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Introduction to aperiodic crystals

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Lecture content

1. Introduction
 - Diffraction by classical 3D periodic crystals
 - The crystal model
2. The end of a convenient paradigm
 - Historical backgrounds and examples
 - The crystal redefined
3. Introduction to the superspace formalism
 - Structure examples
 - Simulation
4. The structure factor (SF) of incommensurate crystals
 - Numerical recipes for the calculation of SF
5. The resolution of aperiodic crystals
 - The charge flipping algorithm
 - Demonstration
6. Conclusion

Diffraction by periodic objects

QM teaches us that the scattering of an object depends on the scattering vector

$$\mathbf{S} = \mathbf{s} - \mathbf{s}_0$$

where \mathbf{s}_0 and \mathbf{s} indicate the direction of the incident resp. scattered beam. Moreover, if λ is the wavelength of the incident beam

$$|\mathbf{s}| = |\mathbf{s}_0| = \frac{1}{\lambda}$$

The total scattering of an object with volume V and density function $\rho(\mathbf{x})$ is given by

$$G_V(\mathbf{S}) = \int_V \rho(\mathbf{x}) \exp(2\pi i \mathbf{S} \cdot \mathbf{x}) d\mathbf{x}$$

Diffraction by periodic objects (2)

The FT of the density function is given by

$$G(\mathbf{S}) = \int_{-\infty}^{\infty} \rho(\mathbf{x}) \exp(2\pi i \mathbf{S} \cdot \mathbf{x}) d\mathbf{x}$$

The difference between the two relations $G(\mathbf{S})$ et $G_v(\mathbf{S})$ resides in the integration domain.

This can be accommodated by defining a new function $h(x)$ which is 1 inside the crystal and 0 everywhere else.

In a one dimensional periodic crystal with N cells, this yields

$$h(x) = \begin{cases} 1 & \text{for } |x| \leq \frac{Na}{2} \\ 0 & \text{everywhere else} \end{cases}$$

Diffraction by periodic objects (3)

It can be shown that

$$\mathcal{F} [h(x)] = H(S) = Na \frac{\sin \pi NaS}{\pi NaS}$$

For large values of N this function is close to the Dirac $\delta(S)$ function.
In three dimensions

$$H(\mathbf{S}) = V \frac{\sin \pi N_1 a_1 S}{\pi N_1 a_1 S} \frac{\sin \pi N_2 a_2 S}{\pi N_2 a_2 S} \frac{\sin \pi N_3 a_3 S}{\pi N_3 a_3 S}$$

Diffraction by periodic objects (4)

Finally we get

$$\begin{aligned} G_V(\mathbf{S}) &= \mathcal{F}[\rho(\mathbf{x}) \cdot h(\mathbf{x})] \\ &= G(\mathbf{S}) * H(\mathbf{S}) \\ &\approx G(\mathbf{S}) \end{aligned}$$

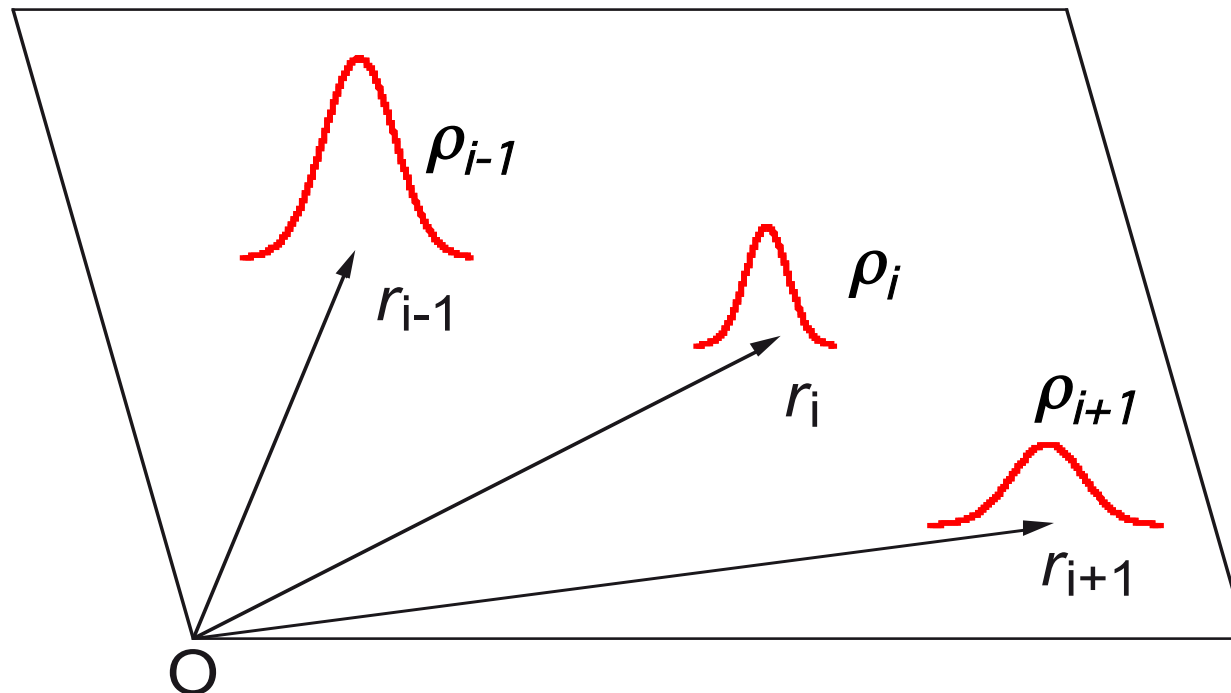
as $H(\mathbf{S}) \rightarrow \delta(\mathbf{S})$ for $N \gg 0$, which is the case here.

The volume factor has been omitted in this expression.

Scattering from assemblies of atoms

The content of a unit cell can be conveniently expressed by the convolution product

$$\rho(\mathbf{r}) = \sum_i \rho_i(\mathbf{r}) * \delta_i(\mathbf{r} - \mathbf{r}_i)$$



Scattering from assemblies of atoms (2)

As the density function $\rho(\mathbf{x})$ is periodic, we can exploit the property of the convolution product and express the density function over the crystal by

$$\rho(\mathbf{x}) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty} \delta\{\mathbf{x} - (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3)\} * \left[\sum_i \rho_i(\mathbf{x}) * \delta(\mathbf{x} - \mathbf{x}_i) \right]$$

\mathbf{a}_i represent the lattice constants and n_i define the lattice nodes. The sum over the ∞ number of terms is justified as seen before.

The FT $\mathcal{F}[\rho(\mathbf{x})] = G(\mathbf{S})$ is given by

$$G(\mathbf{S}) = R(\mathbf{S}).F(\mathbf{S})$$

where $R(\mathbf{S})$ is the FT of the triple sum and $F(\mathbf{S})$ the FT of the unit cell content given between [].

Scattering from assemblies of atoms (3)

The Fourier transform of the unit cell content

$$F(\mathbf{S}) = \int \rho(\mathbf{r}) \exp(2\pi i \mathbf{S} \cdot \mathbf{r}) d\mathbf{r}$$

can be further simplified by replacing the integral by a summation over the atoms contained in the unit cell. By assuming that the electron density around each atom is independent of the compound, we define the atomic scattering factor

$$f^\mu(\mathbf{S}) \equiv \int_{atom} \rho^\mu(\mathbf{r}) \exp(2\pi i \mathbf{S} \cdot \mathbf{r}) d\mathbf{r}$$

and finally obtain the structure factor.

$$\mathcal{F}[\rho(\mathbf{r})] = F(\mathbf{S}) = \sum_{\mu} f^\mu(\mathbf{S}) \exp(2\pi i \mathbf{S} \cdot \mathbf{r}^\mu)$$

Scattering from assemblies of atoms (4)

We still have to evaluate $R(\mathbf{S})$.

$$R(\mathbf{S}) = \sum_{h_1=-\infty}^{\infty} \sum_{h_2=-\infty}^{\infty} \sum_{h_3=-\infty}^{\infty} \delta\{\mathbf{S} - (h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*)\}$$

It turns out that the FT of a Dirac function is also a Dirac function where the basis vectors \mathbf{a}_i^* are the so-called reciprocal lattice vectors satisfying the following relation

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}$$

Consequently $R(\mathbf{S})$ is everywhere 0 except on the nodes h_i of the reciprocal vector \mathbf{h}

$$\mathbf{h} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*$$

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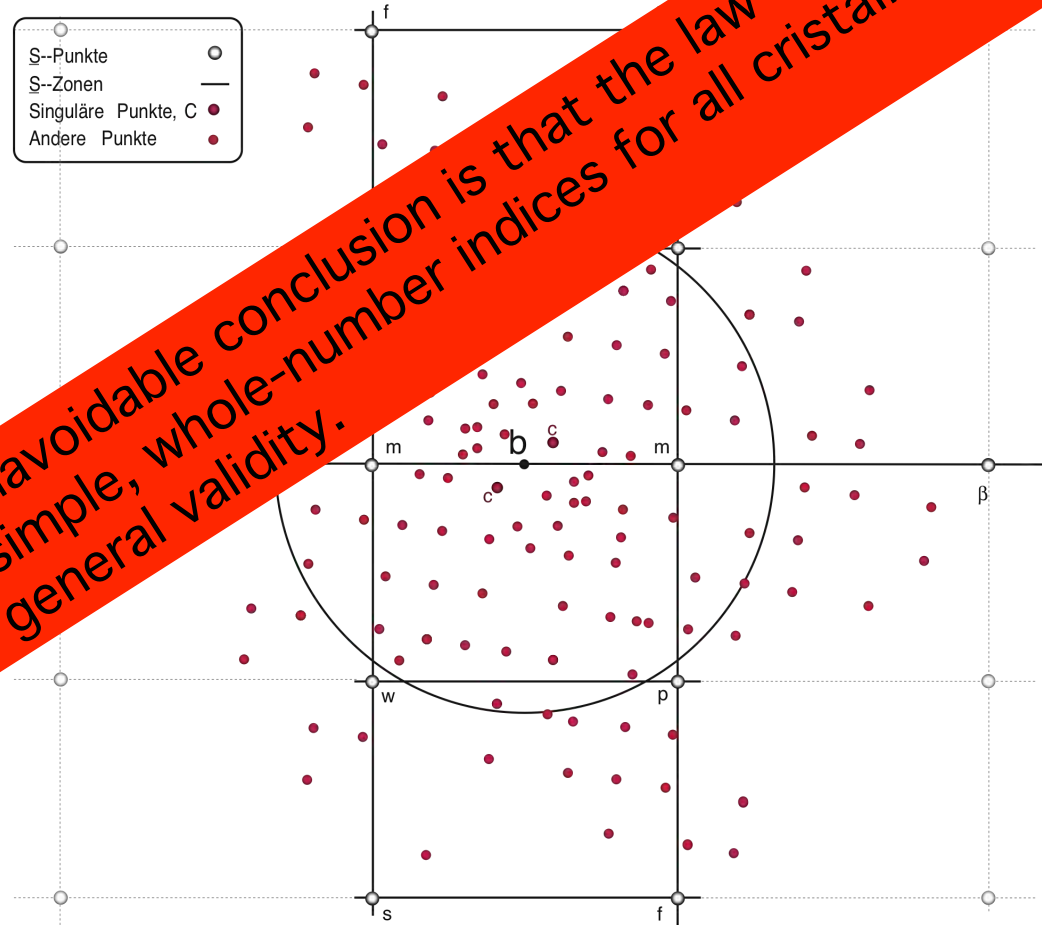
The decisive steps to aperiodic-crystallography

- ... Dehlinger (1927), Preston (1938), Kochendörfer (1939), Chao & Taylor (1940), Daniel & Lipson (1943), Hargreaves (1952),
...
- 1967 Masaaki Korekawa (University of Munich)
 - » Theory of satellite reflections (in german)
- 1972 P.M. de Wolff (IUCr Kyoto)
 - » 4-d space groups of $\gamma\text{-Na}_2\text{CO}_3$ an incommensurate structure
 - A. Janner (IUCr Kyoto, same session as de Wolff !)
 - » Symmetry groups of lattice vibrations
- 1981 Makovicky & Hyde
 - » Composite crystals
- 1984 Shechtman, Blech, Gratias & Cahn
 - » Quasicrystals, Al-Mn alloy with sharp 10-fold symmetry pattern

The Calaverite puzzle

Copy of the original figure from the article
«Über Calaverit»
 von V. Goldschmidt, Ch. Palache and M. Peacock
 in

