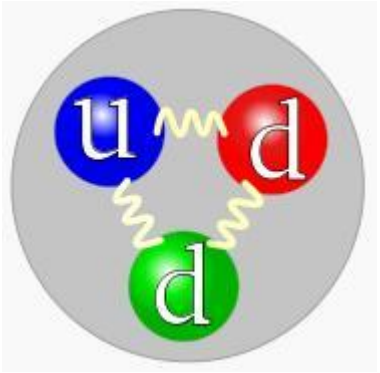
Neutron diffraction

NEUTRONS
FOR SOCIETY

Neutron properties

Discovered in 1932 by Chadwick

At least 50% of the Universe matter



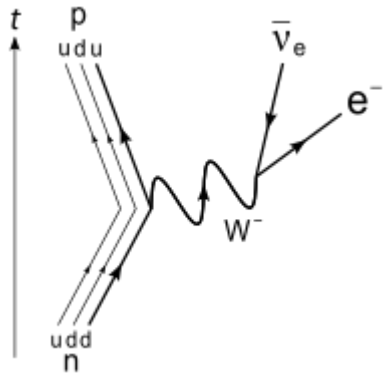
Composed by 3 quarks

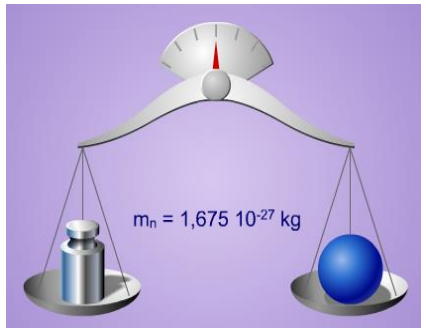
Is not stable outside the nucleus

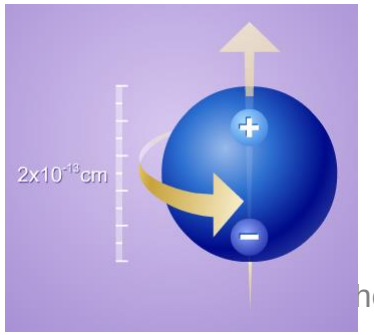
$$n^0 \rightarrow p^+ + e^- + \bar{\nu}_e$$

