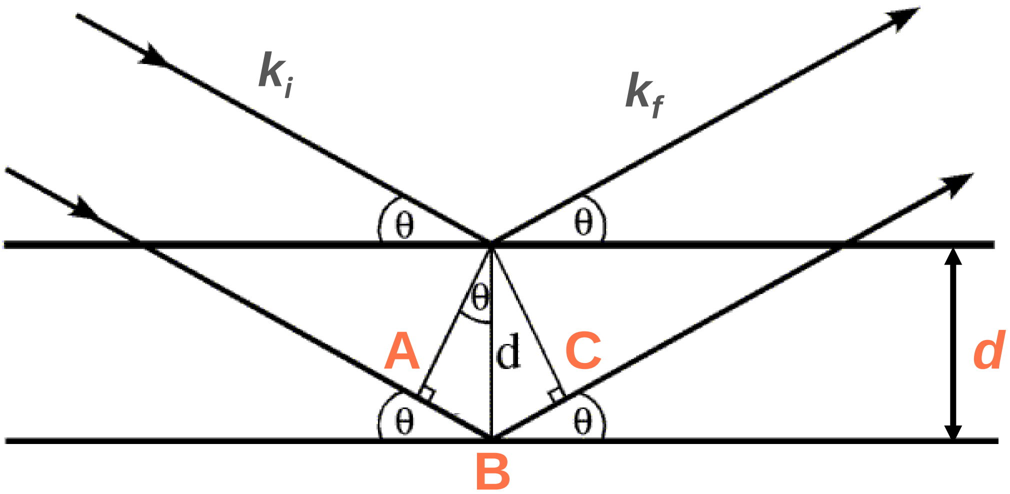
SwedNess practical at IFE

Powder neutron diffraction recap

Magnus H. Sørby

Direction of diffracted beams: Bragg's law

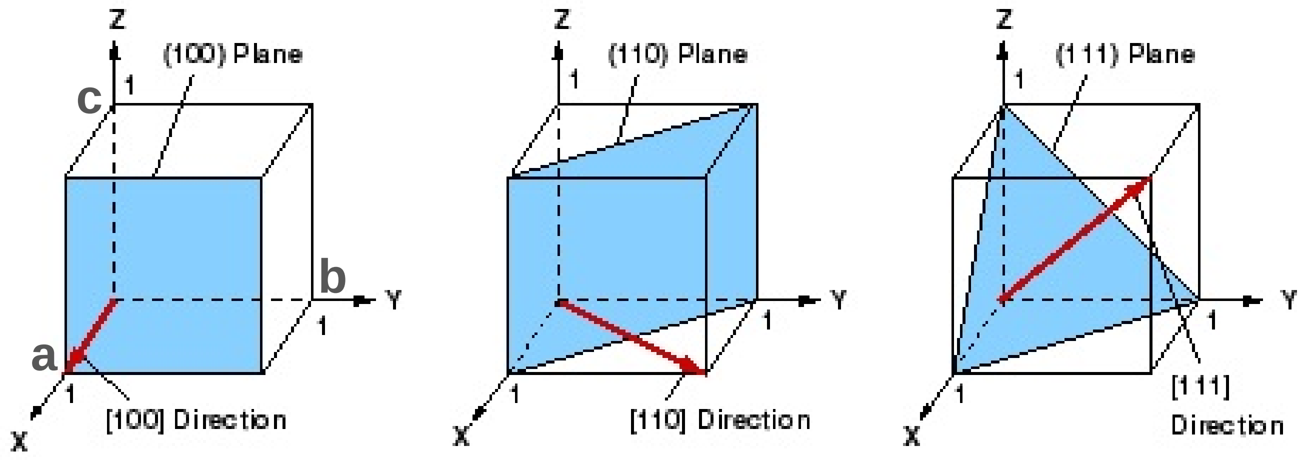


AB + BC = 2*d*sinθ

