

IDENTIFICATION OF THE POINT GROUP OF Si FROM CBED PATTERNS

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IDENTIFICATION OF THE POINT GROUP OF Si FROM CBED

- Method of
B.F. Buxton, J.A. Eades, J.W. Steeds and G.M. Rackham
Phil. Trans. Roy. Soc. London, 1976, A281, 181-184

Four symmetries

- Whole Pattern (WP) symmetry
- Bright Field (BF) symmetry
- Dark Field (DF) symmetry
- +g / -g symmetries

- Multibeam method of Tanaka *et. al* } on high symmetry
zone axis pattern

Tables taken from:

- The symmetry of electron diffraction zone axis patterns
B.F. Buxton, J.A. Eades, J.W. Steeds and G.M. Rackham
Phil. Trans. Roy. Soc. London, 1976, A281, 181-184
- CBED
M. Tanaka and M. Terauchi , Jeol Tokyo, 1985

- Buxton et al method

Identify:

- *the whole pattern*
 - *2D symmetry*
 - *3D symmetry*
- *the bright-field symmetry*
- *the dark-field symmetry*
 - *first pattern*
 - *second pattern*
- *the +/-g symmetry*
 - *first pattern*
 - *second pattern*
- *the projection diffraction group from 2D information*
- *the possible diffraction groups from 3D information*
- *the possible point groups*

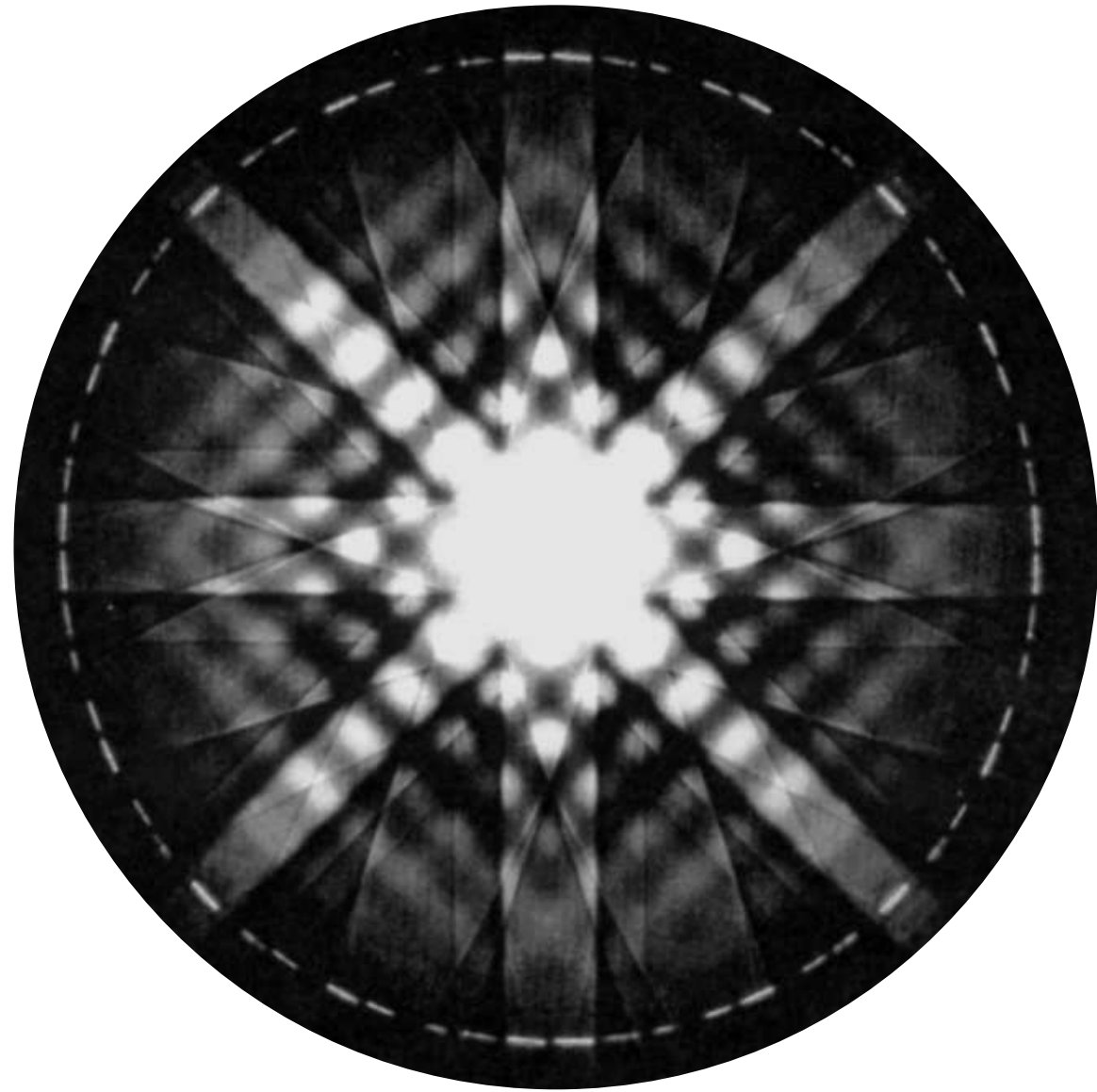
Tanaka multi-beam method

Identify:

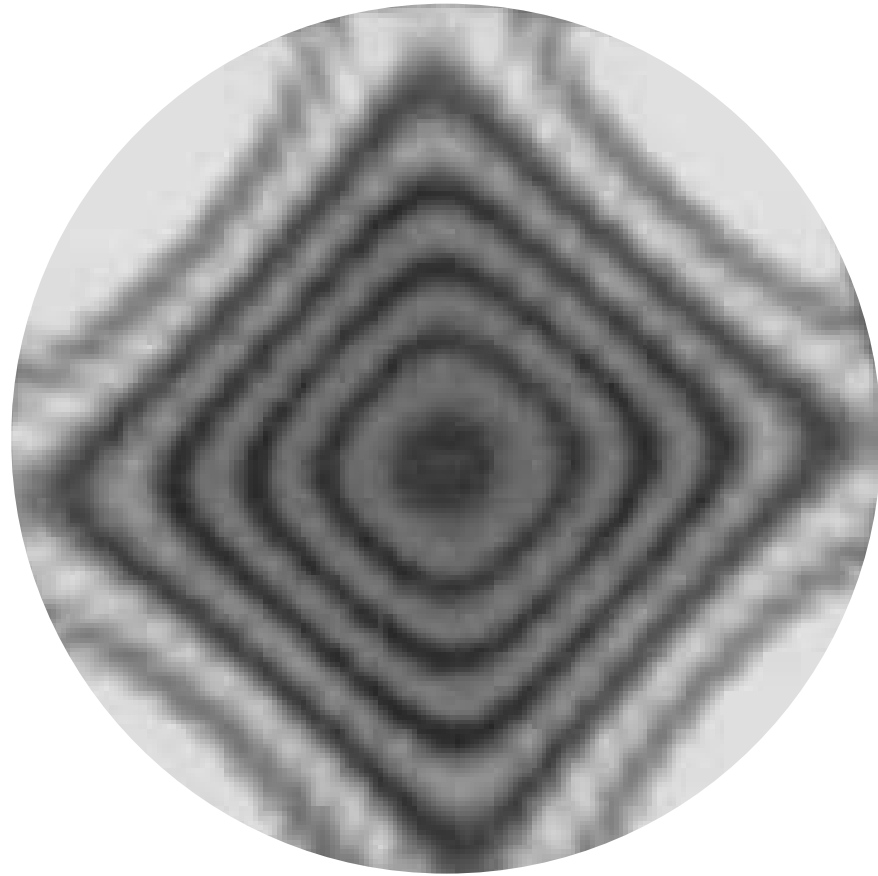
- *the possible diffraction groups*
- *the possible point groups*

Conclusion

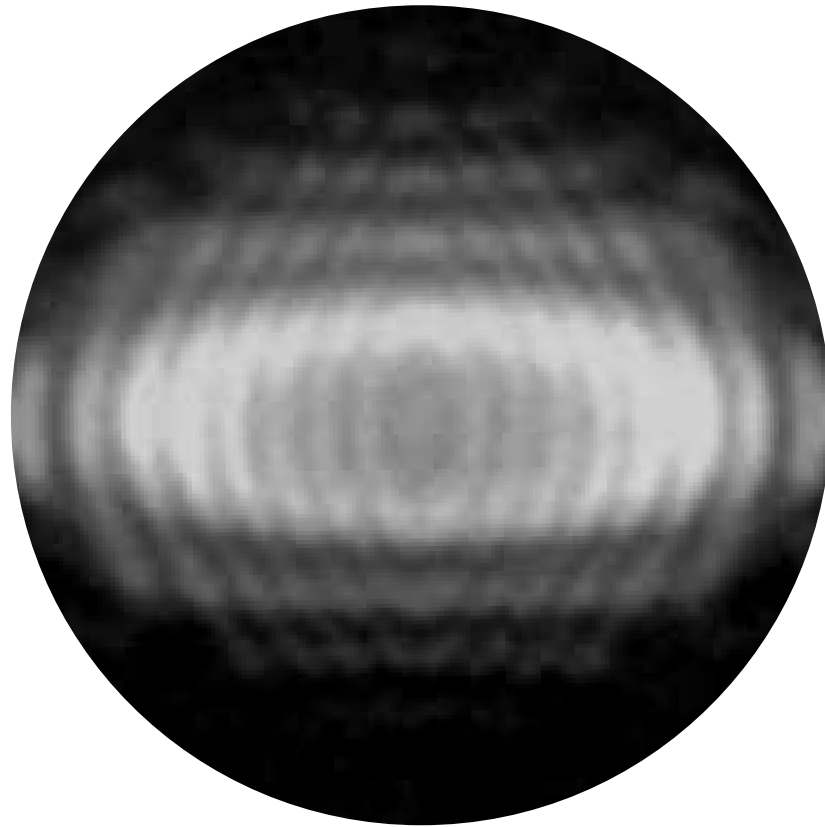
Whole Pattern (WP)