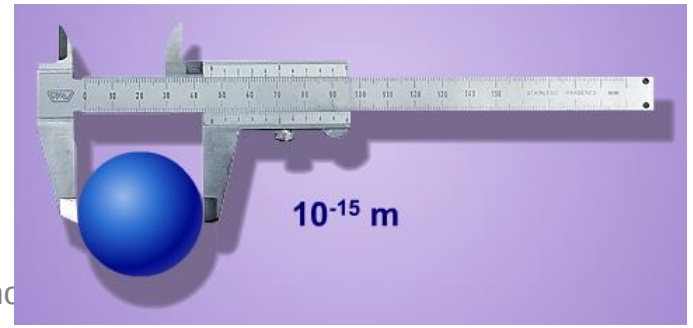
15 min

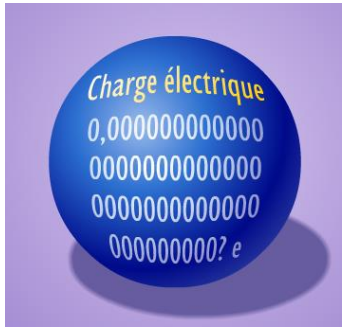
0 min



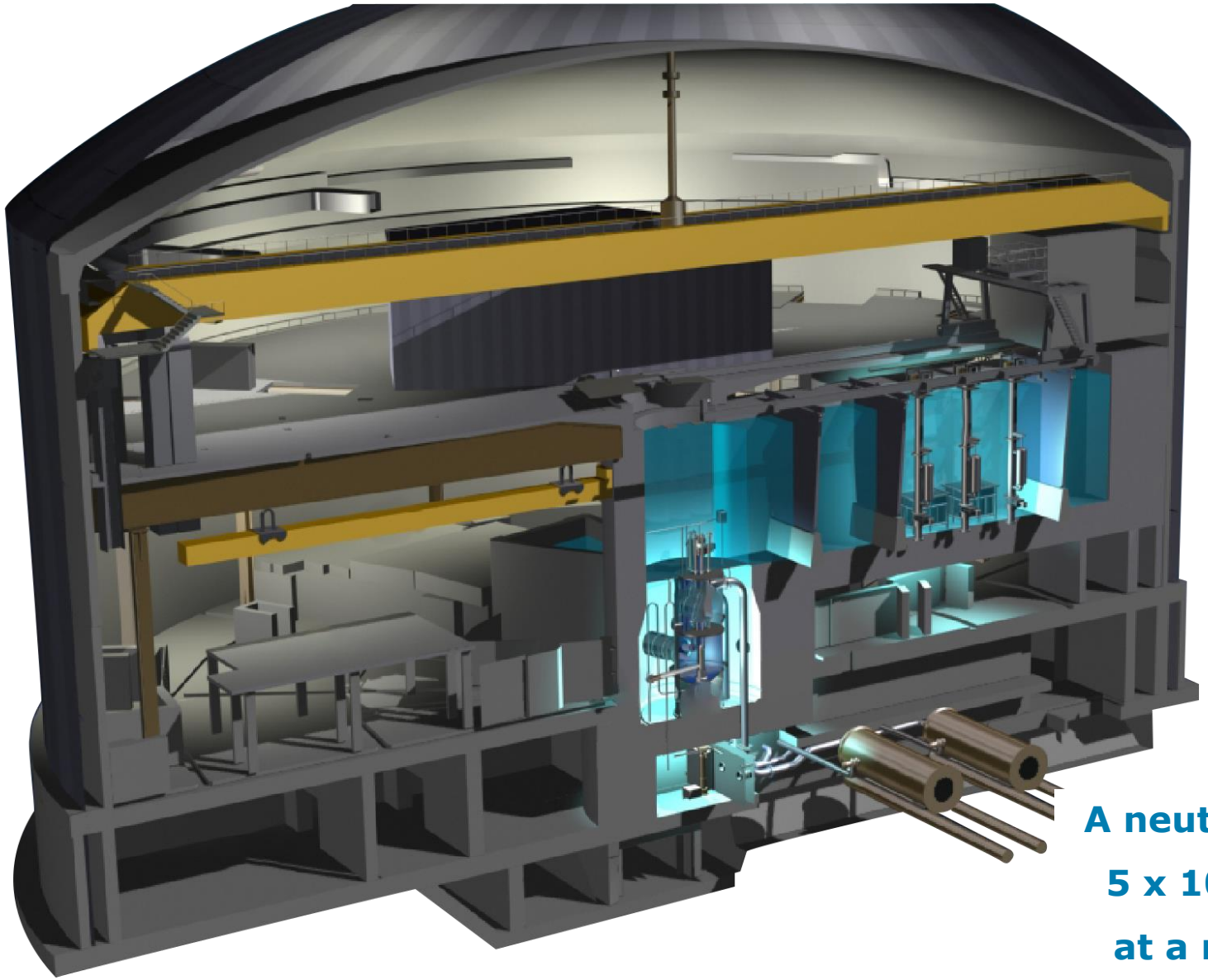


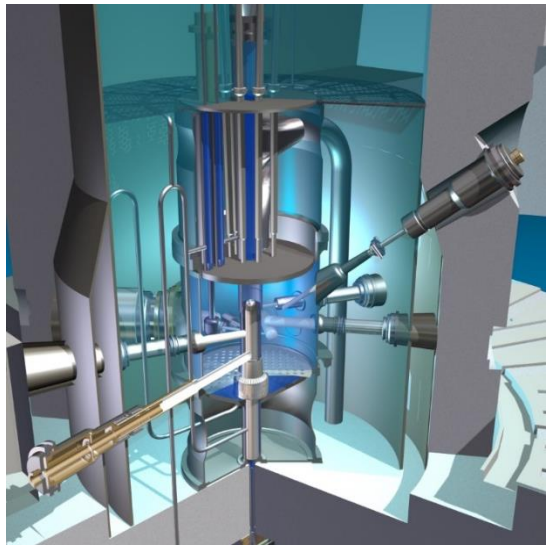


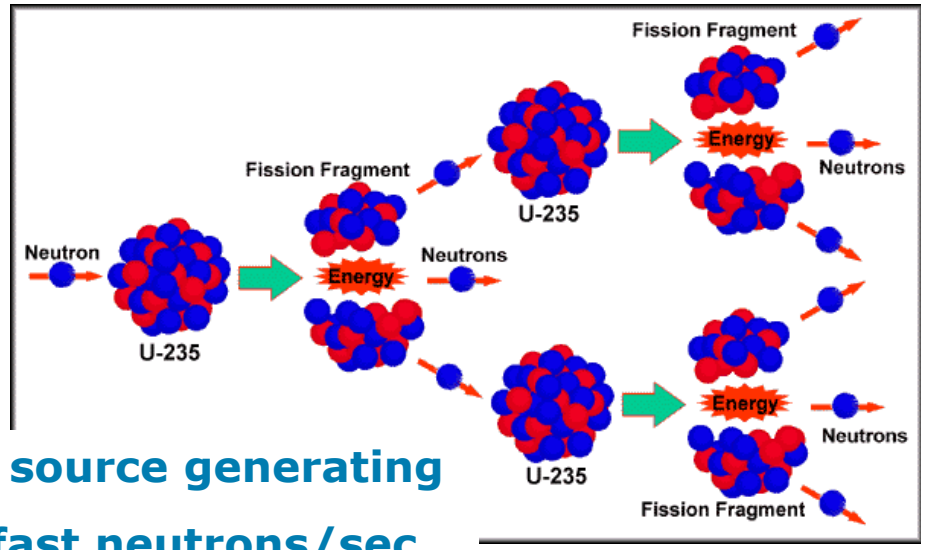




Neutron's generation: The ILL Reactor





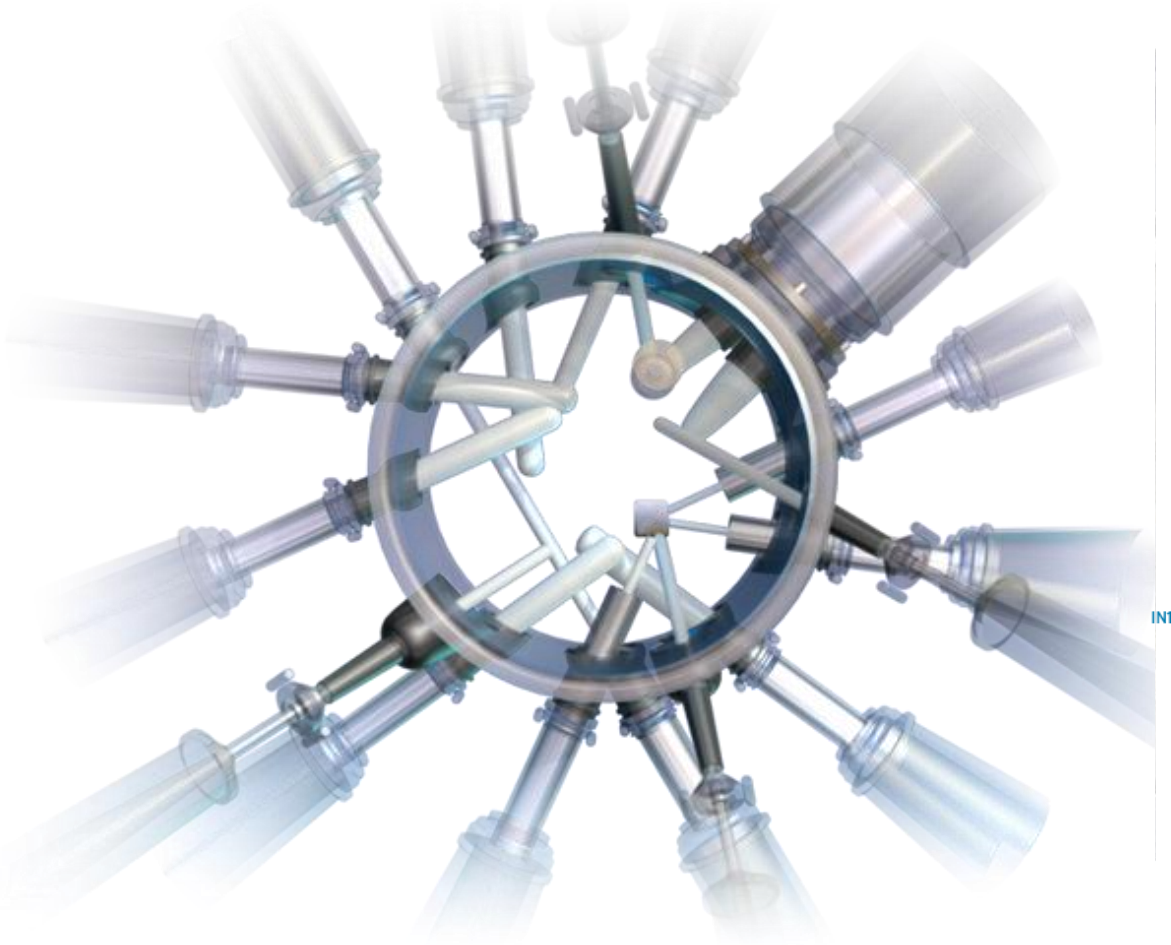


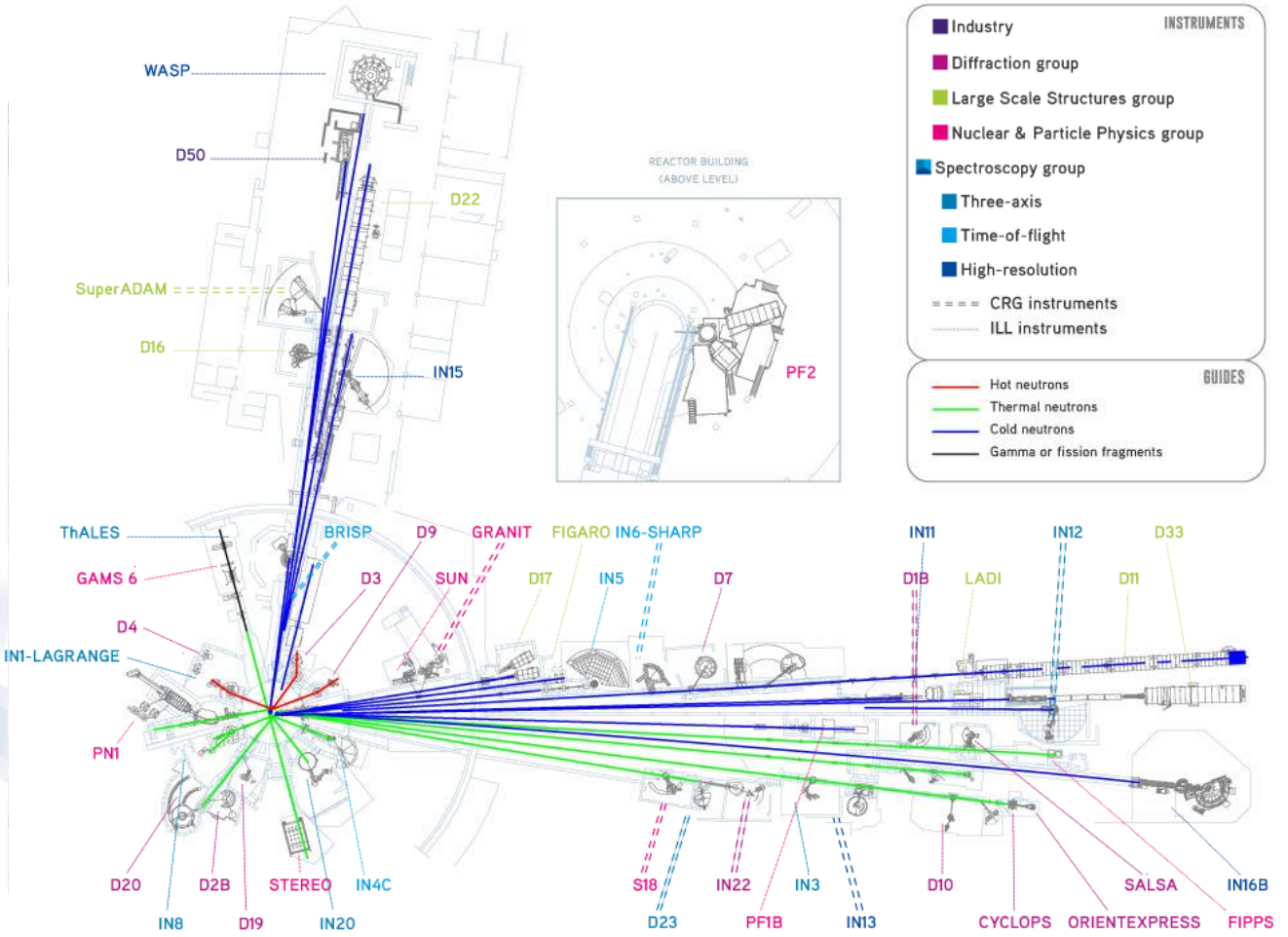
A neutron source generating

5 x 10^{18} fast neutrons/sec

at a max power of 58 MW

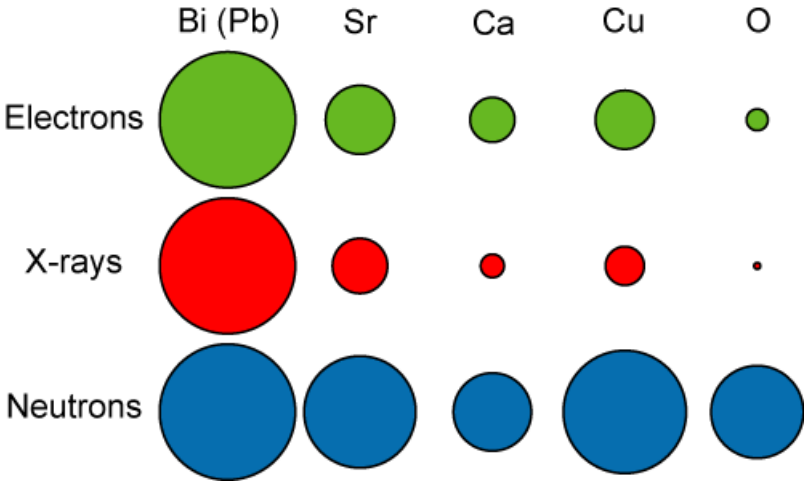
How neutrons are extracted and guided

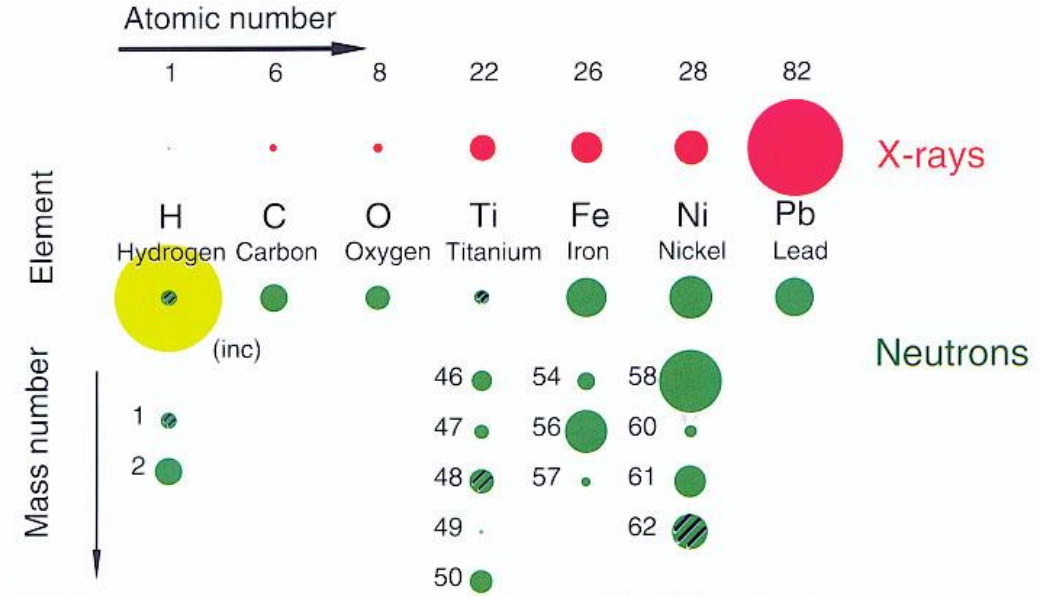




Why Neutrons?

Light atoms, as hydrogen or oxygen, are scattered as much as heavy atoms

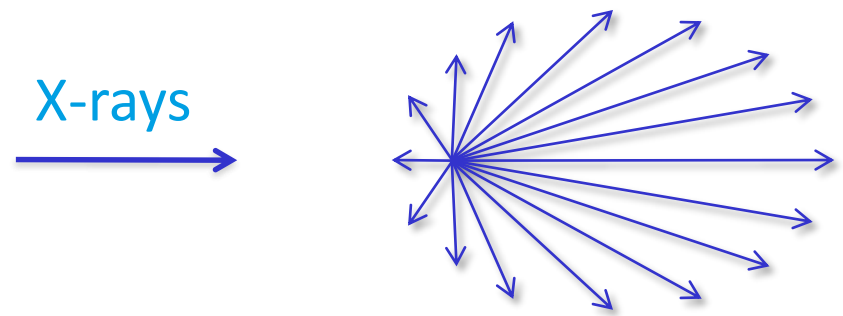


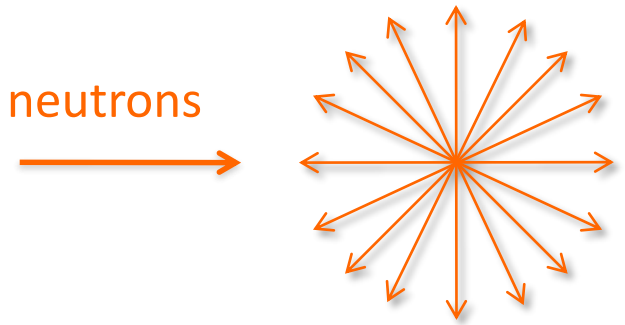


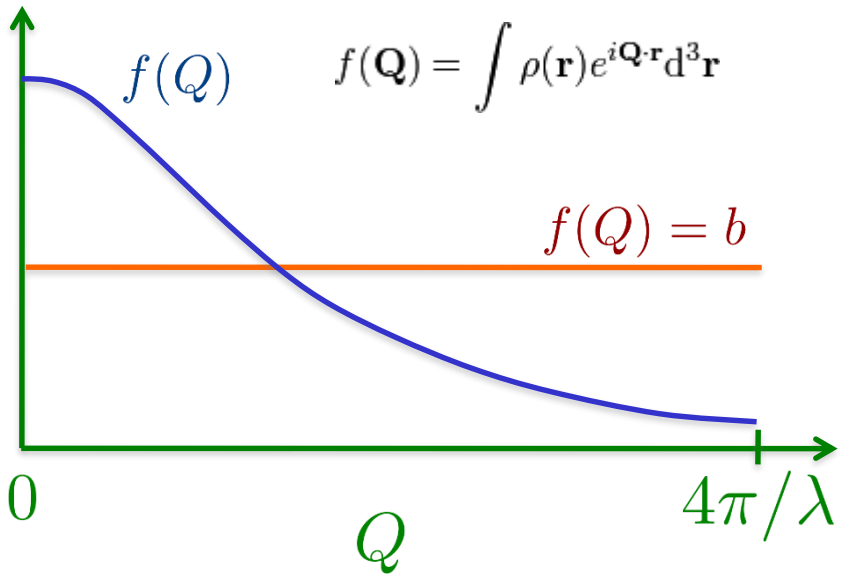
- X-ray scattering is proportional to the number of electrons (Z^2)
- Electron scattering depends on the electric potential
- Neutron scattering is similar for all atoms with a non-clear atomic (or isotopic) dependence.

Form factor

- The nuclear form factor is independent of ***Q (neutrons)***
- The structural form factor is strongly dependent of ***Q (X-ray)***
- High *Q*'s region is better explored using neutron diffraction





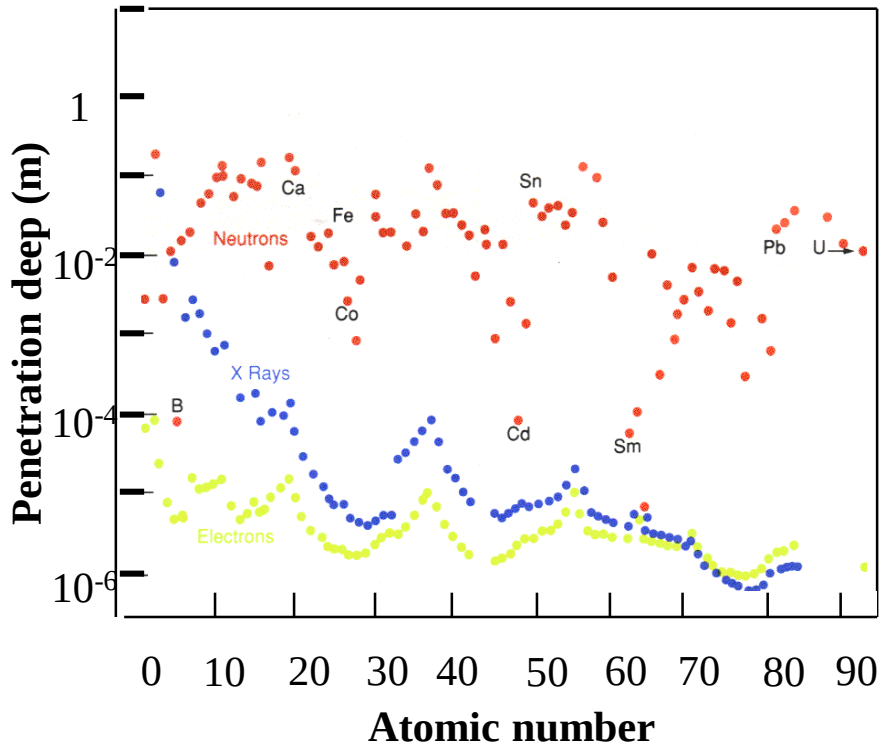


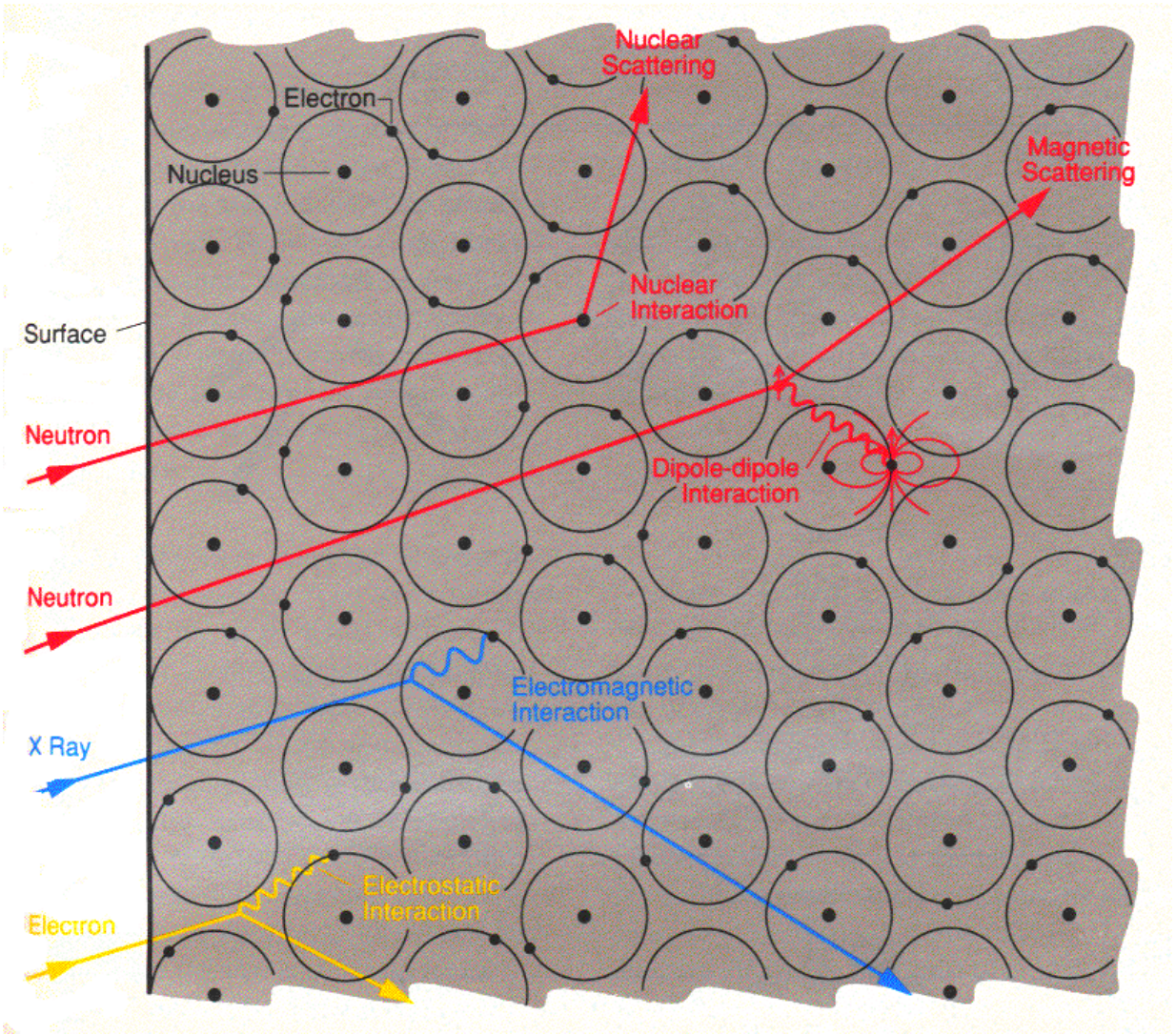
Bragg law $Q = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$

Penetration on the Matter

Neutrons interact with the tiny atomic nuclei and can localise the atoms more precisely

They can penetrate deeper than X-rays





Magnetic Scattering

Neutrons have no charge, but they do have a magnetic moment.

The magnetic moment is given by the neutron's spin angular momentum:

$$-\gamma \mu_N \hat{\sigma}$$

Where:

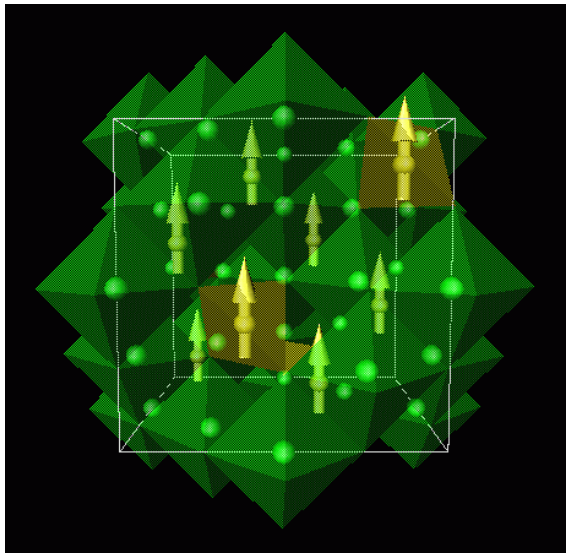
- γ is a constant (=1.913)
- μ_N is the nuclear magneton
- $\hat{\sigma}$ is the quatum mechanical Pauli spin operator

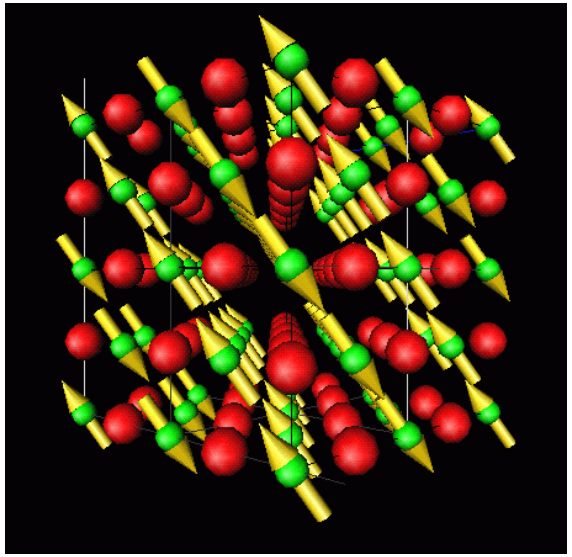
Normally refer to neutron as a spin-1/2 particle

Magnetic Scattering

Neutrons are strongly scattered by magnetic materials

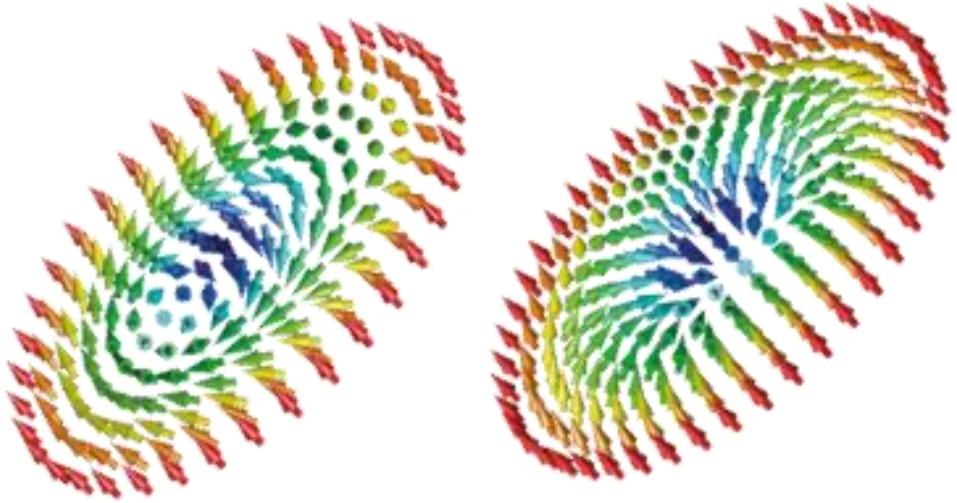
- Neutrons are like small magnets
- The neutron's magnetic moment strongly interacts with the magnetic atomic moments
- Neutrons can determine magnetic structures and measure the magnetization with high precision





Ferromagnetic magnetite Fe_3O_4 and antiferromagnetic manganese oxide MnO

Arrangement of spins in two different types of skyrmions



I. Kezsmarki et al., Nature Materials, 2015, **14**, 1116; DOI: 10.1038/nmat4402ptions.

Overview

- **X-rays**
  - Surface or small samples
  - Diffraction power correlated with *Z*
  - Difficult for determine light atoms
  - Low contrast for atoms close in the Periodic Table
  - High flux
    - Small samples
  - High resolution
- **Neutrons**
  - Bulk meausrements
  - Diffraction power different for different isotopes
  - Can see light atoms (incoherent problem of H)
  - Can distinguish neighbors in in the Periodic Table
  - Low flux
    - Big samples
  - Medium resolution

Magnetic Structures!!!
« Magnetic studies »

Scattering Concepts

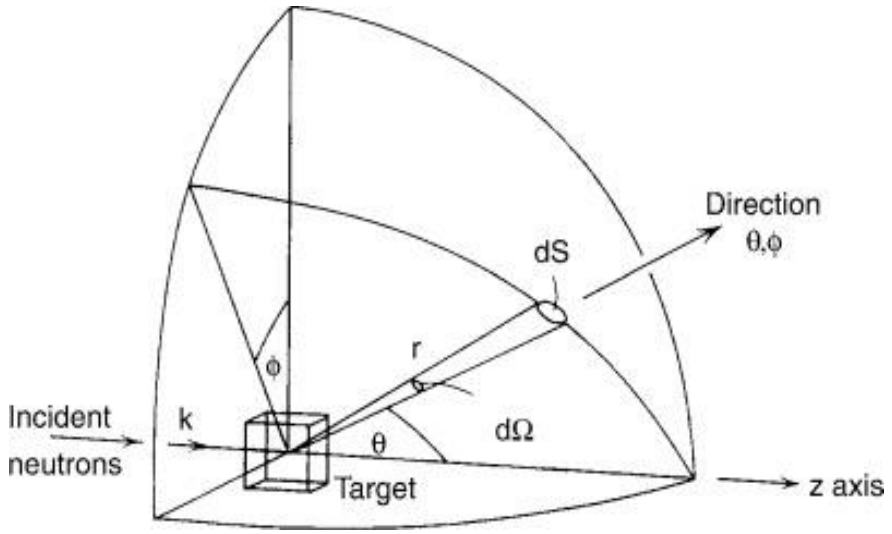
$$\hbar\mathbf{Q} = \hbar(\mathbf{k}' - \mathbf{k}) = h\mathbf{s}$$

The prime (′) superscripts stand for final state of the particle

The differential scattering cross section can be defined based on the fraction of neutrons scattered into a solid angle dΩ, with an angle θ. The incident neutrons have an initial wave vector **k**, which change to **k**′ after the scattering process. The final wave vector, **k**′, lies within the solid angle dΩ.

