Geometric interpretation of reflection conditions

Didactic material for the MaThCryst schools

Massimo Nespolo, Université de Lorraine, France
massimo.nespolo@univ-lorraine.fr

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

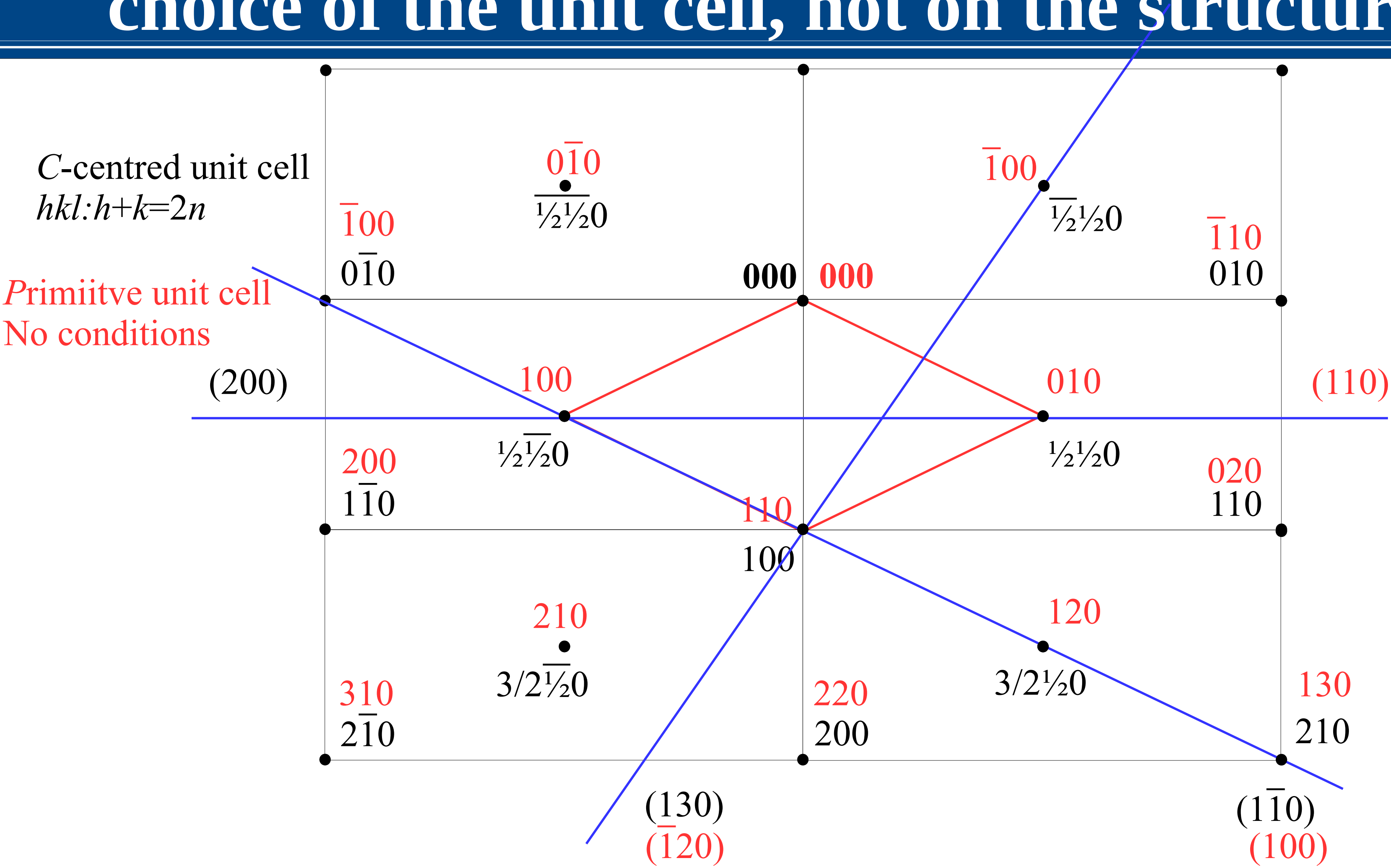
Massimo Nespolo, Université de Lorraine

Integral conditions

They affect the whole reciprocal space and show up when a non-primitive cell is chosen

Massimo Nespolo, Université de Lorraine

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

https://doi.org/10.1107/S1600576715011206

Change of coordinate system

Covariant quantities

$$\left(\mathbf{abc}\right)\mathbf{P} = \left(\mathbf{a'b'c'}\right)$$

$$\left(hkl\right)\mathbf{P} = \left(h'k'l'\right)$$

Row vectors

Contravariant quantites

$$\mathbf{P}^{-1}\begin{pmatrix}\mathbf{a}^*\\\mathbf{b}^*\\\mathbf{c}^*\end{pmatrix} = \begin{pmatrix}\mathbf{a}^{*\prime}\\\mathbf{b}^{*\prime}\\\mathbf{c}^{*\prime}\end{pmatrix}$$

$$\mathbf{P}^{-1}\begin{pmatrix}x\\y\\z\end{pmatrix} = \begin{pmatrix}x'\\y'\\z'\end{pmatrix}$$

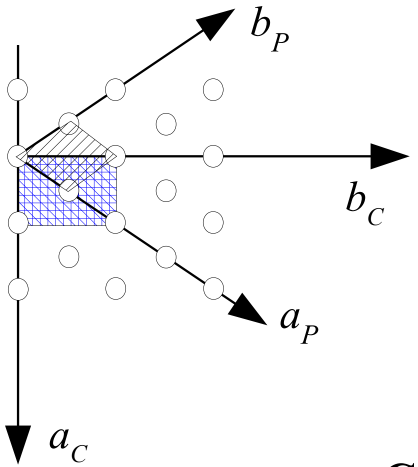
$$\mathbf{P}^{-1}\begin{pmatrix}u\\v\\w\end{pmatrix} = \begin{pmatrix}u'\\v'\\w'\end{pmatrix}$$