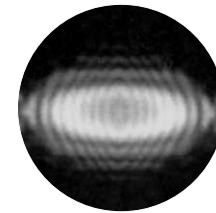
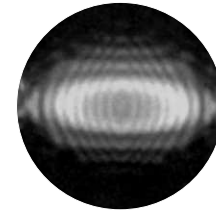
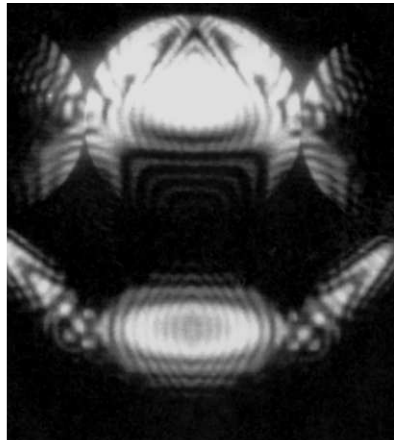
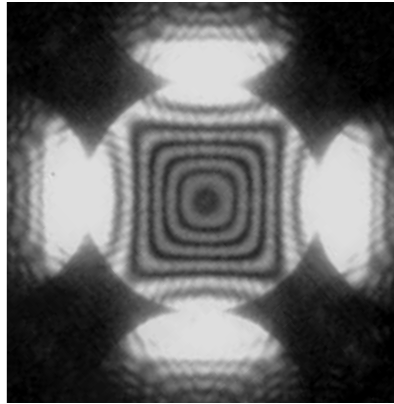
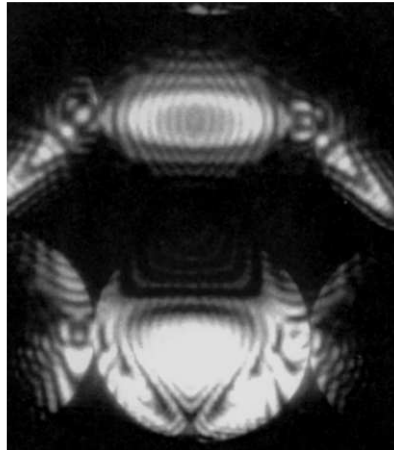
Bright Field (BF)