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

$$\mathbf{2d_{hkl}\sin\theta = \lambda}$$

Miller indices

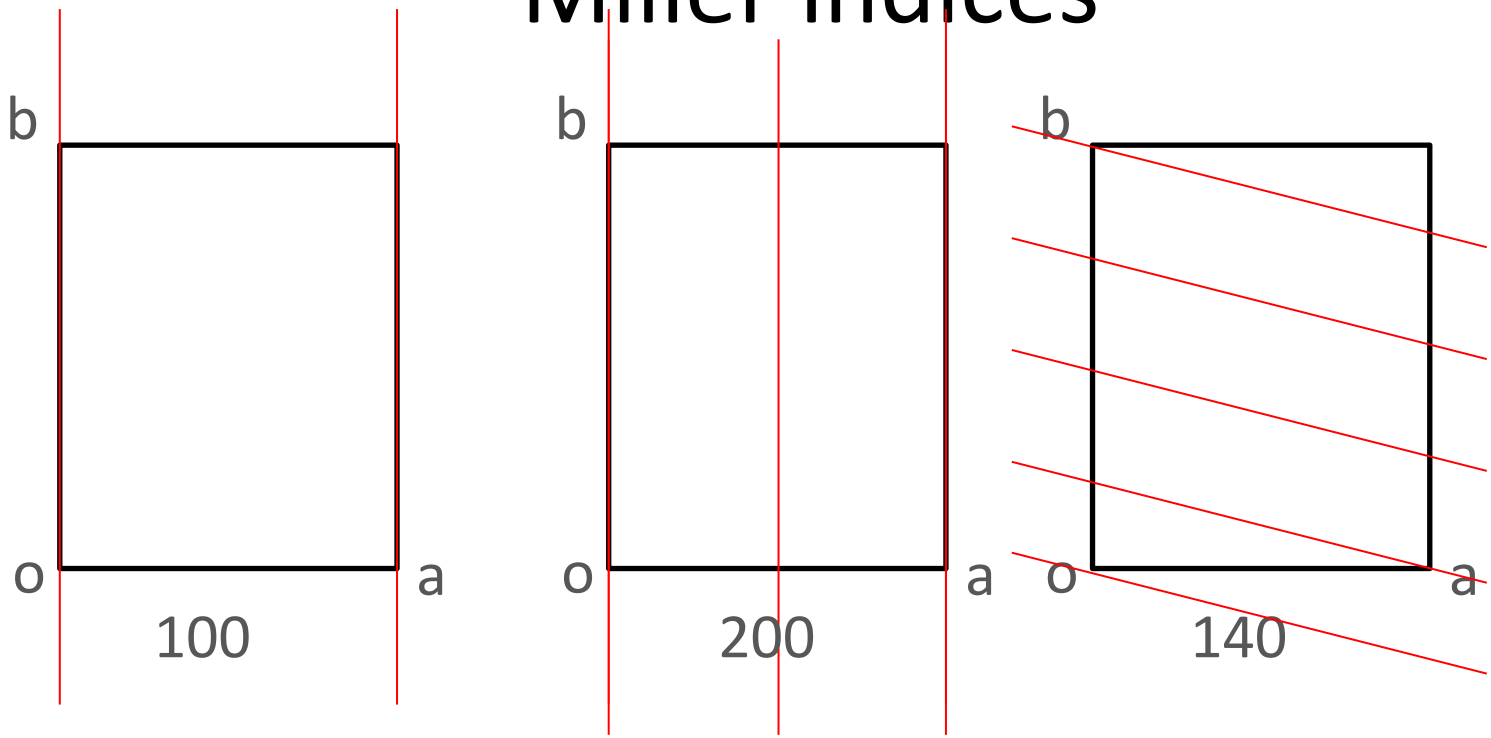


The (*hkl*) plane makes intercepts **a**/*h*, **b**/*k* and ***c***/*l* along the x, y, z axes.