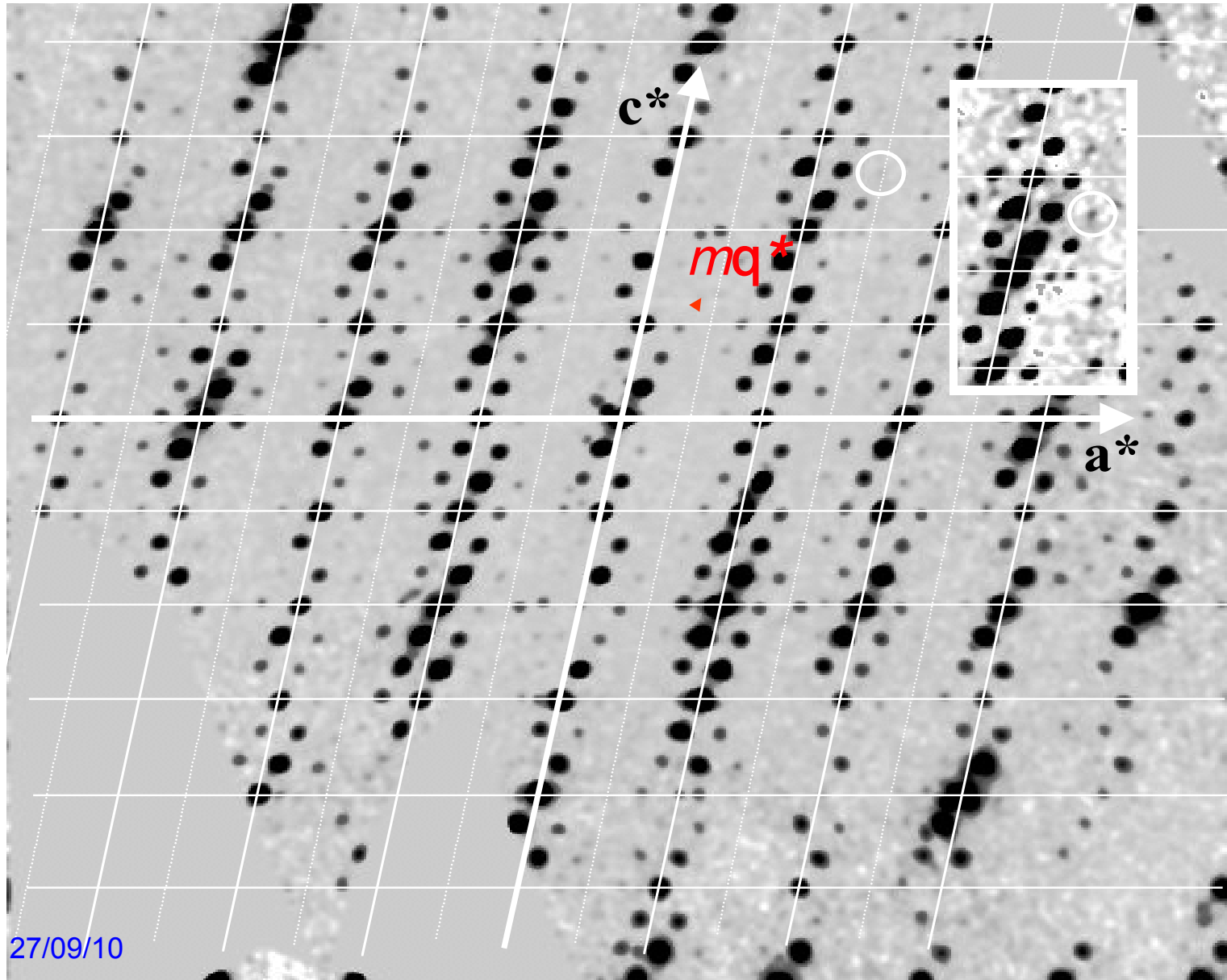
Neues Jahrbuch für Mineralogie, Geologie und Paläontologie, 63. Beilage Band. Abt. A, 1907



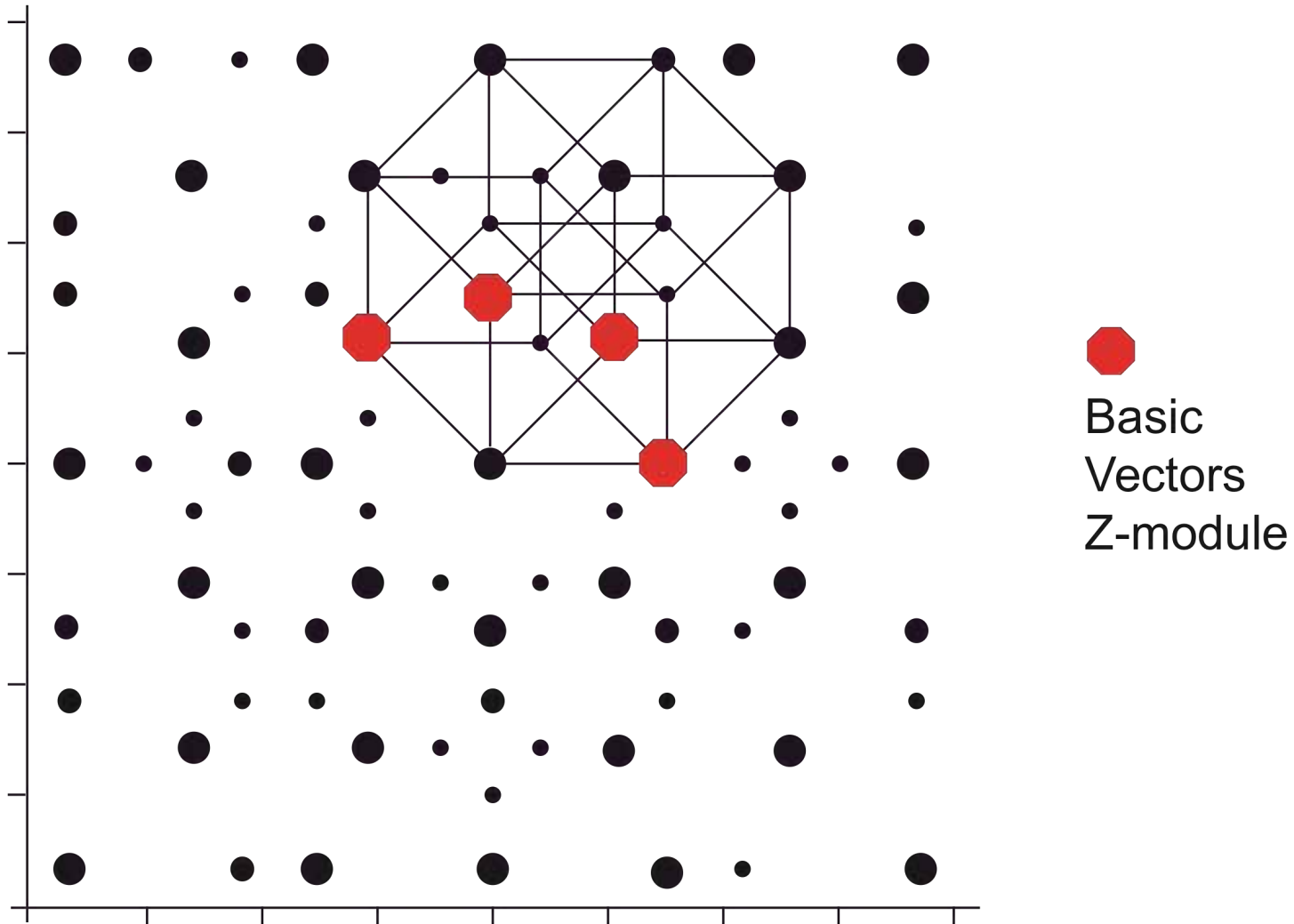
(transl.) “The unavoidable conclusion is that the law of rational indices, i.e. the law of simple, whole-number indices for all crystalline forms, [...] is not of general validity.”

Reconstructed $h2l$ layer of the non-periodic structure $\gamma\text{-Na}_2\text{CO}_3$

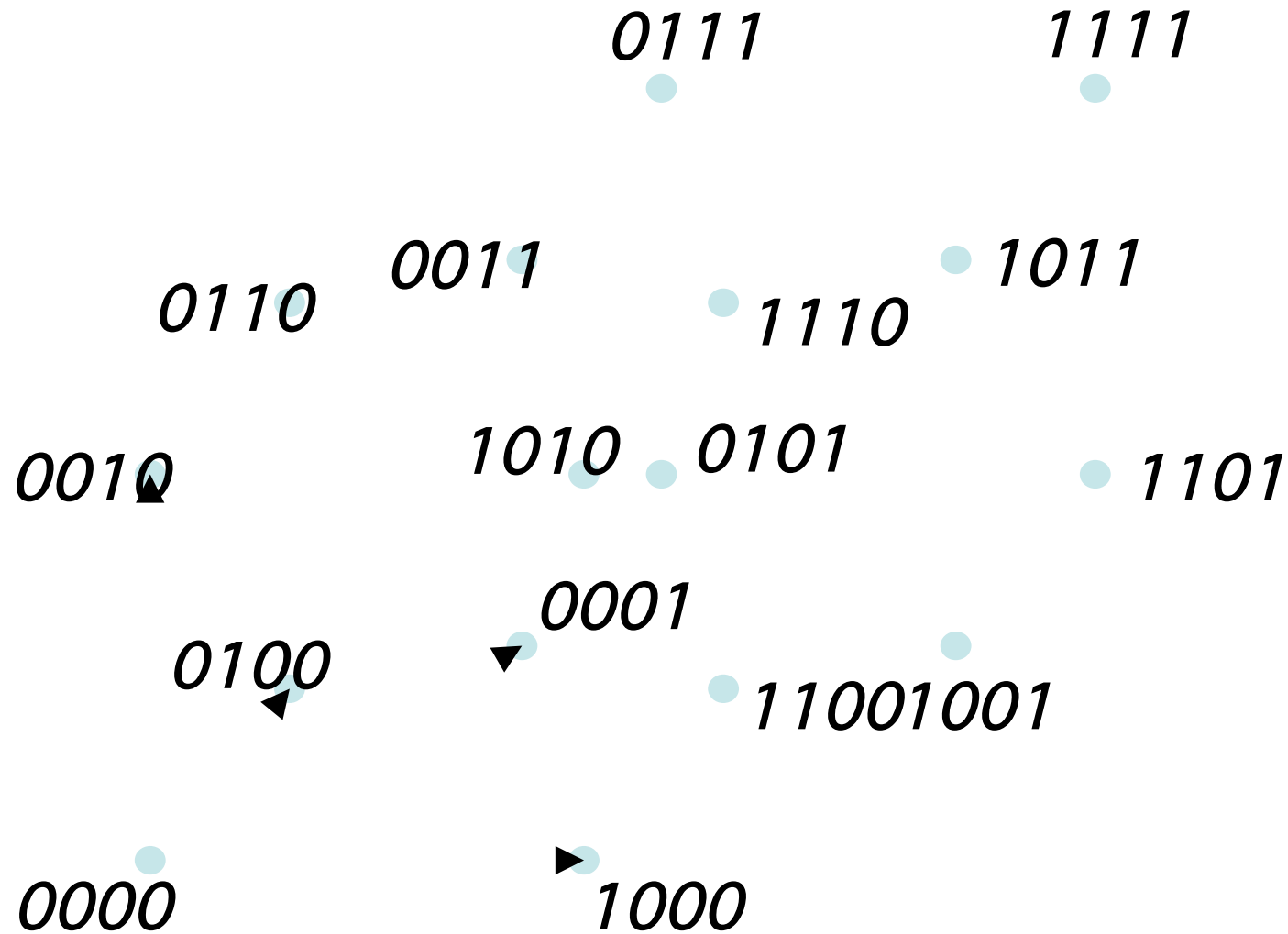
$$H = h_1 a_1^* + h_3 a_3^* + m q^*$$



Layer of a diffraction pattern requesting more than two integers to index the pattern.