Dark Field (DF)
First pattern



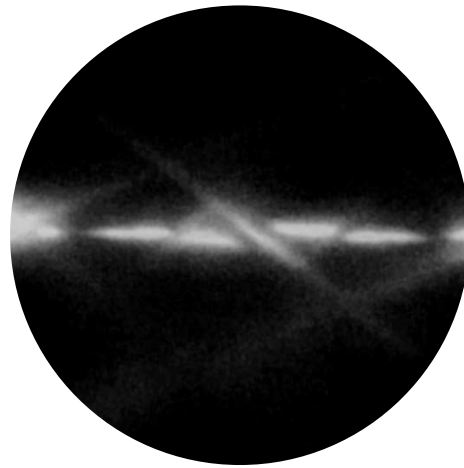
+g / -g patterns



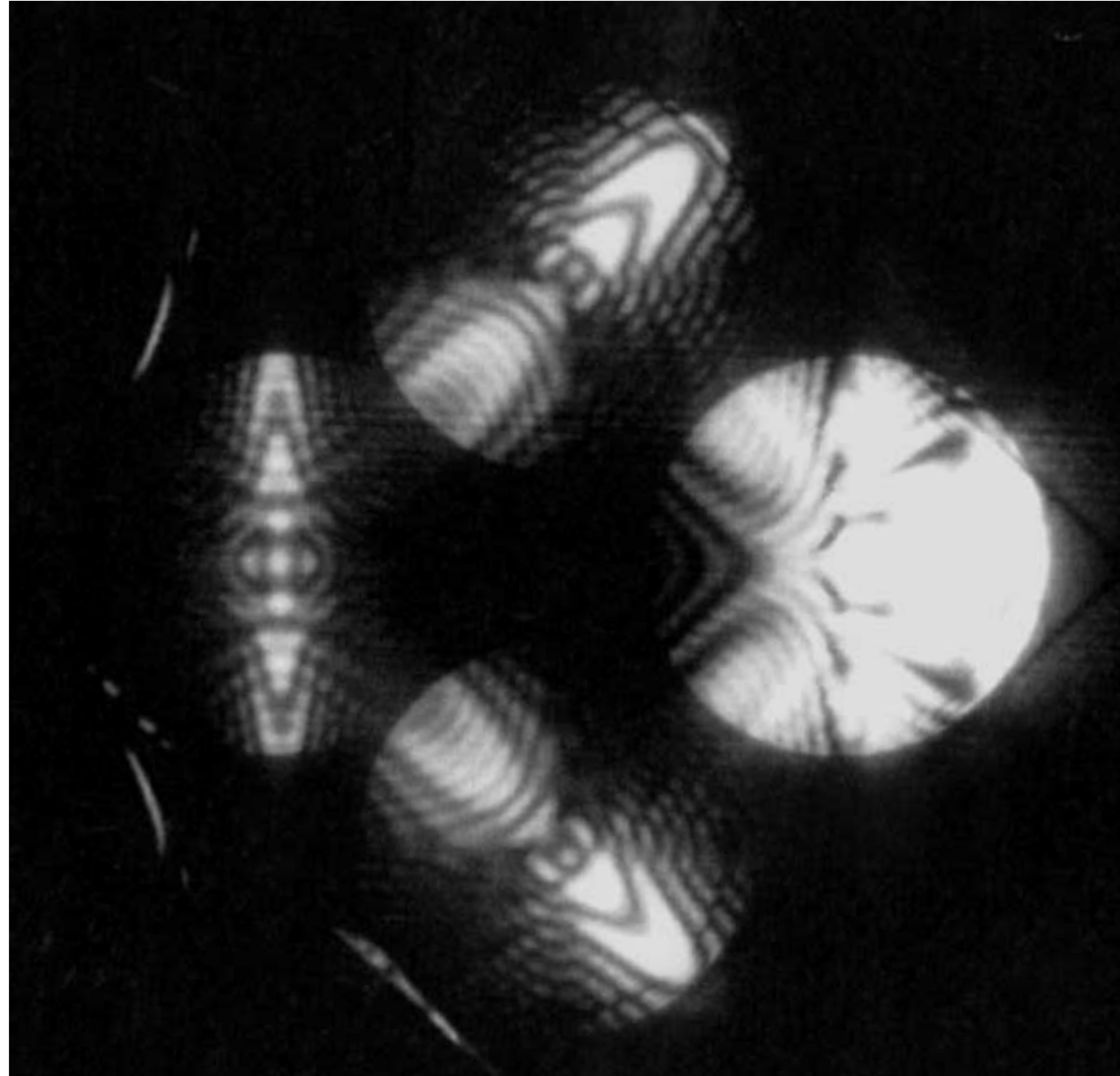
Dark Field (DF)
Second pattern



+g / -g symmetry
Second patterns

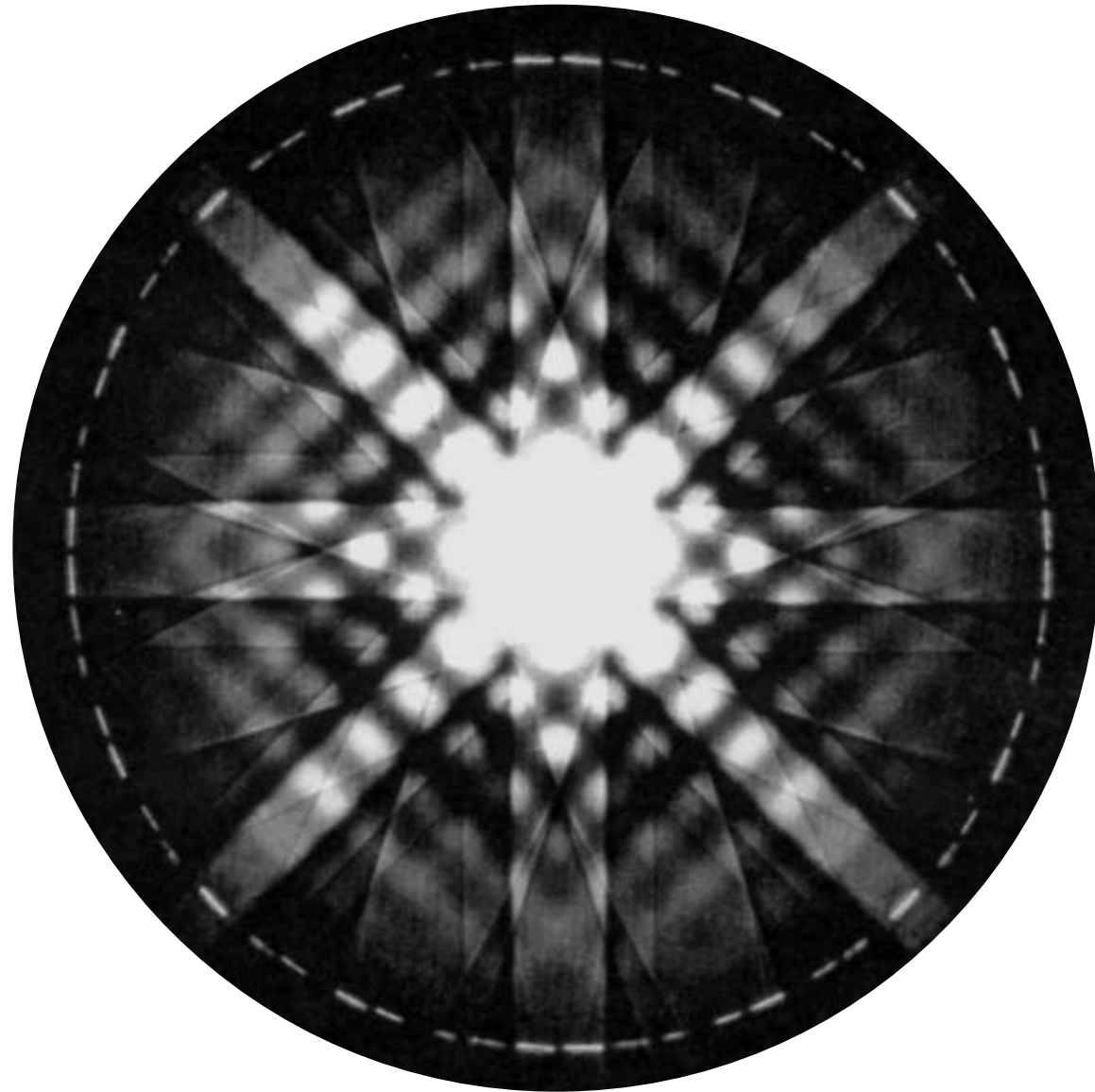


