A few reminders about crystallographic standard notation and symbols

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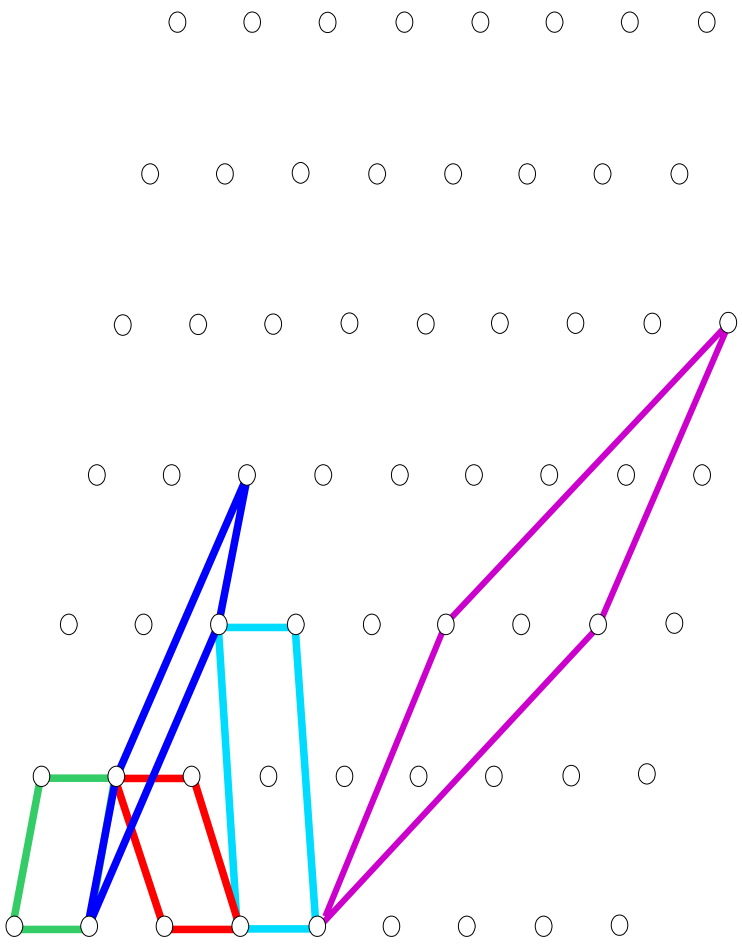
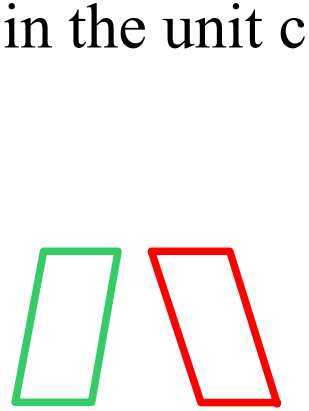
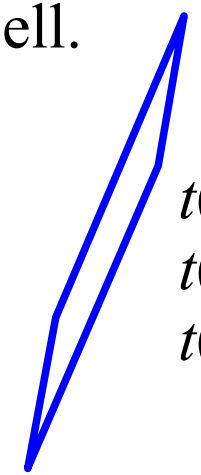
Unit cells

A unit cell is identified by the translations from a lattice node arbitrarily take as the origin to all lattice nodes on or in the unit cell.

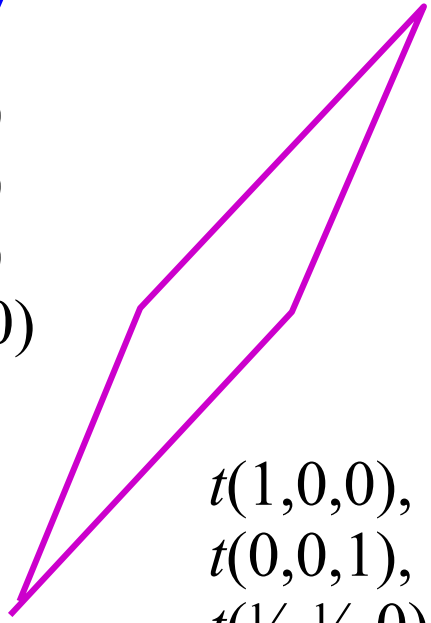






$t(1,0,0)$,
$t(0,1,0)$,
$t(0,0,1)$

$t(1,0,0)$
$t(0,1,0)$
$t(0,0,1)$
$t(\frac{1}{2},\frac{1}{2},0)$



$t(1,0,0)$, $t(0,1,0)$,
$t(0,0,1)$, $t(\frac{3}{4},\frac{1}{4},0)$,
$t(\frac{1}{2},\frac{1}{2},0)$, $t(\frac{1}{4},\frac{3}{4},0)$

Unit cells

For some unit cells, more often adopted, a letter is used which allows to avoid specify the translations

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$: P

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(0,\frac{1}{2},\frac{1}{2})$: A

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{1}{2},0,\frac{1}{2})$: B

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{1}{2},\frac{1}{2},0)$: C

S

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$: I

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(0,\frac{1}{2},\frac{1}{2})$, $t(\frac{1}{2},0,\frac{1}{2})$, $t(\frac{1}{2},\frac{1}{2},0)$: F

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$, $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$: R (obverse setting)

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{2}{3},\frac{1}{3},\frac{2}{3})$, $t(\frac{1}{3},\frac{2}{3},\frac{1}{3})$: R (reverse setting)

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{2}{3},\frac{1}{3},0)$, $t(\frac{1}{3},\frac{2}{3},0)$: H

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$, $t(\frac{1}{3},\frac{1}{3},\frac{1}{3})$, $t(\frac{2}{3},\frac{2}{3},\frac{2}{3})$: D

Unit cells

Problem: how to identify a primitive unit cell?

$t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$: P

But we do not know how the translations are oriented in space!

We need a reference with respect to which any primitive unit cell can be uniquely defined

Solutions:

1. The **conventional** unit cell (uniquely defined only from orthorhombic symmetry upwards)
2. An **orthonormal** unit cell (whose edges do not connect lattice nodes, in general)
3. The **reduced** unit cell, of which we have two types:

   type I: $a \leq b \leq c$, all acute angles

   type II: $a \leq b \leq c$, all non-acute angles

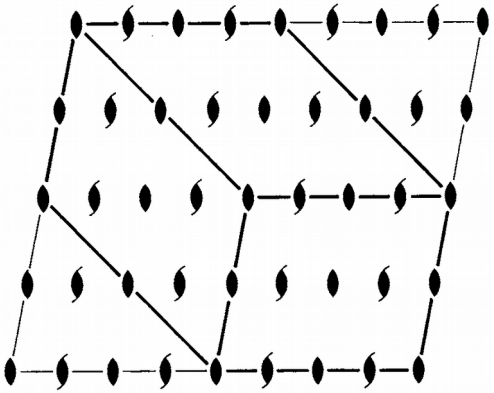
Conventional unit cell

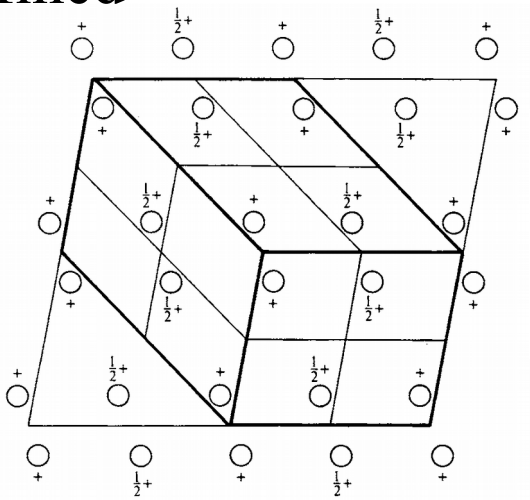
For each lattice, the conventional cell is the cell obeying the following conditions:

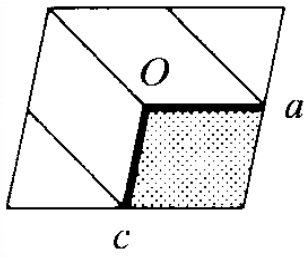
1.its basis vectors define a **right-handed axial setting**;
2.its **edges** are along **symmetry directions of the lattice**;
3.it is the **smallest** cell compatible with the above condition.

Triclinic crystals do not have symmetry directions: the conventional unit cell is not defined

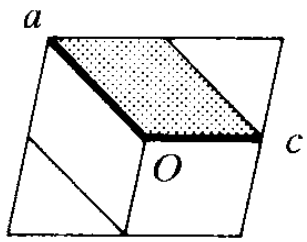
Monoclinic crystals have only one symmetry direction: the conventional unit cell is not uniquely defined



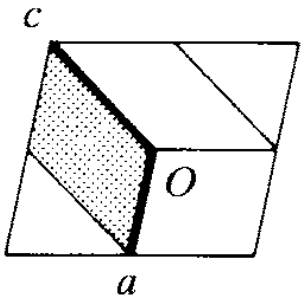




*C*121



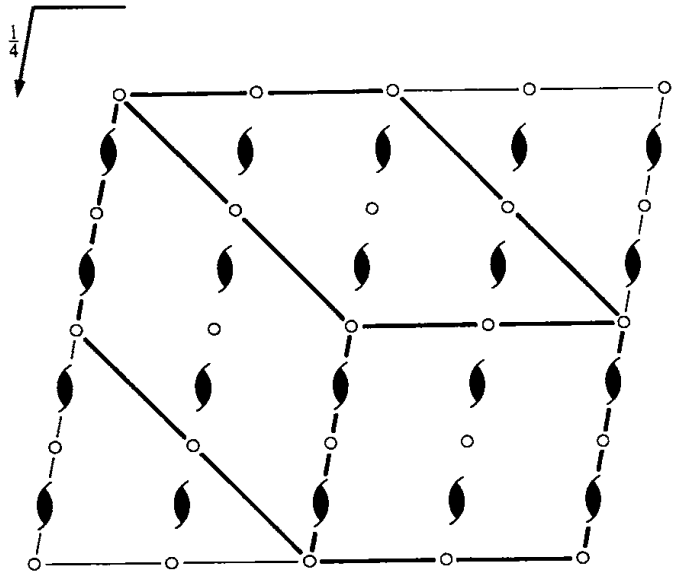
*A*121

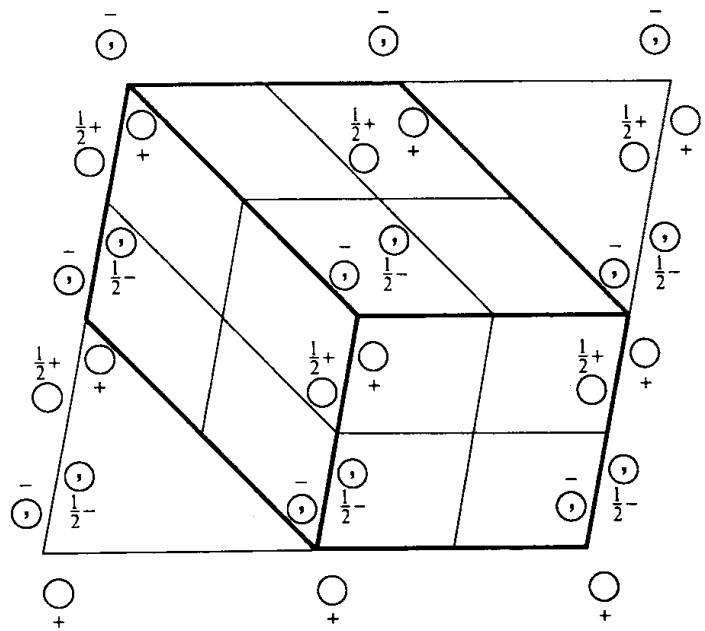


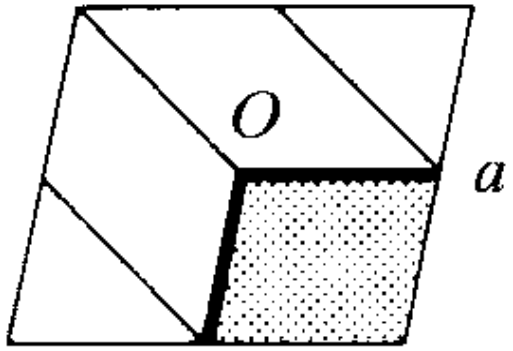
*I*121

A monoclinic angle between 90 and 120° is usually preferred

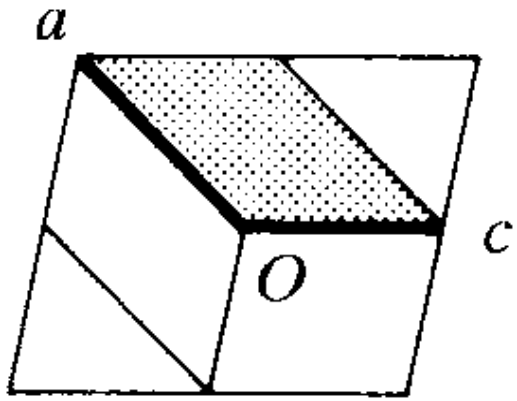
Conventional unit cell



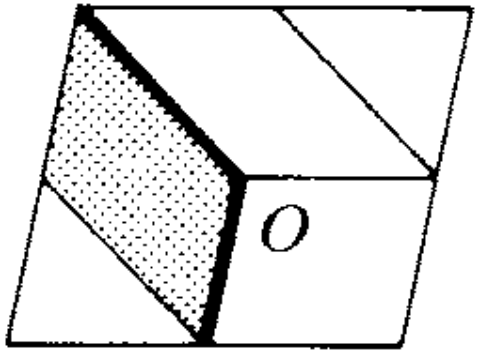




$P12_1/c1$



$P12_1/n1$



$P12_1/a1$

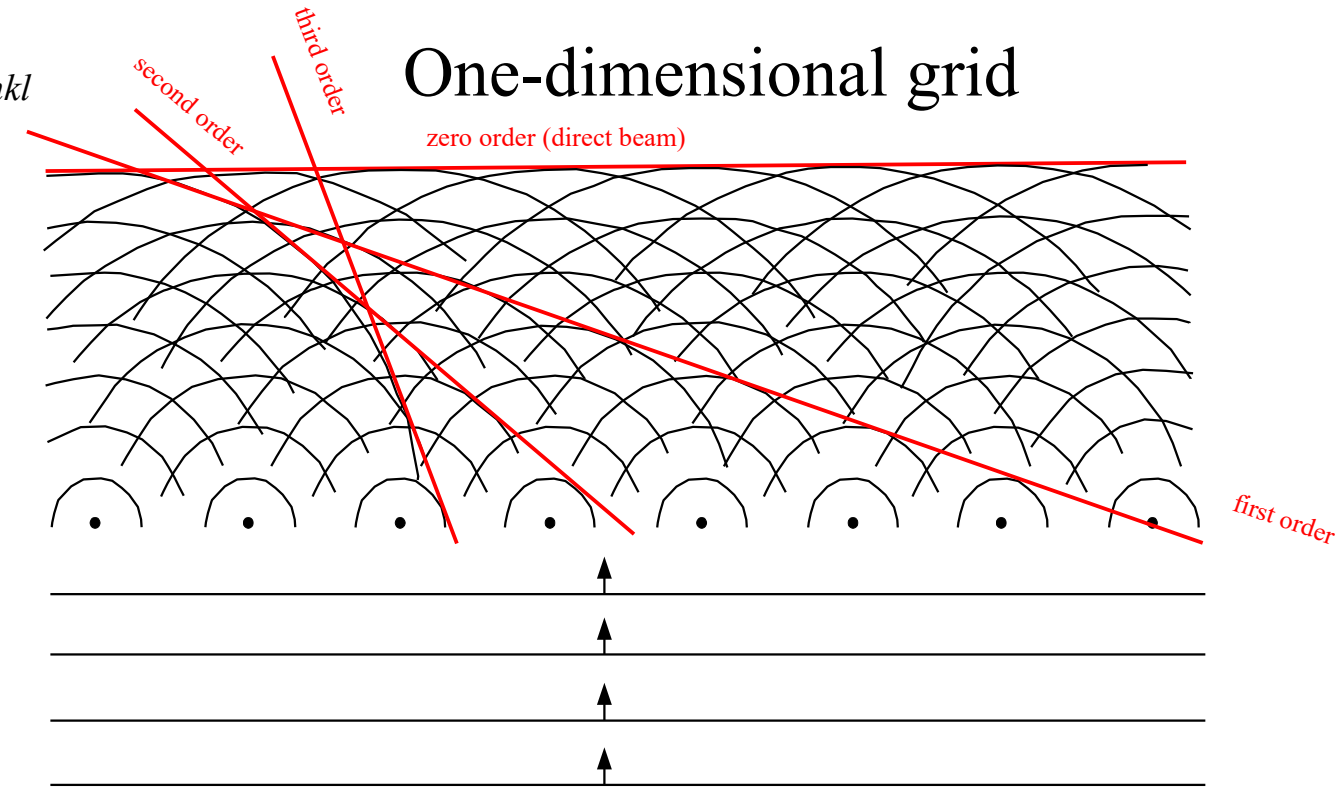
A monoclinic angle between 90 and 120° is usually preferred

Symbols

a,**b**,**c**:	basis vectors (bold)
a,*b*,*c*:	cell parameters (italics)
uvw	Coordinates of a lattice node
[*uvw*]	Indices of direction in direct space
[*UVTW*]	Weber indices for hexagonal lattice (forget them!)
⟨*uvw*⟩	Indices of a set of directions crystallographically equivalent in direct space
[*uvw*]*	Indices of direction in reciprocal space
(*hkl*)	**Miller** indices of a family of lattice planes
(*hkil*)	**Bravais-Miller** indices of a family of lattice planes for the hexagonal lattice
{*hkl*}	**Miller** indices of a crystal form (set of equivalent families of lattice planes)
{*hkil*}	Bravais-Miller indices of a crystal form for the hexagonal lattice
hkl	**Laue** indices of a diffraction, coordinates of a reciprocal lattice node (no parentheses!)
(*hkl*)*	Miller indices of a family of planes in reciprocal space