The direction [*hkl*] is perpendicular to the (*hkl*) plane.

a,**b**,**c**: Unit cell dimensions

Miller indices



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The *hkl* plane intercepts **a**, **b** and **c** *h, k* and *l* times, respectively,

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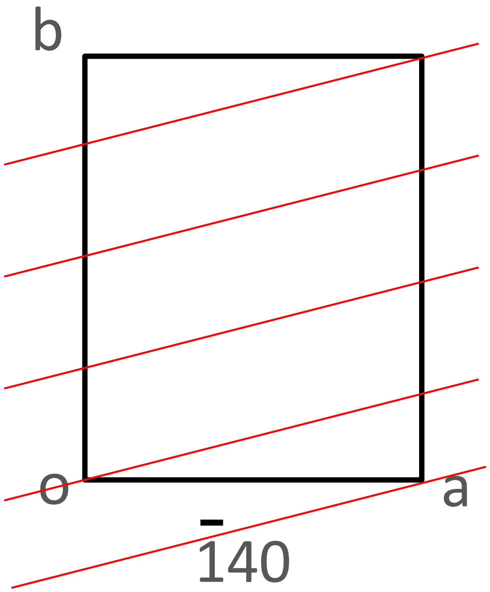

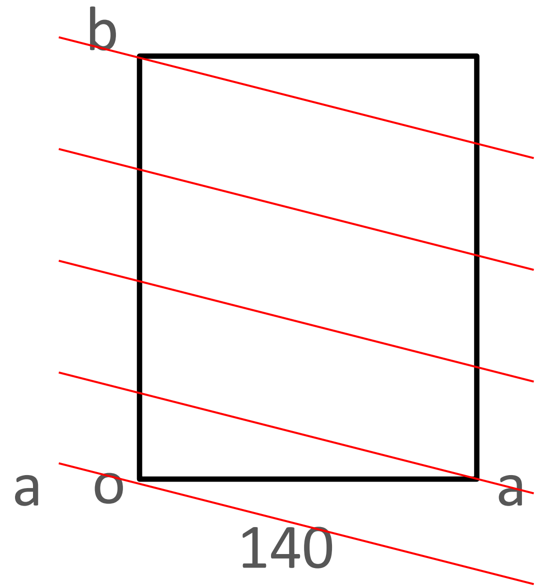

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The structure factor

$$F(\mathrm{Q}) = \sum_j b_j \cdot e^{\mathrm{i}\vec{\mathrm{Q}}\cdot\vec{\mathrm{r}}_j}$$

Neutrons: b_j = scattering length
X-rays: $b_\mathrm{j} = f_{\mathrm{at,j}}$ = atomic form factor

$$F_{hkl} = \sum_{\substack{\text{Unit}\\\text{cell}}} b_\mathrm{j} \cdot e^{2\pi\mathrm{i}(h\cdot\mathrm{x}_\mathrm{j} + k\cdot\mathrm{y}_\mathrm{j} + l\cdot\mathrm{z}_\mathrm{j})}$$

Intensity of scattered beams:

$$I \sim |F|^2$$

Displacement factor (Debye Waller factor, temperature factor):

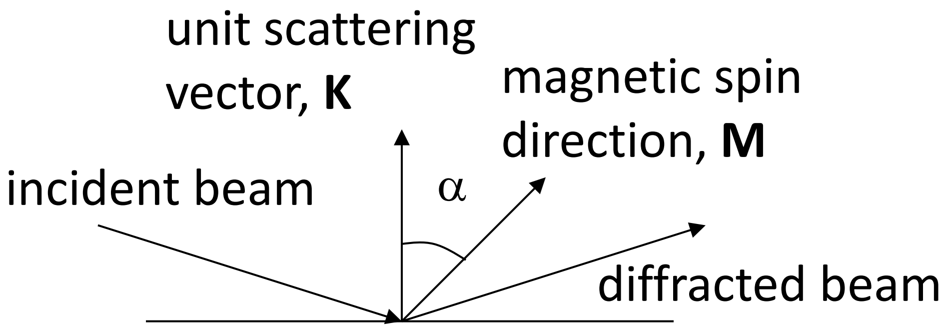
$$T_\mathrm{j} = e^{-W_\mathrm{j}},\ W_\mathrm{j} = 8\pi^2 \langle u_j{}^2 \rangle \frac{\sin^2\theta}{\lambda^2} = 1/2\,\mathrm{Q}^2 \langle u_j{}^2 \rangle$$

