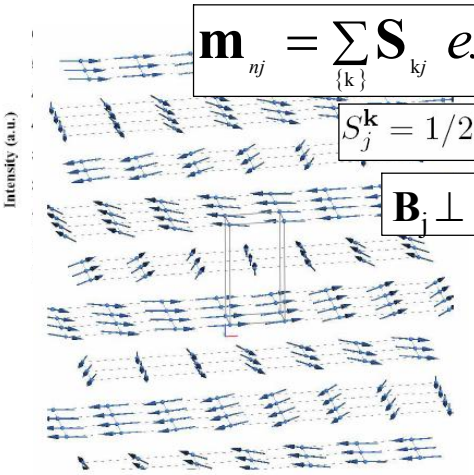
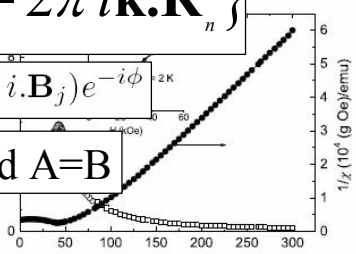
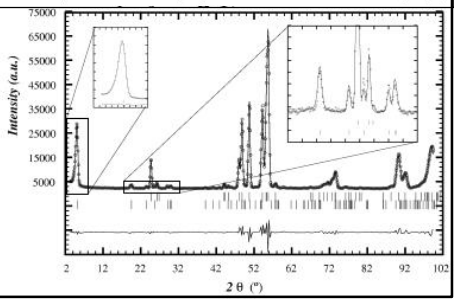


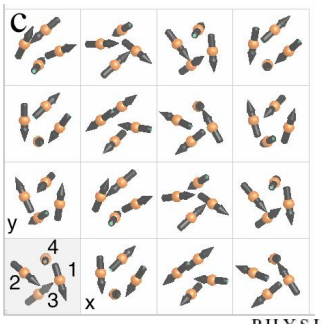
FIG. 4: Magnetic structure of $Cr_{0.5}TiSe_2$. The l = (000) crystallographic cell is indicated.





Antiferromagnetism in the ordered subsystem of Cr ions intercalated into titanium diselenide,
N. V. Baranov, A. N. Titov, V. I. Maksimov,
N. V. Toporova, A. Daoud-Aladine, A. Podlesnyak,
Journal of Physics-Condensed Matter **17**, 5255 (2005).

From simple to complex cases…



Solution/refinement of Single XTAL data
gives a magnetic structure
that shows no AF plaquettes nor dimers,
but canted pairs

VOLUME 93, NUMBER 21 PHYSICAL REVIEW LETTERS week ending 19 NOVEMBER 2004

p. 217206-1

Incommensurate Magnetic Ordering in $Cu_2Te_2O_5X_2$ (X = Cl, Br) Studied by Neutron Diffraction

O. Zaharko,* A. Daoud-Aladine, S. Streule, and J. Mesot
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P.-J. Brown
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H. Berger
Institut de Physique de la Matière Complexe, EPFL, CH-1015 Lausanne, Switzerland

(Received 19 May 2004; revised manuscript received 14 September 2004; published 18 November 2004)

From simple to complex cases…

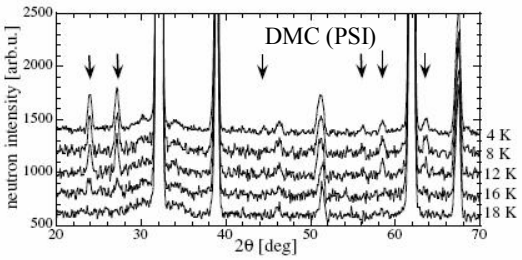
NDP

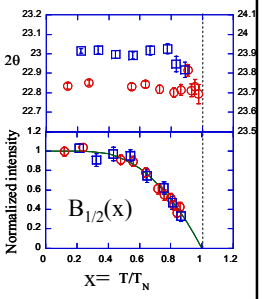
6-8 magnetic peaks

4 Cu atoms per cell

⇒

23 magnetic params





k=(-0.15 0.42 1/2)

