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Twin point groups

Massimo Nespolo, Université de Lorraine, France
massimo.nespolo@crm2.uhp-nancy.fr
What is a twin point group?

- A twin point group is a chromatic crystallographic point group.
- We assign to each individual of a twin a color.
- Symmetry operations of the individual are achromatic; operations mapping the orientation of an individual onto that of another individual are chromatic.
- Twin point groups are thus obtained as extensions of the achromatic $H^*$ intersection group by the chromatic twin operation(s).
Symmetry operations in a chromatic group

- **Achromatic** operation: it does not exchange the colors.
- **Grey** operation: it exchanges the colors without moving the object (no application in twinning).
- **Totally chromatic** operation: it exchanges a number of colors equal to the order of the operation without leaving fixed any color.
- **Partially chromatic** operation: it leaves fixed one or more colors.
Fourfold axis totally chromatic: it exchanges *four colors*. 
Two mirror planes totally chromatic: each of them exchanges *two pairs* of colors.
Two mirror planes partially chromatic: each of them exchanges *one pair* of colors and leaves fixed the other pair.
Categories of chromatic point groups

- **Dichromatic** crystallographic point groups: Shubnikov groups $K^{(2)}$
- **Polychromatic invariant** extension of crystallographic point groups (no partially chromatic operation): Koptsik groups $K^{(p>2)}$
- **Polychromatic non-invariant** extension of crystallographic point groups (with partially chromatic operations): Van der Waerden-Burckhardt groups $K_{WB}^{(p>2)}$
Example of dichromatic (Shubnikov) $K^{(2)}$ groups
A simple exercise on dichromatic (Shubnikov) groups

Three $K^{(2)}$ groups corresponding to the same holohedral achromatic group

- $H^* = 422$
  - $K^{(2)} = 4/m'2/m'2/m'$
- $H^* = \overline{4}2m$
  - $K^{(2)} = 4'/m'2/m'2'/m$
- $H^* = 4/m$
  - $K^{(2)} = 4/m2'/m'2'/m'$
A simple exercise on dichromatic (Shubnikov) groups: obtain the possible $K^{(2)}$ from the given $H^*$

$H^* = 3m1$

$K^{(2)} = 32'/m$

$K^{(2)} = 6'm2'$

$K^{(2)} = 6'mm'$
Exercise

Find the twin point group of two individuals with $H = 222$ related by a twin mirror plane (010). What type of twin is it?
Exercise

Find the twin point group of two individuals with $H = 222$ related by a fourfold twin axis parallel to [001]. What type of twin is it?
Exercise

Find the twin point group of two individuals with $H = mmm$ related by a fourfold twin axis parallel to [001]. What type of twin is it?
Exercise

Find the twin point group of two individuals with $H = 2$ and $\beta = 90^\circ$ related by a twofold twin axis parallel to [100]. What type of twin is it?
Find the twin point group of two individuals with $H = m$ and $\beta = 90^\circ$ related by a twofold twin axis parallel to [100]. What type of twin is it?
Exercise

(210) twinning in hauyne, $H = \overline{43m}$

Twinning by reticular merohedry

What is the twin index?
Exercise

(120) twinning in melilite, $H = \overline{4}2m$

Twinning by reticular polyholohedry

What is the twin index?

$K = H$
Examples of Koptsik $K^{(p)}$ groups for first-order twins

$H^* = 222$

$K^{(3)} = (23^{(3)})^{(3)}$

$K^{(3)} = \overline{3}^{(3)}$

$H^* = \overline{1}$
Examples of Koptsik $K^{(p)}$ groups for higher-order twins

$H^* = 2$

$K^{(2)} = \frac{2}{m'}$

$K^{(4)} = \left( \frac{2^{(2)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2)}} \frac{2}{m^{(2)}} \right)^{(4)}$
Examples of Koptsik $K^{(p)}$ groups for higher-order twins

- $H^* = 3$
- $K^{(2)} = 32'1$
- $K^{(4)} = (6^{(2)} 2^{(2)} 2^{(2)})^{(4)}$
- $K^{(8)} = \left(\frac{6^{(2)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$
A simple exercise on Koptsik groups: obtain the orthorhombic holohedral $K^{(p>2)}$ from $H^* = \frac{2}{m}$. 