In total:

$$F_{hkl} = \sum_{\substack{\text{Unit}\\\text{cell}}} b_\mathrm{j} \cdot e^{2\pi\mathrm{i}(h\cdot\mathrm{x}_\mathrm{j} + k\cdot\mathrm{y}_\mathrm{j} + l\cdot\mathrm{z}_\mathrm{j})} \cdot e^{-1/2 Q^2 \langle u_j{}^2 \rangle}$$

Magnetic neutron scattering

- The neutron has a magnetic moment.
- This will interact with the magnetic moment of atoms with unpaired electrons.



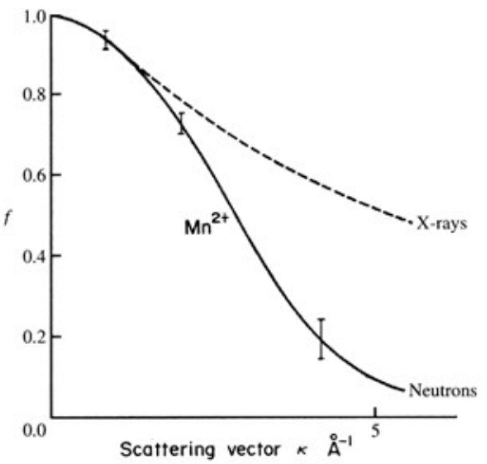
$$\vec{F}_{magnetic,hkl} = \sum_i \vec{m}_i f_i \cdot e^{2\pi i(hx_i + ky_i + lz_i)}$$

$$\vec{m} = \vec{K}(\vec{K} \cdot \vec{M}) - \vec{M}, \qquad |\vec{m}| = \sin\alpha$$