Elementary geometrical model of diffraction

$$n\lambda = 2d_{hkl}\sin\vartheta_{hkl}$$

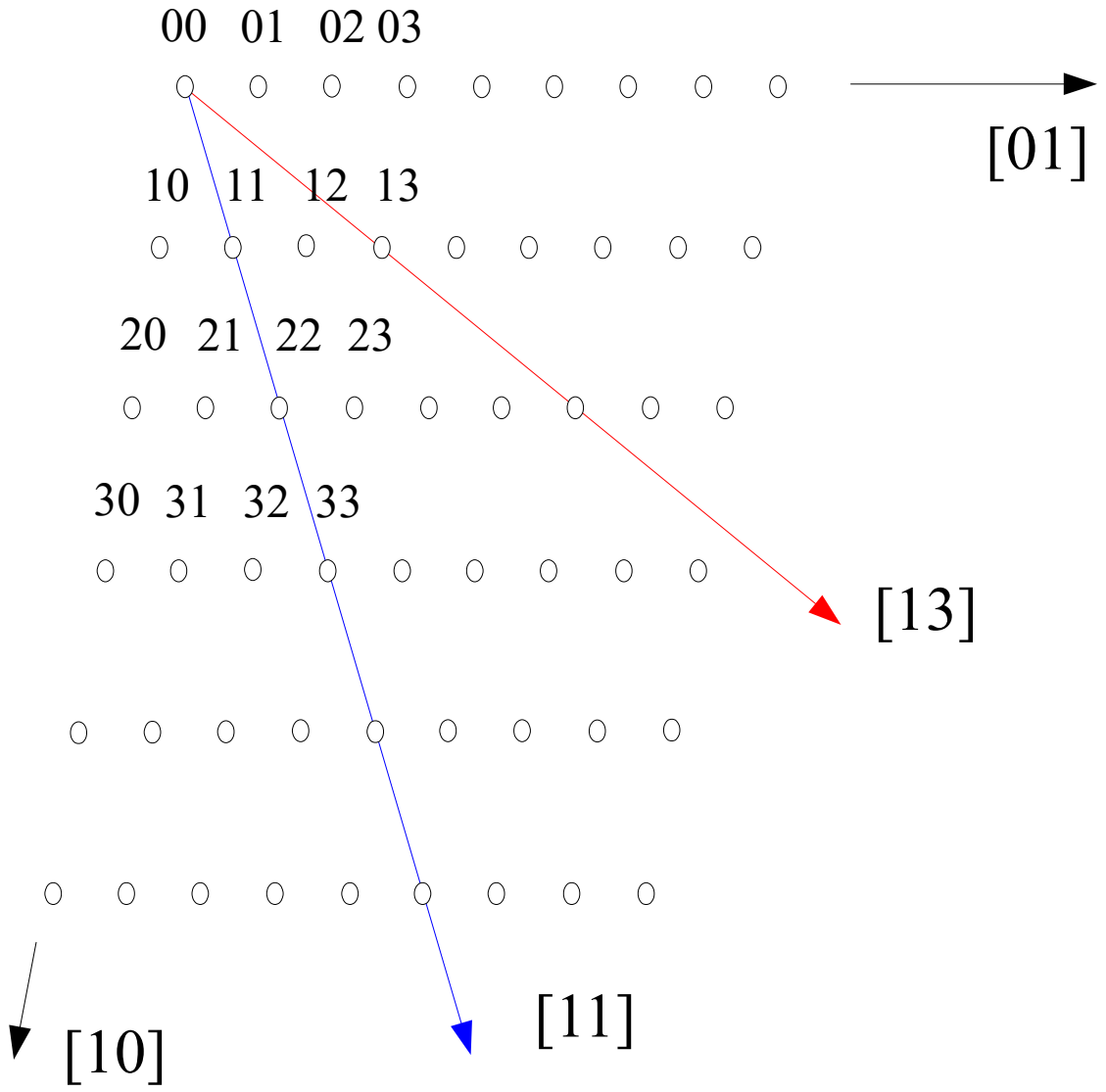


Spherical waves originate at each point of a periodic grid and interfere positively when their phase differs by an integer number of wavelengths. A difference of ***n*** wavelengths corresponds to diffraction of order ***n***.

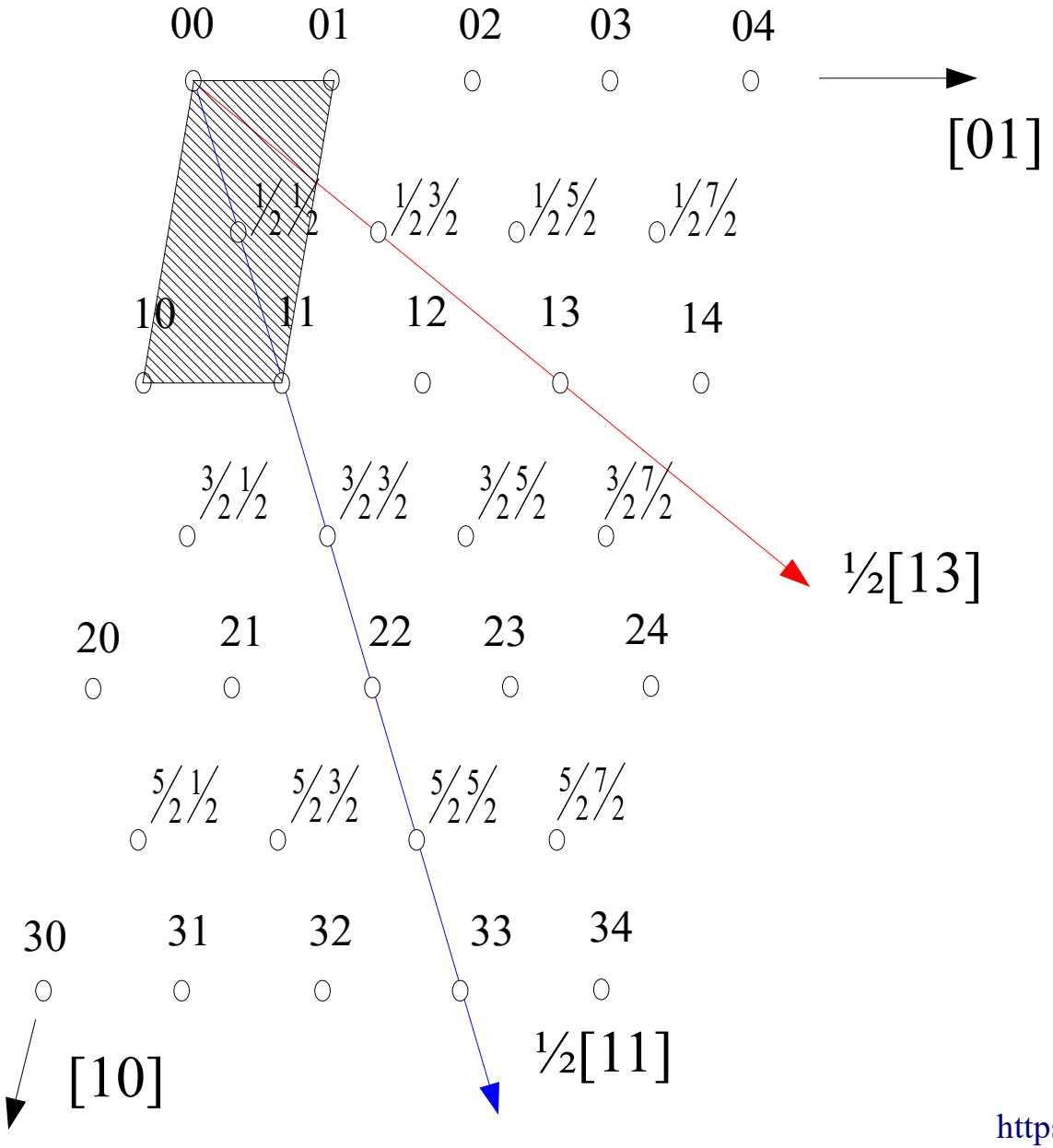
Diffraction *nh*,*nk*,*nl* (**Laue** indices, no parentheses) is the *n*-order diffraction from plane (*hkl*) (**Miller** indices, with parentheses).

Figure modified after M.J. Burger, X-ray crystallography

Coordinates of lattice nodes, direction indices [*uv*]

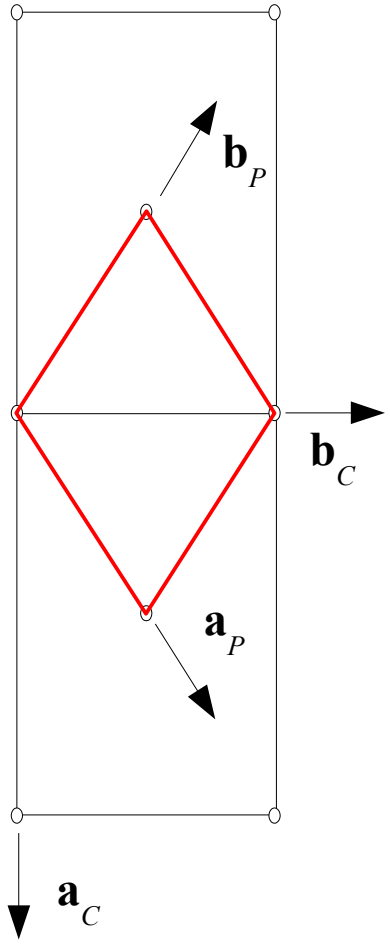


Coordinates of lattice nodes, direction indices [*uv*]



https://doi.org/10.1107/S1600576717010548

Why is it important to use correct indexing?