$H^* = m \quad \Rightarrow \quad K^{(2)} = \frac{2'}{m} \quad \Rightarrow \quad K^{(4)} = \left( \frac{2^{(2)}}{m^{(2)}} \frac{2^{(2)}}{m} \frac{2^{(2)}}{m^{(2)}} \right)^{(4)}$
A simple exercise on Koptsik groups: obtain the tetragonal holohedral $K^{(p>2)}$ from $H^* = m$

$H^* = m$

$K^{(2)} = 2'/m$

$K^{(4)} = \left(\frac{2^{(2)}}{m^{(2)}}, \frac{2^{(2)}}{m^{(2)}}, \frac{2^{(2)}}{m}\right)^{(4)}$

$K^{(8)} = \left(\frac{4^{(4)}}{m}, \frac{2^{(2)}}{m^{(2)}}, \frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$

Note the change of axial setting!
A simple exercise on Koptsik groups: obtain the hexagoanl holohedral $K^{(p>2)}$ from $H^* = m$

$K^{(6)} = \left( \frac{6^{(6)}}{m} \right)^{(6)}$

$K^{(12)} = \left( \frac{6^{(6)} \ 2^{(2)} \ 2^{(2)}}{m \ m^{(2)} \ m^{(2)}} \right)^{(12)}$

$K^{(3)} = 6^{(3)}$

$H^* = m$
Exercise

Find the twin point group of four individuals with H = 2 related by 1) a mirror plane (010) and 2) a twofold twin axis parallel to [100]. What type of twin is it?
Exercise

Find the twin point group of three individuals with $H = 2$ related by a threefold twin axis parallel to $[010]$. What type of twin is it? What happens if one of the individuals does not develop or is chopped off?
Repeat the previous exercise by adding:

➔ a twin mirror plane (001)
➔ a twofold twin axis parallel to [100]

What type of twin is it? What happens if two of the individuals do not develop or are chopped off?
Examples of Van der Waerden-Burckhardt $K^{(p)}_{WB}$ groups

$H^* = 2 \quad \rightarrow \quad K_{WB}^{(3)} = (3^{(3)}2^{(2,1)})^{(3)}$
Examples of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups

$H^* = m$

$K^{(2)} = m'm2'$

$K^{(4)} = \left(\frac{2^{(2)}}{m}, \frac{2^{(2)}}{m^{(2)}}, \frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$

$K_{WB}^{(12)} = \left(\frac{2^{(2)}}{m^{(2,4)}}, \frac{3^{(6)}}{}\right)^{(12)}$
Example of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups for higher-order twins

$H^* = m2m \quad \rightarrow \quad K' = \left( \frac{2'}{m} \quad \frac{2}{m'} \quad \frac{2'}{m} \right) \quad \rightarrow \quad K_{WB}^{(4)} = \left( \frac{4^{(4)}}{m} \quad \frac{2^{(2,2)}}{m^{(2,2)}} \quad \frac{2^{(2)}}{m^{(2)}} \right)^{(4)}$
Obtain the tetragonal holohedral $K_{WB}^{(p>2)}$ from $H^* = m$

\[
K_{WB}^{(4)} = (4^{(4)} m^{(2,2)} m^{(2)})^{(4)}
\]

\[
K_{WB}^{(8)} = \left( \frac{4^{(4)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2,4)}} \frac{2^{(2)}}{m^{(2)}} \right)^{(4)}
\]
Obtain the hexagonal holohedral $K_{\text{WB}}^{(p>2)}$ from $H^* = m$

$K_{\text{WB}}^{(6)} = (6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$

$K_{\text{WB}}^{(12)} = \left( \frac{6^{(6)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2,4)}} \frac{2^{(2)}}{m^{(2)}} \right)^{(12)}$