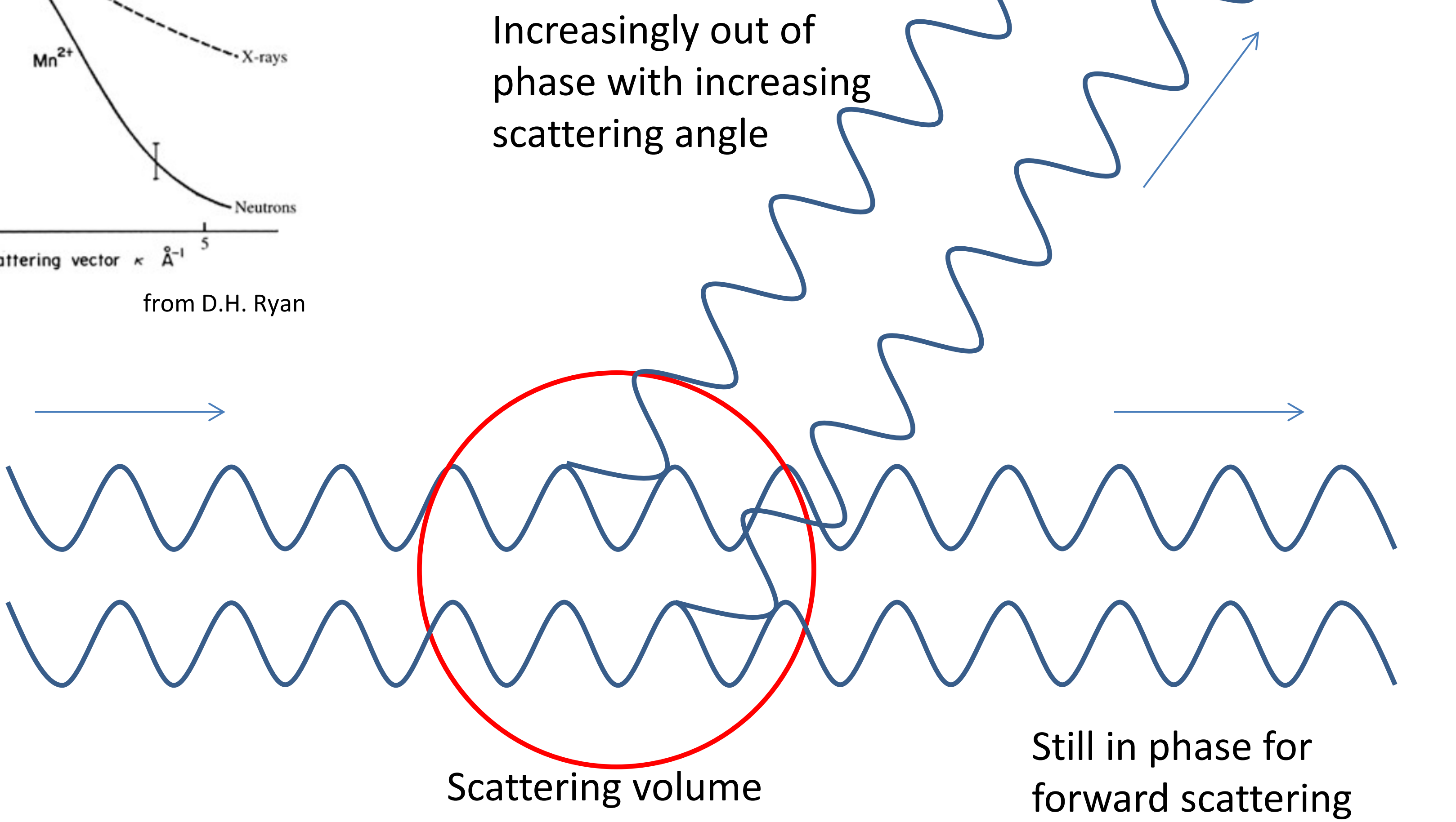
$$|\vec{m}| = 0, \qquad \vec{K} \parallel \vec{M}$$

$$|\vec{m}| = 1, \qquad \vec{K} \perp \vec{M}$$

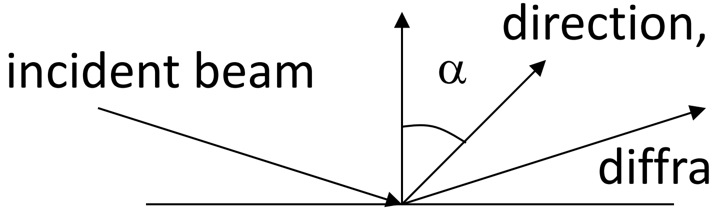
Form factor, f



from D.H. Ryan



Magnetic neutron scattering



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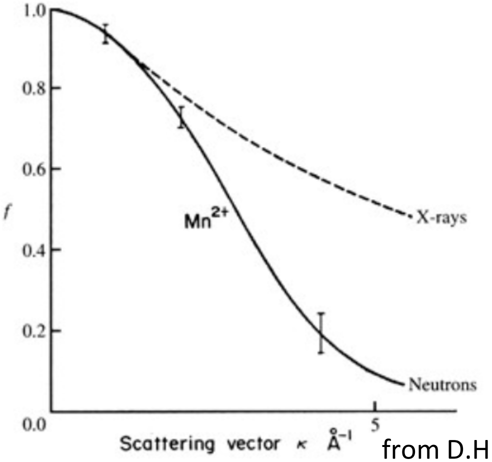