Column vectors

Massimo Nespolo, Université de Lorraine

Integral reflection conditions: *C* type of unit cell

Direct space



Change of coordinate system in direct space (covariant vectors)

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

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

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

$C \rightarrow P$ $\qquad$ $P \rightarrow C$

Change of coordinate system in reciprocal space (contravariant vectors)

$\mathbf{a}^*_C = (\mathbf{a}^*_P-\mathbf{b}^*_P)/2$; $\mathbf{a}^*_P = \mathbf{a}^*_C+\mathbf{b}^*_C$

$\mathbf{b}^*_C = (\mathbf{a}^*_P+\mathbf{b}^*_P)/2$; $\mathbf{a}^*_P = -\mathbf{a}^*_C+\mathbf{b}^*_C$

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

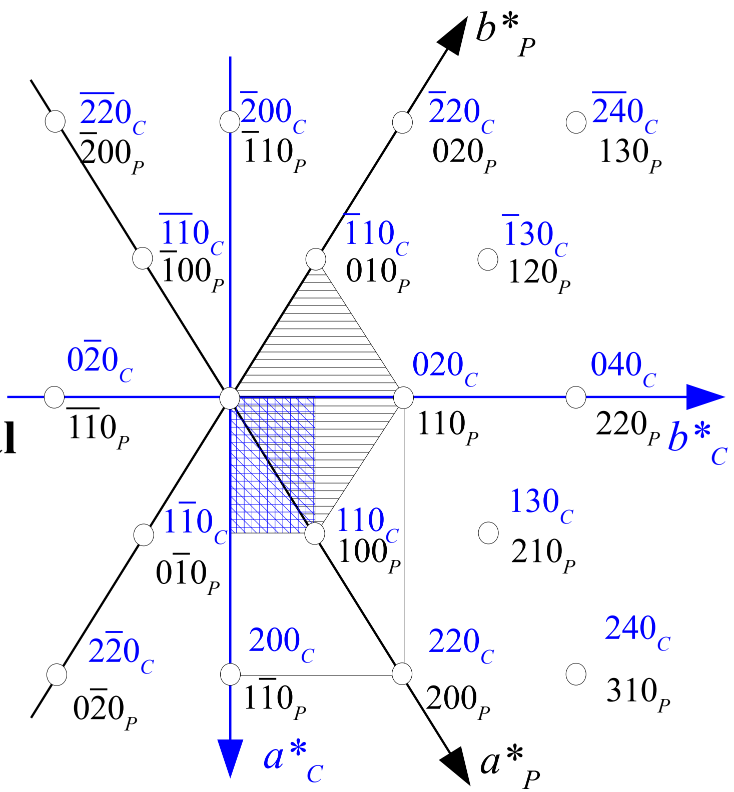
$P \rightarrow C$ $\qquad$ $C \rightarrow P$

P = primitive

C = conventional

$$(hkl)_P \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = (h'k'l')_C \qquad h'+k' = 2h \text{ even}$$

Reciprocal space

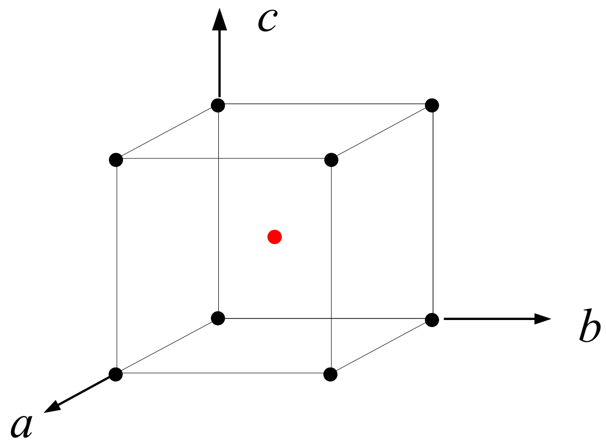


In both direct and reciprocal space, the conventional unit cell is *C*-centred.