Here we will consider only the magnetic interaction between the incident neutrons and the target.

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{s\lambda\to s'\lambda'} = \frac{k'}{k}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 \left|\left\langle \mathbf{k}'s'\lambda'\middle|V_m\middle|\mathbf{k}s\lambda\right\rangle\right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$



Where E_λ and $E_{\lambda'}$ denoting the initial and the final kinetic energy of the probe and and *s* and *s*′ are spin states.

Scattering Concepts

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{s\lambda\to s'\lambda'} = \frac{k'}{k}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 \left|\langle \mathbf{k}'s'\lambda'|V_m|\mathbf{k}s\lambda\rangle\right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

The matrix element, which contain most of the physics

Conservation of the Energy

The square of the matrix element gives the transition probability from the initial to the final state.

This transition probability is related to the probe-target interaction through the potential V_m, which is the potential felt by the neutron due to the magnetic field created by moving electrons of the target.

$$V_m = -\gamma\mu_N\,\hat{\sigma}\cdot\mathbf{B}$$

Where **B** is the magnetic induction

ELASTIC SCATTERING

If the incident neutron energy = the final neutron energy, the scattering is considered as "**elastic**".

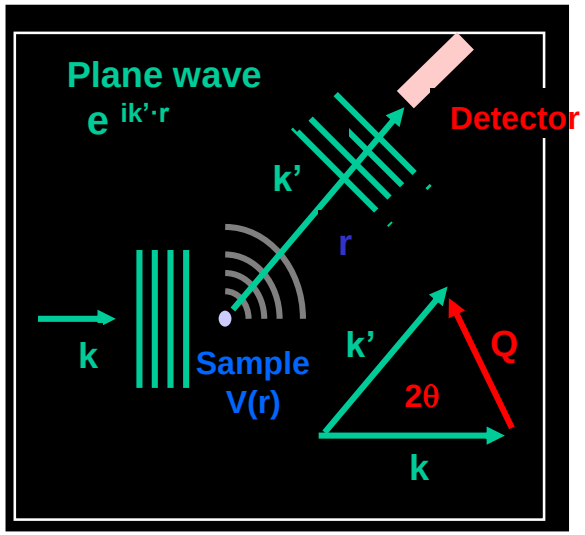
$$\left(\frac{d^2\sigma}{d\Omega}\right)_{s\to s'} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 \left|\langle \mathbf{k}'s'|V_m|\mathbf{k}s\rangle\right|^2$$

If we are using unpolarised neutron scattering we can assume than s = s'.

We can integrate over all volume (**r**)

$$\left|\langle \mathbf{k}'|V_m|\mathbf{k}\rangle\right| = \left|\int V_m e^{i\mathbf{Q}\mathbf{r}} d\mathbf{r}\right| = \left|\mathbf{M}_\perp(\mathbf{Q})\right|$$

with $\mathbf{Q} = \mathbf{k}' - \mathbf{k}$



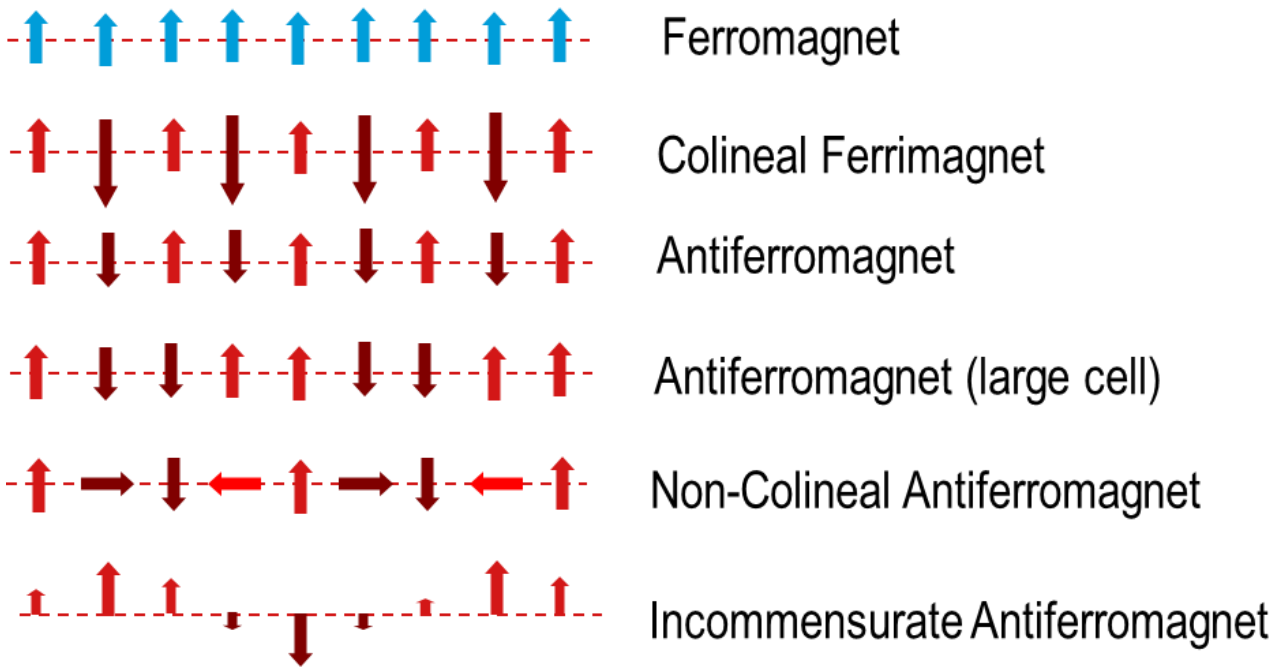
The elastic cross-section is then directly proportional to the **Fourier transform squared** of the potential.
Neutron scattering thus works in Fourier space, otherwise called ***reciprocal space***.

Magnetic Ground State

The magnetic ground state of a spin system, should provide a magnetic structure compatible with the minimum energy of the classical spin Hamiltonian

$$H = \sum_{jl\alpha,im\beta} J^{\alpha\beta}_{jl,im} S_{jl\alpha} S_{im\beta} + \ldots$$

Here below we present some 1D magnetic models:



MAGNETIC FIELD EXPERIENCED BY A TRAVELING NEUTRON:

Magnetism is caused by unpaired electrons or by movement of charges.

The magnetic field felt by the neutron due to the spin (S) and orbital (L) moments of an electron can be expressed using the following equation:

$$\mathbf{B}_j = \mathbf{B}_{jS} + \mathbf{B}_{jL} = \frac{\mu_0}{4\pi}\left\{\nabla \times \left(\frac{\boldsymbol{\mu}_j \times \hat{\mathbf{R}}}{R^2}\right) - \frac{2\mu_B}{\hbar}\frac{\mathbf{p}_j \times \hat{\mathbf{R}}}{R^2}\right\}$$

Spin — Orbital/Movement — Dipolar field — *Biot-Savart law*

Where the two term within braces correspond to the *magnetic vector potential of a dipolar field due to the electron spin moment* and the second correspond to the *Biot-Savart law for a single electron with linear momentum* ***p***.

MAGNETIC FIELD EXPERIENCED BY A TRAVELING NEUTRON:

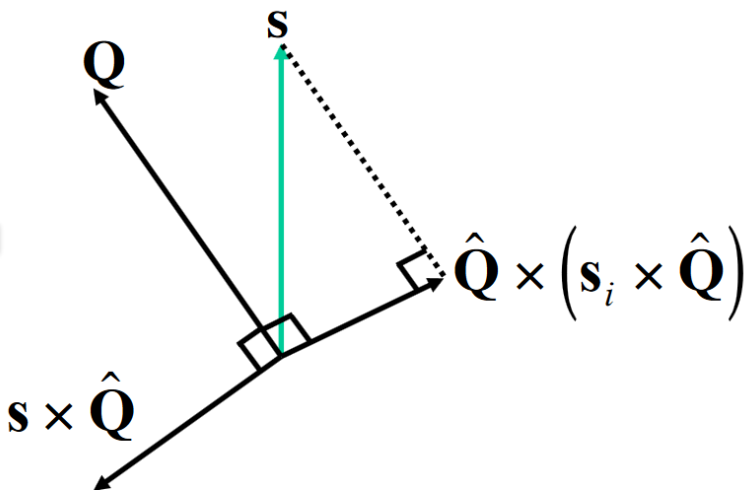
The evaluation of the **spatial part of the transition matrix** element for an electron *j* is described by the following expression:

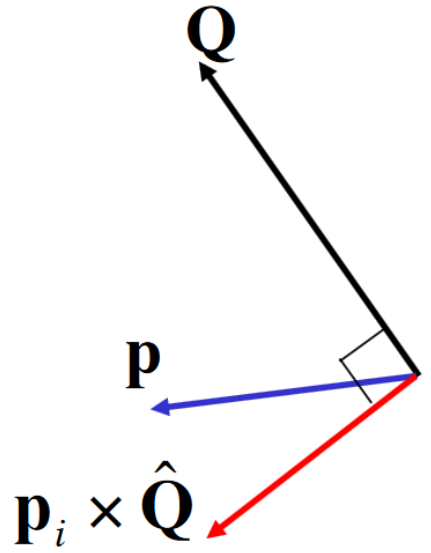
$$\left\langle \mathbf{k}' \left| V_m^j \right| \mathbf{k} \right\rangle \propto 4\pi \exp(i\mathbf{Q}\mathbf{R}_j) \left\{ \hat{\mathbf{Q}} \times (\mathbf{s}_j \times \hat{\mathbf{Q}}) + \frac{i}{\hbar Q} (\mathbf{p}_j \times \hat{\mathbf{Q}}) \right\}$$

Spin contribution

Orbital contribution

Neutrons are only sensible to the component of the local magnetization that is **perpendicular** to the scattering vector !!

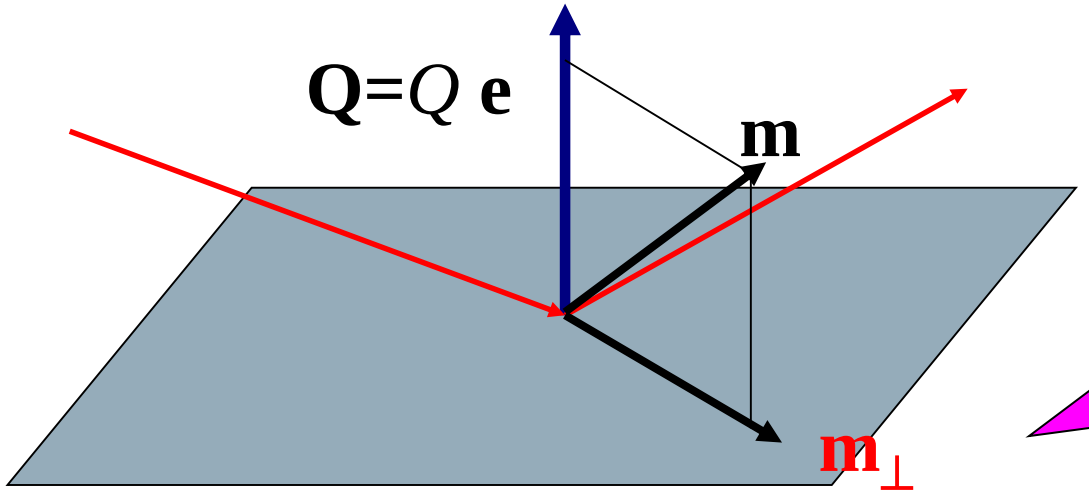




- The interaction between a body characterized by the magnetic density $\rho_m(\boldsymbol{r})$ and a neutron beam provides:

$$f(\mathbf{Q}) = \int_S \rho_m(\boldsymbol{r}) \exp(2\pi\, i\mathbf{Q}.\boldsymbol{r})\, d\boldsymbol{r}$$

- Magnetic form factor, f(**Q**), is the **Fourier transform** of the magnetic density.



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

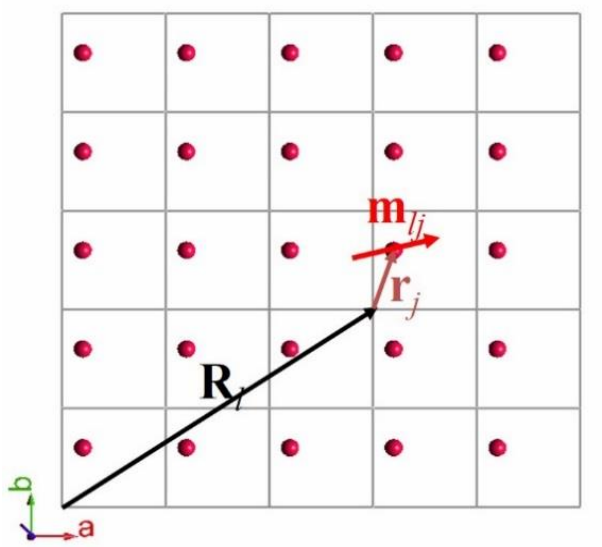
The above formulas are quite general: they can be applied to the cases in which ρ(**r**) represents the electron density of an electron, of an atom, of a molecule, of the unit cell, of the full crystal.