$$\mathbf{a}_P = (\mathbf{a}_C + \mathbf{b}_C)/2 \qquad \mathbf{a}_C = \mathbf{a}_P - \mathbf{b}_P$$
$$\mathbf{b}_P = (-\mathbf{a}_C + \mathbf{b}_C)/2 \qquad \mathbf{b}_C = \mathbf{a}_P + \mathbf{b}_P$$
$$\mathbf{c}_P = \mathbf{c}_C \qquad \mathbf{c}_C = \mathbf{c}_P$$

$$(\mathbf{a}_P\,\mathbf{b}_P\,\mathbf{c}_P) = (\mathbf{a}_C\,\mathbf{b}_C\,\mathbf{c}_C)\begin{pmatrix} \tfrac{1}{2} & \bar{\tfrac{1}{2}} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (\mathbf{a}_C\,\mathbf{b}_C\,\mathbf{c}_C) = (\mathbf{a}_P\,\mathbf{b}_P\,\mathbf{c}_P)\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

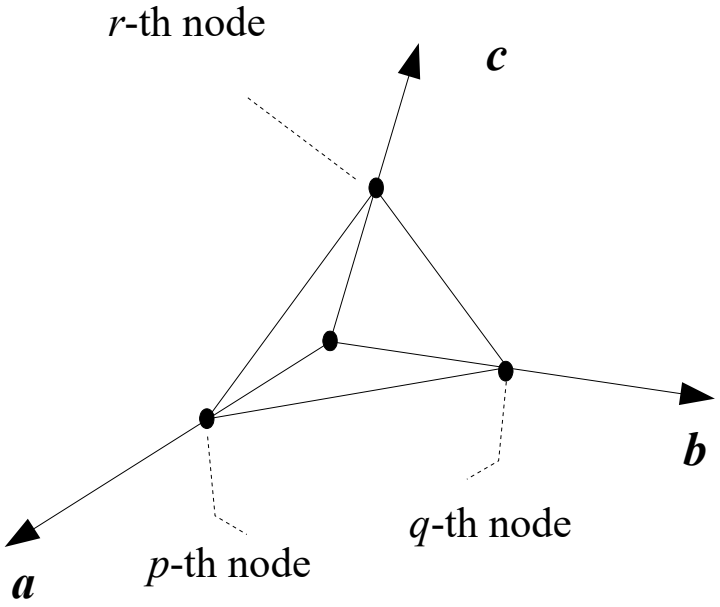
$$\begin{pmatrix} u_C \\ v_C \\ w_C \end{pmatrix} = \begin{pmatrix} \tfrac{1}{2} & \bar{\tfrac{1}{2}} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} \qquad \begin{pmatrix} u_P \\ v_P \\ w_P \end{pmatrix} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} u_C \\ v_C \\ w_C \end{pmatrix}$$

$$\begin{pmatrix} \tfrac{1}{2} \\ \tfrac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} \tfrac{1}{2} & \bar{\tfrac{1}{2}} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 2 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$[100]_P \rightarrow [½½0]_C = ½[110]_C$

[200] is **NOT** correct as a lattice direction, because 200 is not the first lattice node on that direction

Miller indices



The values h, k and l are called the **Miller indices** of the lattice plane and give its **orientation**.

All lattice planes in the same family have the same orientation → (hkl) represents the whole **family of lattice planes**.

Parametric equation of the plane:
$x/p + y/q + z/r = 1$

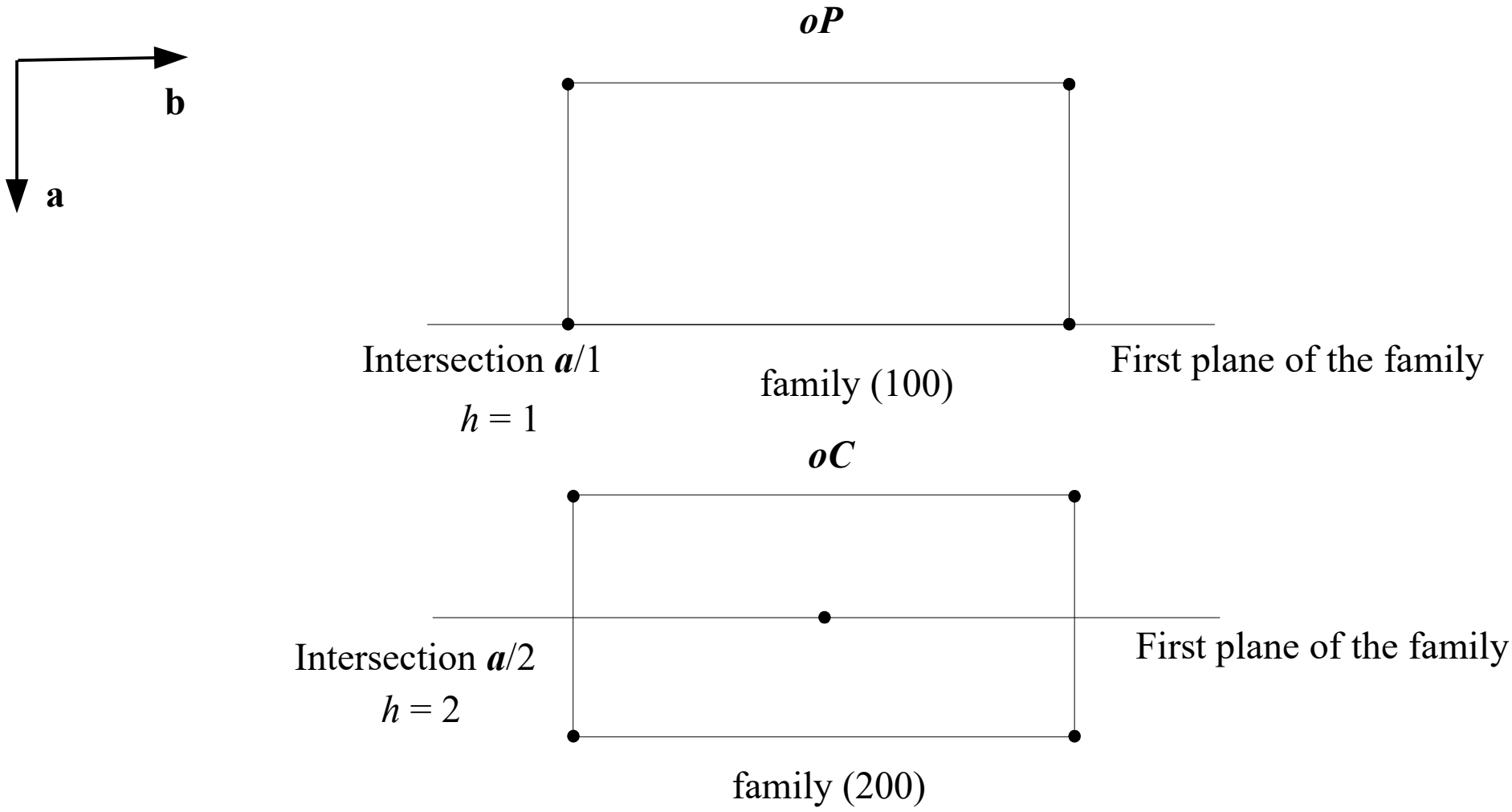
$(qr)x + (pr)y + (pq)z = pqr$
$hx + ky + lz = m$

Making m variable, we obtain a *family* of lattice planes, (hkl), where h, k and l are called the Miller indices.