How to generate an hypercube

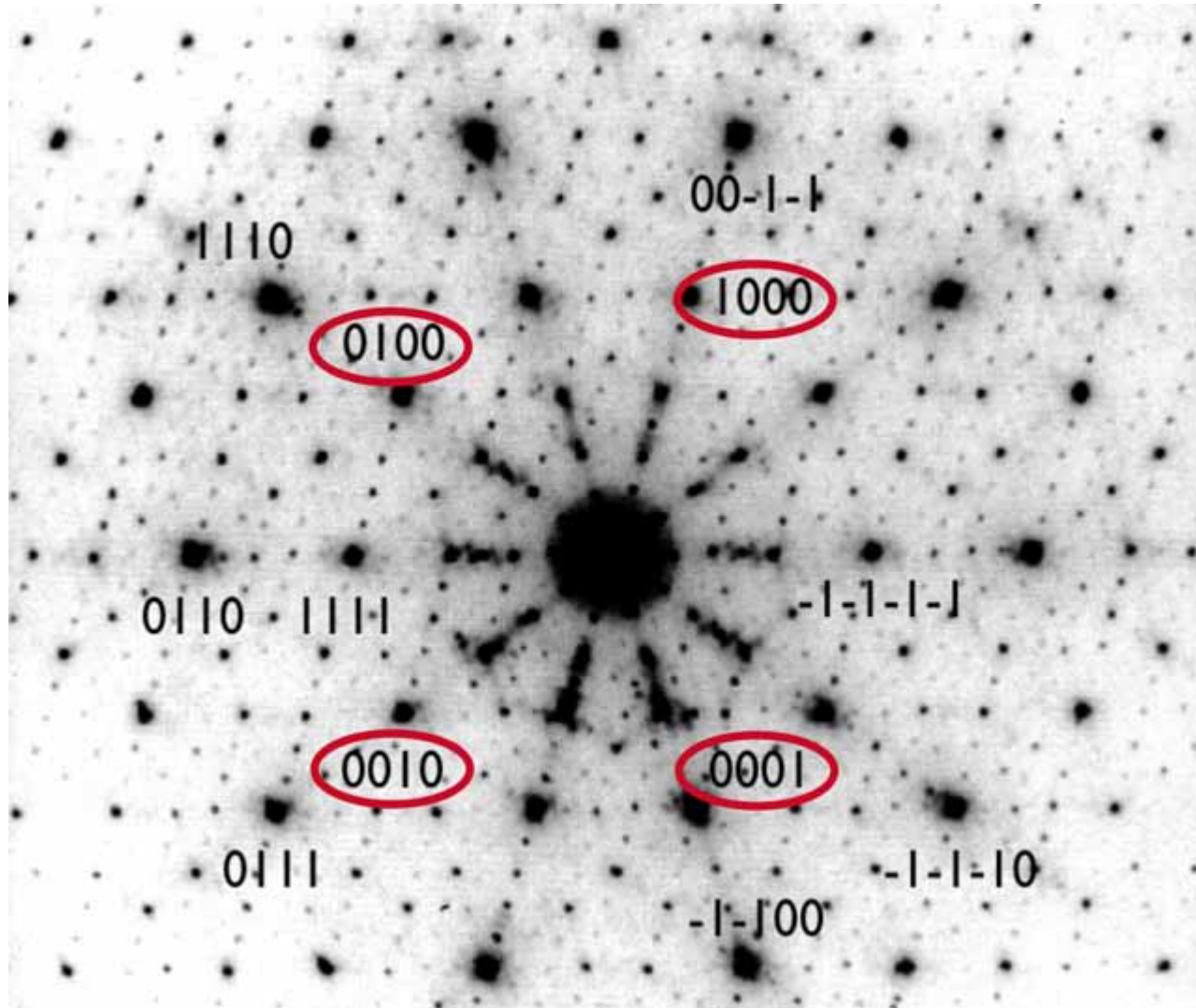


Decagonal
crystal



27/09/10

Another example of a diffraction pattern requesting 4 integer indices to index each spot



What is a crystal?

What is an aperiodic crystal?

What is a crystal?

A material is a crystal if it has essentially a **sharp diffraction pattern**. The word essentially means that most of the intensity of the diffraction is concentrated in relatively sharp Bragg peaks, besides the always present diffuse scattering. In all cases, the positions of the diffraction peaks can be expressed by

$$\mathbf{H} = h_1 \mathbf{a}_1^* + h_2 \mathbf{a}_2^* + \cdots + h_n \mathbf{a}_n^* \quad (n > 3)$$

Here \mathbf{a}_i^* and h_i are the reciprocal lattice vectors and integer coefficients respectively and the number n is the minimum for which the positions of the peaks can be described with integer coefficient h_i . The conventional crystals are a special class, though very large, for which $n = 3$.

What is an aperiodic crystal?

If \mathbf{h} is a reciprocal vector with rank = n

$$\mathbf{h} = h_1 \mathbf{a}_1^* + h_2 \mathbf{a}_2^* + h_3 \mathbf{a}_3^* + \dots + h_n \mathbf{a}_n^*$$

\mathbf{h} describes a periodic crystal if its space is equal to its rank

\mathbf{h} describes an aperiodic crystal if its rank is larger than its space

A short break to solve exercise 1

In the printed version, the text is given at the end of the file

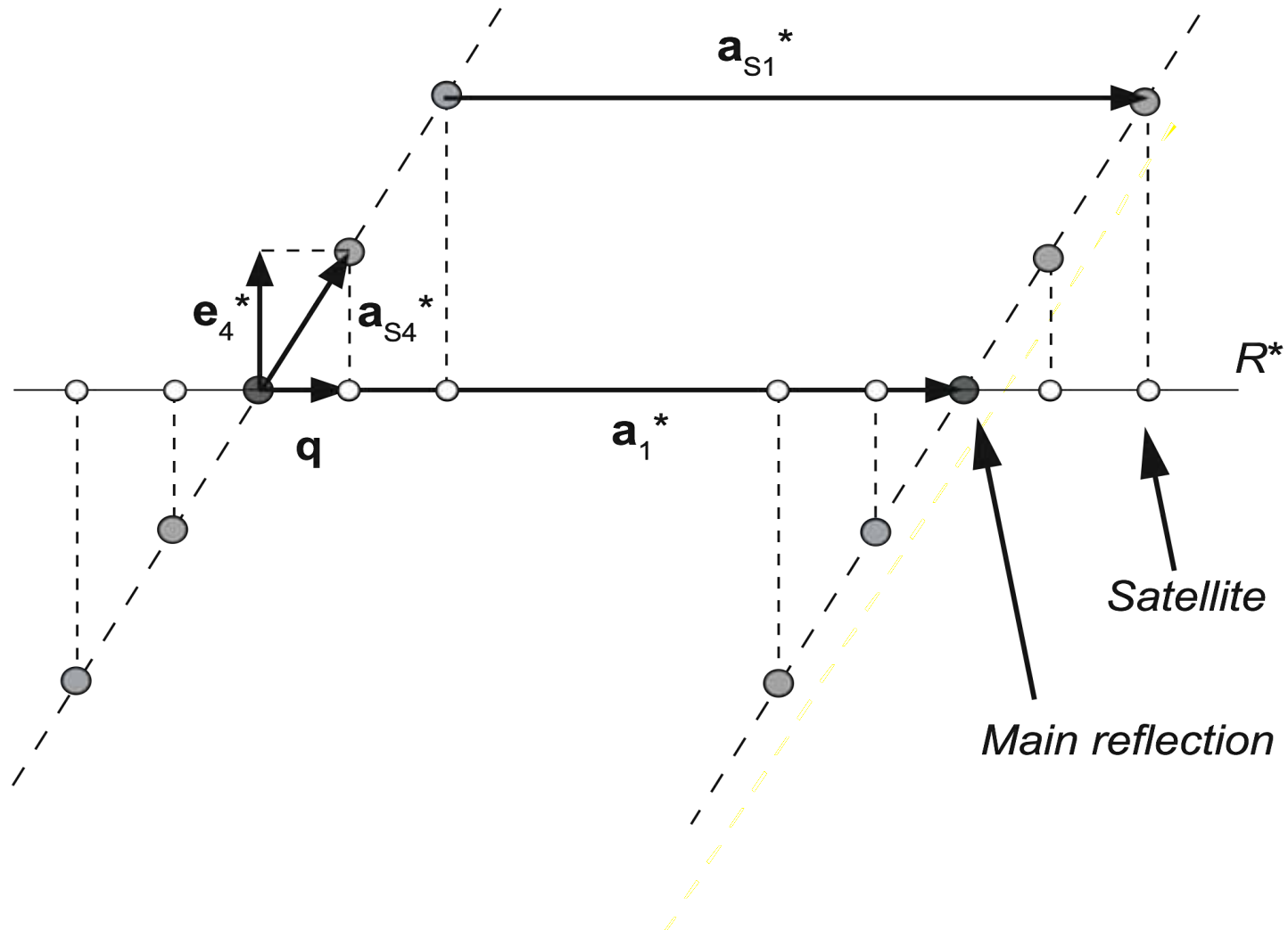
Where do aperiodic crystals occur?

- In all types of crystalline materials
 - Minerals
 - Metals, alloys (quasicrystals)
 - Organic, inorganic materials
 - Proteins, macro-molecules
- In pressure or temperature induced phase transitions
 - $\alpha \rightarrow \text{inc} \rightarrow \beta$ quartz
- ...

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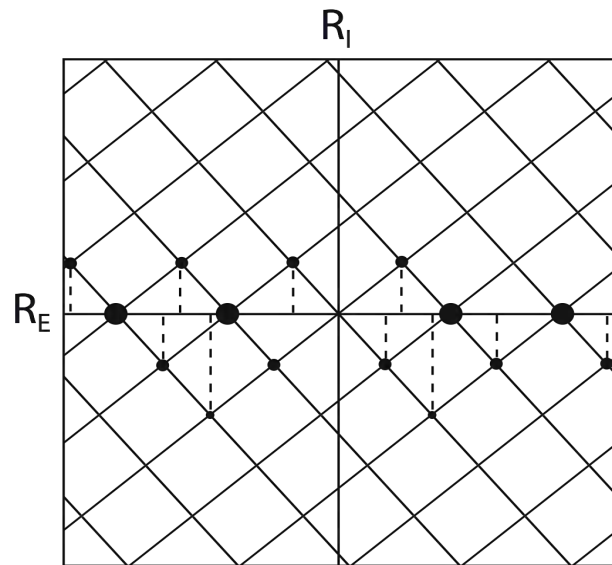
(3+1)-dimensional extension of the reciprocal space with satellite reflections



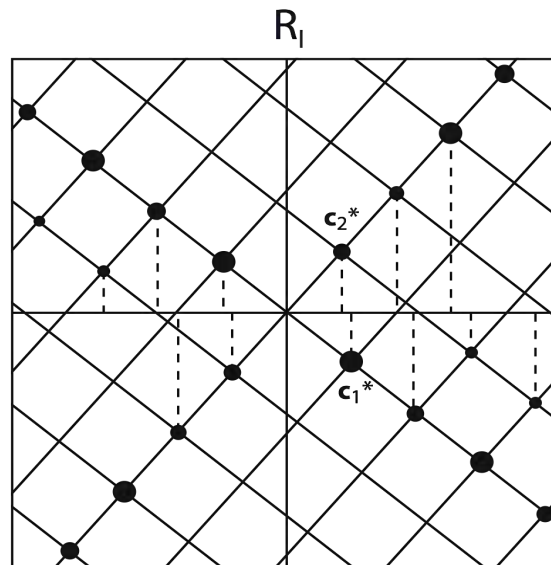
Variants of aperiodic structures (according to A. Yamamoto)