Reflection conditions: *hkl* : $h+k = 2n$

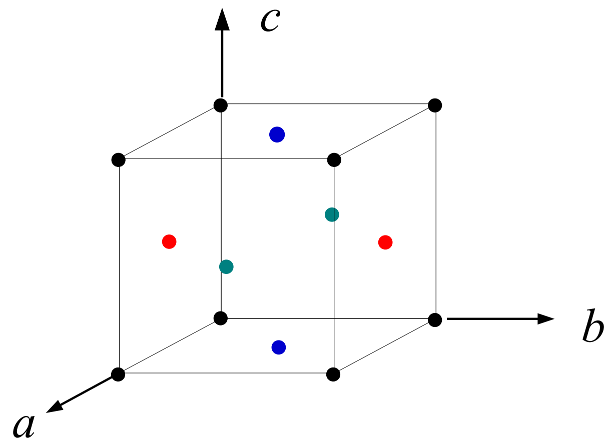
Reminder : *I* vs. *F* cell

I-centred cell



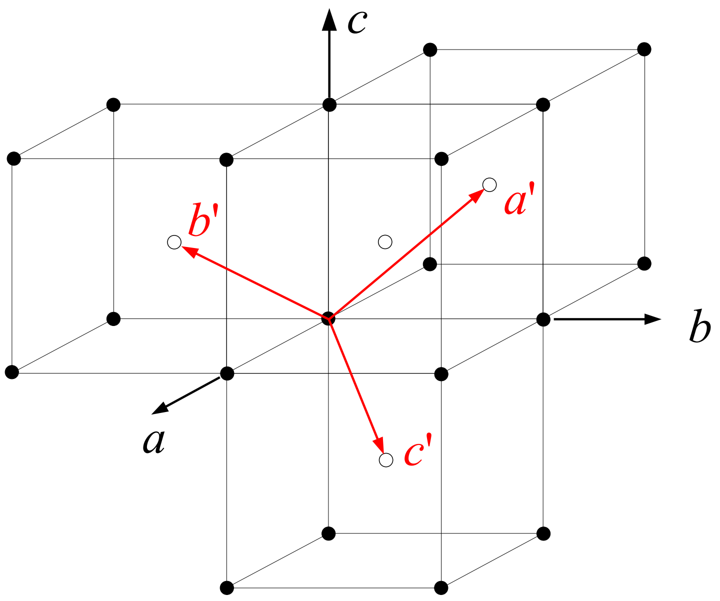
t(½½½)

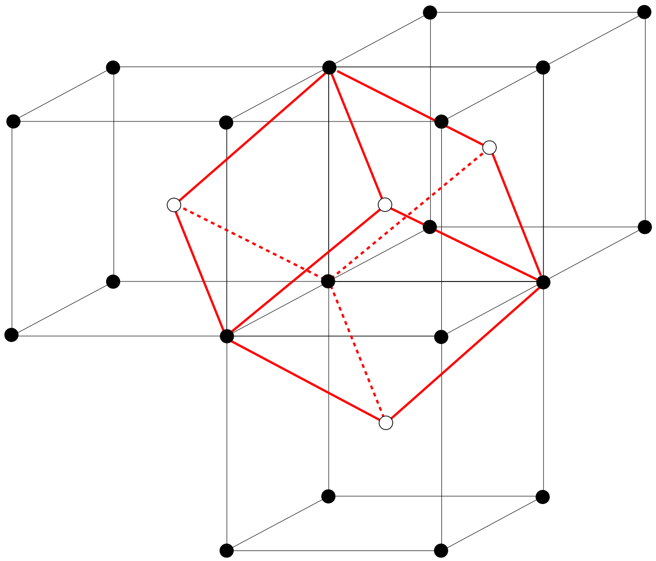
F-centred cell



t(½½0),t(½0½),t(0½½)

Transformation of an *I*-centred cell to a primitive cell





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

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

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

$\mathbf{a}_I = \mathbf{b}_P+\mathbf{c}_P$

$\mathbf{b}_I = \mathbf{a}_P+\mathbf{c}_P$

$\mathbf{c}_I = \mathbf{a}_P+\mathbf{b}_P$

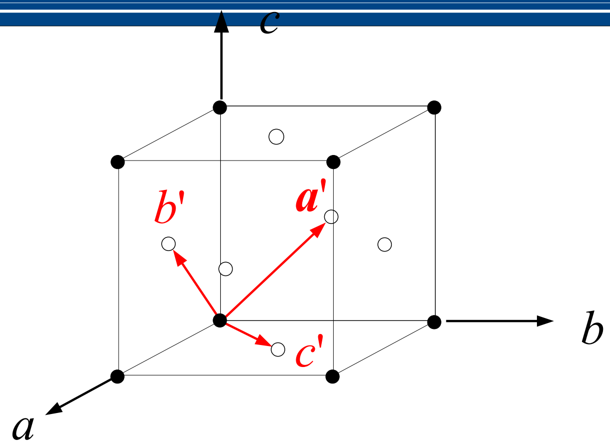
$$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$$

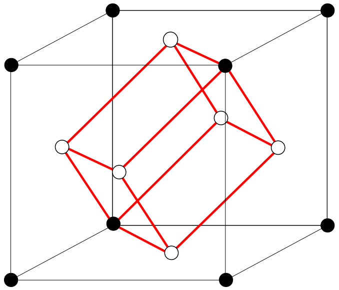
$I \rightarrow P$

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$P \rightarrow I$

Transformation of an F-centred cell to a primitive cell





$\mathbf{a}_P = (\mathbf{b}_F+\mathbf{c}_F)/2$
$\mathbf{b}_P = (\mathbf{a}_F+\mathbf{c}_F)/2$
$\mathbf{c}_P = (\mathbf{a}_F+\mathbf{b}_F)/2$

$$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$F \rightarrow P$

$\mathbf{a}_F = -\mathbf{a}_P+\mathbf{b}_P+\mathbf{c}_P$
$\mathbf{b}_F = \mathbf{a}_P-\mathbf{b}_P+\mathbf{c}_P$
$\mathbf{c}_F = \mathbf{a}_P+\mathbf{b}_P-\mathbf{c}_P$

$$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$$

$P \rightarrow F$

Direct space

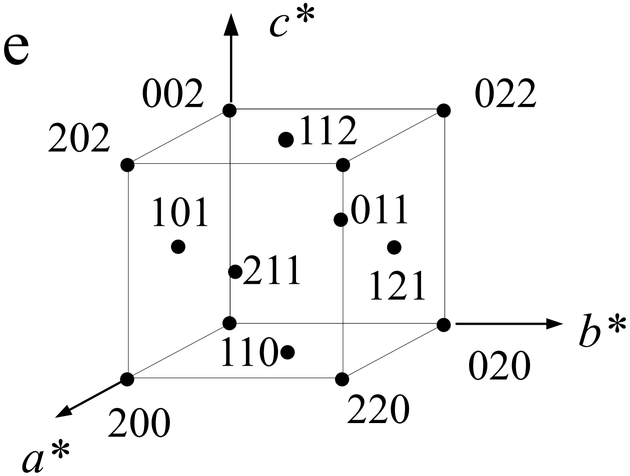
$$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$I \rightarrow P$ $\qquad$ $P \rightarrow I$