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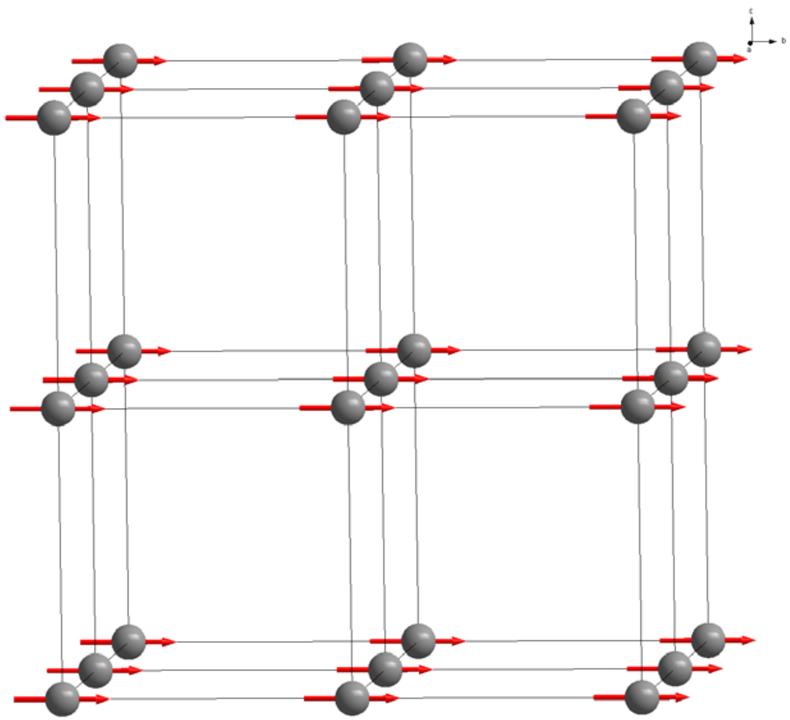

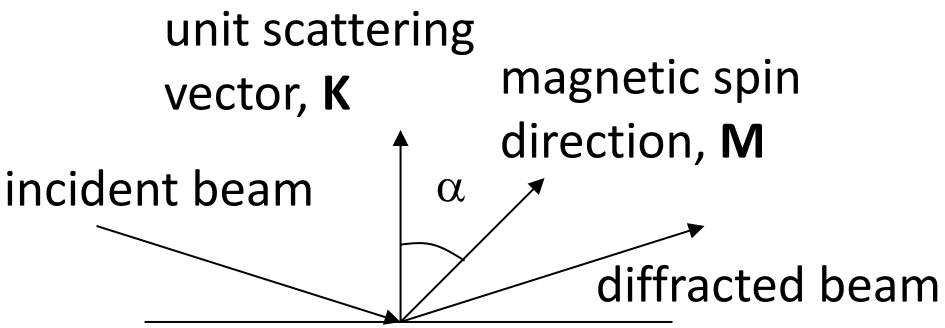

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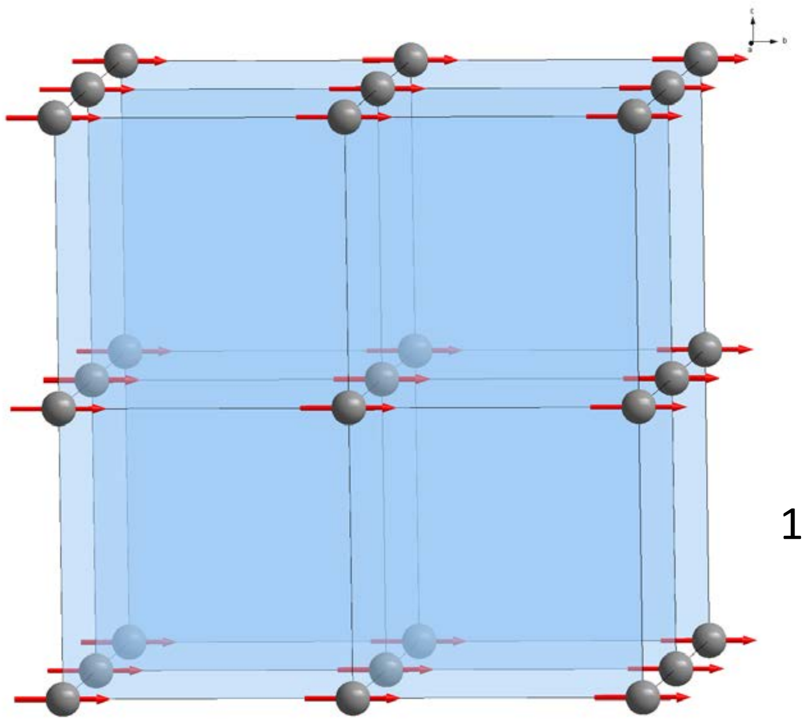