Diffraction pattern extensions of aperiodic crystals

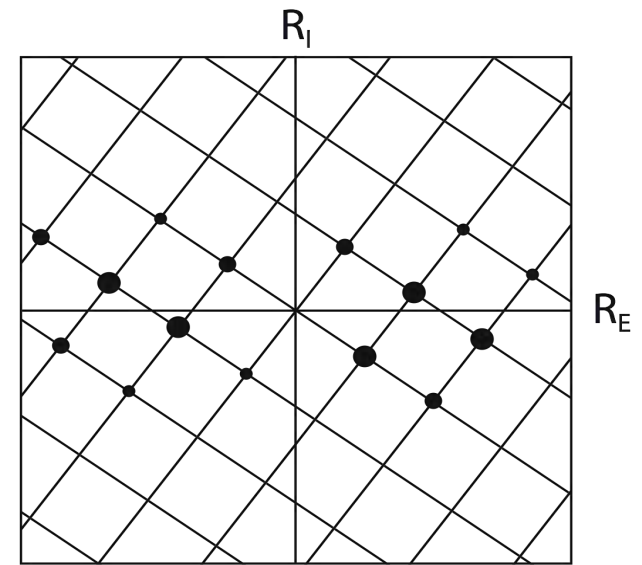
modulated crystal



composite crystal



quasicrystal



From reciprocal to direct superspace

(3+1)d example

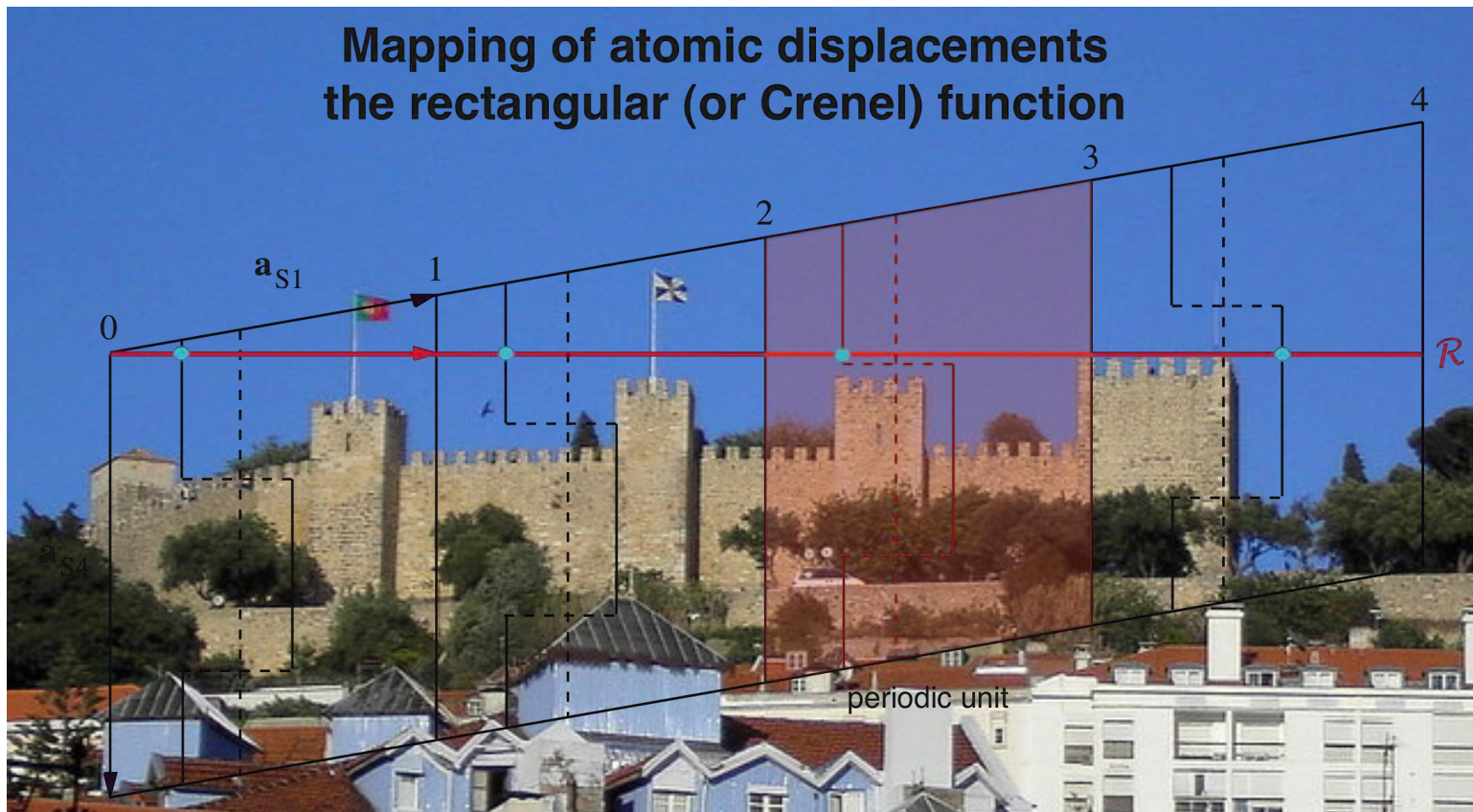
$$\begin{array}{l} a_{S1}^* = (\mathbf{a}_1^*, 0) \\ a_{S2}^* = (\mathbf{a}_2^*, 0) \\ a_{S3}^* = (\mathbf{a}_3^*, 0) \\ a_{S4}^* = (\mathbf{q}, 1) \end{array} \longrightarrow a_{Si}^* \cdot a_{Sj} = \delta_{ij} \longrightarrow \begin{array}{l} a_{S1} = (\mathbf{a}_1, -\mathbf{q} \cdot \mathbf{a}_1) \\ a_{S2} = (\mathbf{a}_2, -\mathbf{q} \cdot \mathbf{a}_2) \\ a_{S3} = (\mathbf{a}_3, -\mathbf{q} \cdot \mathbf{a}_3) \\ a_{S4} = (0, 1) \end{array}$$

Which in 3d is equivalent to

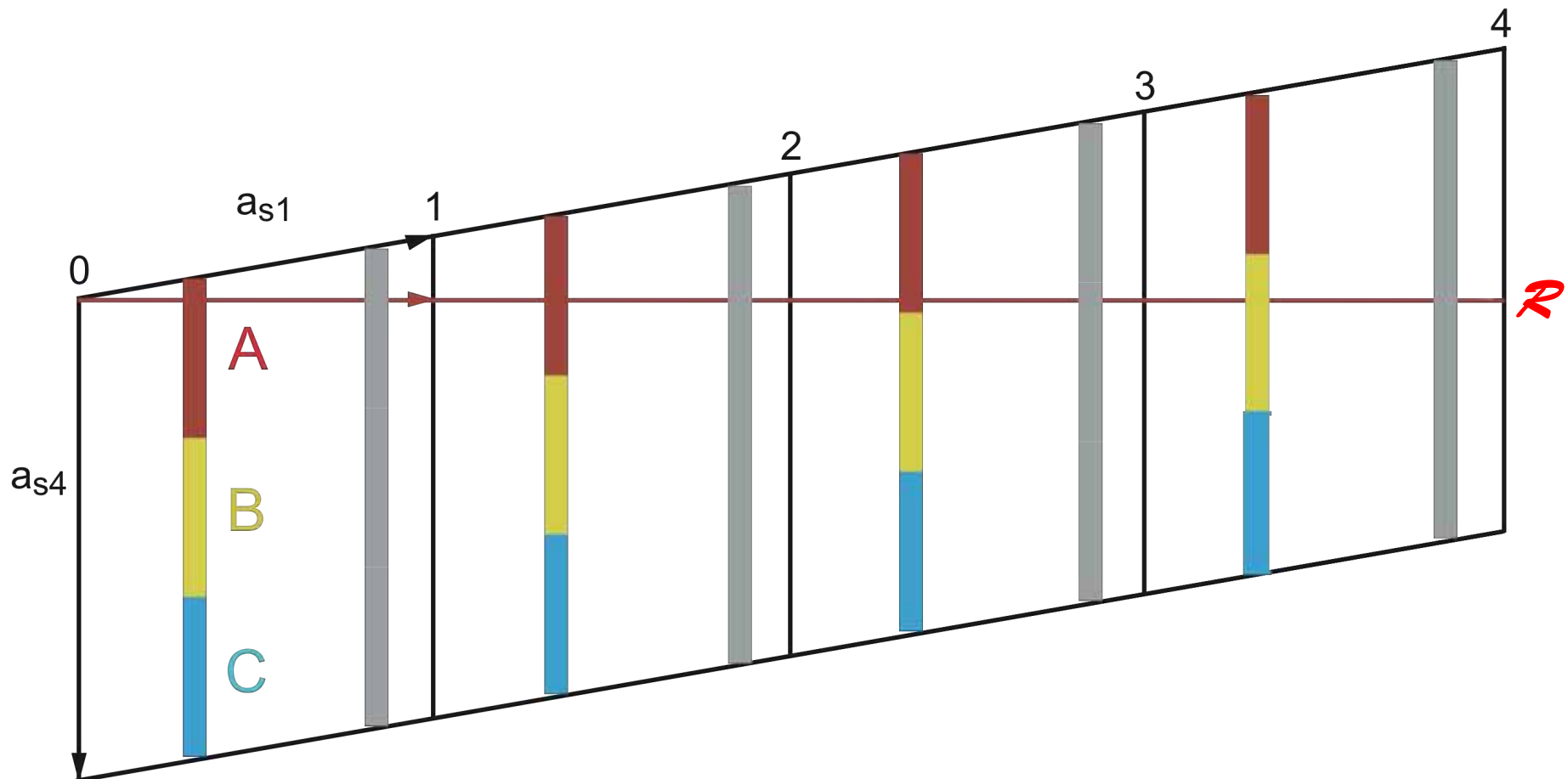
$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}; \quad \mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V}; \quad \mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

$$V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$

Mapping of atomic displacements the rectangular (or Crenel) function



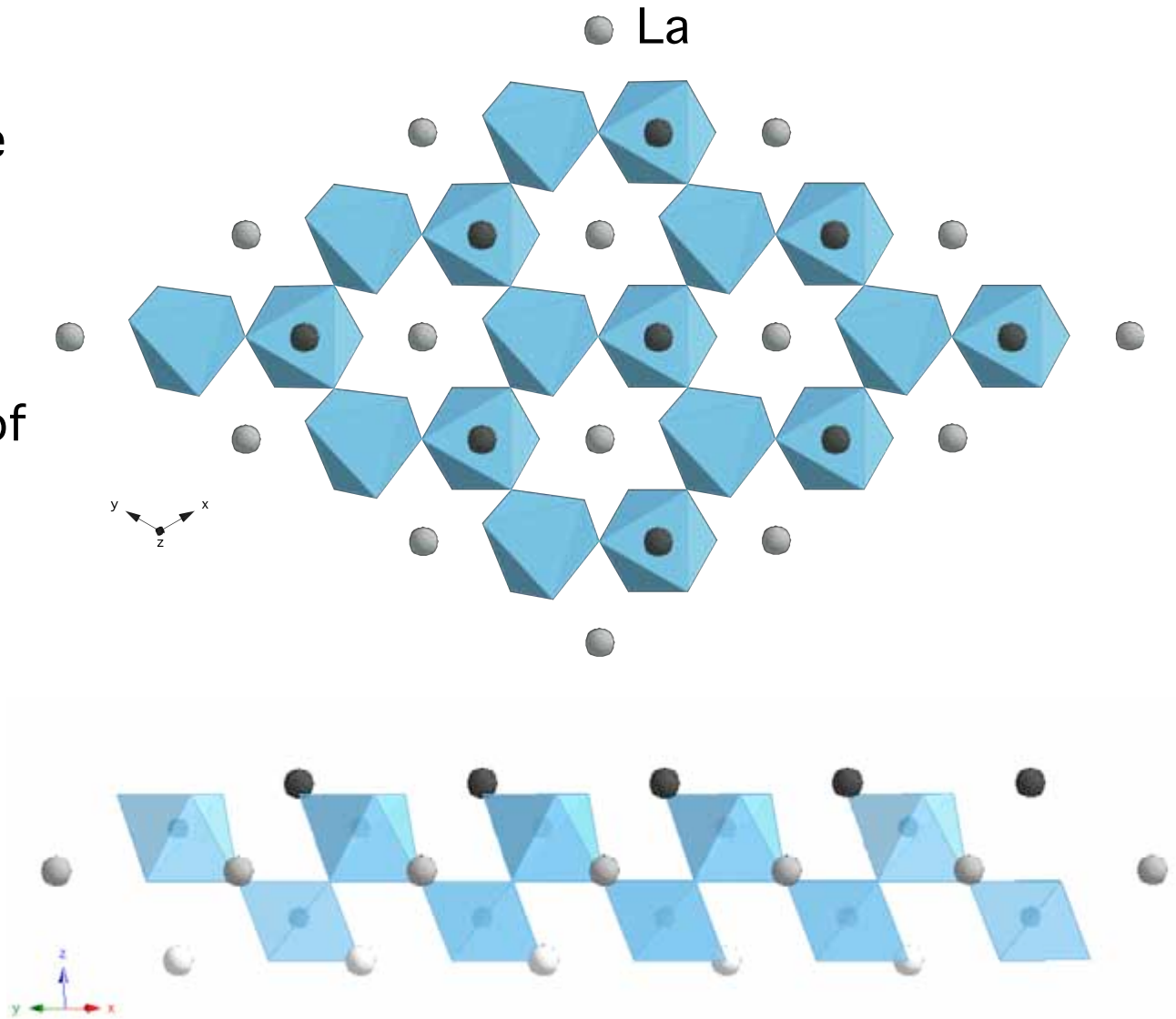
Mapping of atomic displacements by density modulation function example: layer structure