Reciprocal space

$$\frac{1}{2}\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$$

$P \rightarrow F$



In the reciprocal space, the conventional cell is *F*-centred

$$(hkl)_P \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} = (h'k'l')_I$$

$h'+k'+l' = 2h+2k+2l$ even

Reflection conditions

$hkl : h+k+l = 2n$

Reciprocal of an *F*-centred cell

Direct space

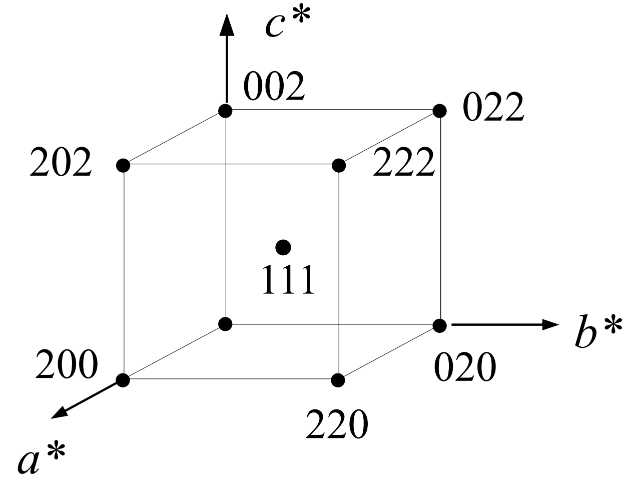
$$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$$

$$F \rightarrow P \qquad P \rightarrow F$$

Reciprocal spae

$$\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$P \rightarrow I$$



In the reciprocal space, the conventional cell is *FI*-centred**

$$\left(hkl\right)_P \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix} = \left(h'k'l'\right)_F$$

$h'+k' = 2l$ even
$h'+l' = 2k$ even
$k'+l' = 2h$ even

Reflection conditions

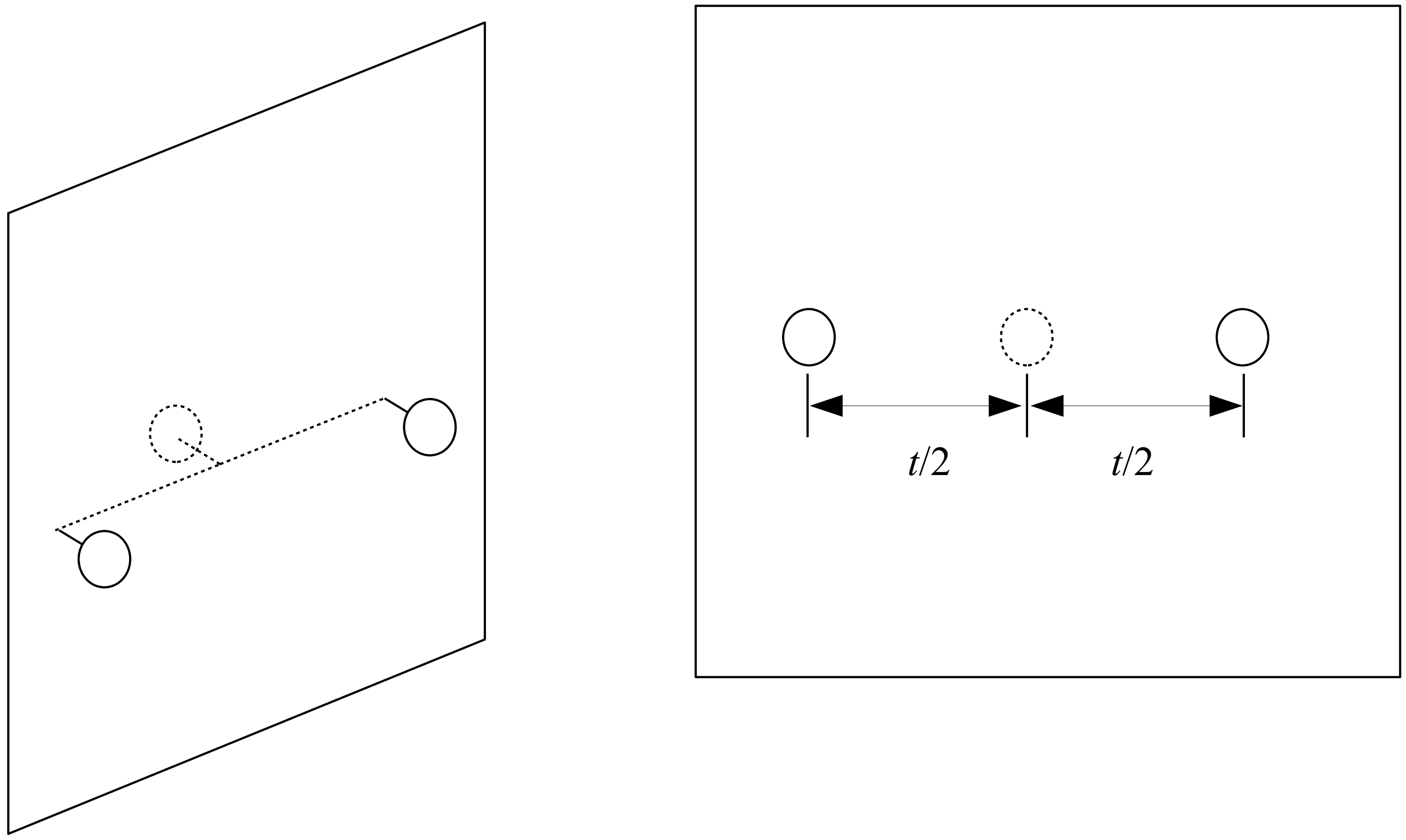
$hkl : h+k = 2n \; ; \; h+l = 2n \; ; \; k+l = 2n$