- Tanaka "multibeam" pattern



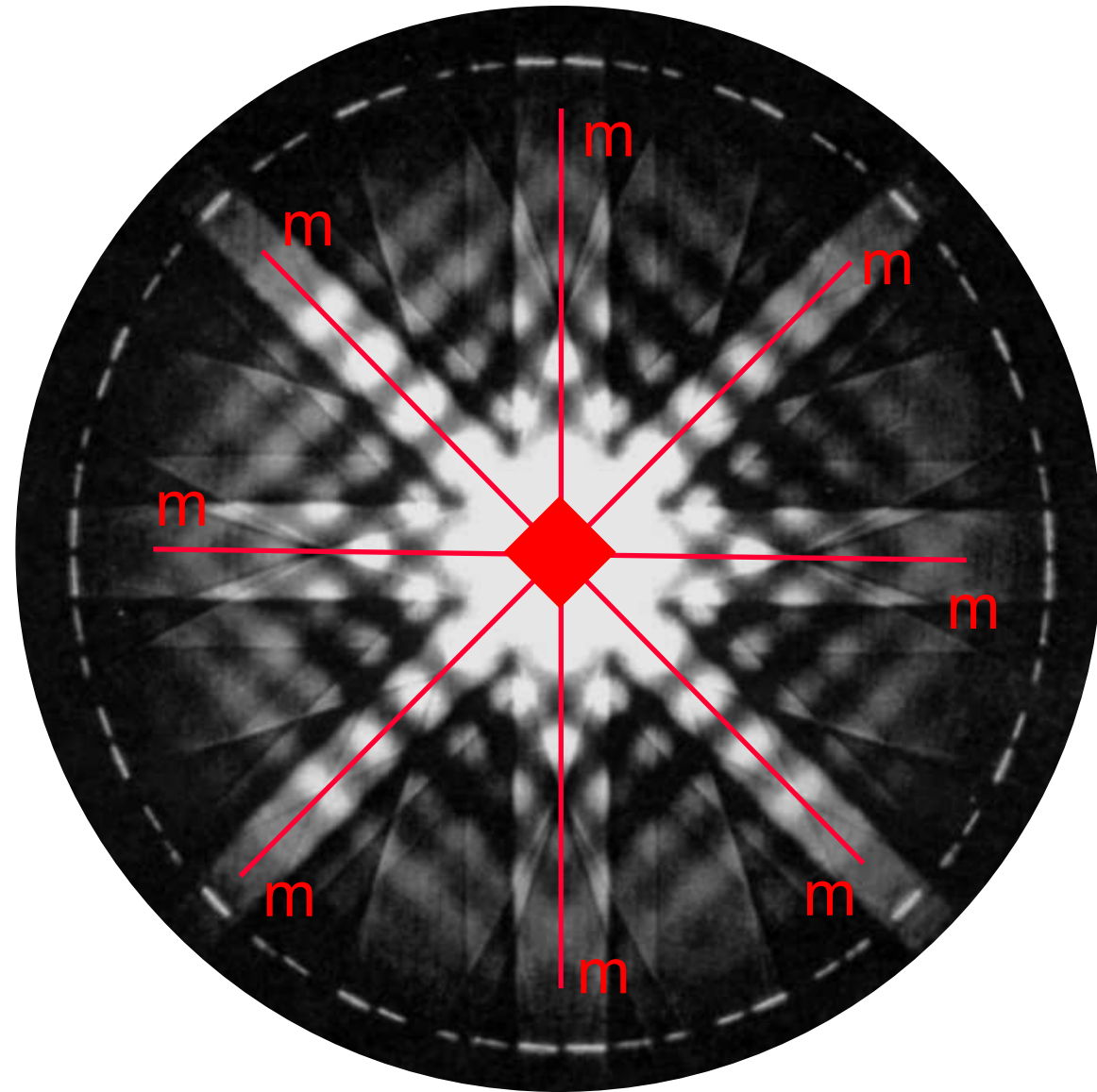
Whole Pattern (WP) symmetry ?

2D Information
(FOLZ not taken
into account)



Whole Pattern (WP) symmetry

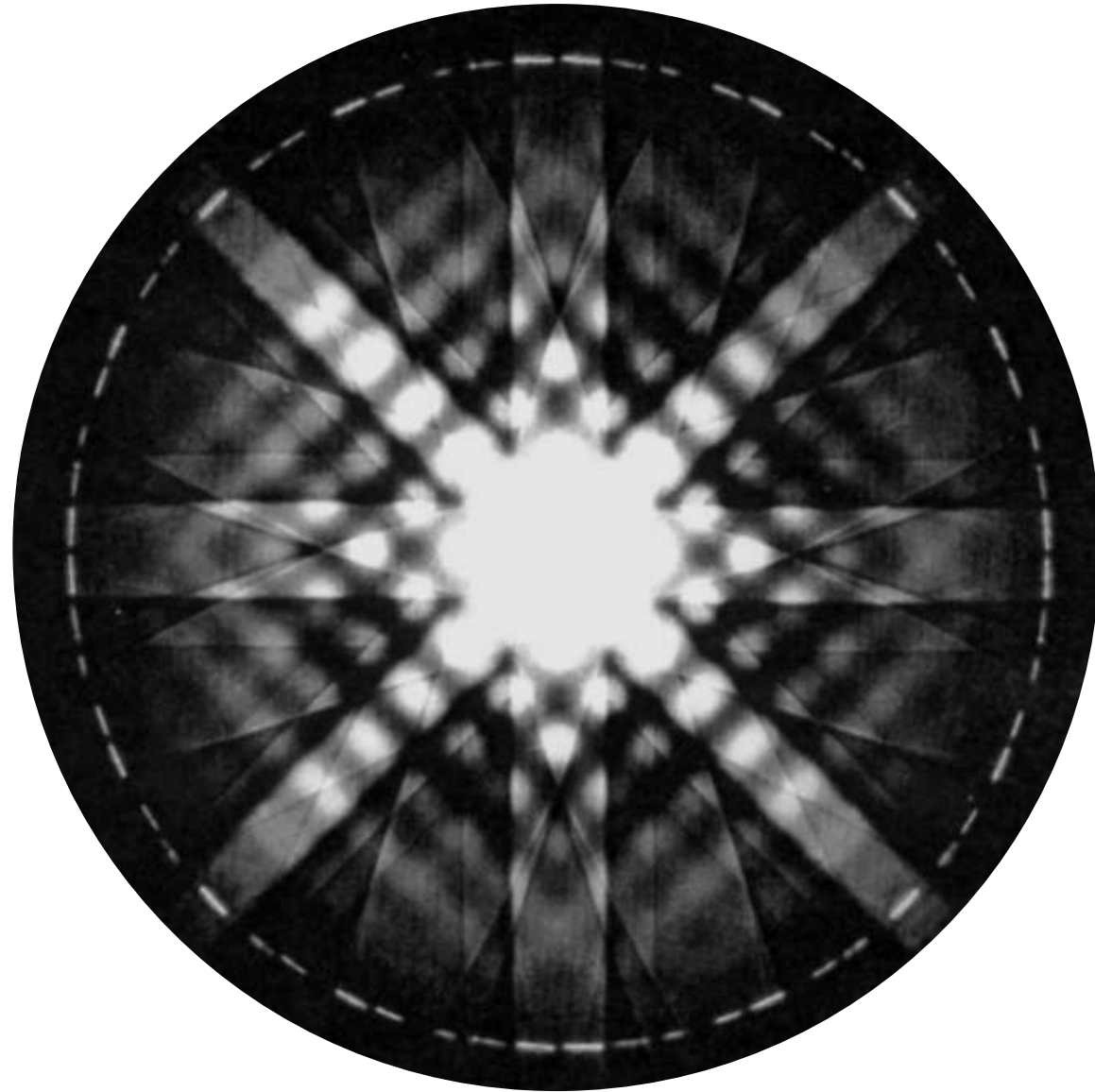
2D Information
(FOLZ not taken
into account)