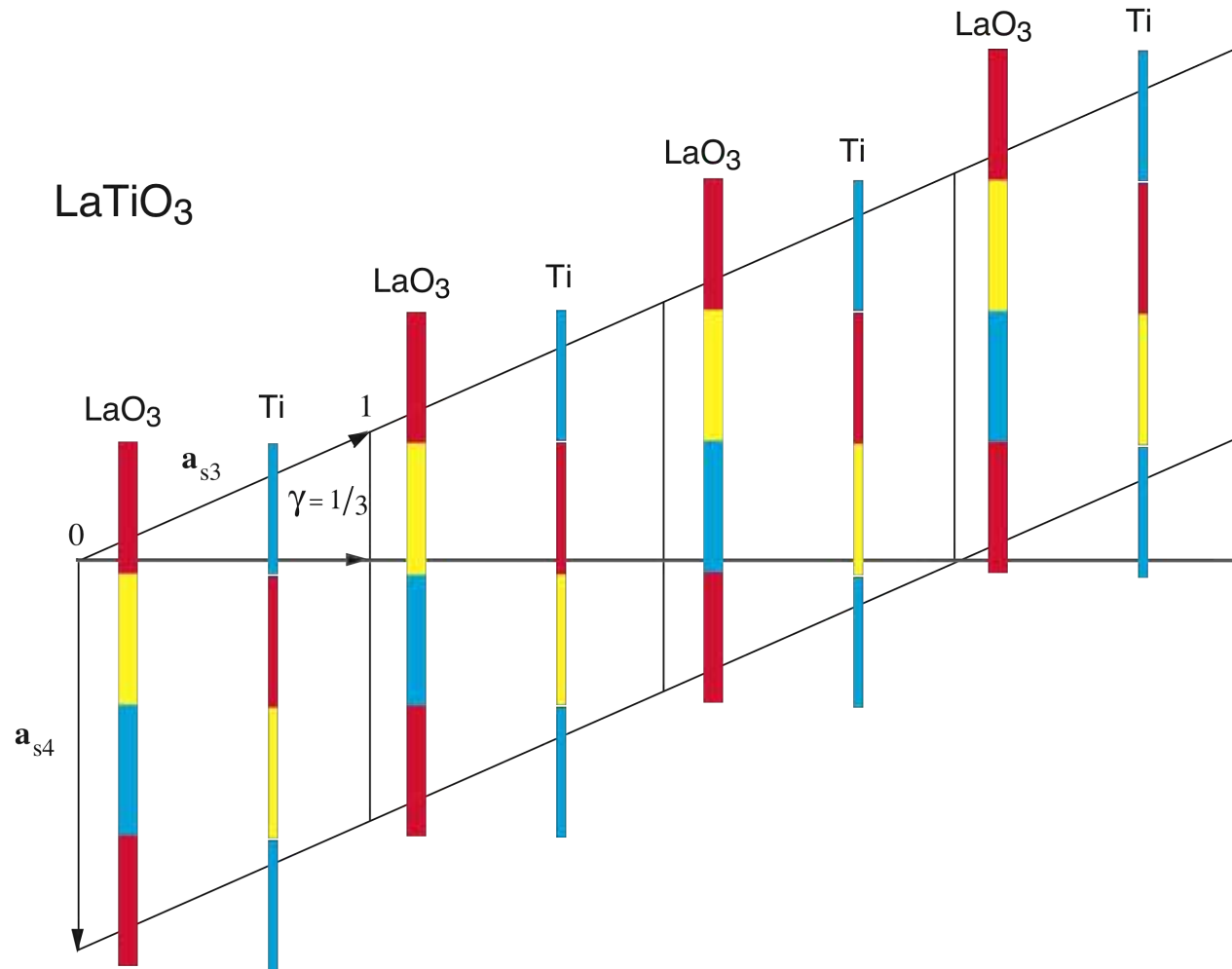
Example: the layer structure of LaTiO_3

Two projections of the LaTiO_3 layer.

The structure can be considered as an alternating sequence of LaO_3 and Ti layers



The layer structure of LaTiO_3 represented in the superspace

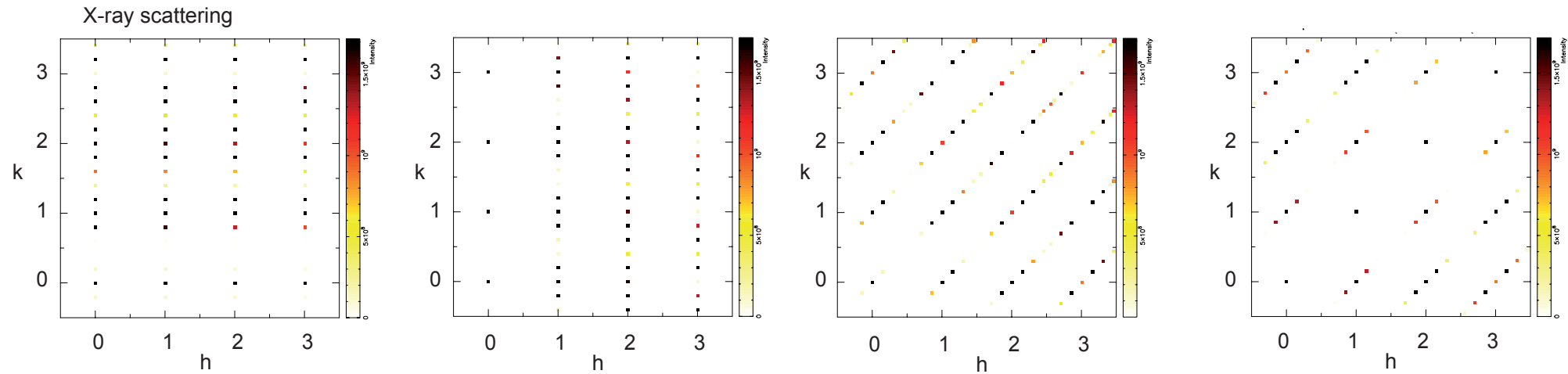
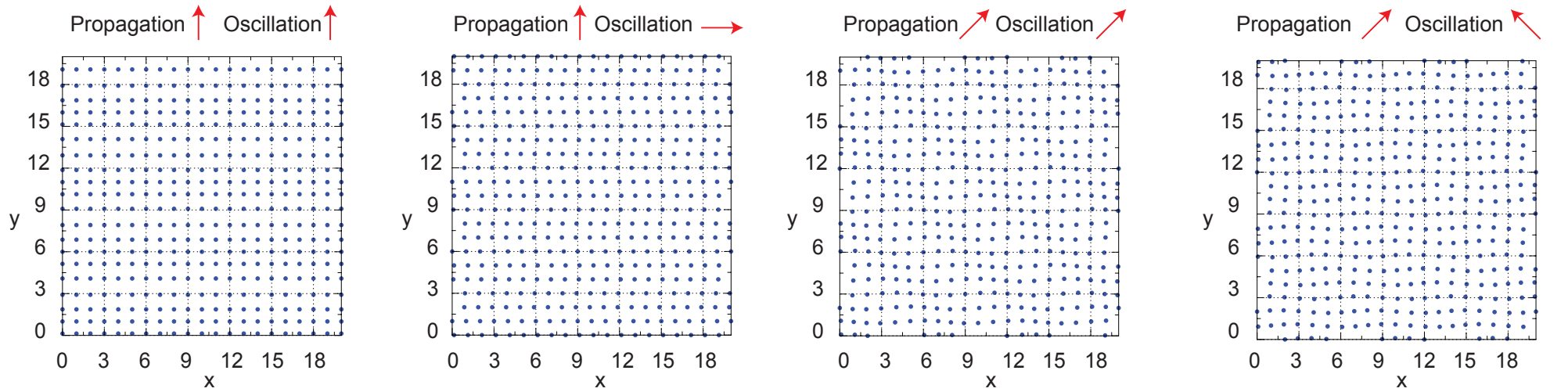


Simulation: from superspace to real structure

Simulation of diffraction patterns from modulation waves

Authors: Th. Proffen and R.B. Neder

Effect of different modulations on diffraction



Do we have space group equivalent in superspace?

- Yes!
- (3+1) dimensional superspace groups are four-dimensional space groups having some additional properties
- 775 inequivalent groups which are called superspace groups
- Listed in IT vol C.
- Also freely available from open databases on Internet

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The structure factor of a (3+1)d crystal
(Paciorek *et al.* J. Appl. Cryst. 1992)

$$F_{\mathbf{H}} = \sum_{\mu} f_{\mathbf{H}}^{\mu} \exp(2\pi i \mathbf{H} \cdot \mathbf{r}^{\mu}) \\ \times \int_0^1 dt p^{\mu}(t) \exp\{2\pi i (\mathbf{H} \cdot \mathbf{u}^{\mu}(t) + h_4 t)\}$$

Where \mathbf{r}^{μ} represents the basic atomic positions on which the modulation displacements \mathbf{u}^{μ} are applied.

$$\mathbf{H} = \sum_1^4 h_i \mathbf{a}_i^* \quad \text{and} \quad t = x_4 - \mathbf{q} \cdot \mathbf{r}$$

The structure associated to \mathbf{r}^{μ} is called the basic structure whereas the complete structure is the modulated structure.

The split basis expressions

It is convenient to introduce the split basis notation in order to separate the physical space from the internal space

$$a_{S_i}^* = (\mathbf{a}_i^*, 0) \quad i = 1, 2, 3,$$
$$a_{S_4}^* = (\mathbf{q}, 1)$$

which in direct translates space to

$$a_{S_i} = (\mathbf{a}_i, -q_i) \quad i = 1, 2, 3,$$
$$a_{S_4} = (0, 1)$$

These expression satisfies the condition if we limit to (3+1)D

$$a_{S_i} \cdot a_{S_j}^* = \delta_{ij}, \quad i, j = 1, \dots, 4$$

The split basis expressions (2)

Any spot on the diffraction pattern is given by

$$H_S \equiv (\mathbf{H}, H_I) = \mathbf{h} + h_4 \mathbf{q}, h_4) = \sum_1^4 h_i a_{Si}^*$$

in direct space any vector can be written

$$r_S \equiv (\mathbf{r}, r_I) = (\mathbf{r}, t) = \sum_1^4 x_i a_{Si}$$

With the conditions

$$\mathbf{r} = \sum_1^3 x_i a_{Si}$$

$$x_4 = \mathbf{q} \cdot \mathbf{r} + t$$

The split basis expressions (3)

The scalar product between the two vectors can be expressed in a variety of equivalent forms

$$\begin{aligned}H_S \cdot r_S &\equiv (\mathbf{H}, H_I) \cdot (\mathbf{r}, r_I) \\ &= \mathbf{H} \cdot \mathbf{r} + H_I t \\ &= \mathbf{h} \cdot \mathbf{r} + h_4 x_4 \\ &= \sum_{i=1}^4 h_i x_i\end{aligned}$$

All these forms can be found in the literature and are the source of many ambiguities.

The most general form of the structure factor given in IT

$$F_{\mathbf{H}} = \sum_{\mu} f_{\mathbf{H}}^{\mu} \int_{\Omega_I} dt p^{\mu}(\mathbf{t}) \\ \times \exp\{2\pi i(\mathbf{H}, \mathbf{H}_I) \cdot (\mathbf{r}^{\mu} + \mathbf{u}^{\mu}(\mathbf{t}), \mathbf{t})\}$$

Which can be transformed to the more appropriate expression in (3+1)D

$$F_{\mathbf{H}} = \sum_{\mu} f_{\mathbf{H}}^{\mu} \exp(2\pi i \mathbf{H} \cdot \mathbf{r}^{\mu}) \\ \times \int_0^1 dt p^{\mu}(t) \exp\{2\pi i(\mathbf{H} \cdot \mathbf{u}^{\mu}(t) + h_4 t)\}$$

The most general form of the structure factor given in IT (2)

The modulation parameters (displacement and population) must satisfy the following conditions for real valued parameters

$$\mathbf{u}^\mu(t) = \sum_n \mathbf{u}_n^\mu \exp(2\pi i n t), \quad \mathbf{u}_{-n}^\mu = \mathbf{u}_n^{\mu*}$$

$$p^\mu(t) = \sum_n p_n^\mu \exp(2\pi i n t), \quad p_{-n}^\mu = p_n^{\mu*}$$

The structure factor of a (3+1)D adapted for LS refinement

The following basis functions are frequently used in this expansion

$$t_n(x) = \begin{cases} 1, & n = 0 \\ \cos(2\pi nx), & n = 2m - 1, \quad n = 0, \dots, N \\ \sin(2\pi nx), & n = 2m \end{cases}$$