Massimo Nespolo, Université de Lorraine

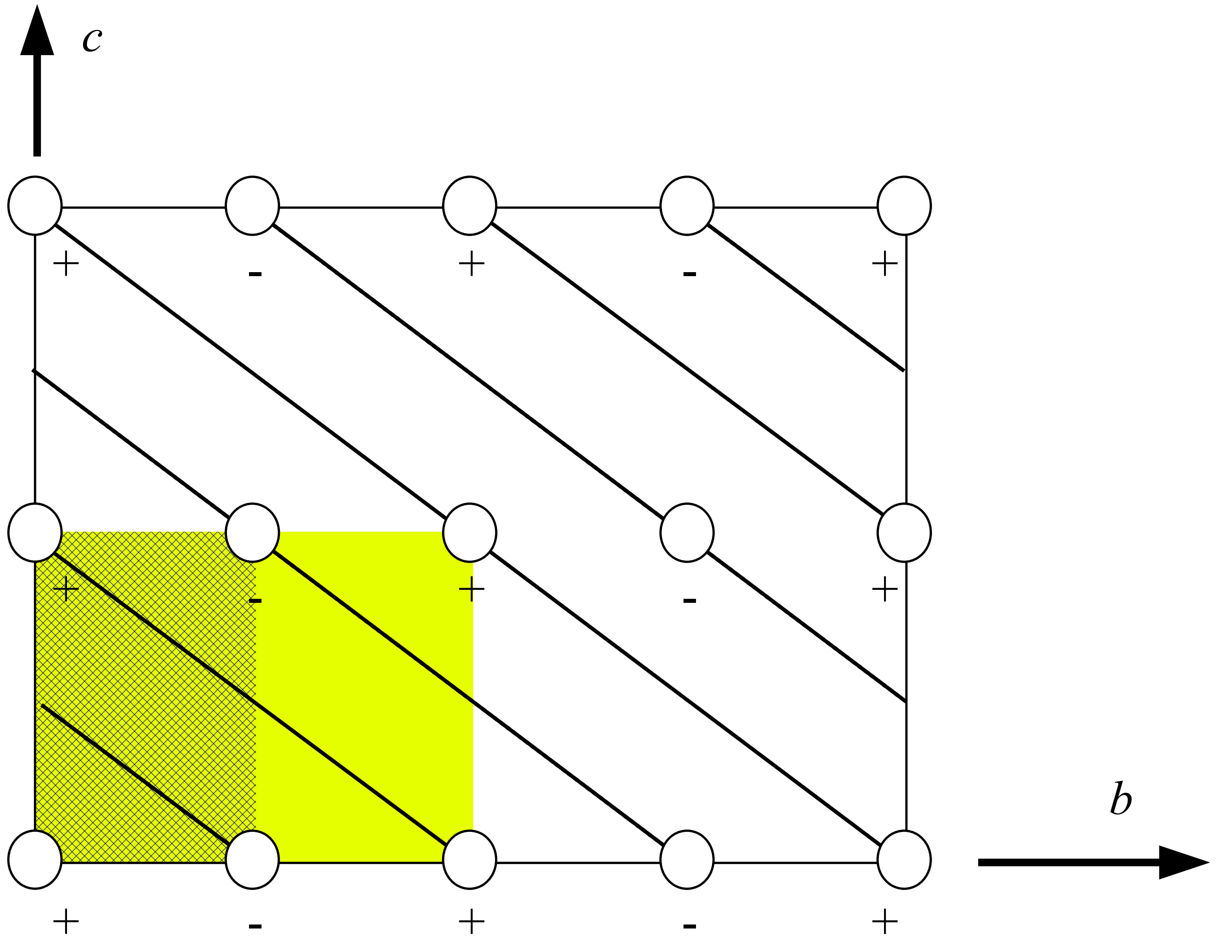
Zonal reflection conditions

They affect one plane of the reciprocal space and show up in presence of a glide plane