2D symmetry
4mm

Whole Pattern (WP) symmetry ?

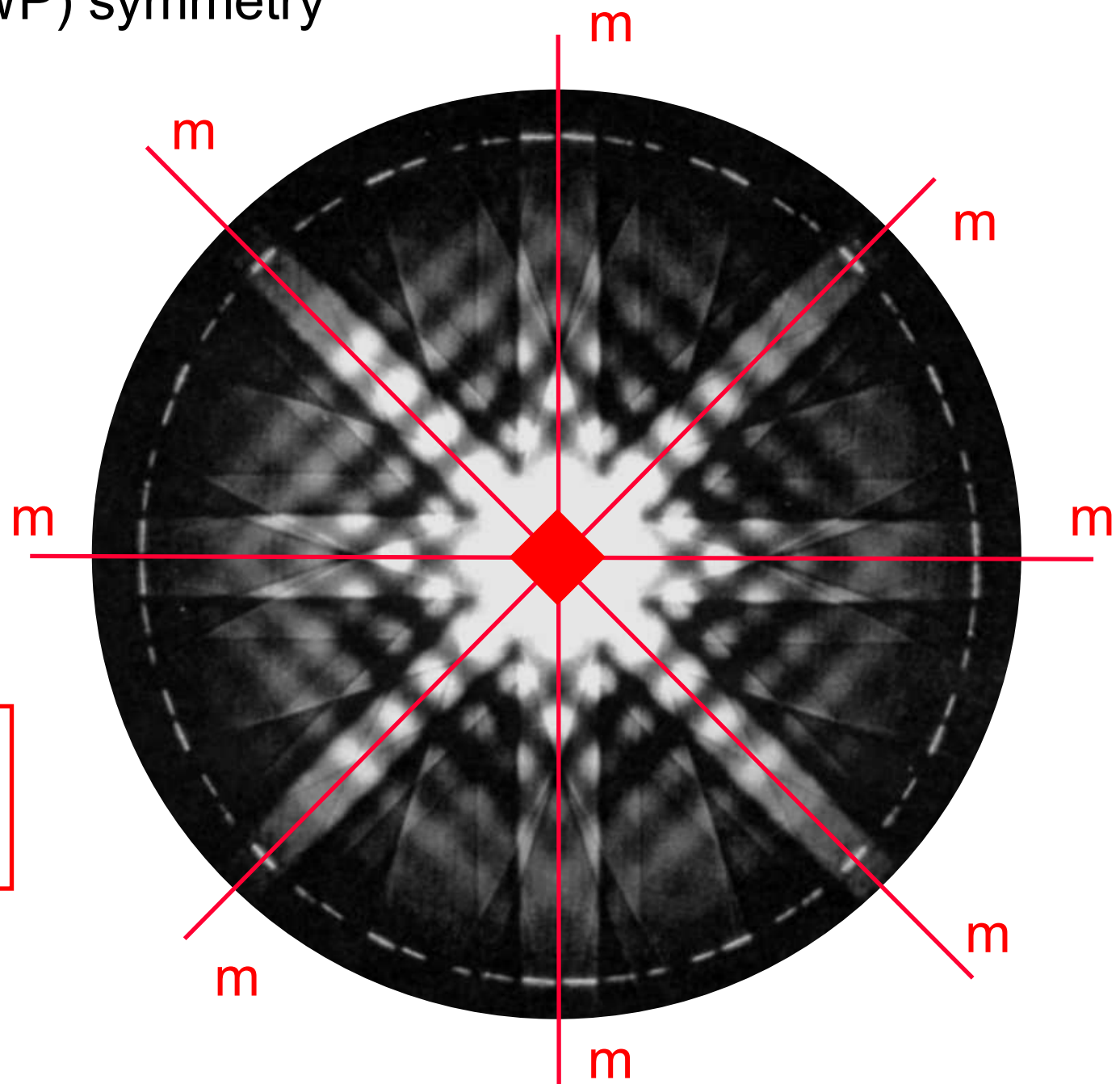
3D Information
(FOLZ taken
into account)