The atomic coordinates, anisotropic displacement parameters and occupational parameters are all periodic functions of the internal coordinate \bar{x}_4

$$x_i^\mu(\bar{x}_4) = \bar{x}_i^\mu + \sum_{n>0} u_{i,n}^\mu t_n(\bar{x}_4), \quad i = 1, \dots, 3$$

$$B_{ij}^\mu(\bar{x}_4) = \sum_{n \geq 0} B_{ij,n}^\mu t_n(\bar{x}_4), \quad \bar{B}_{ij}^\mu \equiv B_{ij,0}^\mu, \quad i, j = 1, \dots, 3$$

$$P^\mu(\bar{x}_4) = \sum_{n \geq 0} P_n^\mu t_n(\bar{x}_4), \quad \bar{P}^\mu \equiv P_0^\mu$$

The structure factor of a (3+1)D adapted for LS refinement (2)

The geometrical part of the SF for an atom μ generated by the (3+1)D superspace symmetry operation s depends on the internal coordinate and is given by

$$G^{\mu,s}(\bar{x}_4) = \exp \left(2\pi i \left\{ \sum_{i=1}^3 [h_i^s \bar{x}_i^\mu + H_i^s u_i^\mu(\bar{x}_4) + h_i \tau_i^s] + h_4^s \bar{x}_4 + h_4 \tau_4^s \right\} \right)$$

The rotational part of the symmetry element (R^s, τ^s) is applied to the reflection indices:

$$h_i^s = \sum_{j=1}^4 R_{ji}^s h_j, \quad i = 1, \dots, 4$$

$$H_i^s = h_i^s + h_4^s q_i, \quad i = 1, \dots, 4$$

q_j are the components of the modulation vector

The structure factor of a (3+1)D adapted for LS refinement (3)

The anisotropic Debye-Waller terms are given by

$$T^{\mu,s}(\bar{x}_4) = \exp \left[- \sum_{i,j=1}^3 H_i^s H_j^s B_{ij}(\bar{x}_4) \right]$$

It is convenient to introduce quantities describing the contribution to the SF from all atoms related by symmetry to atom μ :

$$\bar{F}^{\mu}(\bar{x}_4) = \sum_s \bar{F}^{\mu,s}(\bar{x}_4) \equiv \sum_s T^{\mu,s}(\bar{x}_4) G^{\mu,s}(\bar{x}_4)$$

$$F^{\mu}(\bar{x}_4) = \sum_s F^{\mu,s}(\bar{x}_4) \equiv P^{\mu}(\bar{x}_4) \sum_s \bar{F}^{\mu,s}(\bar{x}_4)$$

The structure factor of a (3+1)D adapted for LS refinement (4)

Finally, the SF is the sum of integrals over a period of the internal coordinate:

$$F(\mathbf{H}) = \sum_{\mu} M^{\mu} f^{\mu} \int_0^1 d\bar{x}_4 F^{\mu}(\bar{x}_4) \equiv \sum_{\mu} M^{\mu} f^{\mu} \langle F^{\mu} \rangle$$

Each atom contribution is multiplied by an appropriate multiplicity M^{μ} and scattering factor f^{μ} .

This form is particularly adapted for numerical recipes with very fast and efficient algorithms. We only focus on the expression in $\langle \rangle$.

The structure factor of a (3+1)D adapted for LS refinement (5)

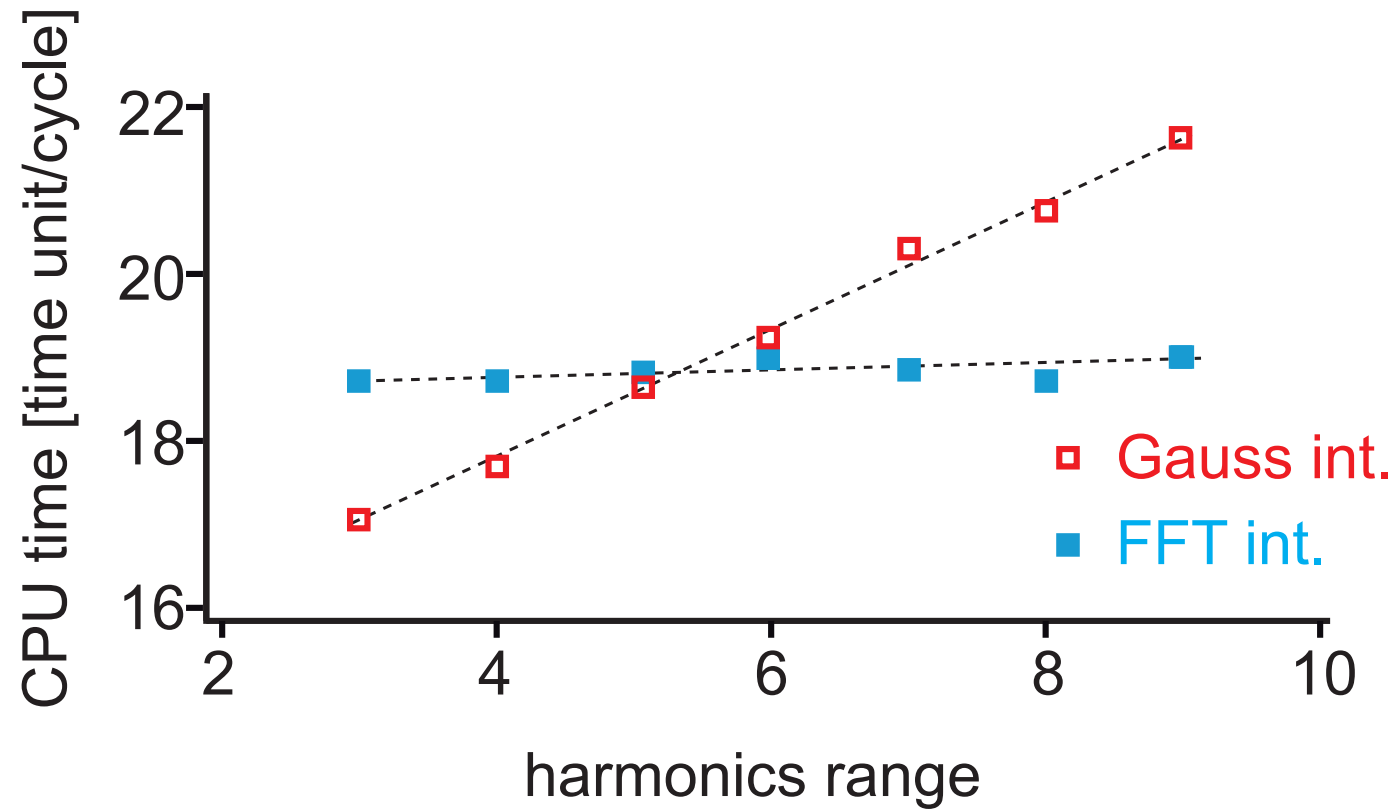
The last expression of the SF is a very convenient form to obtain partial derivatives where the expression in $\langle \rangle$ can easily be estimated numerically by discrete Fourier transform (DFT)

$$\frac{\partial F}{\partial \bar{x}_i^\mu} = f^\mu M^\mu \sum_s 2\pi i h_i^s \langle t_0 F^{\mu,s} \rangle$$

$$\frac{\partial F}{\partial u_{i,n}^\mu} = f^\mu M^\mu \sum_s 2\pi i H_i^s \langle t_n F^{\mu,s} \rangle$$

$$\frac{\partial F}{\partial B_{ij,n}^\mu} = -f^\mu M^\mu \sum_s H_i^s H_j^s \langle t_n F^{\mu,s} \rangle$$

The efficiency of the DFT algorithm for the calculation of the derivatives



Other algorithm for simple harmonic function

In some particular cases, it is possible to use some approximation based on the Jacobi-Auger expansion using Bessel functions

$$\exp(iz \sin \alpha) = \sum_{m=-\infty}^{\infty} \exp(-im\alpha) J_{-m}(z)$$

In this case the SF associated with atom μ can be expressed (up to a phase factor) by

$$F^{\mu}(h, k, l, m) = f^{\mu}(\mathbf{H}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_0^{\mu}) \times J_m(2\pi i \mathbf{H} \cdot \mathbf{U}^{\mu})$$

With the atomic modulation function expressed by

$$\mathbf{u}^{\mu} = \mathbf{U}^{\mu} \cos(2\pi \mathbf{q} \cdot \mathbf{r}^{\mu})$$

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The phase problem in any dimension

The electron density of a structure is obtained from the relation

$$\rho(\mathbf{x}_S) = \frac{1}{V_S} \sum_{\mathbf{H}} F(\mathbf{H}) \exp(-2\pi i \mathbf{H} \mathbf{x}_S)$$

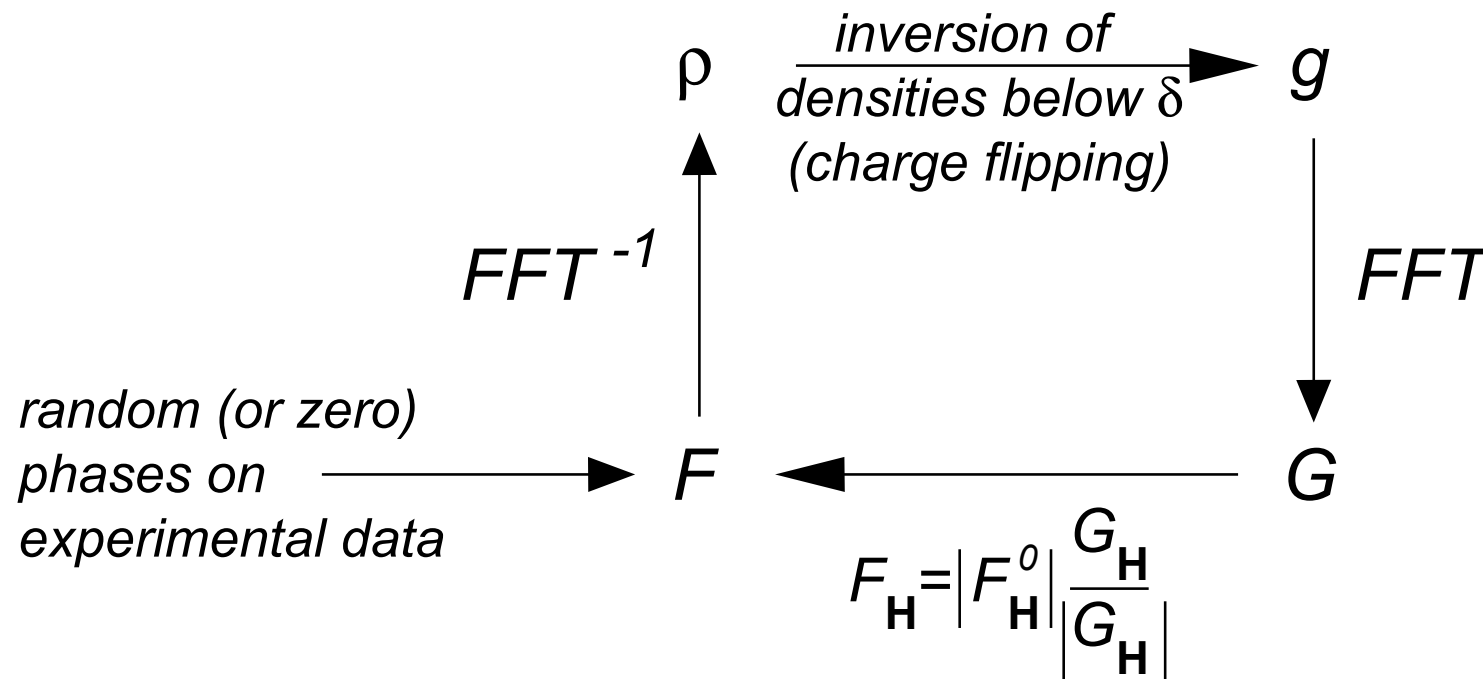
\mathbf{x}_S represent the atomic position in any dimension (usually up to 6). The structure factor is a complex magnitude and only the module can be retrieved from experiment

$$F(\mathbf{H}) = \sum_{j=1}^n f_j(\mathbf{H}) \exp(2\pi i \mathbf{H} \mathbf{x}_{S_j}) = |F(\mathbf{H})| \exp(i\phi_{\mathbf{H}})$$
$$I(\mathbf{H}) \propto |F(\mathbf{H})|^2$$