Zonal reflection conditions: witness of glide planes



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 : $0kl : k = 2n$

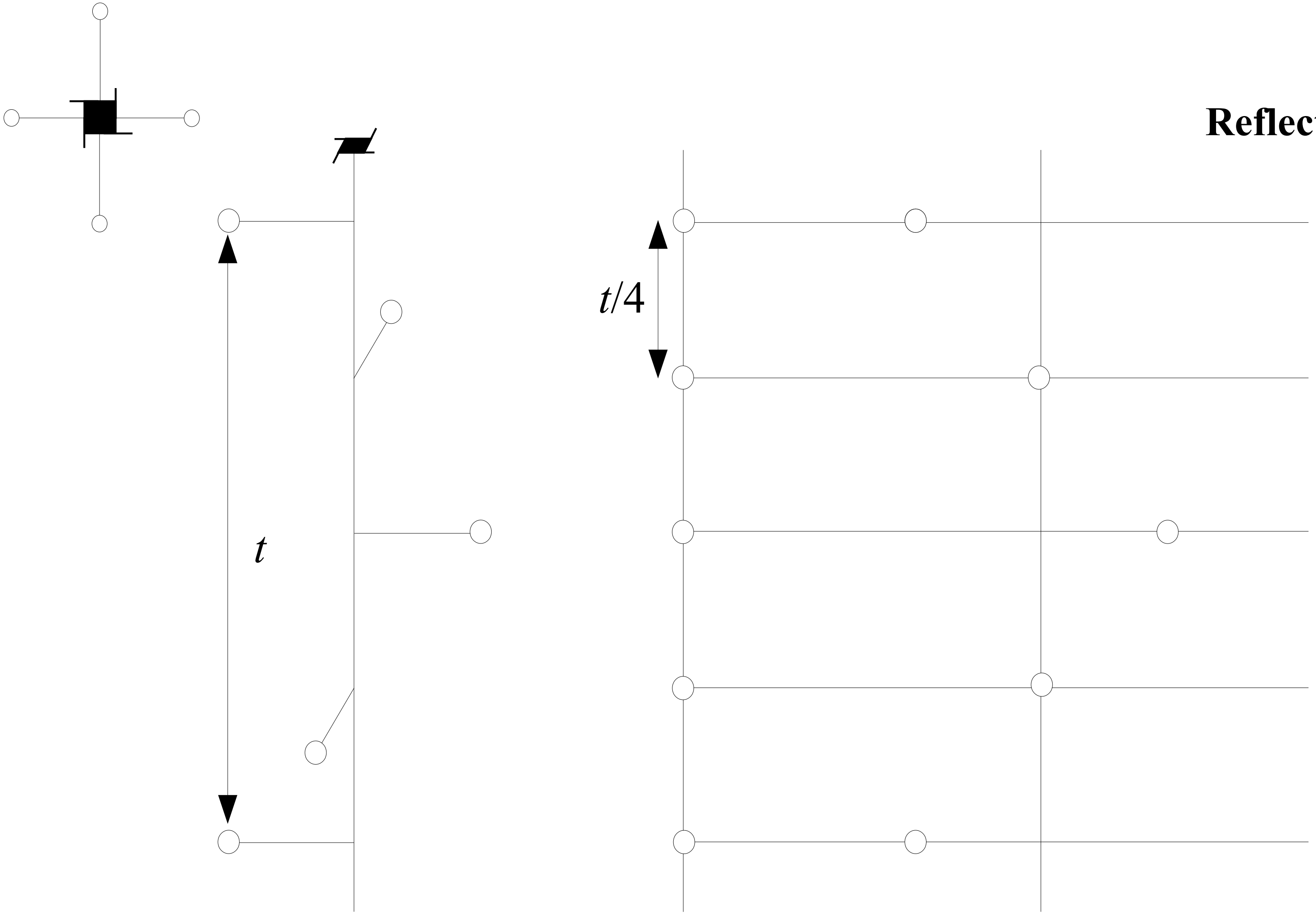
Serial reflection conditions

They affect one row of the reciprocal space and show up in presence of a screw axis

Massimo Nespolo, Université de Lorraine

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.

From reflections conditions to space groups (absence of metric specialisation is assumed hereafter)

Massimo Nespolo, Université de Lorraine

Example 1: *a*, *b*, *c*; $\alpha = \beta = \gamma = 90°$

$hkl: k+l = 2n$ → Integral reflection conditions: centred cell → *oA*

$0kl: k+l = 2n$

$h0l: l = 2n$

$hk0: h = 2n$ → Zonal reflection conditions: glide plane → $hk0$: perpendicular to [001]; h even : a glide → $a_{[001]}$

$hk0: k = 2n$

$h00: h = 2n$

$0k0: k = 2n$

$00l: l = 2n$

Extinction symbol : *A*--*a*

Possible space-group types : $Am2a$, $A2_1ma$, $Amma$

Massimo Nespolo, Université de Lorraine

Example 2: $a = b, c; \alpha = \beta = \gamma = 90°$

No integral reflection condition → tP

$hk0: h+k = 2n$
$0k0: k = 2n$
→ Zonal reflection conditions: glide plane
→ $hk0$: perpendicular to [001]
→ $h+k$ even : n glide
→ $n_{[001]}$

$hhl: l = 2n$
$00l: l = 2n$
→ Zonal reflection conditions: glide plane
→ hhl: perpendicular to $[1\bar{1}0]$
→ l even : c glide
→ $c_{\langle 1\bar{1}0 \rangle}$

Non-independent

Extinction symbol : $Pn\text{-}c$

Possible space-group type: $P4_2/nmc$

Example 3: $a = b = c$; $\alpha = \beta = \gamma = 90°$

$hkl: h+k+l = 2n$ ► Integral reflection condition — cI

$0kl: k = 2n$

$0kl: l = 2n$

$h0l: h = 2n$

$h0l: l = 2n$

$hk0: h = 2n$

$hk0: k = 2n$

► Zonal reflection condition

- $0kl$: perpendicular to [100], k even — $b_{[100]}$
- $0kl$: perpendicular to [100], l even — $c_{[100]}$
- $h0l$: perpendicular to [010], h even — $a_{[010]}$
- $h0l$: perpendicular to [010], l even — $c_{[010]}$
- $hk0$: perpendicular to [001], h even — $a_{[001]}$
- $hk0$: perpendicular to [001], k even — $b_{[001]}$