Diffraction Equations for crystals

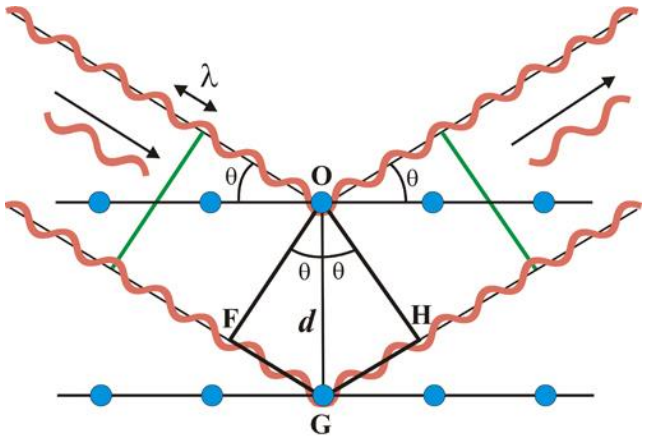
Laue conditions: the scattering vector is a reciprocal lattice vector of the crystal

$$\mathbf{s} = \mathbf{H}$$

The Laue conditions have as a consequence the Bragg Law

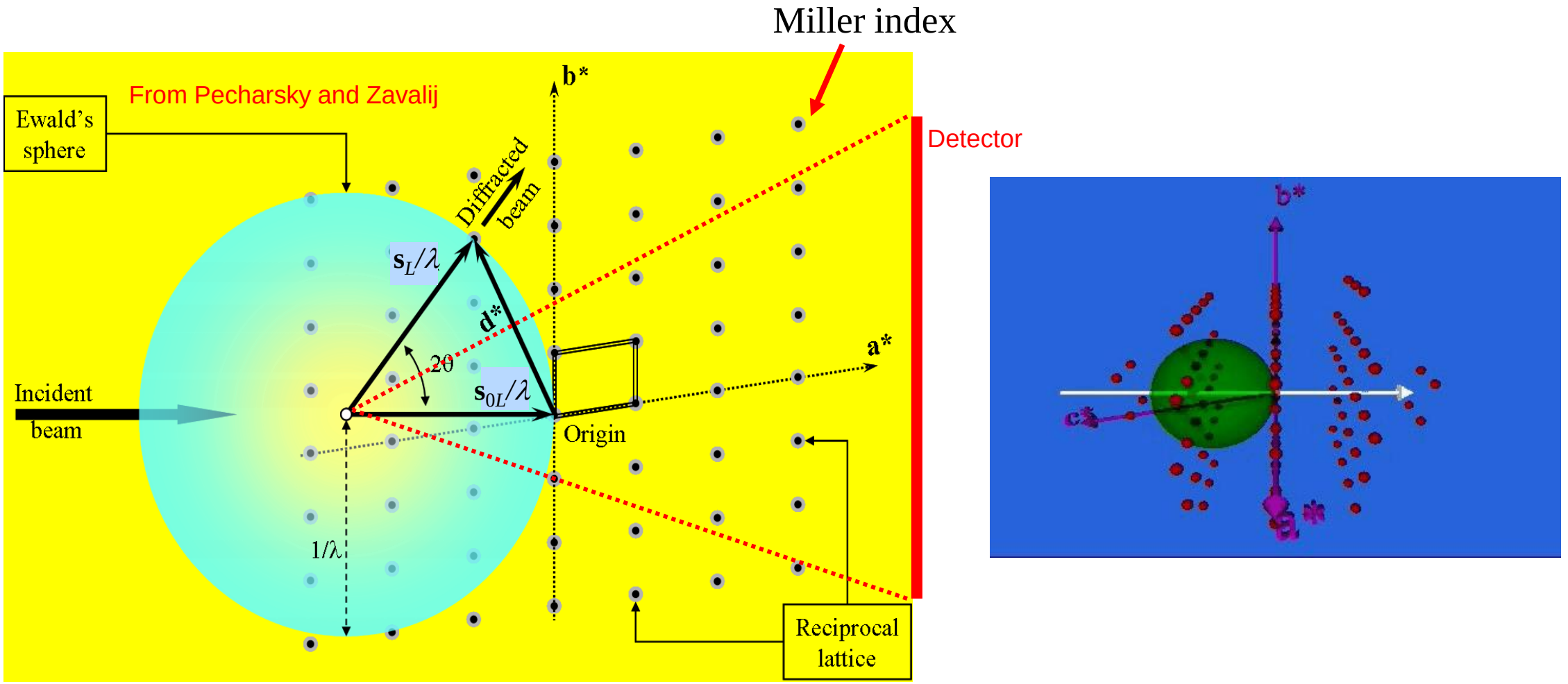


$$|\mathbf{s}| = \frac{2\sin\theta}{\lambda} \quad |\mathbf{H}| = \frac{1}{d_{hkl}} \quad \Rightarrow \quad 2d_{hkl}\sin\theta = \lambda$$

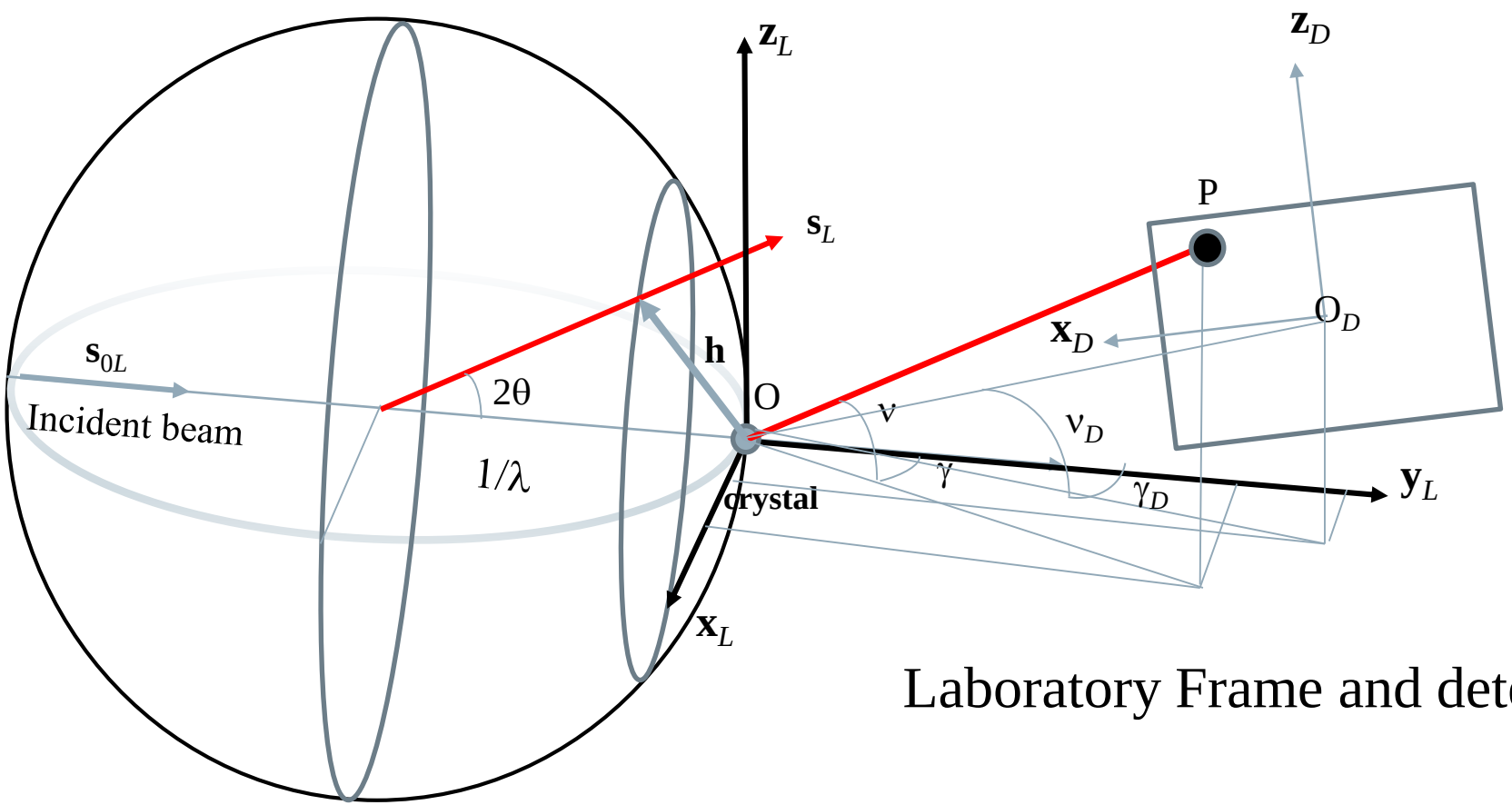


$$I_N(\mathbf{H}) \propto \left| \sum_{j=1,n} b_j \exp(2\pi i \mathbf{H}\cdot\mathbf{r}_j) \right|^2 = |F(\mathbf{H})|^2$$

Ewald construction

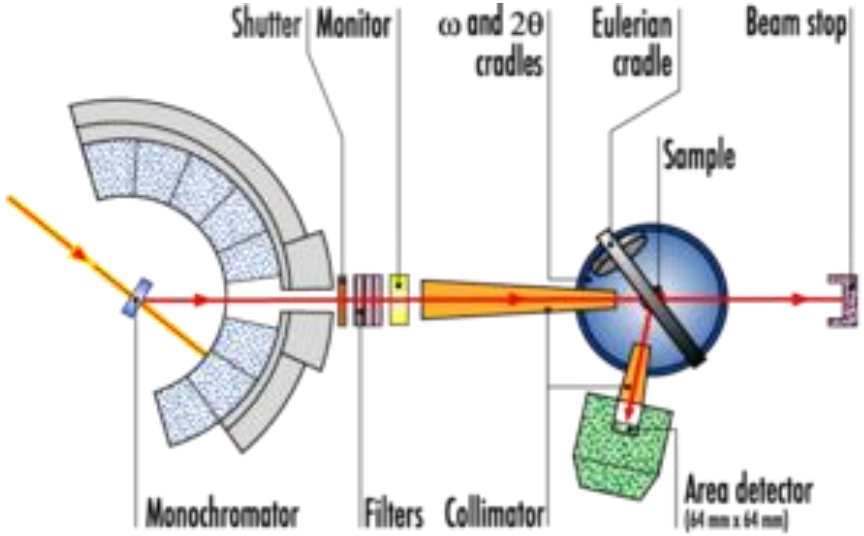


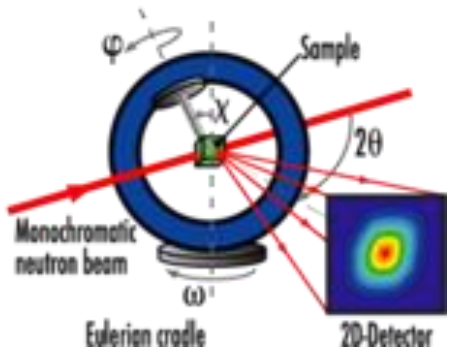
Ewald construction: single crystal case



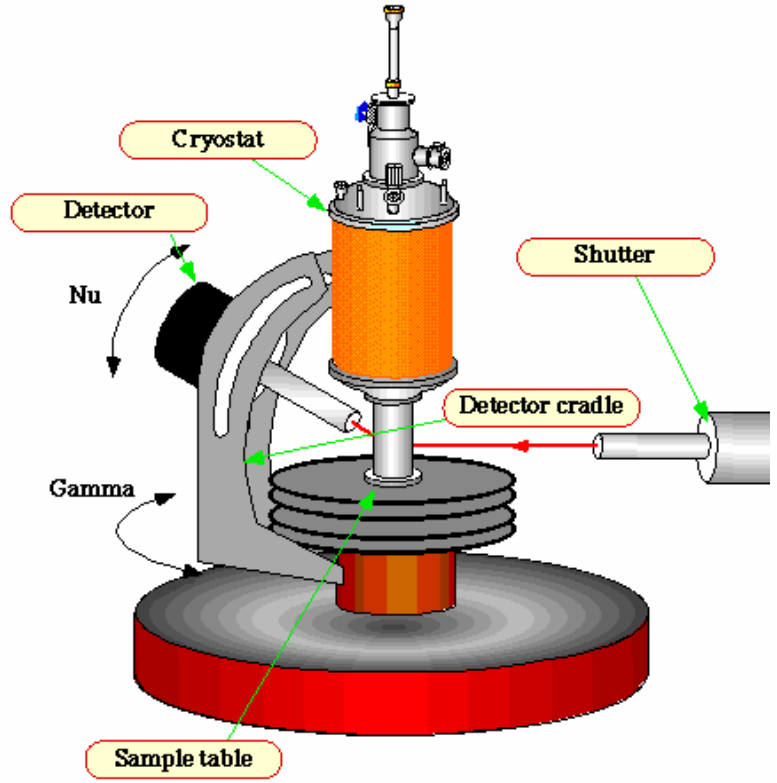
Laboratory Frame and detector

Four-circle configuration





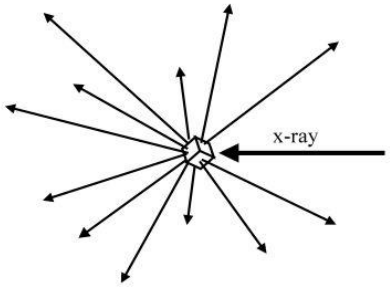
Normal-beam configuration



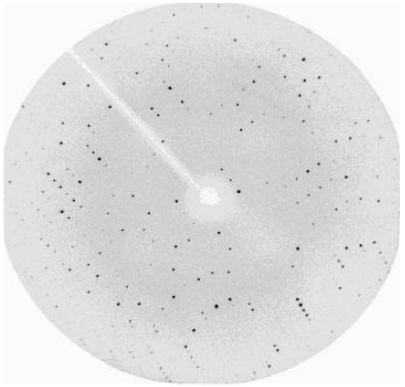
Diffraction patterns

Single Xtal - 2D image + scan –> 3D Int vs 2θ

Powder - 2D image –> 1D Int vs 2θ



(a)



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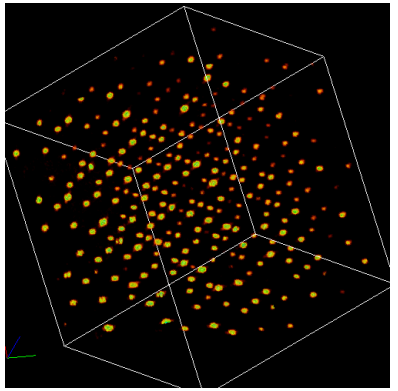
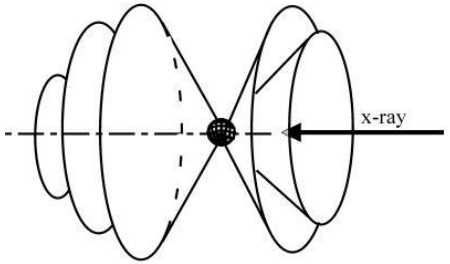
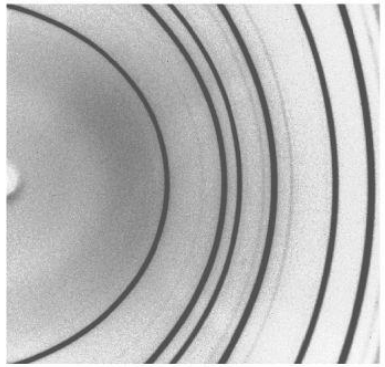


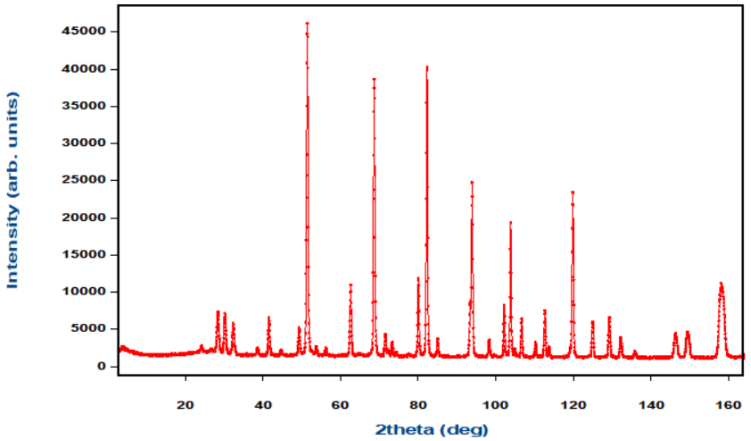
Single Crystal



(c)



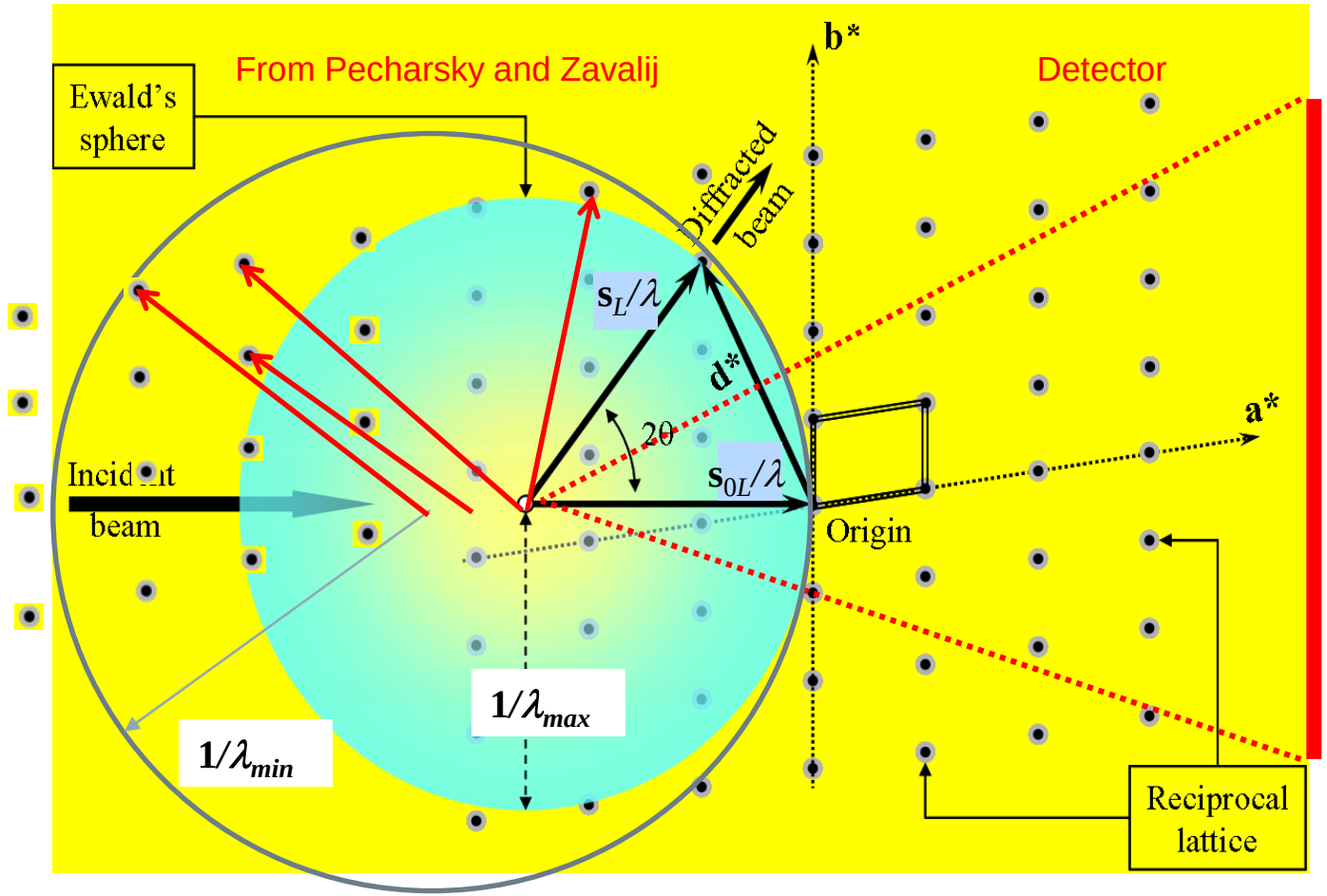
(d)