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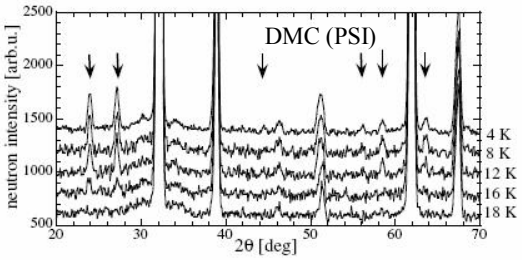
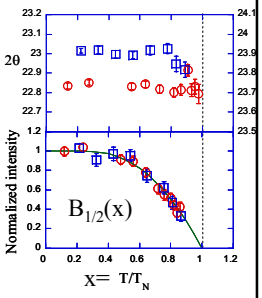


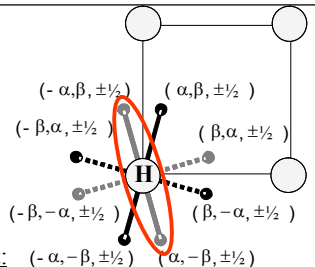


k=(-0.15 0.42 1/2)

Single XTAL

50 magnetic reflections

Structure solution:
Simulated annealing
Structure refinement:
Least squares



Star of the wave vector
⇒ Complex domain structure

Even **focusing on one arm** of the star (i.e on one domain)...

at TRICS (PSI) and D15 (ILL):

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From simple to complex cases…

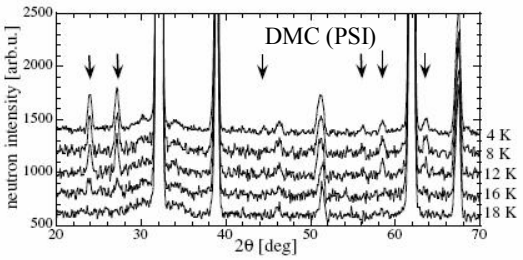
NDP

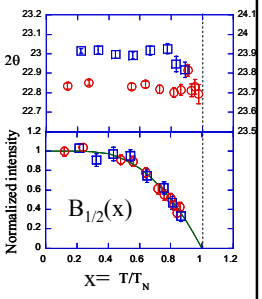
6-8 magnetic peaks

4 Cu atoms per cell

⇒

24 magnetic params





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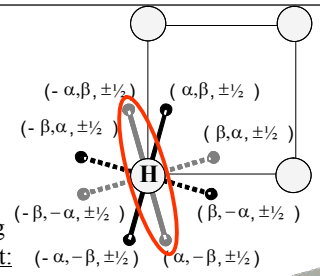
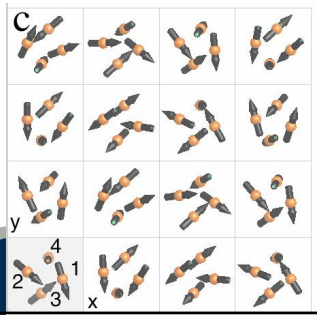