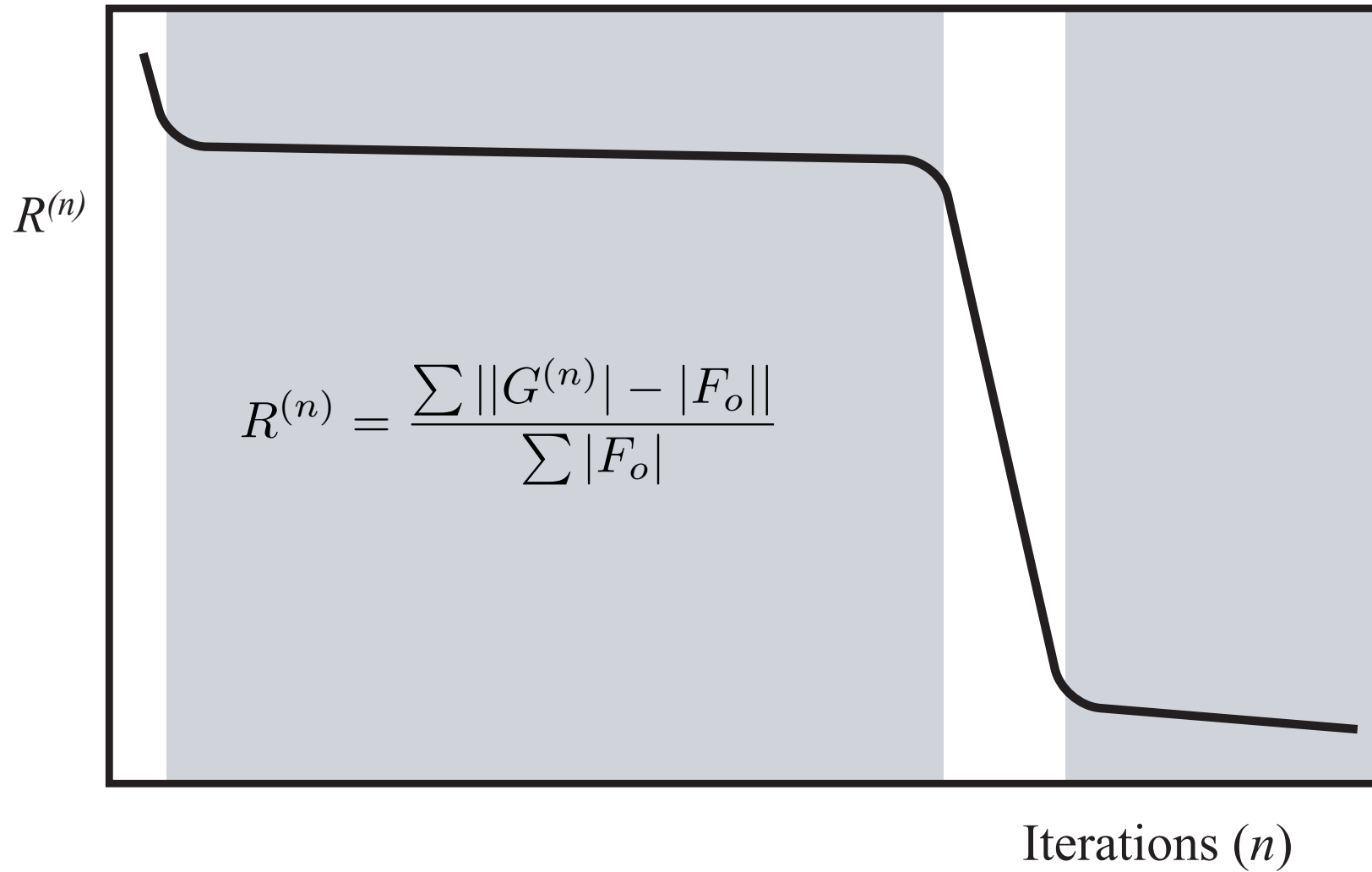
The reciprocal vector is of dimension N

$$\mathbf{H} = h_1 \mathbf{a}_1^* + h_2 \mathbf{a}_2^* + \cdots + h_N \mathbf{a}_N^*$$

The charge flipping (CF) algorithm (Oszlanyi & Sütö, Acta Cryst. 2004, 2005)