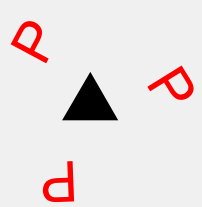
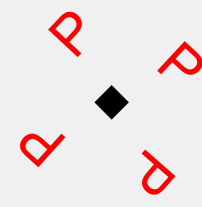
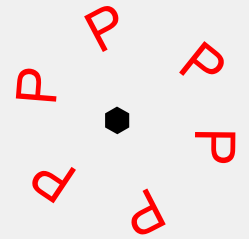
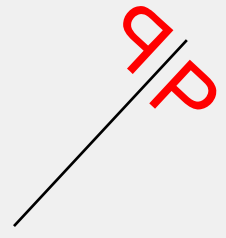
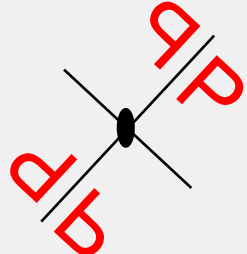
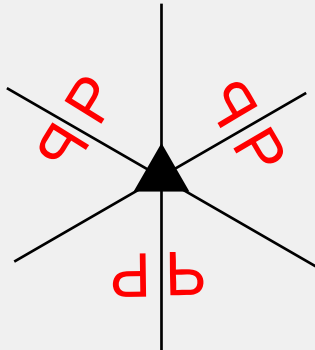
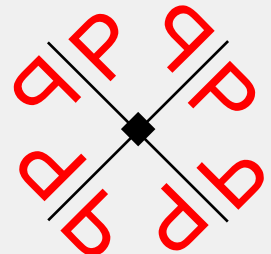
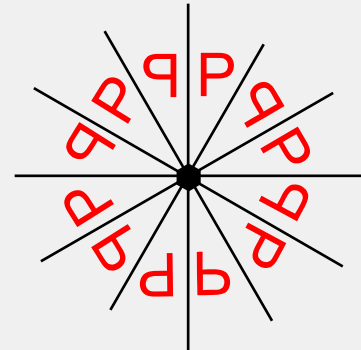
Whole Pattern (WP) symmetry

3D Information
(FOLZ taken
into account)



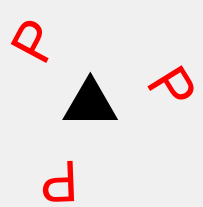
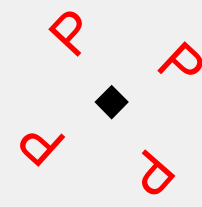
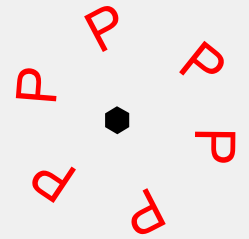
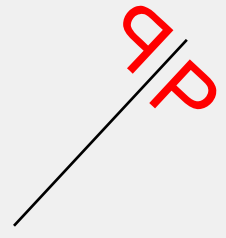
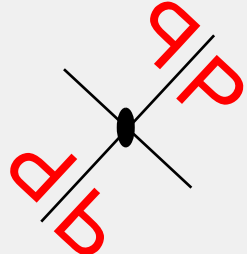
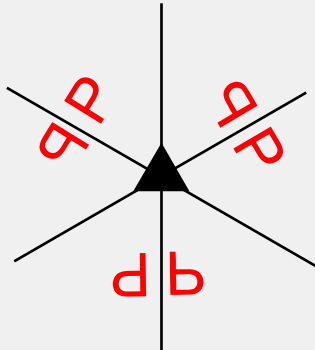
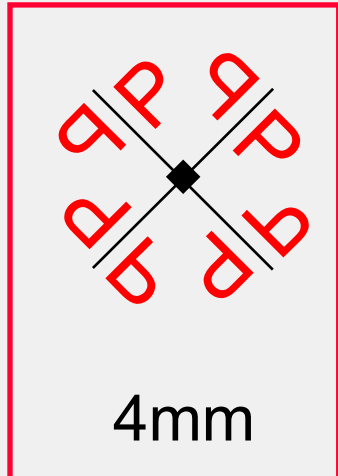
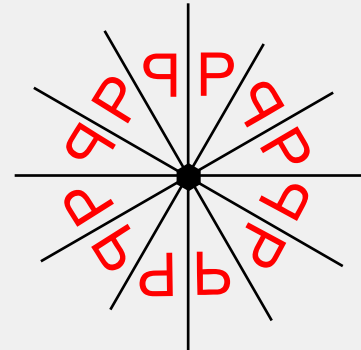
3D symmetry
4mm



- Whole Pattern (WP) symmetry

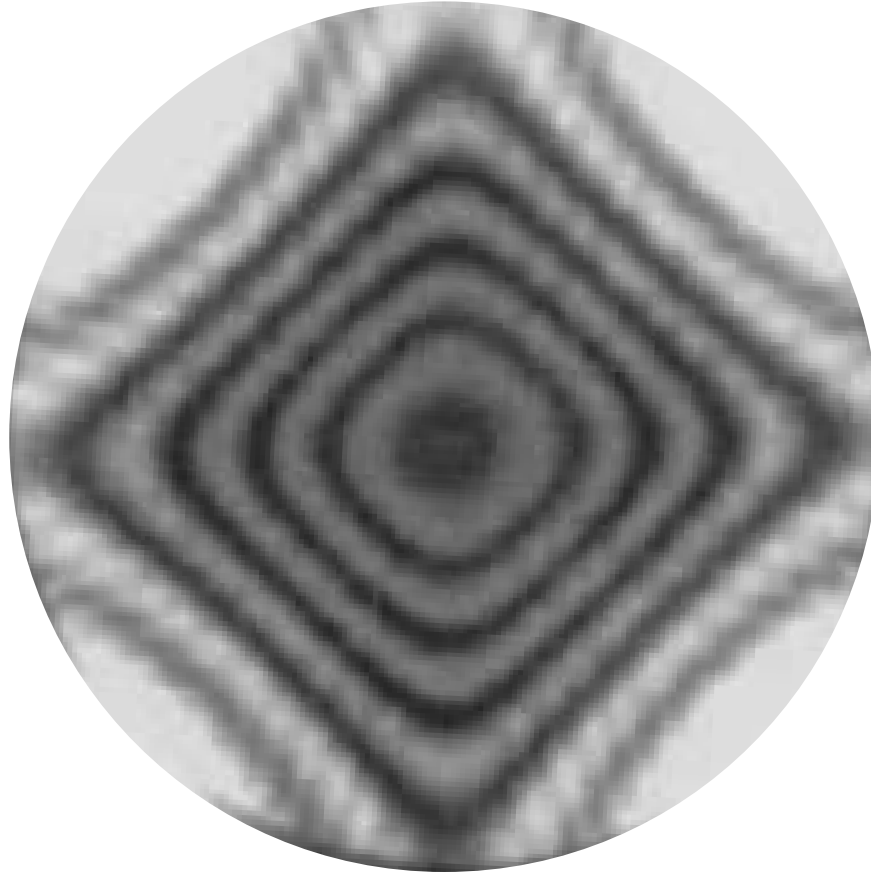
 <p>1</p>	 <p>2</p>	 <p>3</p>	 <p>4</p>	 <p>6</p>
 <p>m</p>	 <p>2mm</p>	 <p>3m</p>	 <p>4mm</p>	 <p>6mm</p>

