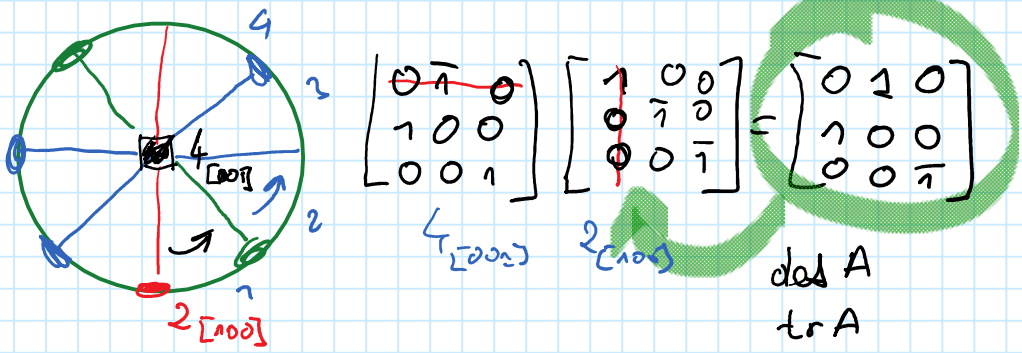
Składanie elementów sym. a reprezentacja macierzowa

Płaszczyzna symetrii	Macierz	Płaszczyzna symetrii	Macierz	Płaszczyzna symetrii	Macierz
$m_{(100)}$	$\begin{matrix}-1&0&0\\0&1&0\\0&0&1\end{matrix}$	$m_{(010)}$	$\begin{matrix}1&0&0\\0&-1&0\\0&0&1\end{matrix}$	$m_{(001)}$	$\begin{matrix}1&0&0\\0&1&0\\0&0&-1\end{matrix}$
$m_{(110)}$	$\begin{matrix}0&-1&0\\-1&0&0\\0&0&1\end{matrix}$	$m_{(\bar{1}10)}$	$\begin{matrix}0&1&0\\1&0&0\\0&0&1\end{matrix}$	$m_{(011)}$	$\begin{matrix}1&0&0\\0&0&-1\\0&-1&0\end{matrix}$
$m_{(101)}$	$\begin{matrix}0&0&-1\\0&1&0\\-1&0&0\end{matrix}$	$m_{(\bar{1}01)}$	$\begin{matrix}0&0&1\\0&1&0\\1&0&0\end{matrix}$	$m_{(0\,\bar{1}1)}$	$\begin{matrix}1&0&0\\0&0&1\\0&1&0\end{matrix}$

Oś symetrii	Macierz	Oś symetrii	Macierz	Oś symetrii	Macierz
$2_{[100]}$	$\begin{matrix}1&0&0\\0&-1&0\\0&0&-1\end{matrix}$	$2_{[010]}$	$\begin{matrix}-1&0&0\\0&1&0\\0&0&-1\end{matrix}$	$2_{[001]}$	$\begin{matrix}-1&0&0\\0&-1&0\\0&0&1\end{matrix}$
$2_{[110]}$	$\begin{matrix}0&1&0\\1&0&0\\0&0&-1\end{matrix}$	$2_{[101]}$	$\begin{matrix}0&0&1\\0&-1&0\\1&0&0\end{matrix}$	$2_{[011]}$	$\begin{matrix}-1&0&0\\0&0&1\\0&1&0\end{matrix}$
$2_{[\bar{1}10]}$	$\begin{matrix}0&-1&0\\-1&0&0\\0&0&-1\end{matrix}$	$2_{[\bar{1}01]}$	$\begin{matrix}0&0&-1\\0&-1&0\\-1&0&0\end{matrix}$	$2_{[0\,\bar{1}1]}$	$\begin{matrix}-1&0&0\\0&0&-1\\0&-1&0\end{matrix}$
$4_{[100]}$	$\begin{matrix}1&0&0\\0&0&-1\\0&1&0\end{matrix}$	$4_{[010]}$	$\begin{matrix}0&0&1\\0&1&0\\-1&0&0\end{matrix}$	$4_{[001]}$	$\begin{matrix}0&-1&0\\1&0&0\\0&0&1\end{matrix}$
$3_{[001]}$	$\begin{matrix}-\frac{1}{2}&-\sqrt{3}/2&0\\-\sqrt{3}/2&-\frac{1}{2}&0\\0&0&1\end{matrix}$	$3_{[111]}$	$\begin{matrix}0&0&1\\1&0&0\\0&1&0\end{matrix}$	$3_{[\bar{1}11]}$	$\begin{matrix}0&-1&0\\0&0&1\\-1&0&0\end{matrix}$
$3_{[1\,\bar{1}1]}$	$\begin{matrix}0&-1&0\\0&0&-1\\1&0&0\end{matrix}$	$3_{[11\,\bar{1}]}$	$\begin{matrix}0&1&0\\0&0&-1\\-1&0&0\end{matrix}$	$6_{001]}$	$\begin{matrix}\frac{1}{2}&\sqrt{3}/2&0\\-\sqrt{3}/2&\frac{1}{2}&0\\0&0&1\end{matrix}$