First plane of the family (hkl) for $m = 1$
$hx + ky + lz = 1$

Intercepts of the first plane of the family (hkl) on the axes
$p = pqr/qr = m/qr = 1/h$
$q = pqr/pr = m/pr = 1/k$
$r = pqr/pq = m/pq = 1/l$

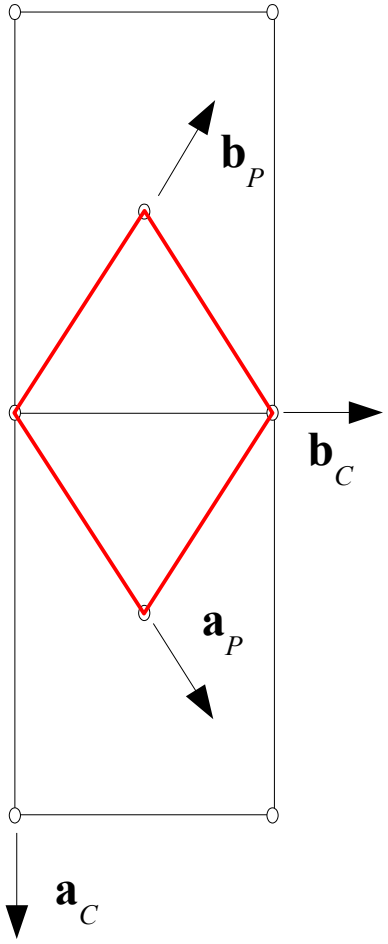
Miller indices for different types of lattice : (*h*00) in *oP* and *oC* (projection on ab)



In morphology, we do not see the lattice and thus the Miller indices of a face are usually coprime integers

http://dx.doi.org/10.1107/S1600576715011206

Why is it important to use correct indexing?



$$\mathbf{a}_C = \mathbf{a}_P - \mathbf{b}_P \qquad \mathbf{a}_P = (\mathbf{a}_C + \mathbf{b}_C)/2$$
$$\mathbf{b}_C = \mathbf{a}_P + \mathbf{b}_P \qquad \mathbf{b}_P = (-\mathbf{a}_C + \mathbf{b}_C)/2$$
$$\mathbf{c}_C = \mathbf{c}_P \qquad \mathbf{c}_P = \mathbf{c}_C$$

$$(\mathbf{a}_C \mathbf{b}_C \mathbf{c}_C) = (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P)\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (\mathbf{a}_P \mathbf{b}_P \mathbf{c}_P) = (\mathbf{a}_C \mathbf{b}_C \mathbf{c}_C)\begin{pmatrix} \tfrac{1}{2} & \tfrac{\bar{1}}{2} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(h_C k_C l_C) = (h_P k_P l_P)\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (h_P k_P l_P) = (h_C k_C l_C)\begin{pmatrix} \tfrac{1}{2} & \tfrac{\bar{1}}{2} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(020) = (110)\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (\tfrac{1}{2}\tfrac{1}{2}0) = (010)\begin{pmatrix} \tfrac{1}{2} & \tfrac{\bar{1}}{2} & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(110)_P \rightarrow (020)_C$$

Miller indices are **NEVER** fractional (a fractional index means that the plane taken as reference is not the first one of the family!)

Classification of reflection conditions

- **General**: apply to all Wyckoff positions.
- **Special**: ： apply to special Wyckoff positions. In particular, in presence of non-characteristic and extraordinary orbits one gets additional special reflection conditions.
- **Integral**: appear when a non-primitive unit cell is selected.
- **Zonal**: appear in presence of glide planes.
- **Serial**: appear in presence of screw axes.

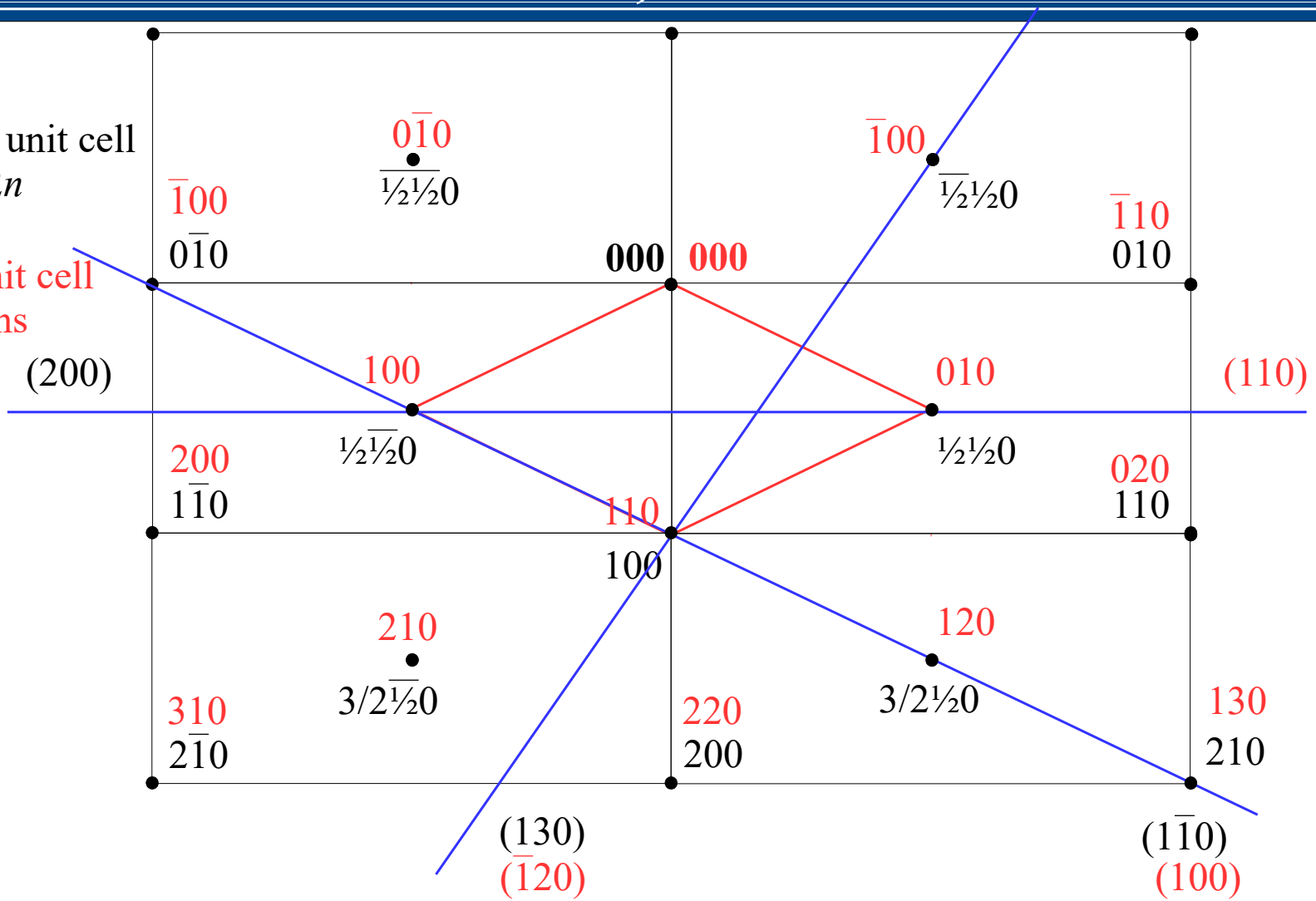
Warning!