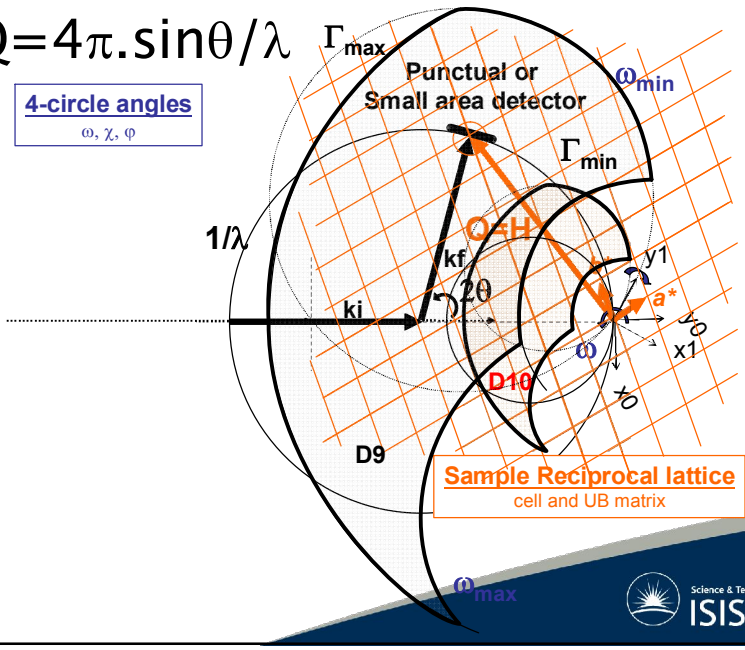
at TRICS (PSI) and D15 (ILL):



Single crystal diffraction: 4-circles

$Q=4\pi.\sin\theta/\lambda$

4-circle angles
ω, χ, φ



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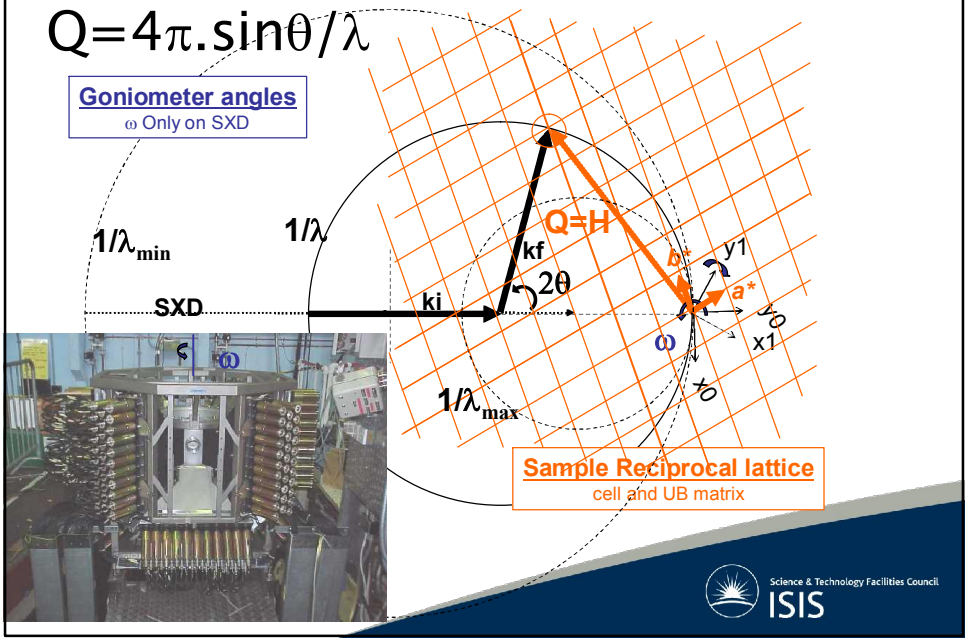
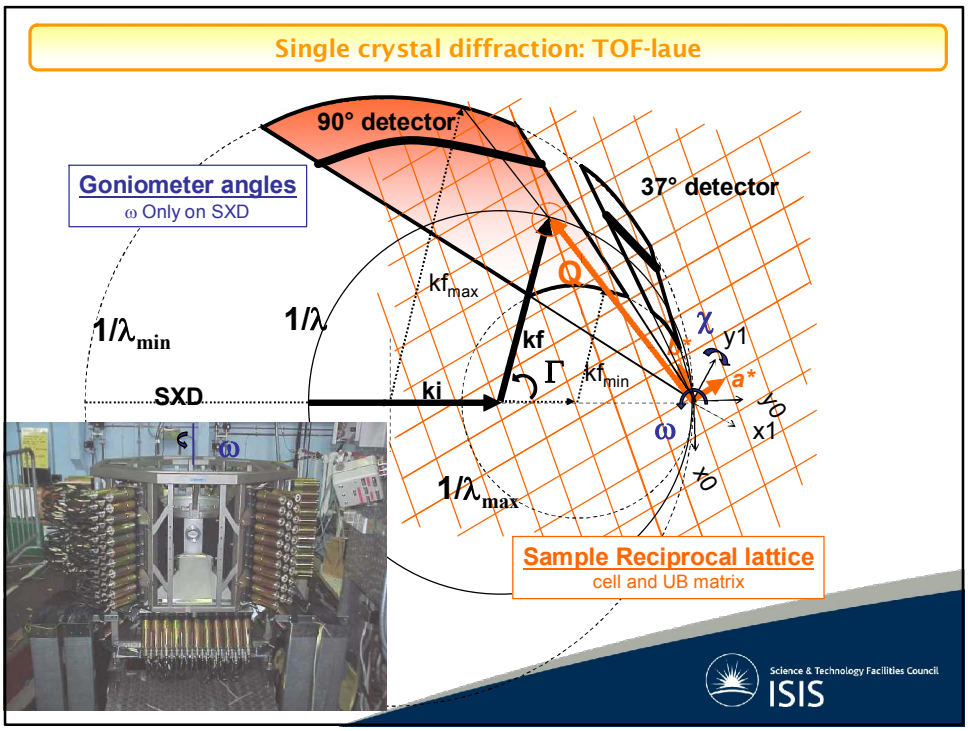
Single crystal diffraction: TOF-laue