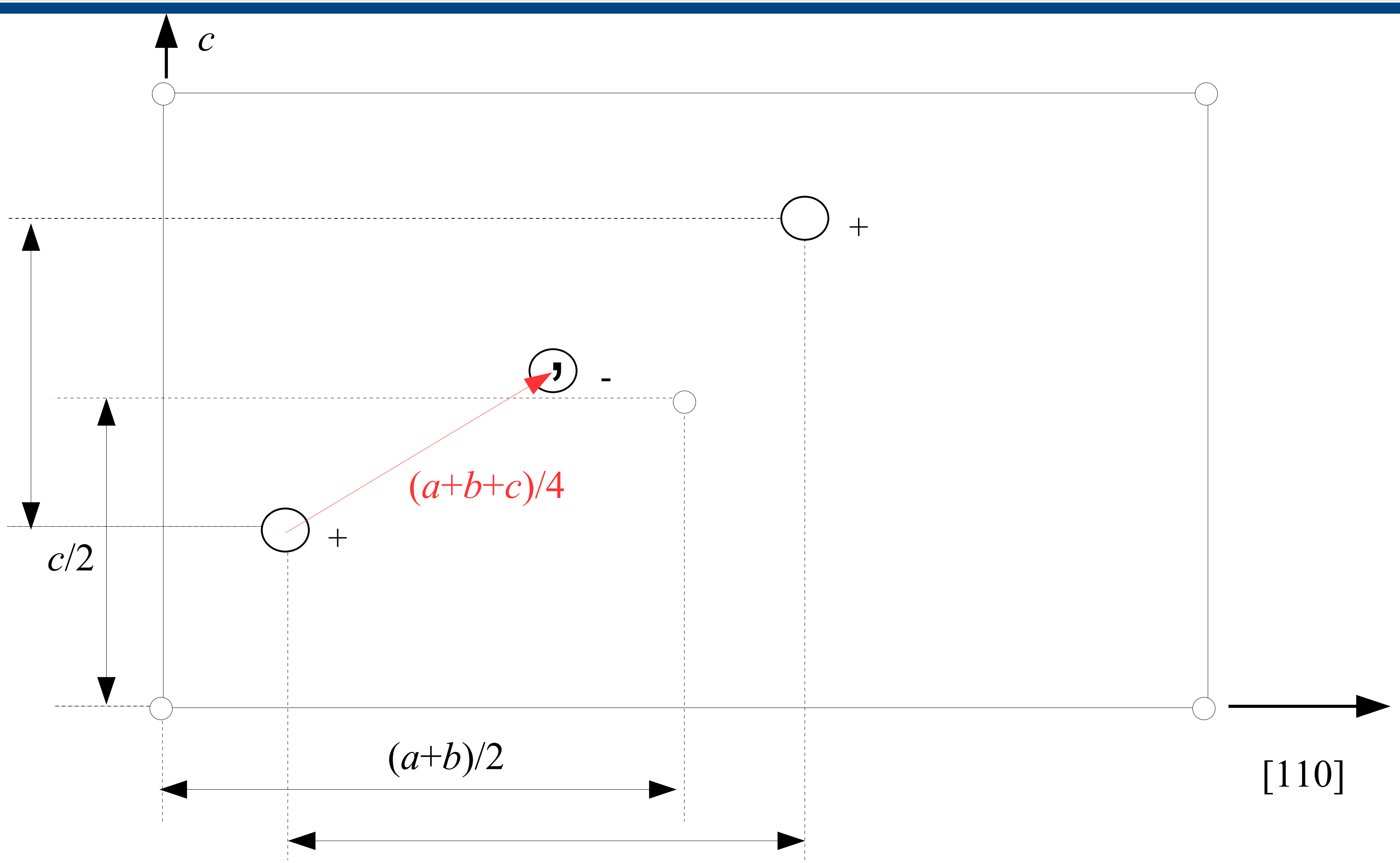
$hhl: 2h+l = 4n$ ► Zonal reflection condition — hhl: perpendicular to $[1\bar{1}0]$, $2h+l = 4n$??

$hhl: l = 2n$

$00l: l = 4n$

Massimo Nespolo, Université de Lorraine

Example 3: $a = b = c$; $\alpha = \beta = \gamma = 90°$



Direct lattice: $(a+b+c)/4$ Reciprocal lattice: $h+k+l = 4n$ $\xrightarrow{(110) \Rightarrow h = k}$ $h+h+l = 4n$

$hhl{:}2h+l = 4n$ $d_{[1\bar{1}0]}$

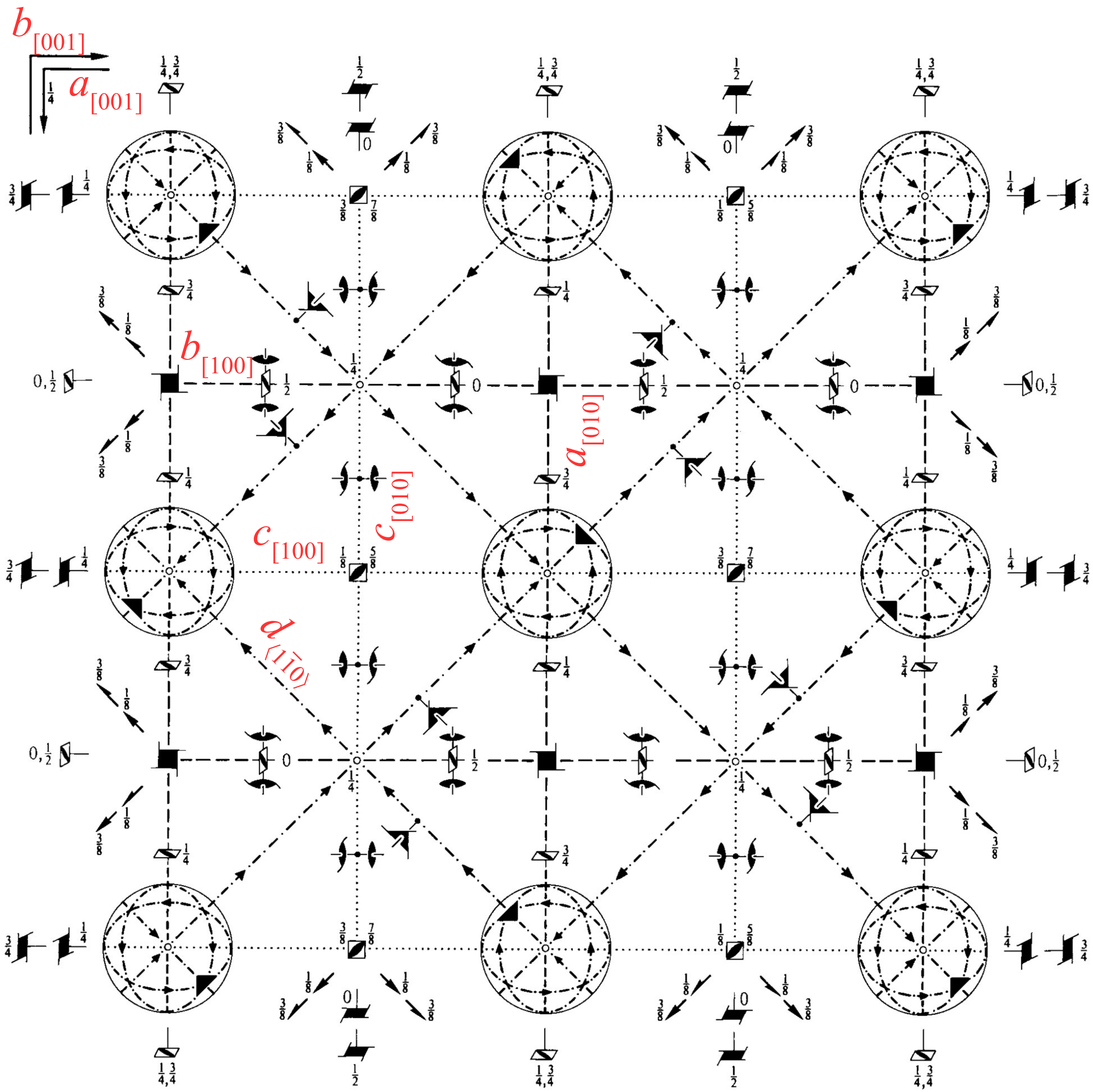
Example 3: $a = b = c$; $\alpha = \beta = \gamma = 90°$