Powder or polycrystalline solid

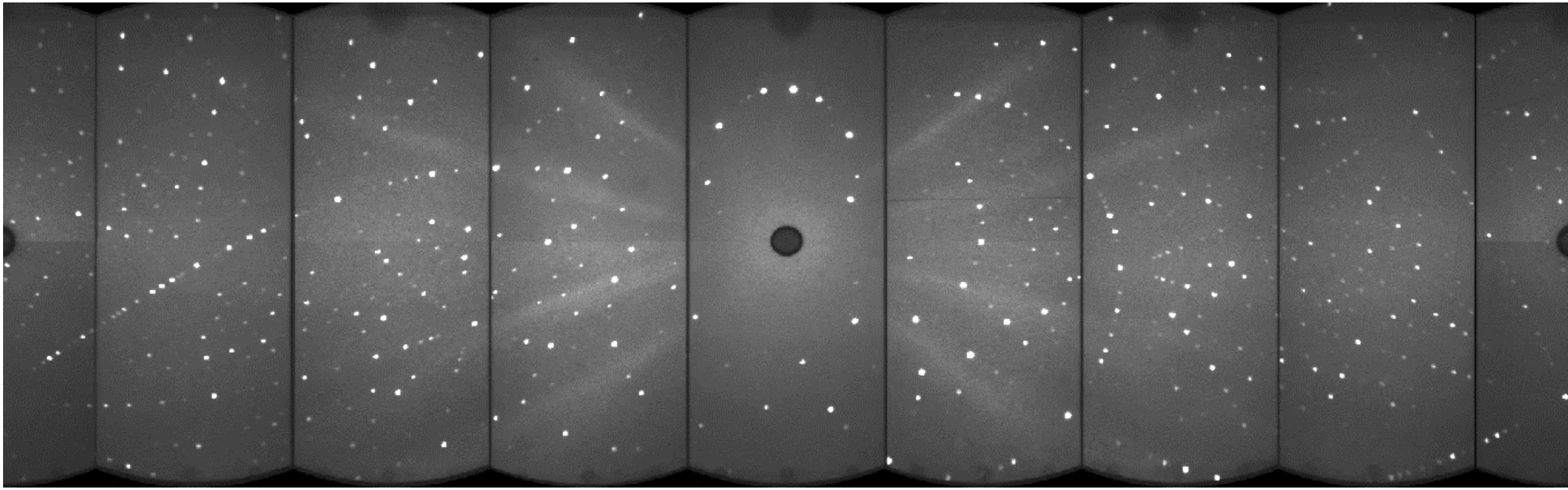
Courtesy of Jim Britten

Ewald construction Laue



$[NH_3CH_3]_N[Co^{II}(HCOO)_6]_N$

Cyclops



Cooling down from RT up to 20K

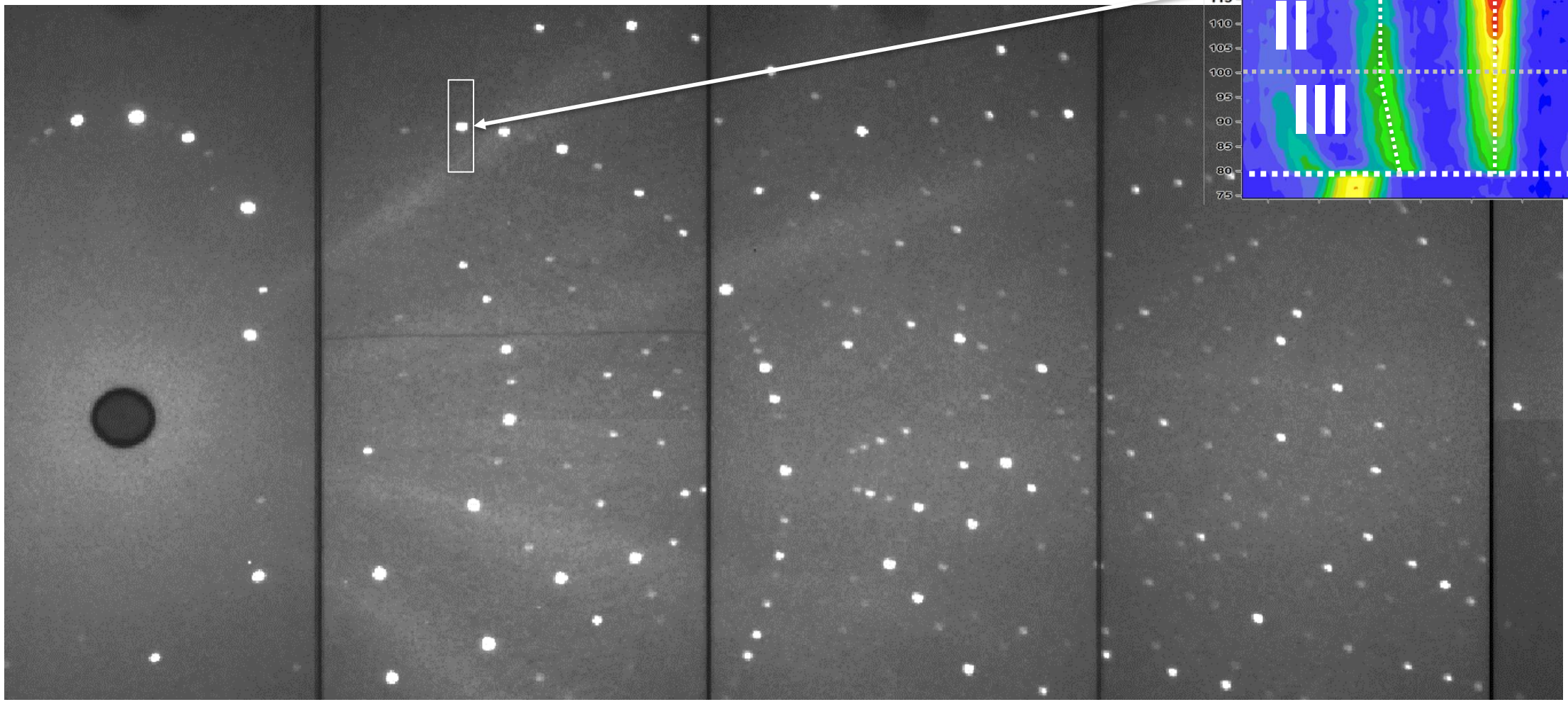
I. Conmensurate structure

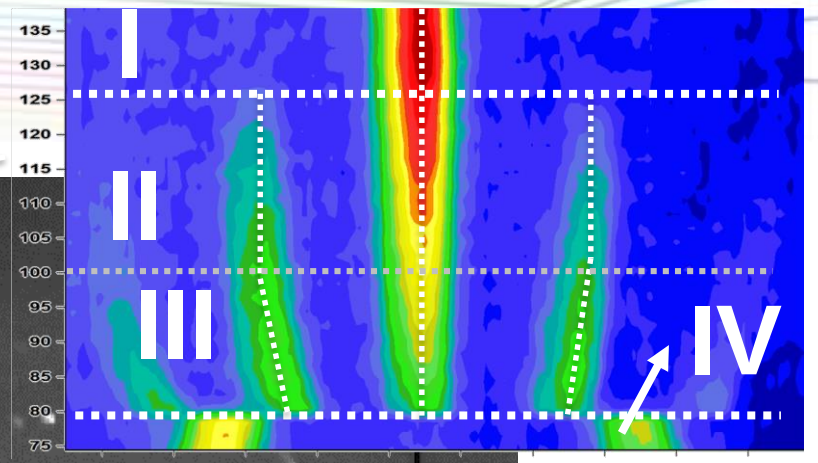
II & III. Inconmensurate structures

IV. Conmensurate structure ↔ Twinned crystal

$[NH_3CH_3]_N[Co^{II}(HCOO)_6]_N$

Cyclops





128K **I. Conmensurate structure**

II & III. Inconmensurate structures

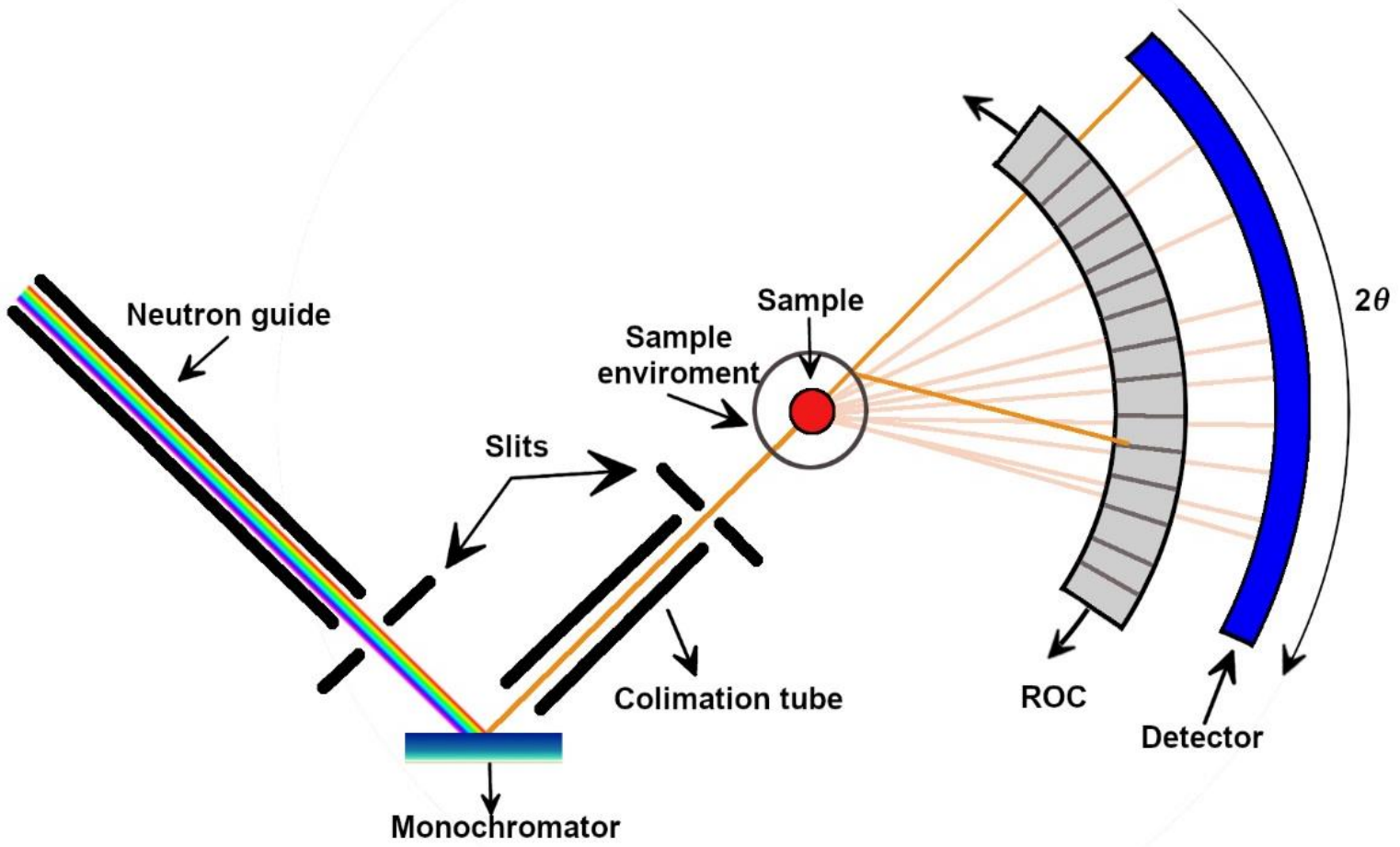
77K **IV. Conmensurate structure ↔ Twinned crystal**

Single Crystal and Powder Diffraction

Single Crystal diffraction allows to get with high precision subtle structural details: thermal parameters, anharmonic vibrations.
Drawbacks: big crystals for neutrons, extinction, twinning
Data reduction: Needs only the indexing and integration of Bragg reflection and obtain structure factors. List: $h\ k\ l$ F^2 $\sigma(F^2)$
Data Treatment: SHELX, FullProf, JANA, GSAS, …

Powder diffraction no problem with extinction or twinning.
Data reduction: minimalistic, needs only the profile intensities and their standard deviations
Data Treatment: FullProf, JANA, GSAS, TOPAS, …

POWDER DIFFRACTOMETER



$$2d = n\lambda sen(\theta)$$

Magnetic Powder Diffraction

Based on the Rietveld Method

$$y_i = \sum_{\mathbf{H}} I_{\mathbf{H}} \, \Omega(T_i - T_{\mathbf{H}}) \; + \; D_i + \; B_i$$

Where y_i is the number of counts, the subscript "i" represents a discrete observation at the scattering variable T_i

The T variable to describe either, the scattering angle 2θ, the time of flight t or the scattering vector modulus **Q** or **s**.

H corresponds to Bragg peaks contributing to the channel "*i*"

I_H is the integrated intensity of the reflection **H**

$\Omega(T_i - T_{\mathbf{H}})$ is the value of the normalised profile function of the Bragg reflection at the position T_i due to the reflection **H** at the position T_H

D_i is the diffuse scattering due to defects

B_i is the background

Magnetic Powder Diffraction

The intensity of each magnetic reflection is affected by other parameters than should be taken into account in the previous equation:

$$I_{M,\mathbf{H}}(\mathbf{h}) \approx \{ j \cdot L \cdot A \cdot O \cdot E \cdot \mathbf{M}_{\perp}(\mathbf{h}) \cdot \mathbf{M}_{\perp}^{*}(\mathbf{h}) \}_{\mathbf{H}}$$

j is the multiplicity of the reflection **H**. *L* is the Lorentz factor. *A* is the absorption correction. *O* is to handle with preferred orientations and *E* is the primary extinction correction.

The $I_{M,\mathbf{H}}(\mathbf{h})$ should be determined experimentally and fitted using theoretical models.

In order to achieve to measure adequately the intensity of magnetic reflections some consideration are needed.

CAGLIOTI'S EQUATION

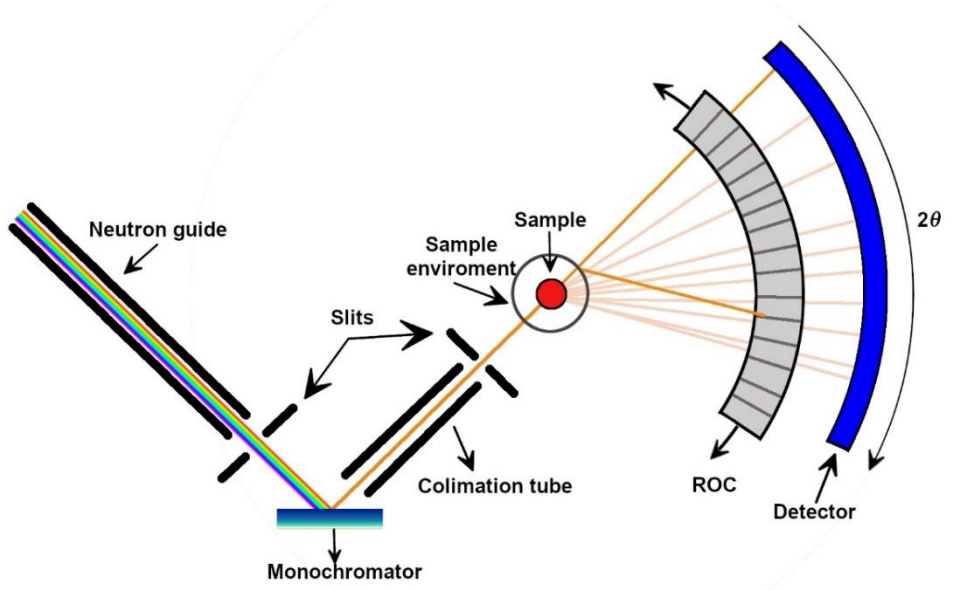
The Caglioti's relations is generally used to calculate an approximate resolution function of the two axis diffractometer.

$$FWHM = (U \tan^2 \theta + V \tan \theta + W)^{1/2}$$

The full width at half maximum (FWHM) of Bragg reflections varies with the scattering angle.

U, V and W are parameter that the user should be provide to the refinement program (FullProf, Jana, Topas, etc…).

Why does on powder diffractometers the detector is placed on the positives values of θ (right side from sample to detector)?