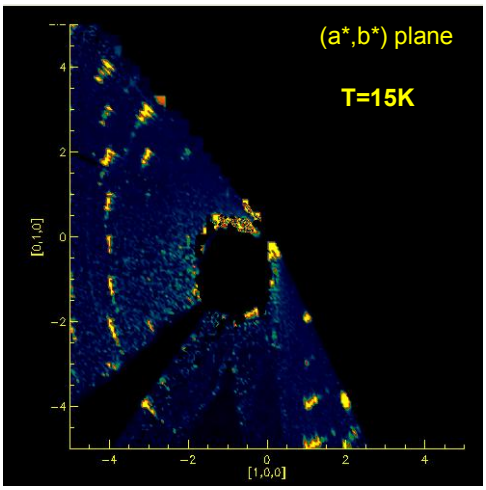
$Q=4\pi.\sin\theta/\lambda$

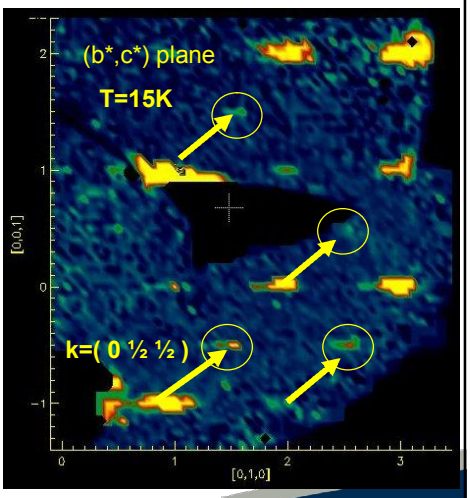


Single crystal diffraction: TOF-laue



CaV_2O_4
Quasi one dimensional magnet V^{3+} S=1





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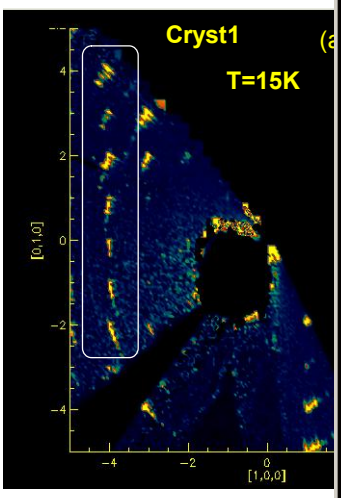