$hkl: h+k+l = 2n$	→ Integral reflection condition		cI
$0kl: k = 2n$	→ Zonal reflection condition	$0kl$: perpendicular to [100], k even	$b_{[100]}$
$0kl: l = 2n$		$0kl$: perpendicular to [100], l even	$c_{[100]}$
$h0l: h = 2n$		$h0l$: perpendicular to [010], h even	$a_{[010]}$
$h0l: l = 2n$		$h0l$: perpendicular to [010], l even	$c_{[010]}$
$hk0: h = 2n$		$hk0$: perpendicular to [001],h even	$a_{[001]}$
$hk0: k = 2n$		$hk0$: perpendicular to [001],k even	$b_{[001]}$
$hhl: 2h+l = 4n$	→ Zonal reflection condition	hhl: perpendicular to $[1\bar{1}0]$, $2h+l = 4n$	$d_{\langle 1\bar{1}0\rangle}$
$hhl: l = 2n$			
$00l: l = 4n$			

Extinction symbol: *Ia-d*

Possible space-group type: $Ia\bar{3}d$

Example 3: $a = b = c$; $\alpha = \beta = \gamma = 90°$



Reflection conditions

h, k, l permutable

General:

hkl : $h+k+l = 2n$

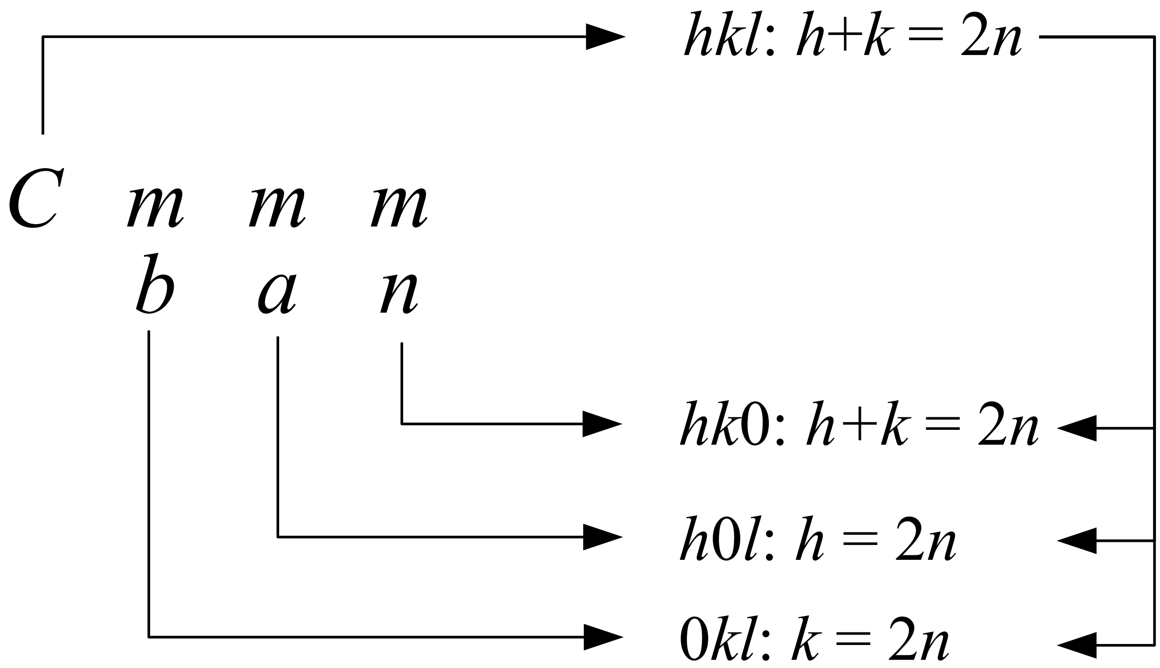
$0kl$: $k, l = 2n$

hhl : $2h+l = 4n$

$h00$: $h = 4n$

Massimo Nespolo, Université de Lorraine

Symmorphic space groups (1)



Symmorphic space groups (2)

$P\ \ 4\ \ m\ \ m$

g → *hhl*: $h+h = 2n$

However, $h+h = 2h$ always true!