Evolution of the iterative algorithm

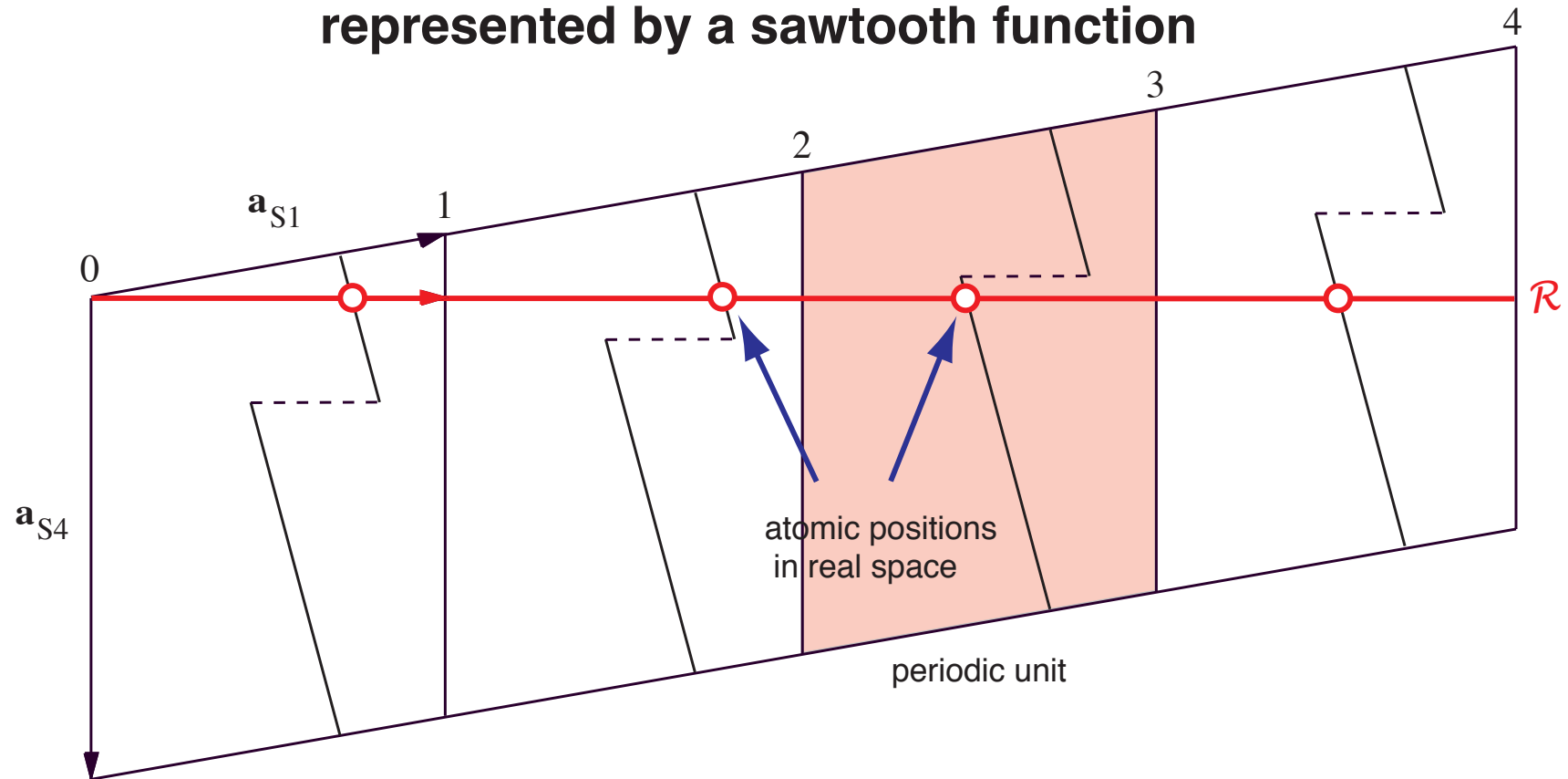


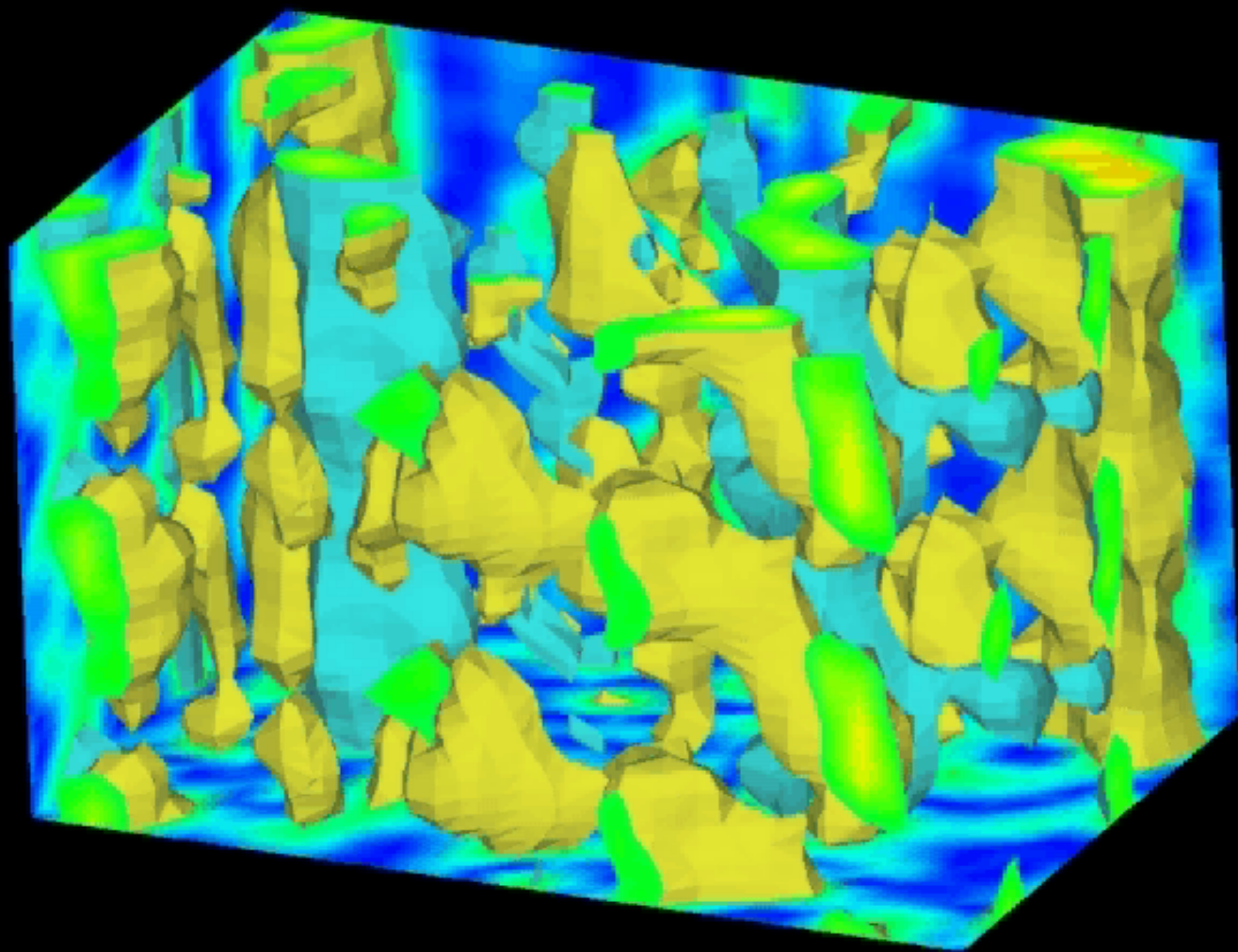
CF in real time

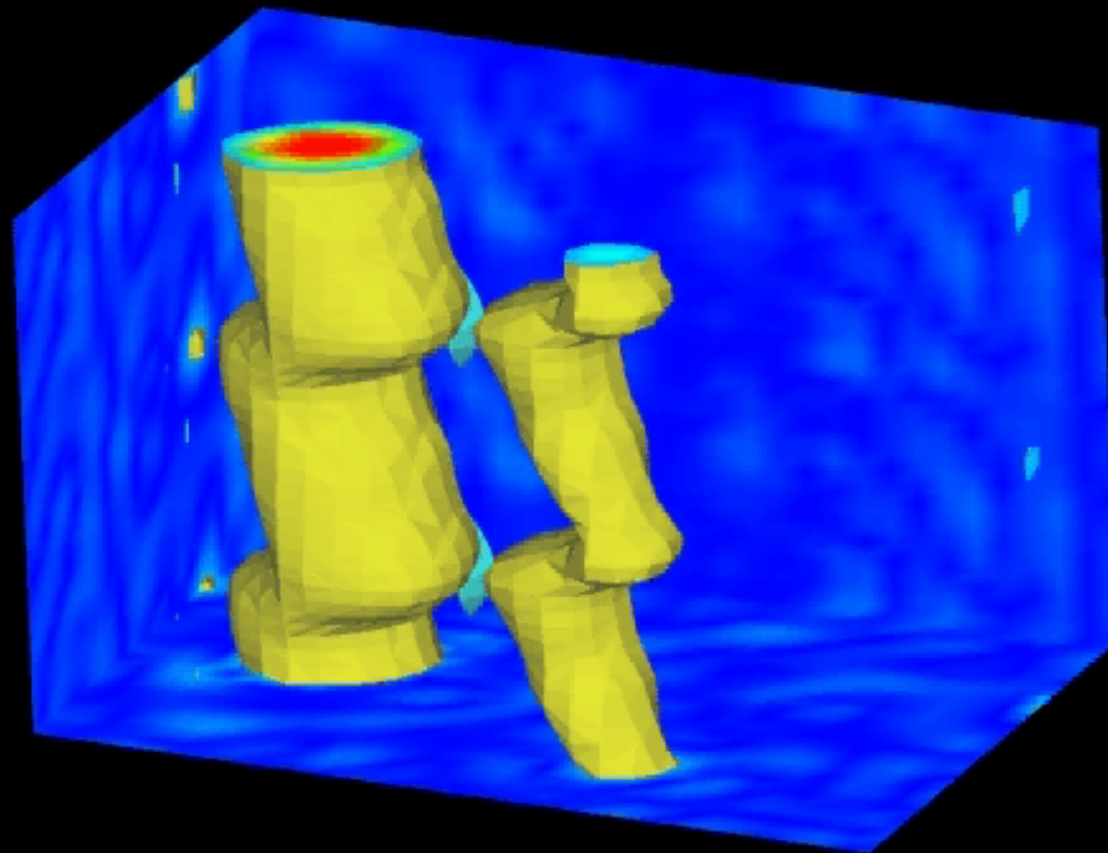
- Live demonstration from our [CF applet](http://escher.epfl.ch/flip/) (<http://escher.epfl.ch/flip/>) directly available on the web
- ([alternatively offline version](#))
 - Create your structure with a drawing tool
 - Calculate the modulus of the structure factor
 - Apply CF to solve the structure

CF in action

Example of a (1+1)D aperiodic structure with one atom represented by a sawtooth function







Conclusions

- Aperiodic crystals are much more than some exceptional and interesting objects for curious scientists.
- They are of great help to understand the subtle interactions in matter.
- We shall see later that the superspace concept is of great help for a better understanding of structure-property relations.
- Efficient tools have been (and still are) developed to deal with aperiodic structures.
- Diffractometer and structure refinement software have been adapted to deal with aperiodic materials.

Introduction to aperiodic crystals

Gervais Chapuis

Exercise 1

The structure of the mineral Calaverite ($\text{Au}_{1-x}\text{Ag}_x$) Te_2 has been a challenge for mineralogists for about hundred years, starting 1895.

1895-1902	Penfield, Ford Face-indexing difficulties, unreasonably high indices Monoclinic crystal
1902	Smith Indexing of the faces assuming 3 interpenetrating lattices 2 monoclinic + 1 triclinic
1931	Goldschmid, Palache, Peacock 105 specimen studied 92 crystal forms Law of Rational Indices given up
1964	Buerger, Letter to P.M. de Wolff suggesting possible incommensurate modulation
1983	Van Tendeloo, Gregoriades & Amelinckx HREM: Incommensurate modulation with wave-vector $\mathbf{q} = (\alpha, 0, \gamma)$

The **gnomonic projection** of the mineral resulting from a series of more than 100 samples from different origins is illustrated in Table 1. The gnomonic projection of the normal to the crystalline faces can be considered has an undistorted representation of a reciprocal layer plane.

Goldschmid, Palache and Peacock (GPP) realised that the so-called S-Punkte (open circles on the figure) from a reciprocal monoclinic grid normal to the monoclinic axis b .

The lattice constants of the unit cell derived from the S points are

$$a = 7.195, b = 4.415, c = 5.070 \text{ (\AA)} \text{ and } \beta = 90.038(4)^\circ$$

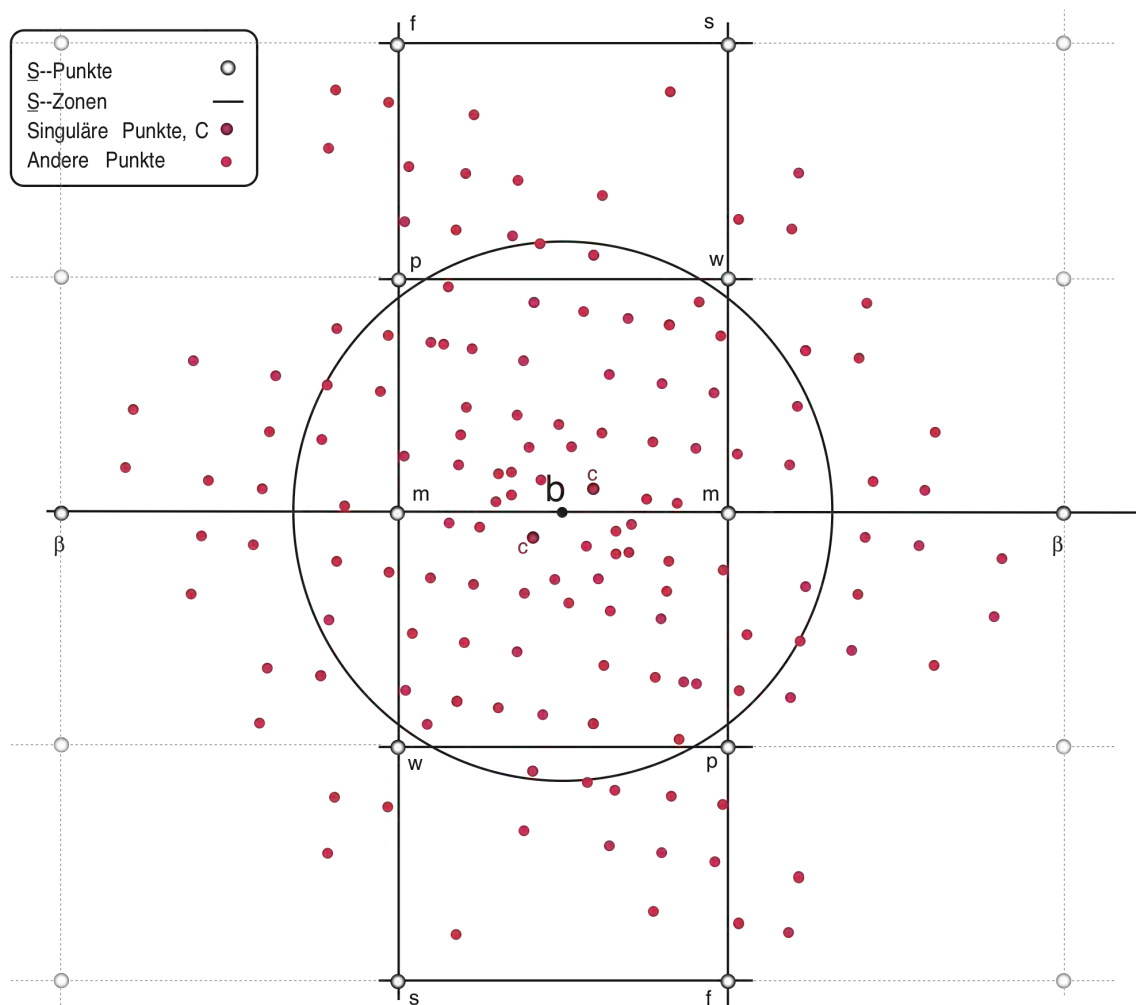
1. Find the reciprocal vectors a^* and c^* and the corresponding indices of the S-points (including the open grey circles which I introduced for the sake of clarity).
2. Assuming that all the red dots correspond to satellite reflections, find the modulation vector q permitting the indexing of all the reflexions with four integers.
3. Estimate the value of the q vector.

Table 1, Gnomonic projection of the reliable forms

Copy of the original figure from the article
«Über Calaverit»

von V. Goldschmidt, Ch. Palache and M. Peacock
 in

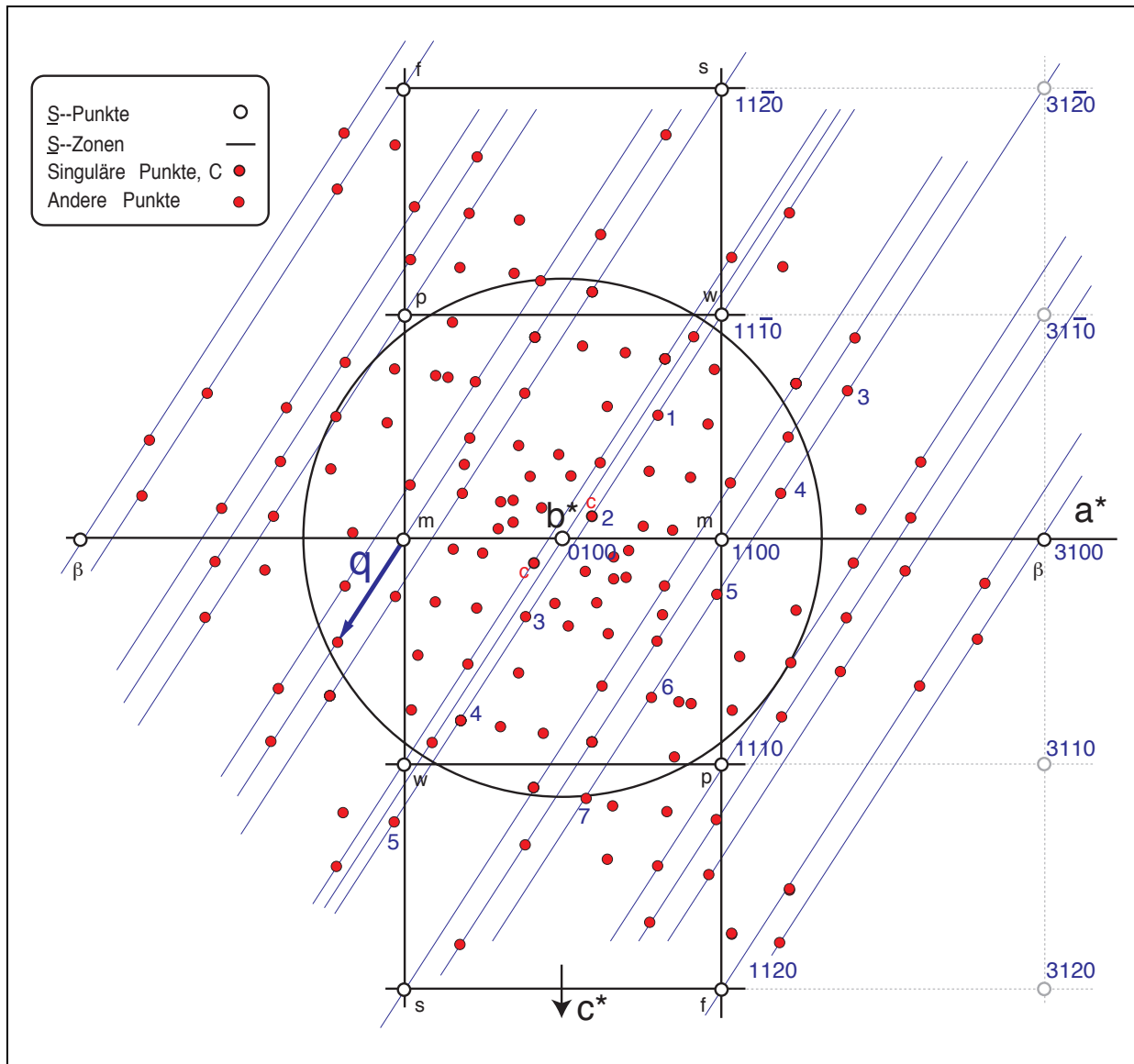
Neues Jahrbuch für Mineralogie, Geologie und Paläontologie, 63. Beilage Band. Abt. A, 1931



Solution 1

The vector \mathbf{a}^* and \mathbf{c}^* can be easily found remembering their reciprocal properties relative to \mathbf{a} and \mathbf{c} .

All the points represented in the gnomonic projection can be found on a series of parallel lines as represented in the figure below. Moreover, each line can be associated with the S-points indicated by a letter. Thus all the points can be indexed with four integers, the fourth index of the S-points being 0.



The additional vector \mathbf{q} has the approximate components (-.40; +.45) relative to \mathbf{a}^* respectively \mathbf{c}^* .