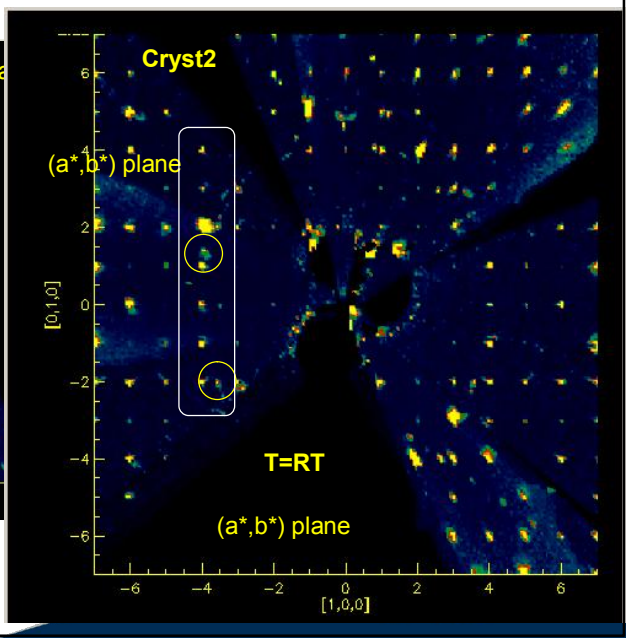

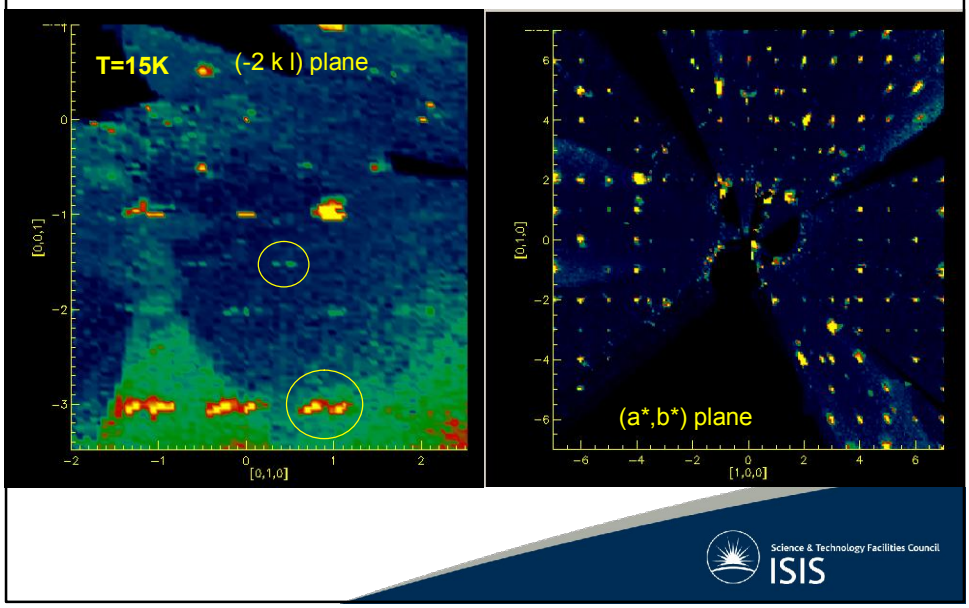

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Structure determination methods

Except for simple cases, the Rietveld "refinement" can only be a final stage of a magnetic structure determination

Before using it, a maximum number of constraints on the magnetic model are desirable (ex: symmetry analysis), or starting models can be obtained using structure solution approaches

Single crystal data are always better, but can be tricky!

For advanced topics:
see the Fullprof Suite documentation and tutorials at:

http://www.ill.fr/dif/Soft/fp/php/tutorials.html

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