Generowanie kolejnych elementów symetrii jest iloczynem macierzowym.

Grupa operacji symetrii

1. $a \circ b = c \quad , \quad a, b, c \in G$

Istnieje operacja zwana iloczynem "$\circ$" która z wyniku złożenia elementu a i b generuje element c, który również należy do grupy.

2. $(a \circ b) \circ c = a \circ (b \circ c)$ ← łączności elementów

$a \circ b \neq b \circ c$

↖ nieprzemienności istnieje w grupach abelowych a zbiór elementów symetrii nie jest grupą abelową.

3. $a \circ \mathbb{1} = \mathbb{1} \circ a = a$

Istnienie elementu neutralnego.

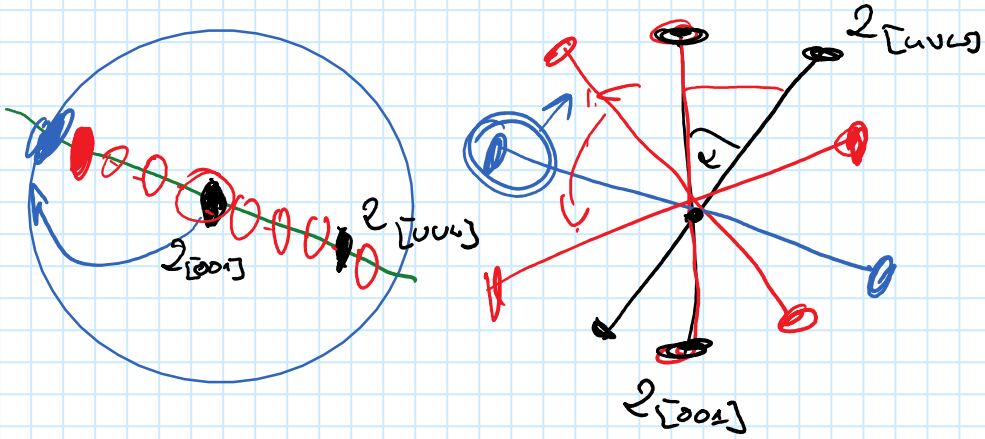
4. $a \circ a^* = a^* \circ a = \mathbb{1}$

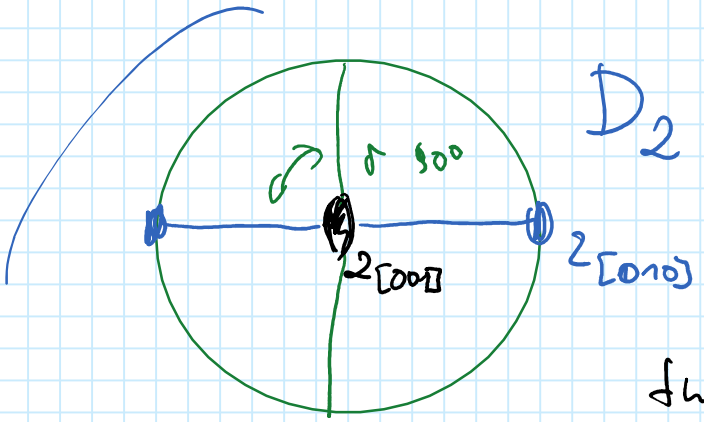
$a^* \rightarrow a^{-1}$

Istnienie elementu przeciwnego.