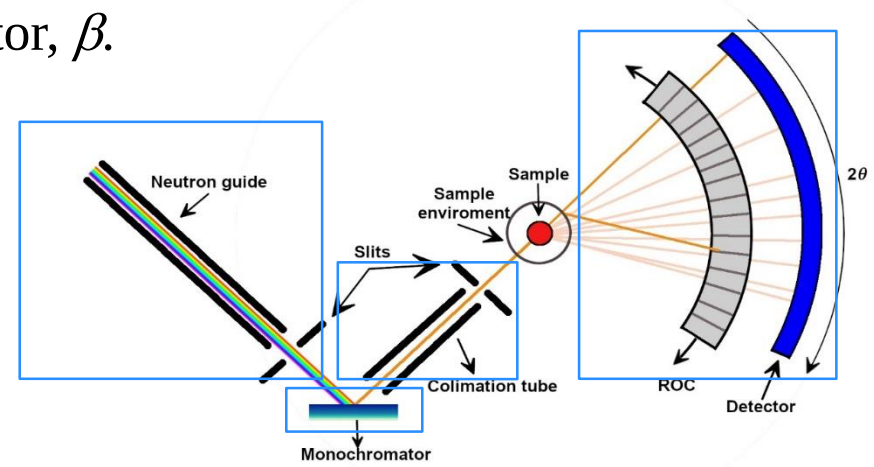


CAGLIOTI'S EQUATION

$$FWHM = (U\tan^2\theta + V\tan\theta + W)^{1/2}$$

The resolution on powder diffraction is defined as the ability to distinguish between two adjacent reflections.
This is correlated with the value of the full width at half maximum (FWHM) at each scattered position.

U, V and W are parameters can be correlated with angular divergence of the incoming neutrons to the monochromator, α_1, the angular aperture of a monochromator-to-sample collimator, α_2, the collimation between sample and detector, α_3, the take-off angle of the monochromator, $2\theta_m$ and the mosaicity of the monochromator, β.



CAGLIOTI-PAOLETTI-RICCI EQUATIONS

The Caglioti-Paoletti-Ricci equations are able to determine U, V and W through angular divergences α_1, α_2 and α_3, the take-off angle and the mosaicity of the monochromator, β.

$$U = 4\left(\alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 + \alpha_2^2\beta^2\right) / \left[\tan^2\theta_m\left(\alpha_1^2 + \alpha_2^2 + 4\beta^2\right)\right]$$

$$V = -4\alpha_2^2(\alpha_1^2 + 2\beta^2) / [\tan\theta_m\ (\alpha_1^2 + \alpha_2^2 + 4\beta^2)]$$

$$W = [\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2 + 4\beta^2(\alpha_2^2 + \alpha_3^2)] / (\alpha_1^2 + \alpha_2^2 + 4\beta^2)$$

For a powder diffractometer used to determine magnetic structures, typically we look for:

- long wavelengths (to separate nuclear and magnetic reflections),
- maximum of resolution on the low angle region (magnetic form factor)
- High flux

CAGLIOTI-PAOLETTI-RICCI EQUATIONS

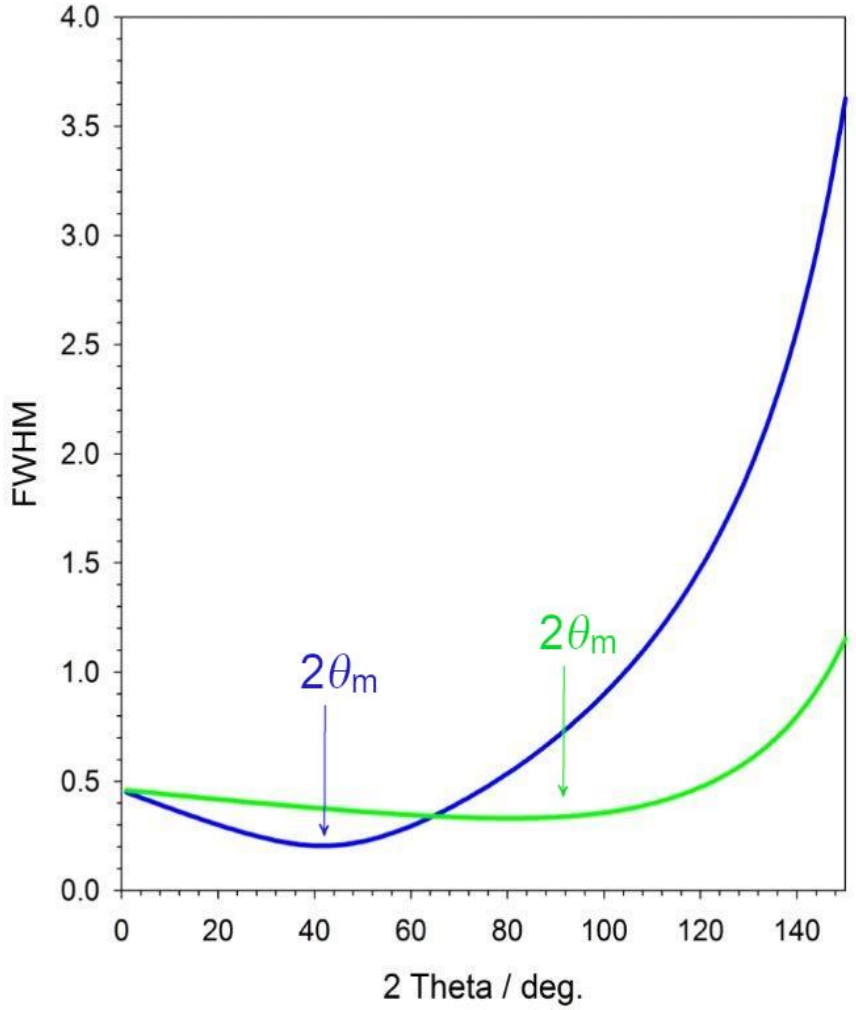
$$U = 4\left(\alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 + \alpha_2^2\beta^2\right) / \left[\tan^2\theta_m\left(\alpha_1^2 + \alpha_2^2 + 4\beta^2\right)\right]$$

$$V = -4\alpha_2^2(\alpha_1^2 + 2\beta^2) / [\tan\theta_m\ (\alpha_1^2 + \alpha_2^2 + 4\beta^2)]$$

$$W = [\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2 + 4\beta^2(\alpha_2^2 + \alpha_3^2)] / (\alpha_1^2 + \alpha_2^2 + 4\beta^2)$$

Here a comparison of two instrument configuration the **blue** one correspond with a instrument configuration dedicated to **magnetism** while the **green** one is dedicated to **structural crystallography**.

There is always a price to paid!!



MAGNETIC DIFFRACTION

The **integrated intensity** of a magnetic Bragg reflections is **proportional** to the **square** of the so called **magnetic interaction vector.**

$$I_M(\mathbf{h}) \approx \left|\mathbf{M}_\perp(\mathbf{h})\right|^2 = \left|\mathbf{M(h)} - (\mathbf{M(h)}\cdot\mathbf{e})\,\mathbf{e}\right|^2$$

Magnetic Interaction Vector

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

Magnetic Structure Factor

$$\mathbf{M}(\mathbf{h}) = p\sum_{j=1}^{n} O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}js}\, exp\left\{2\pi i\left[(\mathbf{H}+\mathbf{k})\left\{S\middle|\mathbf{t}\right\}_s \mathbf{r}_j\right]\right\} \qquad 1/2\cdot r_e\cdot\gamma = p = 0.2696\ 10^{-12}\ \mathrm{cm}/\mu_B$$

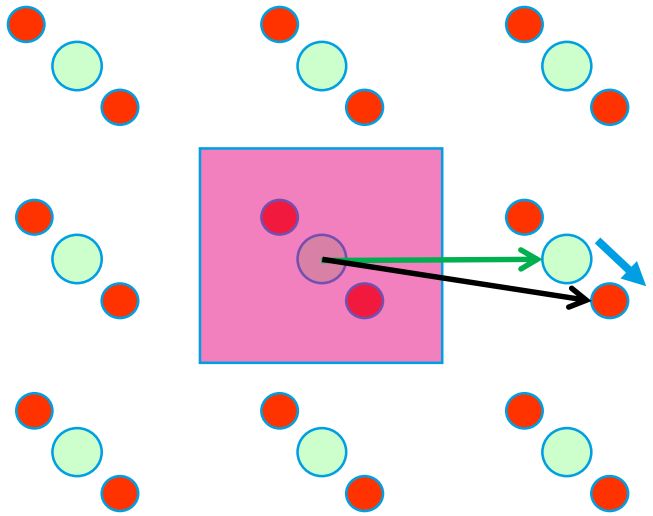
j : index running for all magnetic atom sites in the magnetic asymmetric unit (j =1,…n)

s : index running for all atoms of the orbit corresponding to the magnetic site j (s=1,… n_j). Total number of atoms: N = Σ n_j

$\left\{S\middle|\mathbf{t}\right\}_s$ Symmetry operators of the propagation vector group

Diffraction Patterns of magnetic structures

Portion of reciprocal space



Magnetic reflections

Nuclear reflections

h = **H**+**k**

Magnetic reflections: indexed by a set of propagation vectors {**k**}

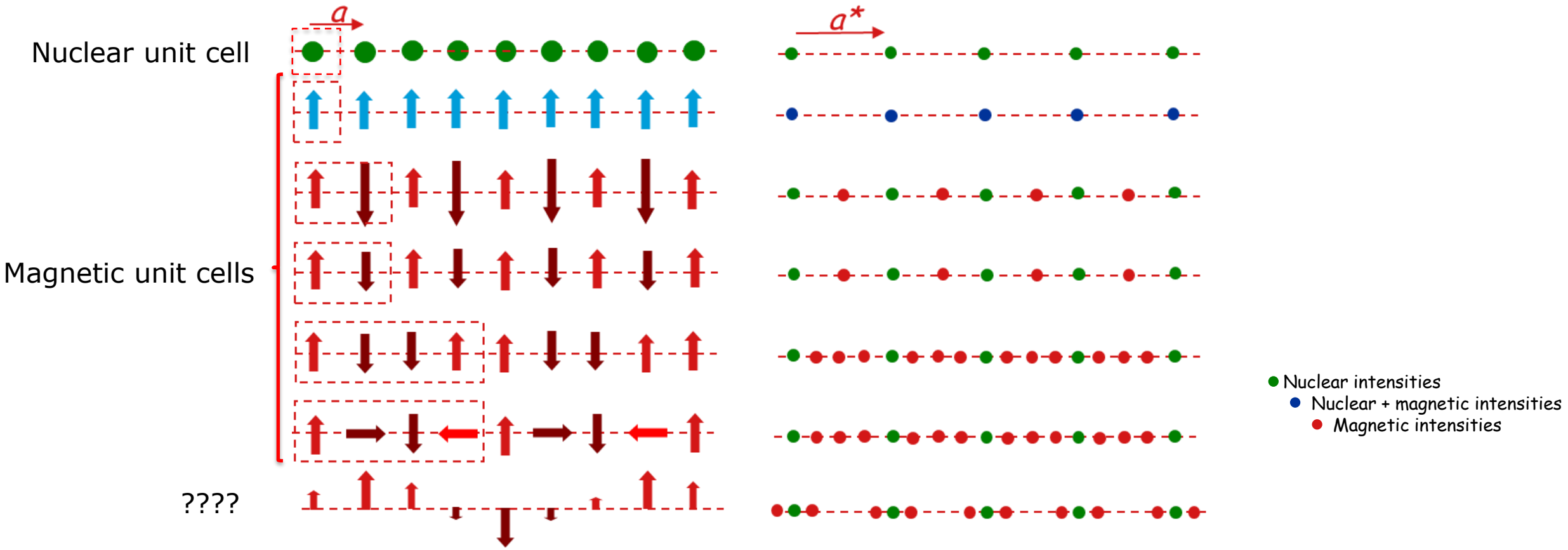
h is the scattering vector indexing a magnetic reflection

H is a reciprocal vector of the crystallographic structure

k is one of the propagation vectors of the magnetic structure

(**k** is reduced to the Brillouin zone)

Propagation Vector

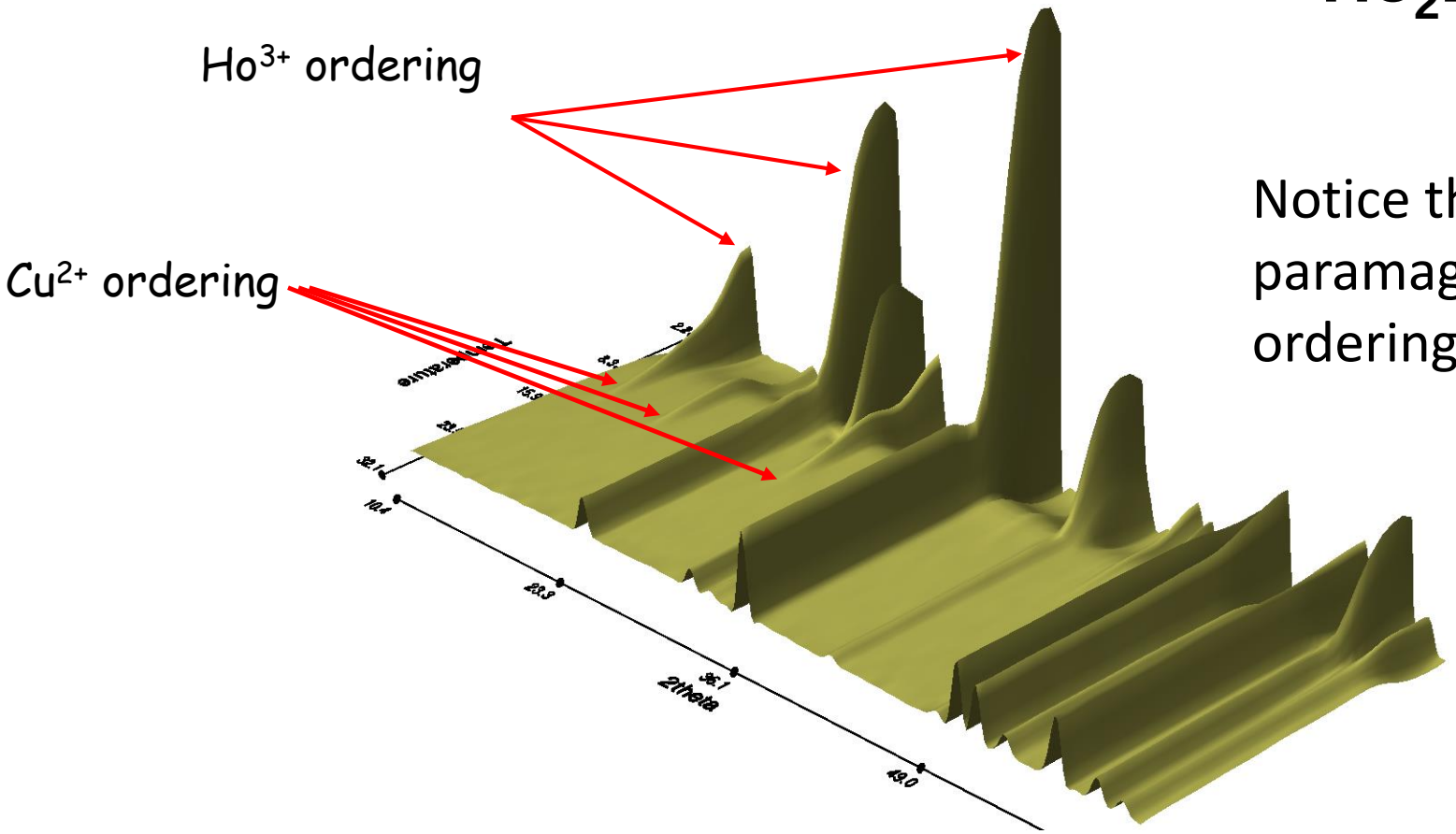


Propagation Vector

Commensurate Magnetic structures can be described by the periodic repetition of a magnetic unit cell, just as crystal structures are described by translation of a nuclear unit cell

We are going to use a description based on the **nuclear unit cell** and a '**propagation vector**', **k**, that describes the relation between moment orientations of equivalent magnetic atoms in different nuclear unit cells

Diffraction Patterns of magnetic structures



Ho_2BaCuO

Notice the decrease of the paramagnetic background on Ho^{3+} ordering

PROPAGATION VECTOR

The magnetic moment "$\mathbf{m}_{lj}$" associated with the atom "j" at the unit cell with origin in $\mathbf{R}_l$, is determined by the Fourier series:

$$\mathbf{m}_{lj} = \sum_{\mathbf{k}} \mathbf{S}_{\mathbf{k}j} \; exp\left\{-2\pi i \mathbf{k}\mathbf{R}_l\right\}$$

Where $\mathbf{S}_{\mathbf{k}j}$ are the Fourier components (linear combination of Basis vectors of irreps) with propagation vector **k** corresponding to the atom j in the zeroth unit cell.