~~Systematic extinctions~~

Systematic absences（ actually, presences! ）

Reflection conditions

Integral reflection condition: depend on the choice of the unit cell, not on the structure



When you choose a primitive unit cell you do not see integral reflection conditions

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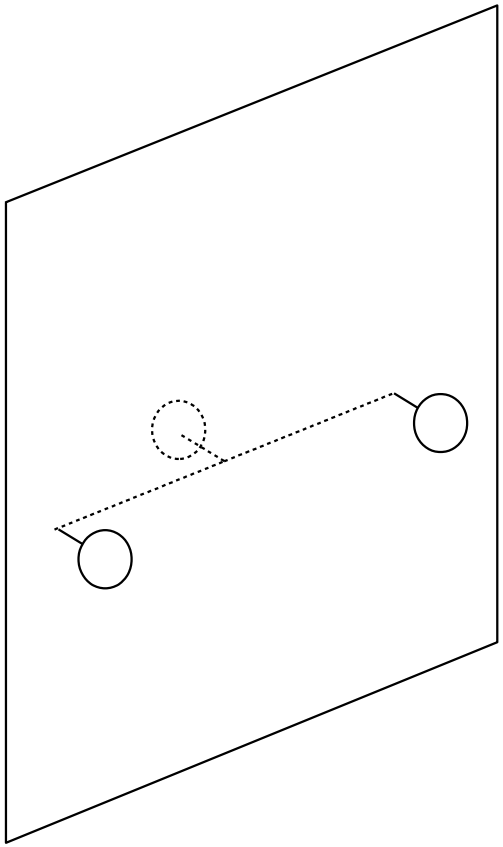
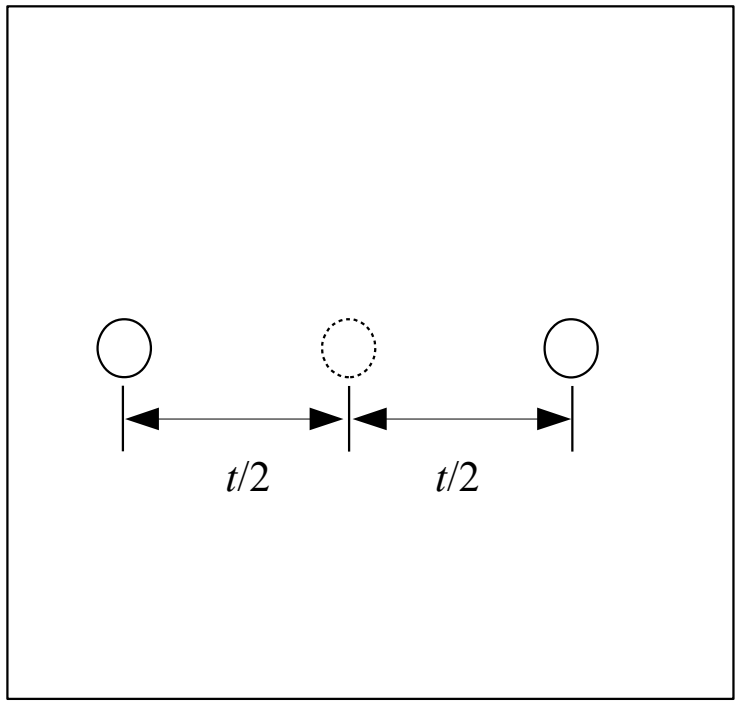
Zonal reflection conditions: witness of glide planes





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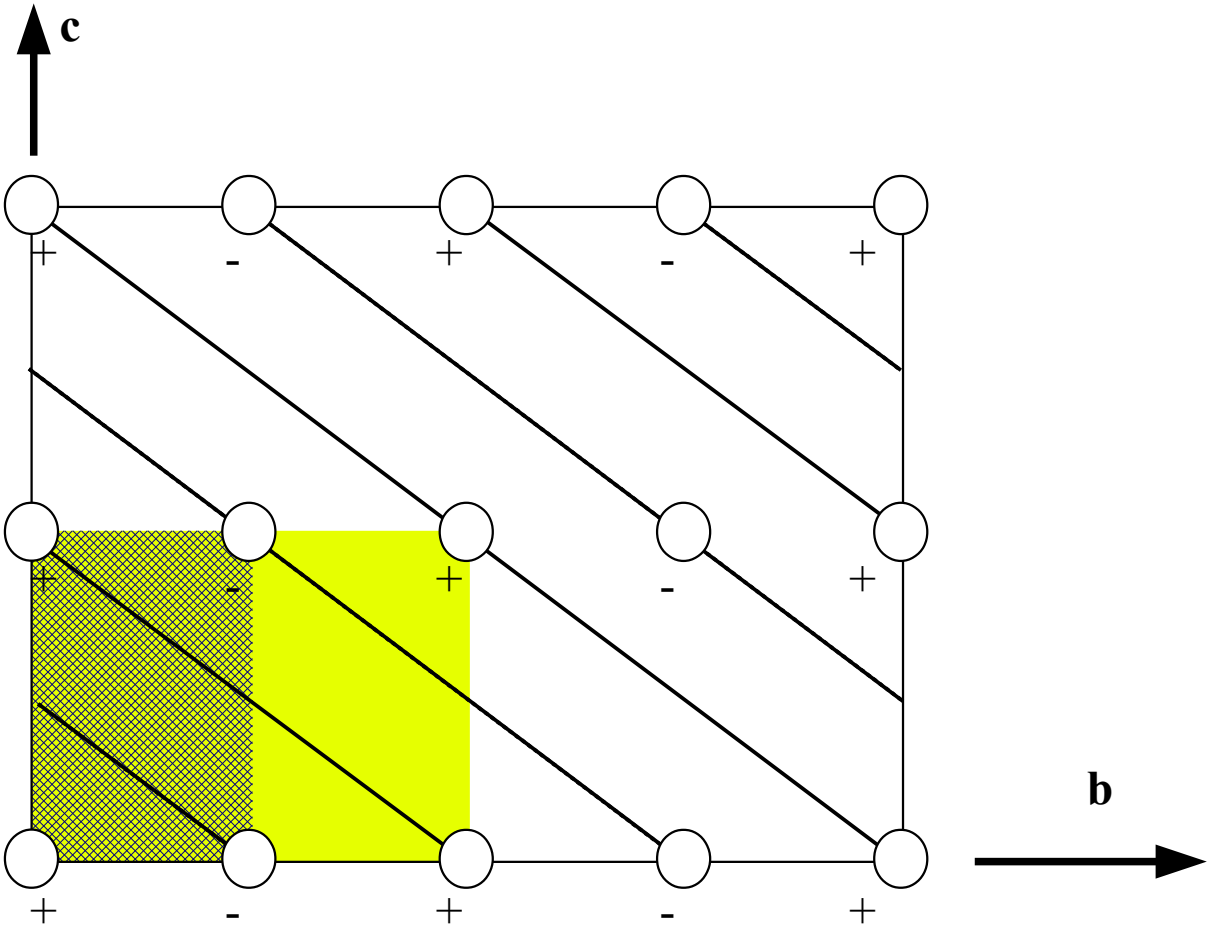
Zonal reflection conditions: witness of glide planes