Każdy element symetrii jest dla siebie elementem odwrotnym.

Kombinacje elementów symetrii





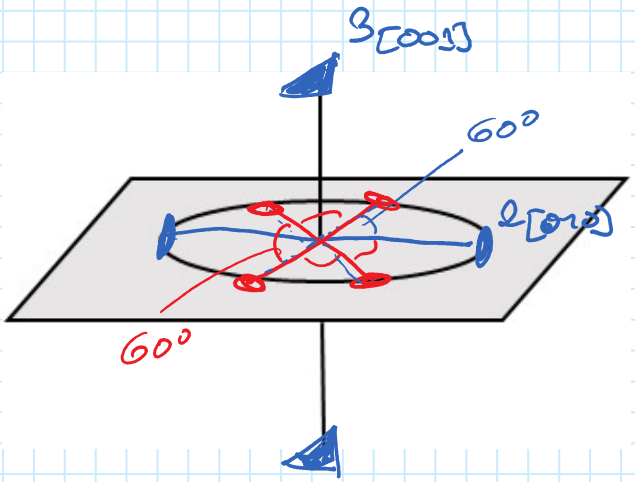
D_2

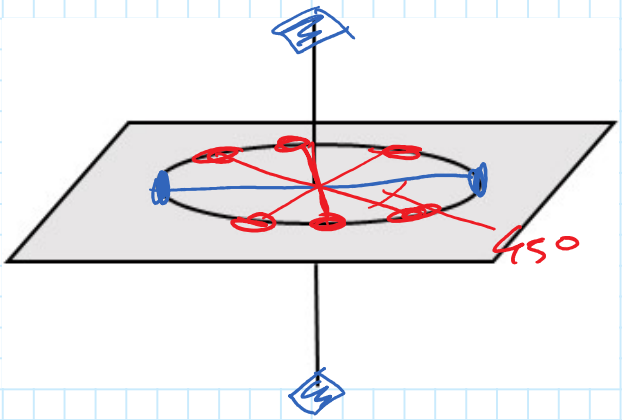
y

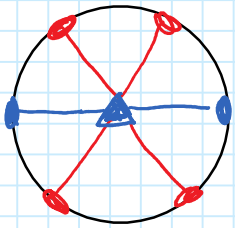
dwa prostopadłe osie 2-krotne generują zawsze grupy