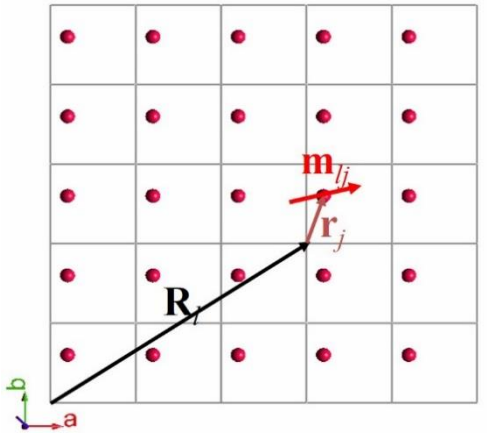
For getting $\mathbf{m}_{lj}$ as real vectors $\mathbf{S}^*_{\mathbf{k}j} = \mathbf{S}_{-\mathbf{k}j}$ should be satisfied

The summation is taken over a discrete set of wavevectors that are confined to the first Brillouin zone of the Bravais lattice of the nuclear cell

Propagation Vector

The magnetic moment can also be written using the next formulation:

$$\mathbf{m}_{lj} = \sum_{\mathbf{k}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k}\,\mathbf{R}_l\} = \sum_{\mathbf{k}} \mathbf{T}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k}\,\mathbf{R}_{lj}\}$$



Where:

$$\mathbf{R}_{lj} = \mathbf{R}_l + \mathbf{r}_j = l_1\mathbf{a} + l_2\mathbf{b} + l_3\mathbf{c} + x_j\mathbf{a} + y_j\mathbf{b} + z_j\mathbf{c}$$

With $\mathbf{R}_l=(l_1, l_2, l_3)$ being a translation vector and (x_j, y_j, z_j) being the fractional coordinates of atom *j* within the unit cell.

One can use whatever of the two formulae keeping in mind the relation: $\mathbf{S}_{\mathbf{k}j} = \mathbf{T}_{\mathbf{k}j}\exp\{-2\pi i\,\mathbf{r}_j\}$

The $\mathbf{S}_{\mathbf{k}j}$ (or $\mathbf{T}_{\mathbf{k}j}$) correspond to the *Fourier components* of the magnetic moment of atom *j.* $\mathbf{S}_{\mathbf{k}j}$ is a complex vector so *6 components are needed.*

Propagation Vector

A magnetic structure could be fully described by:

- Wave-vector(s) or propagation vector(s) {**k**}.

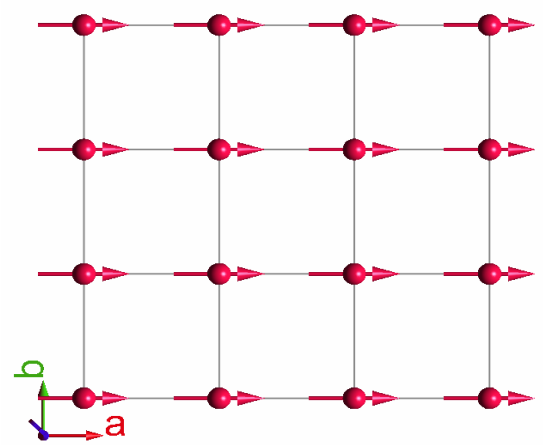
- Fourier components $\mathbf{S}_{\mathbf{k}j}$ for each magnetic atom *j* and **k**-vector $\mathbf{S}_{\mathbf{k}j}$ is a complex vector.

General expression of the Fourier coefficients (complex vectors) for an arbitrary site when $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent can be written as:

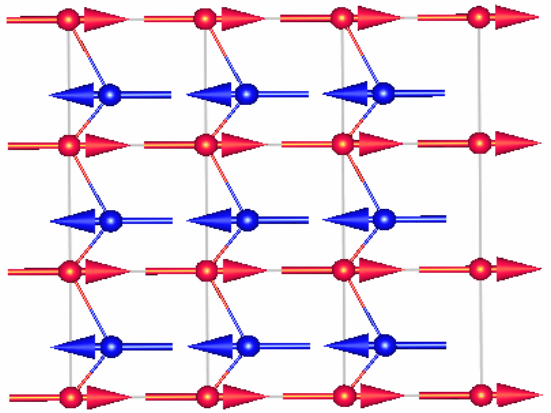
$$\mathbf{S}_{\mathbf{k}} = \frac{1}{2}(\mathbf{R}_{\mathbf{k}} + i\mathbf{I}_{\mathbf{k}})\exp\{-2\pi i\phi_{\mathbf{k}}\}$$

Only six parameters are independent. The writing above is convenient when relations between the vectors $\mathbf{R}$ and $\mathbf{I}$ are established (e.g. when $|\mathbf{R}|=|\mathbf{I}|$, or $\mathbf{R} \cdot \mathbf{I} = 0$). A phase ϕ is also added to handle the possible shift among different magnetic sites.

Simple propagation vector k = (0, 0, 0)



Single magnetic site



Two magnetic sites

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j}\, exp\left\{-2\pi i \mathbf{k}\mathbf{R}_l\right\} = \mathbf{S}_{\mathbf{k}j}$$

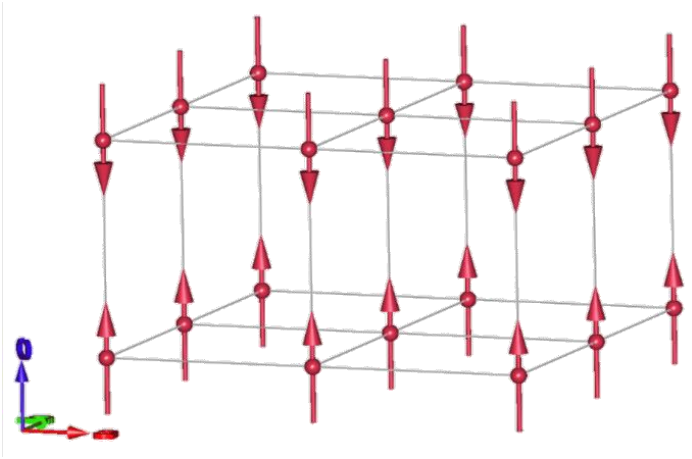
k = (0, 0, 0)

- **Fourier coefficients are real and equal to magnetic moments**
- **The magnetic cell is identical to the crystallographic unit cell**
- **Magnetic symmetry: conventional crystallography plus spin reversal operator → crystallographic magnetic groups**

SINGLE PROPAGATION VECTOR K=1/2 H

The propagation vector is ½ a vector of the reciprocal space vector

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j}\, exp\left\{-2\pi i\, \mathbf{k}\, \mathbf{R}_l\right\} = \mathbf{S}_{\mathbf{k}j}\left(-1\right)^{n(l)}$$



$\mathbf{k} = (0, 0, 1/2)$

$\mathbf{S}_{\mathbf{k}j} = \mathbf{m}_{0\,j}$ corresponds, in this case, to the magnetic moment of the atom j within the zeroth (nuclear) cell.

- REAL Fourier coefficients ≡ magnetic moments
- The magnetic symmetry may also be described using conventional crystallographic magnetic space groups

FOURIER COEFFICIENTS OF SINUSOIDAL STRUCTURES

- **k** interior of the Brillouin zone (pair **k**, **-k**). In other words **k**-(**-k**) is not a reciprocal space vector

- Real $\mathbf{S_k}$, or imaginary component in the same direction as the real one

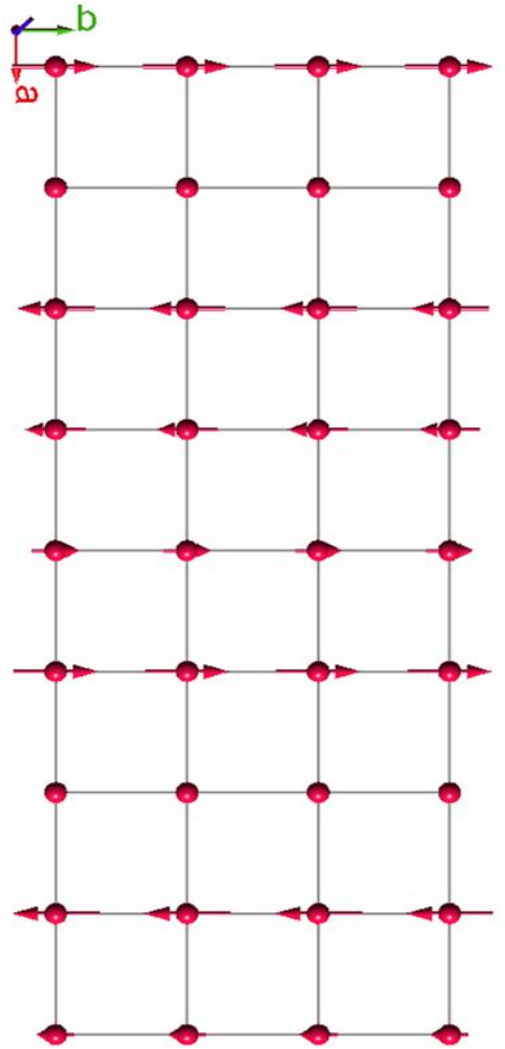
$$\mathbf{m}_{lj} = \mathbf{S}_{\mathbf{k}j} \; exp(-2\pi i \mathbf{k}\mathbf{R}_l) + \mathbf{S}_{\mathbf{-k}j} \; exp(2\pi i \mathbf{k}\mathbf{R}_l)$$

$$\mathbf{S}_{\mathbf{k}j} = \frac{1}{2} m_j \mathbf{u}_j exp(-2\pi i \phi_{\mathbf{k}j})$$

$$\mathbf{m}_{lj} = \frac{1}{2} m_j \mathbf{u}_j exp(-2\pi i \phi_{\mathbf{k}j}) \cdot exp(-2\pi i \mathbf{k}\mathbf{R}_l) + \frac{1}{2} m_j \mathbf{u}_j exp(2\pi i \phi_{\mathbf{k}j}) \cdot exp(2\pi i \mathbf{k}\mathbf{R}_l)$$

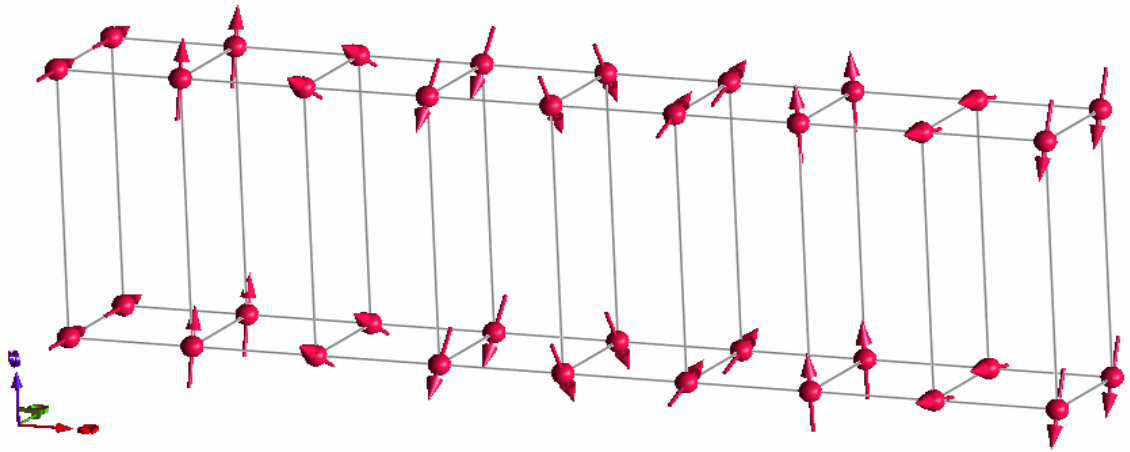
$$\mathbf{m}_{lj} = \frac{1}{2} m_j \mathbf{u}_j \, exp(-2\pi i(\mathbf{k}\mathbf{R}_l + \phi_{\mathbf{k}j})) + \frac{1}{2} m_j \mathbf{u}_j \, exp(2\pi i(\mathbf{k}\mathbf{R}_l + \phi_{\mathbf{k}j}))$$

$$\mathbf{m}_{lj} = m_j \mathbf{u}_j \cos 2\pi(\mathbf{k}\mathbf{R}_l + \phi_{\mathbf{k}j})$$



FOURIER COEFFICIENTS OF HELICAL STRUCTURES

- **k** interior of the Brillouin zone
- Real component of $\mathbf{S_k}$ perpendicular to the imaginary component



$$\mathbf{S}_{\mathbf{kj}} = \frac{1}{2}\left[m_{uj}\mathbf{u}_j + i m_{vj}\mathbf{v}_j \right] exp(-2\pi i \phi_{\mathbf{kj}})$$

$$\mathbf{m}_{lj} = m_{uj}\mathbf{u}_j \cos 2\pi(\mathbf{kR}_l + \phi_{\mathbf{kj}}) + m_{vj}\mathbf{v}_j \sin 2\pi(\mathbf{kR}_l + \phi_{\mathbf{kj}})$$

Representation analysis

A reducible representation of the propagation vector group can be constructed by selecting the atoms of a Wyckoff position and applying the symmetry operators to both positions and axial vectors (spins).

This gives rise to the so called Magnetic Representation of dimension: $3n_a$ (being n_a the number of atoms in the primitive cell)

The basis functions, for each Irrep and each sublattice of a Wyckoff site, can be calculated by using the projection operator formula. The basis functions are constant vectors of the form (1,0,0), (0.5, 1,0) … with components referred to the crystallographic unitary frame: {**a**/a, **b**/b, **c**/c} attached to each sublattice.

Representation analysis

SARAh (Spin and Representation Analysis How-To) – SARAh is widely used for magnetic symmetry analysis.

I**SODISTORT** – Part of the ISOTROPY software suite. ISODISTORT is widely used for symmetry analysis in structural refinements.

BasIreps – BasIreps is part of the FullProf suite and allows for the calculation of irreducible representations of space groups for structural and magnetic systems.

Bilbao Crystallographic Server. It provides tools for representation analysis specifically focused on coupling magnetic symmetry with crystallographic data, useful for magnetic structure analysis.

Suite of diffraction instruments at ILL

Powder Diffractometers:

D1B 2-axis diffractometer (CRG)
D2B high-resolution 2-axis diffractometer
D4 diffractometer for liquids and amorphous substances
D7 diffuse scattering spectrometer (polarized neutrons)
D20 high-flux 2-axis diffractometer
SALSA the strain imager
XtremD diffractometer for extreme conditions experiments (CRG)

D1B 2-axis diffractometer

PHYSICAL REVIEW B **109**, 104411 (2024)

Exploring magnetism and magnetoelectric properties in the green phase of R_2BaCuO_5 (R = Er, Eu, Y, Tm, and Lu): The role of 4f-3d exchange coupling

Premakumar Yanda,[1] N. Boudjada,[2] Juan Rodríguez-Carvajal,[3] and A. Sundaresan[1]

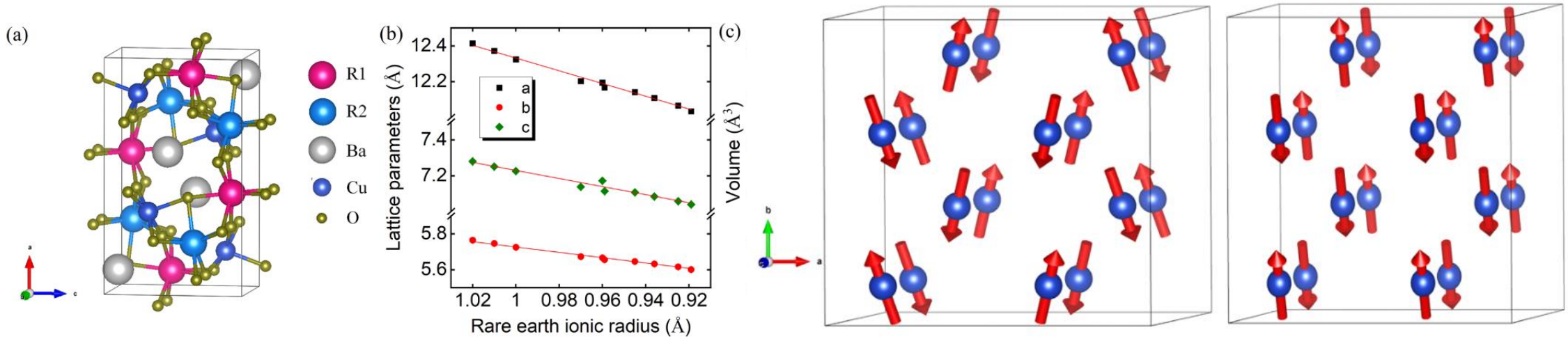
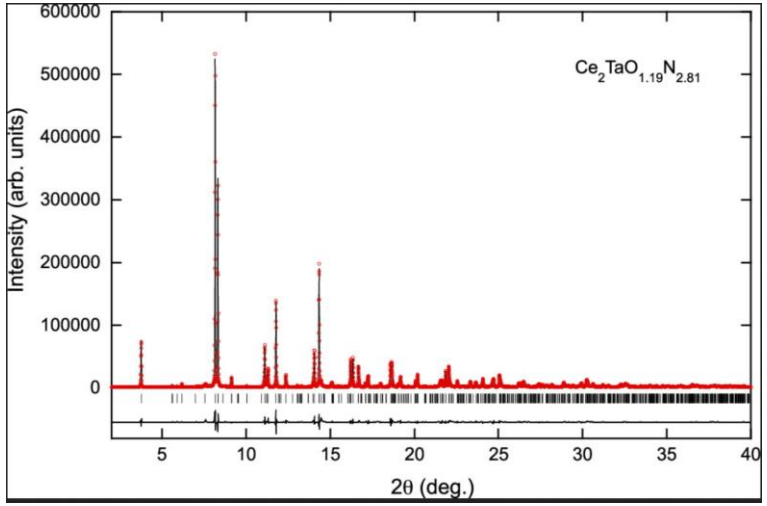
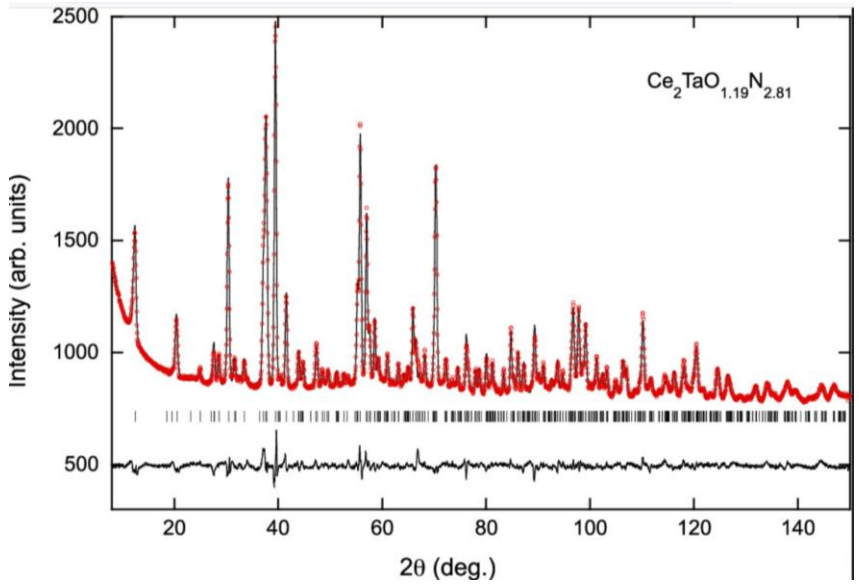


FIG. 1. (a) Crystal structure of R_2BaCuO_5 where R is rare-earth metal ion. (b) Lattice parameters with Vegard's law fitting and (c) Unit cell volume with respect to rare earth ionic radius.