Direct space

In projection along the **a** axis the period along **b** seems halved

Reciprocal space

On the (0*kl*)*plane the period along the **b*** axis appears doubled.

Reflection conditions : $0kl : k = 2n$

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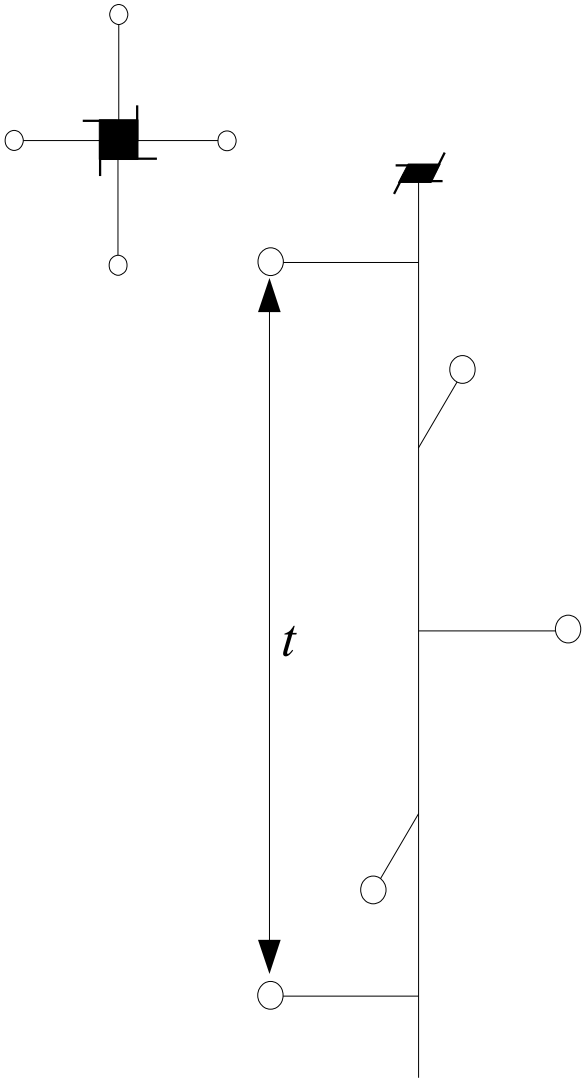
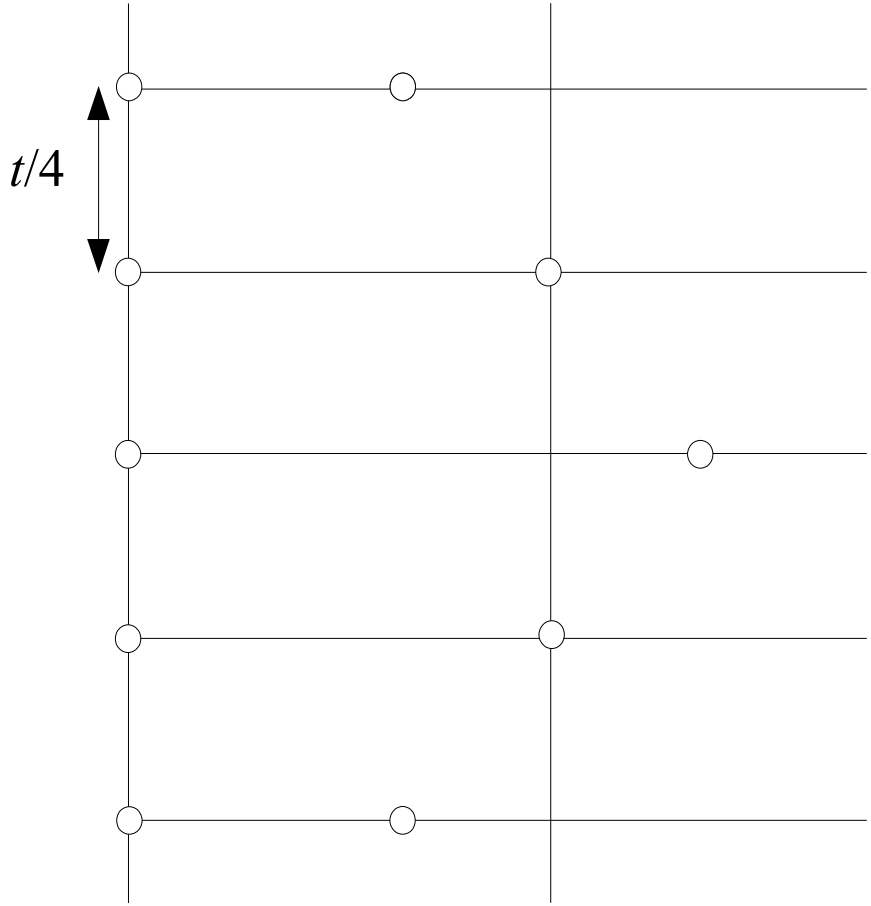
Serial reflection conditions: witness of screw axes





Reflection conditions :
$00l$: $l = 4n$

Direct space
In the projection on the **c** axis the period appear reduced to ¼.

Reciprocal space
In the [001]* direction the period appears multiplied by four.

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Subperiodic groups

Dimension of the space	Periodicity of the object	Type of group
1	0	G^1_0: 1D-point group
1	1	G^1_1: line group
2	0	G^2_0: 2D-point group
2	1	G^2_1: frieze group (2D monoperiodic group)
2	2	G^2_2: plane group
3	0	G^3_0: 3D-point group
3	1	G^3_1: rod group (3D monoperiodic group)
3	2	G^3_2: layer group (3D diperiodic group)
3	3	G^3_3: space group