GRUPY PUNKTOWE KRYSTALOGRAFICZNE
||
KLASY SYMETRII

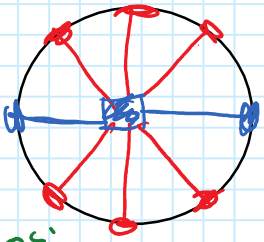
Osiowe klasy symetrii





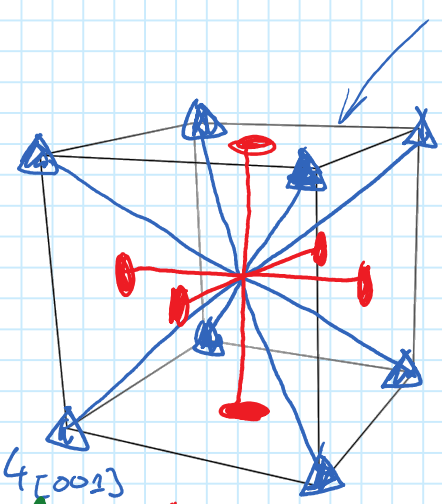
D_2  D_3

D_N ← N osi n-krotnych

 D_4 D_6

GENERATORY: $3_{[001]}$ $2_{[010]}$ $4_{[001]}$ $2_{[010]}$

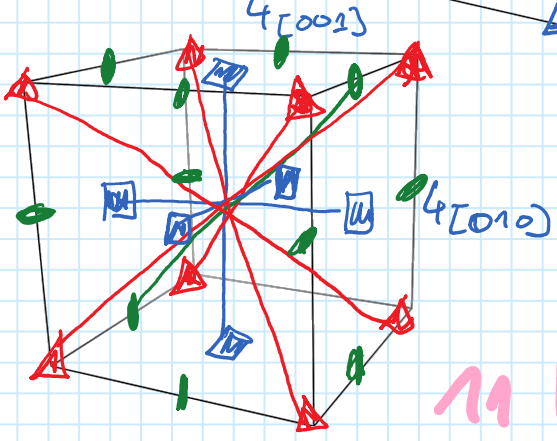
C_1, C_2, C_3, C_4, C_6 → trywialne klasy symetrii



Zaczepiamy od dwóch osi 3-krotnych

GEN.: 3_1 3_2

T

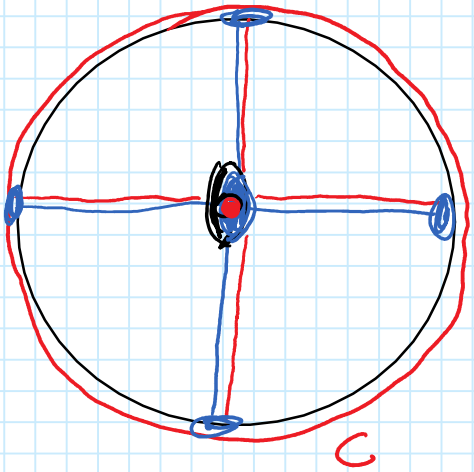


$4_{[001]}$ $4_{[010]}$

O (oktaedr)

11 klas osiowych

Grupy główne (centrosymetryczne)