D20 2-axis diffractometer





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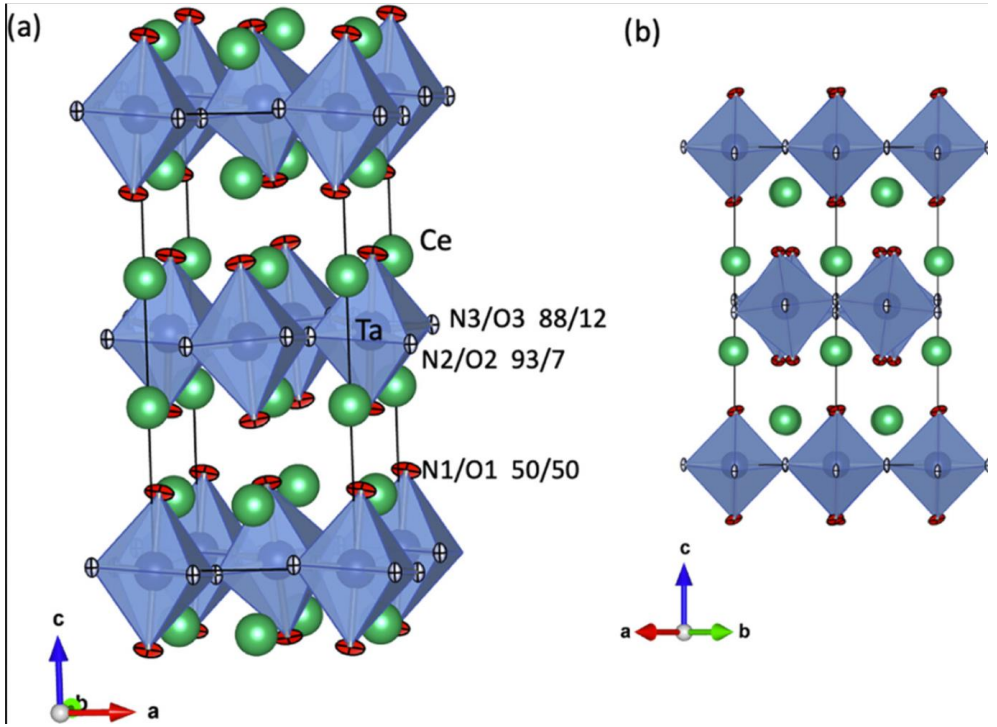
Article

Anionic and Magnetic Ordering in Rare Earth Tantalum Oxynitrides with an $n = 1$ Ruddlesden–Popper Structure

Published as part of the Chemistry of Materials virtual special issue "C. N. R. Rao at 90".

Jhonatan R. Guarín, Carlos Frontera, Judith Oró-Solé, Bastian Colombel, Clemens Ritter, François Fauth, Josep Fontcuberta,* and Amparo Fuertes*

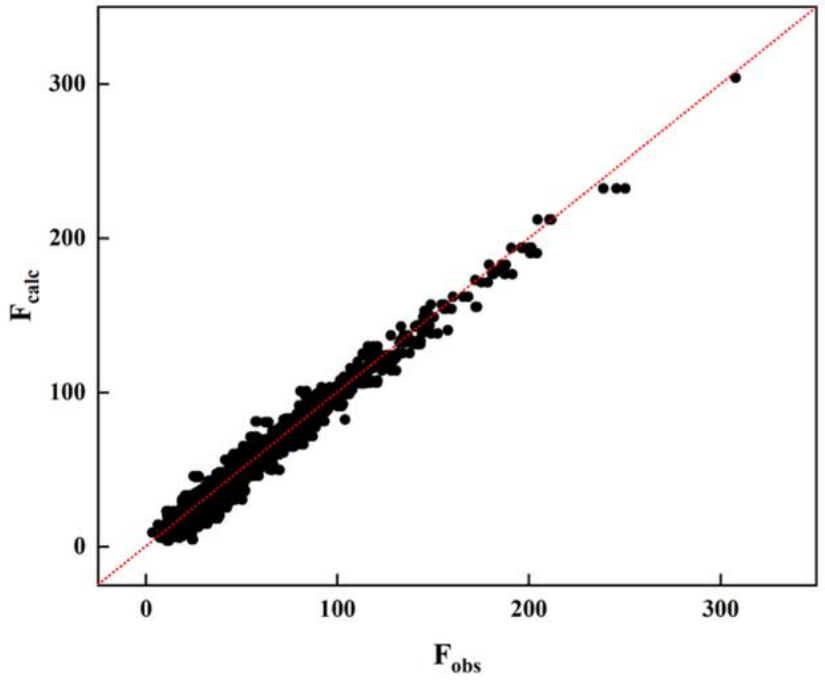


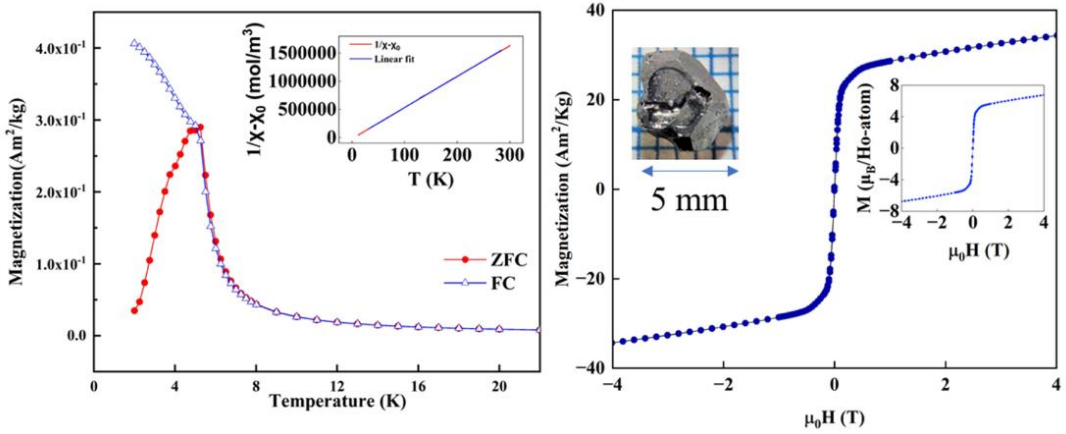
SUITE OF DIFFRACTION INSTRUMENTS AT ILL

Single Crystal Diffractometers:

D3 polarised hot-neutron diffractometer
D9 hot neutrons
D10 4-circle & 3-axis
D23 2-axis spectrometer (CRG)
Orient Express Laue diffractometer for align and check samples

D9 hot neutron





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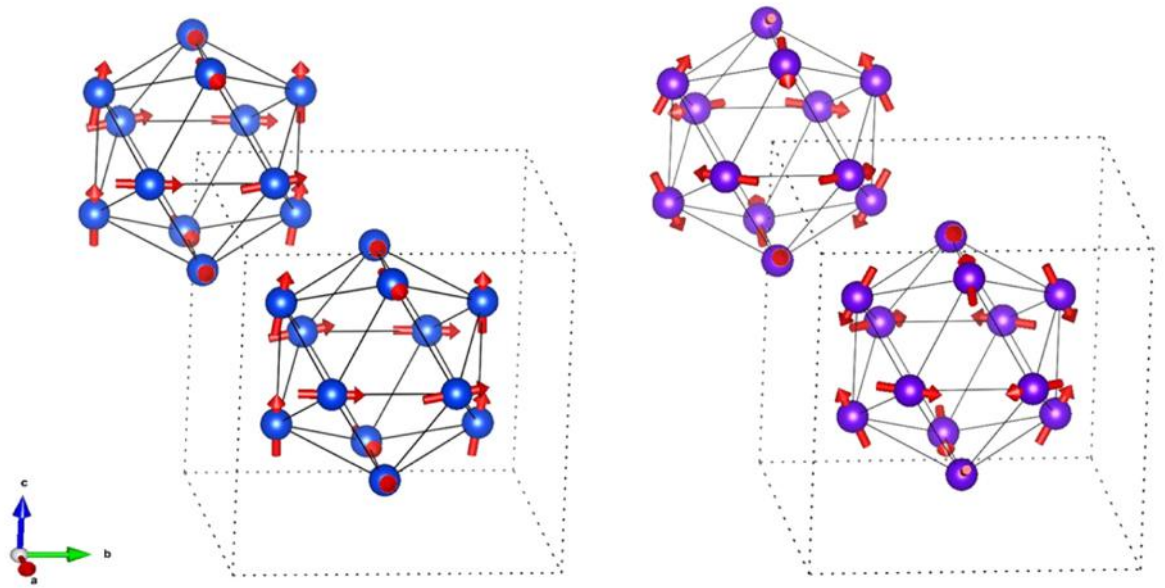
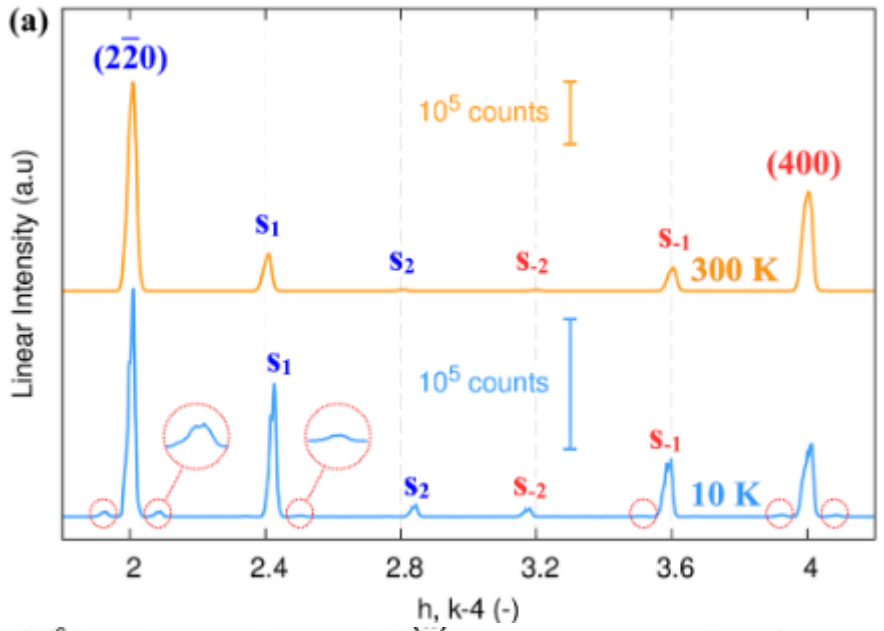
Single-crystal neutron diffraction study on the $Ho_{13.6}Au_{61.1}Al_{25.3}$ quasicrystal approximant

Karthika K. Thilakan [a,*], Fernand Denoel [b], Yu-Chin Huang [a], Oscar Fabelo [c], Roland Mathieu [b], Cesar Pay Gómez [a], Martin Sahlberg [a]



D10 thermal neutron diffractometer



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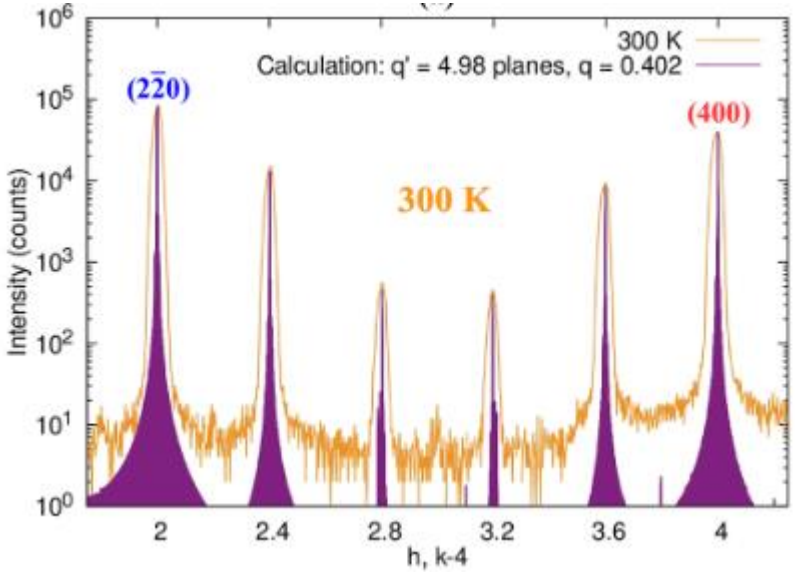
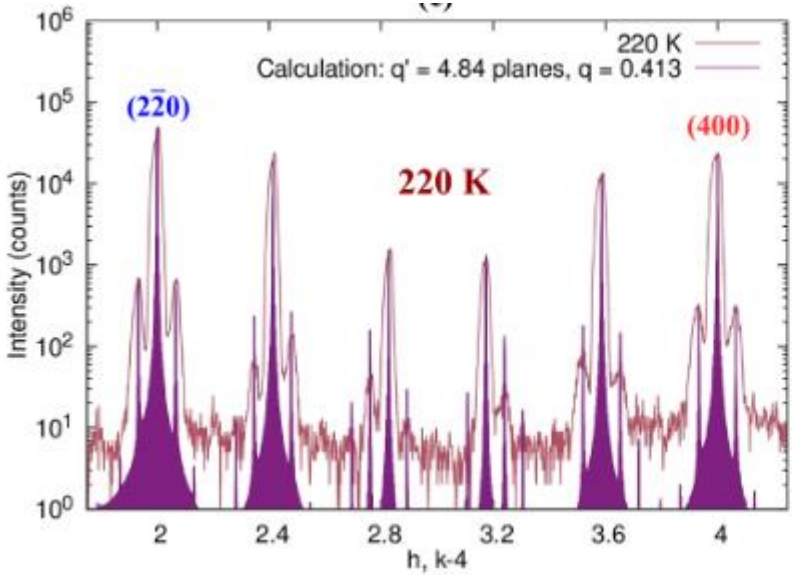
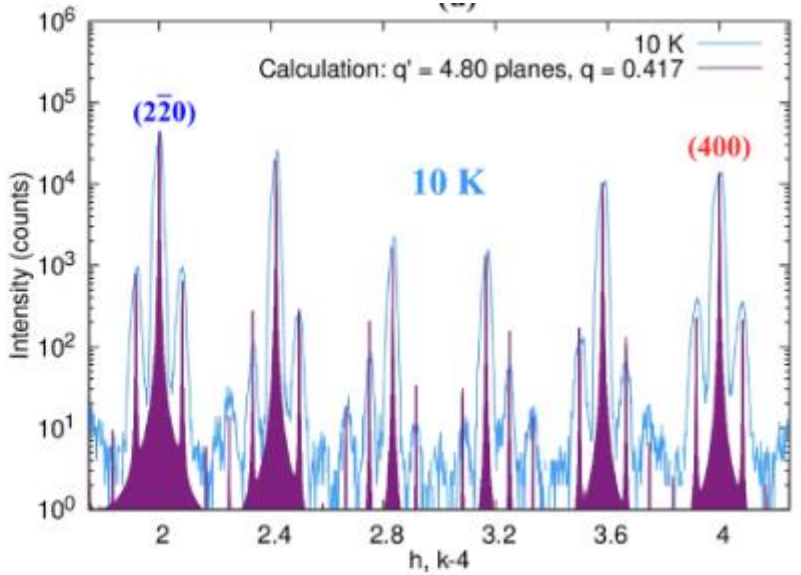
Anharmonic incommensurate structure modulation in Ni-Mn-Ga martensite exhibiting highly mobile twin boundaries

P. Veřtát [a,*], M. Klicpera [b], O. Fabelo [c], O. Heczko [a], L. Straka [a]







Thank you for your kind attention

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