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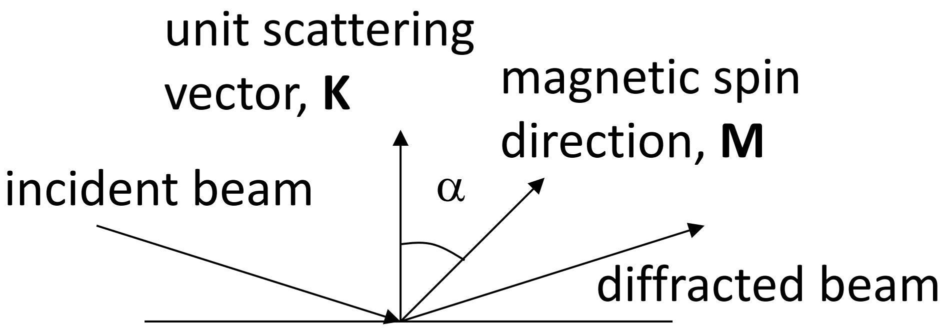

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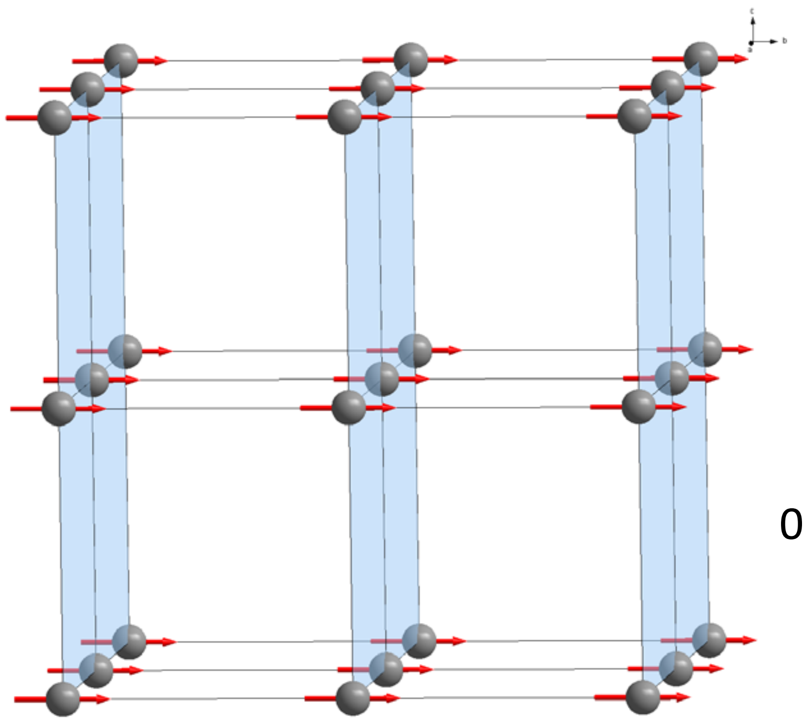