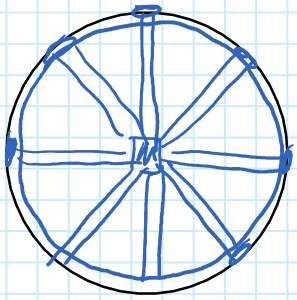


$D_2 + C_i \Rightarrow D_{2h}$

$\bar{1}$

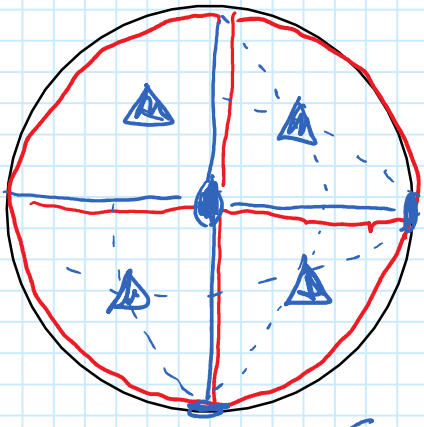
$2_{[001]}$

↑ generatory

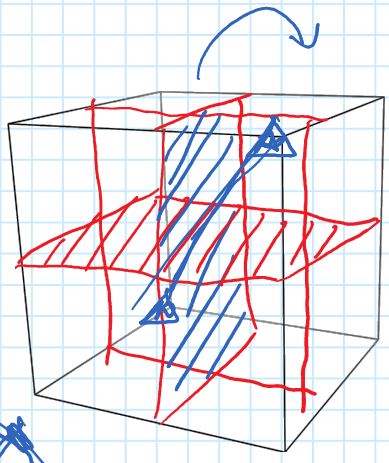


$D_4 + C_i \Rightarrow D_{4h}$

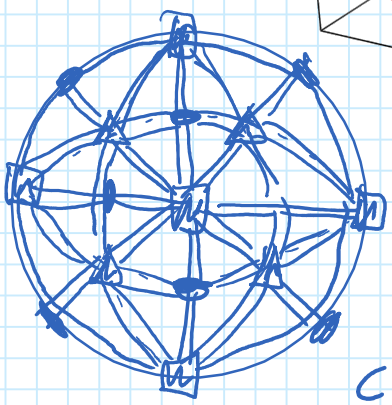
D_{6h}



$T + C_i \Rightarrow T_h$

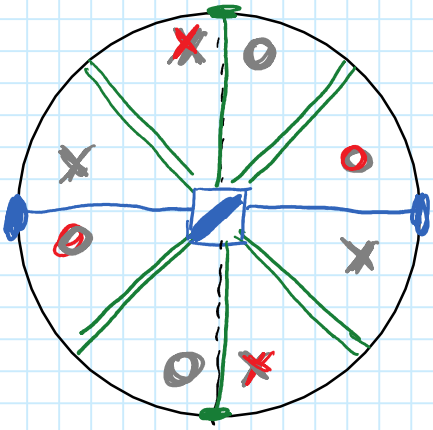


$O + C_i \Rightarrow O_h$



17 klas symetrii grupy głównej

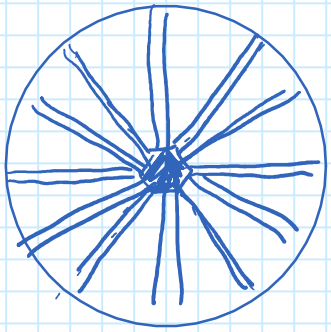
Klasy symetrii z inwersją (np. $\bar{4}$)



D_{2d}

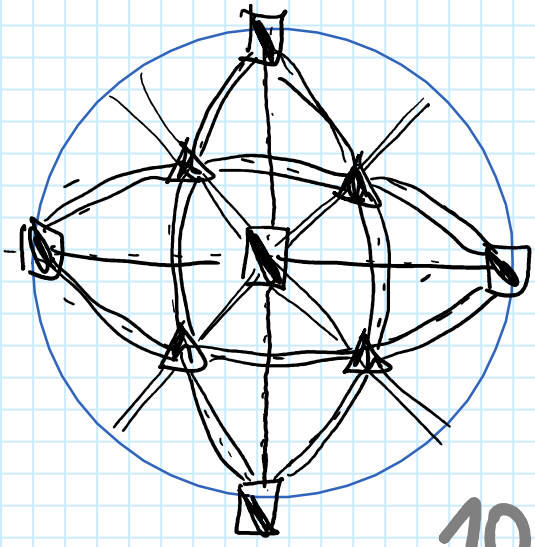
Generatory:

$\bar{4}_{[001]}$: $2_{[010]}$



C_{6v}

$6_{[001]}$: $m_{[010]}$



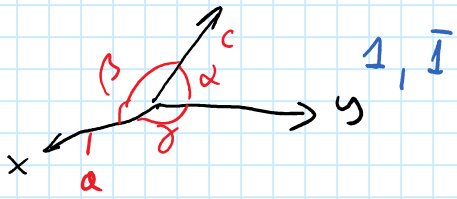
T_d

$\bar{4}_{[001]}$: $\bar{4}_{[010]}$

10 iloczynowych klas symetrii

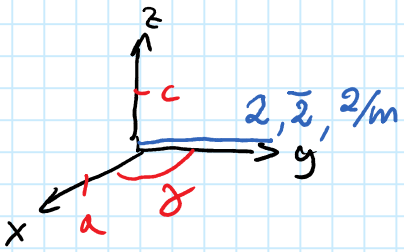
Klasy symetrii a układ krystalograficzny

Selekcja 32 klas symetrii w obrębie układów krystalograficznych:

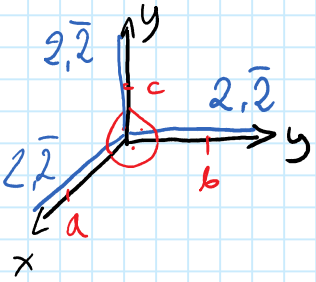


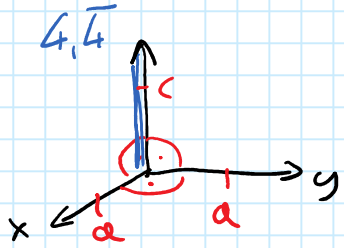
UKŁAD TRÓJSKOŚNY

UKŁAD JEDNOSKOŚNY



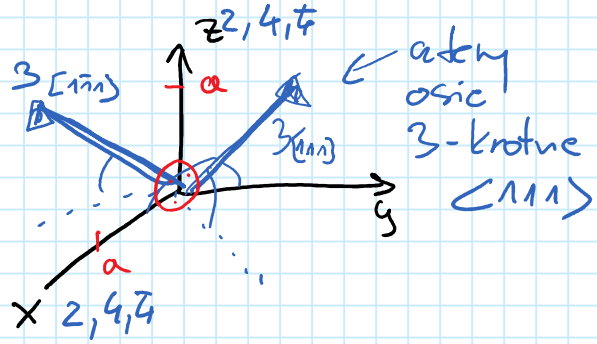
UKŁAD ROMBOWY

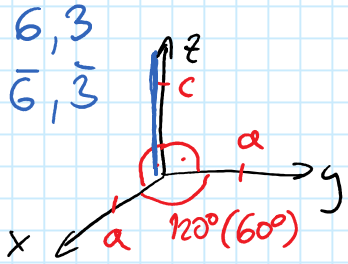




UKŁAD TETRAGONALNY

UKŁAD REGULARNY

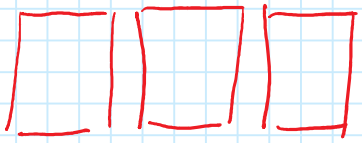




UKŁAD HEKSAGONALNY

Symbolika międzynarodowa klas symetrii

TRZY MOŻLIWE POŁOŻENIE W SYMBOLU



$6, 4, 3, 2, m, \bar{1}, \bar{4}, \bar{6}...$

TRÓJSKOŚNY $1, \bar{1}$

JEDNOSKOŚNY $2\ m\ 2/m$ [X] [Y] [Z]