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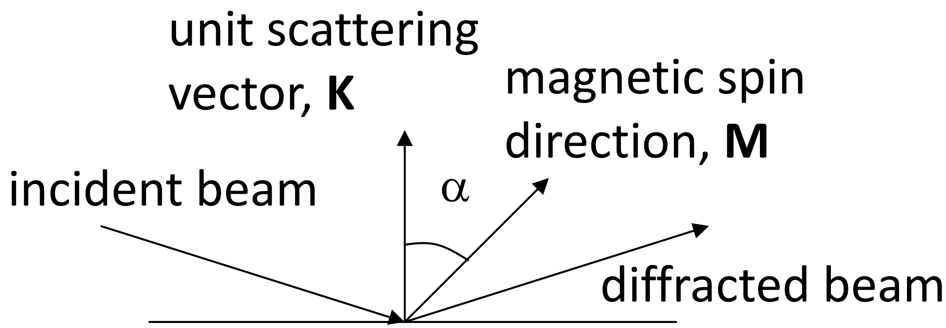

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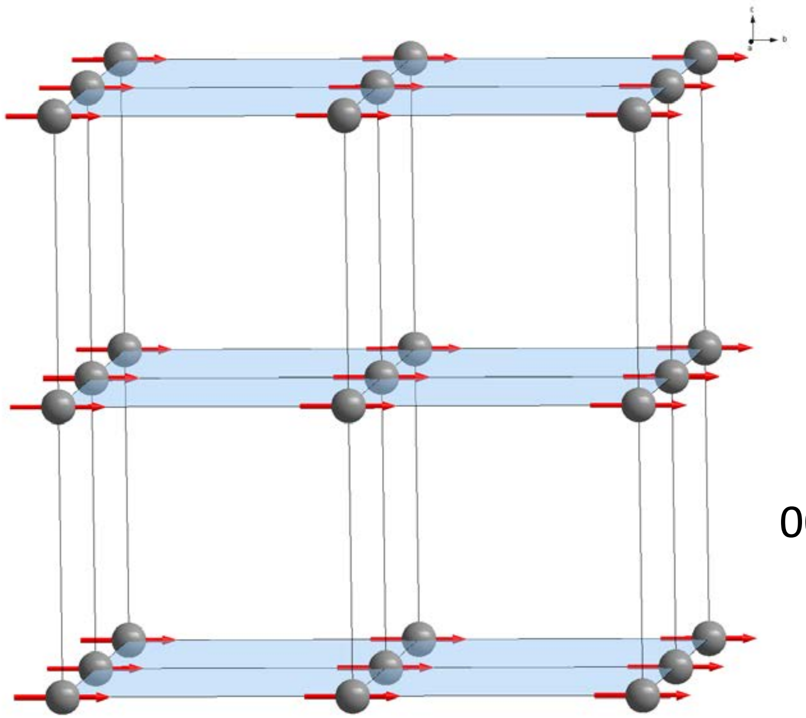

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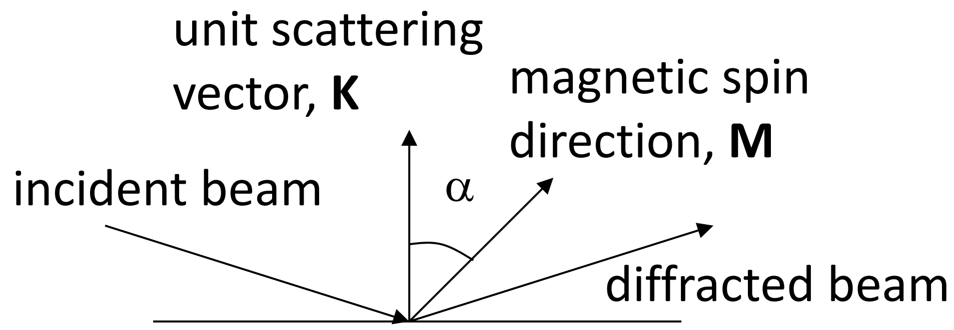

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