KIERUNEK PREFEROWANY TO OŚ Y

RÓMBOWY

X	Y	Z
2	2	2
m	m	2
2/m	2/m	2/m

TETRAGONALNY

Z	X i Y	[110] [1$\bar{1}$0]
4	2	2
$\bar{4}$	m	m
4/m	2/m	2/m

→ DWUSIECZNA OSI X i Y

HEKSAGONALNY

Z	X i Y	[100] [1$\bar{1}$0]
$6, \bar{6}$	2	2
$3, \bar{3}$	m	m
6/m	2/m	2/m

→ DWUSIECZNE OSI X i Y

REGULARNY

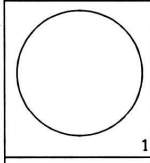
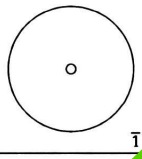
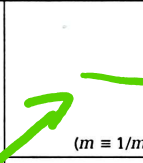
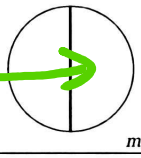
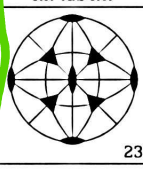
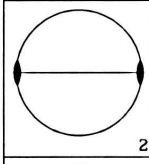
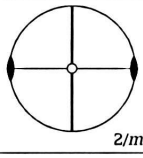
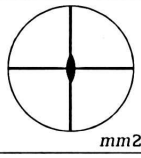
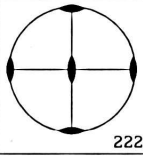
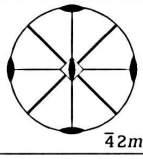
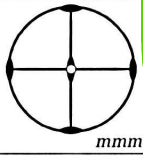
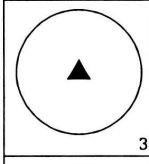
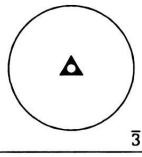
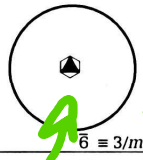
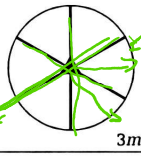
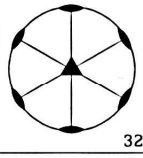
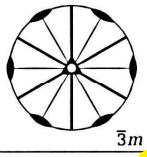
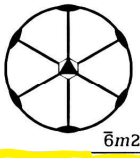
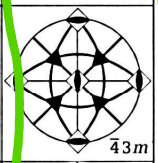
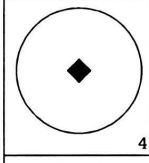
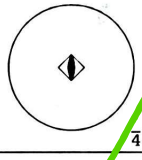
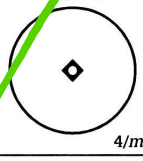
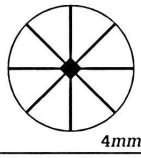
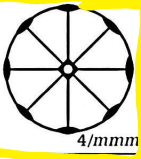
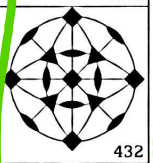
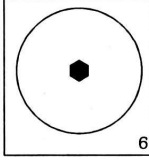
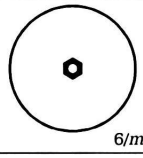
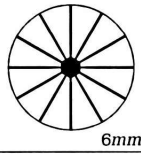
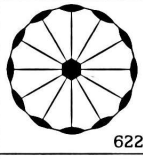
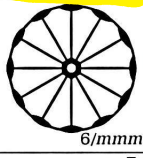
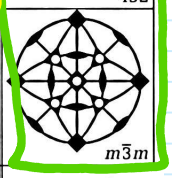
X Y Z	<111>	[110] [1$\bar{1}$0] [101] [10$\bar{1}$] [011] [01$\bar{1}$]
$2, 4, \bar{4}$	$3, \bar{3}$	
2/m, 4/m		

[111] [1$\bar{1}$1] [$\bar{1}$11] [11$\bar{1}$]

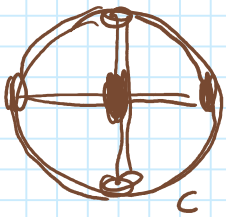
→ X/Y/Z

Zestawienie wszystkich 32 klas symetrii

UKŁADY REGULARNE

n	$\bar{n}$	n/m	nm	$n/2$	$\bar{n}m$	n/mm	nn lub $\bar{n}n$
 1	 $\bar{1}$	 $(m \equiv 1/m)$	 m	$(2 \equiv 12)$	$(2/m \equiv \bar{1}\,m)$	$(mm2 \equiv 1/mm)$	 23
 2	$(\bar{2} \equiv m)$	 2/m	 $mm2$	 222	 $\bar{4}2m$	 mmm	$m\bar{3}$
 3	 $\bar{3}$	 $\bar{6} \equiv 3/m$	 $3m$	 32	 $\bar{3}m$	 $\bar{6}m2$	 $\bar{4}3m$
 4	 $\bar{4}$	 4/m	 $4mm$	422	$(\bar{4}2m)$	 $4/mmm$	 432
 6	$(\bar{6} \equiv 3/m)$	 6/m	 $6mm$	 622	$(\bar{6}m2)$	 $6/mmm$	 $m\bar{3}m$
				(23)		$(m\bar{3})$	
				(432)	$(\bar{4}3m)$	$(m\bar{3}m)$	

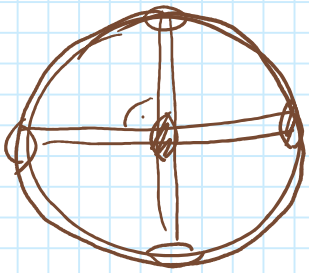
mmm ?

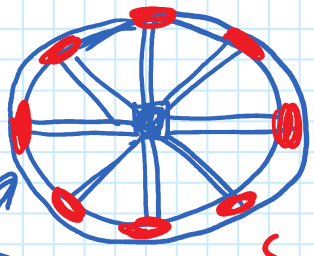


c

X Y Z

2/m 2/m 2/m ⇒ mmm





c

4/mmm ≡ 4/m mm ≡ 4/m mm

II

4/m 2/m 2/m