- Whole Pattern (WP) symmetry

 <p>1</p>	 <p>2</p>	 <p>3</p>	 <p>4</p>	 <p>6</p>
 <p>m</p>	 <p>2mm</p>	 <p>3m</p>	 <p>4mm</p>	 <p>6mm</p>

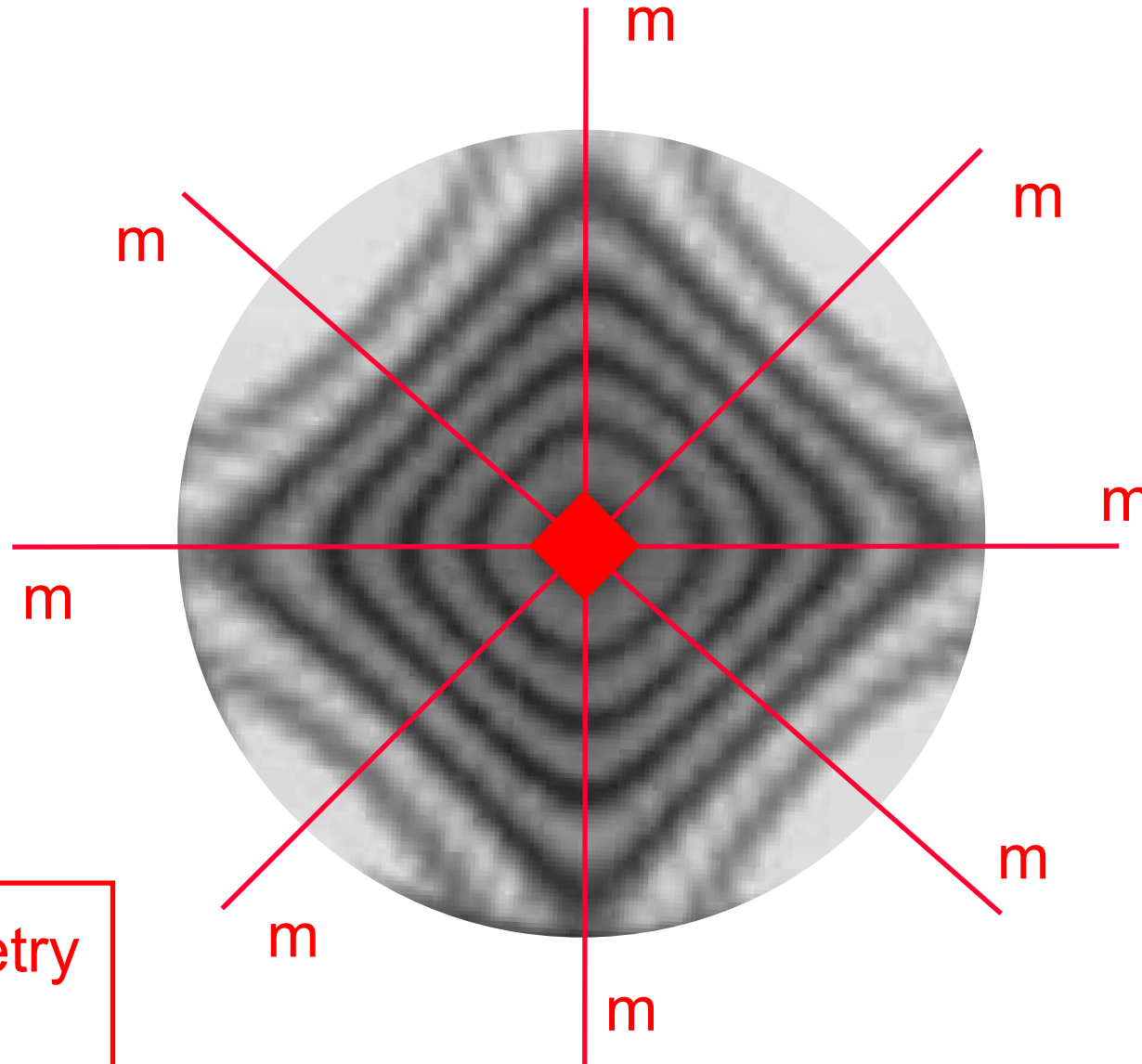
Bright Field (BF) symmetry ?

2D Information



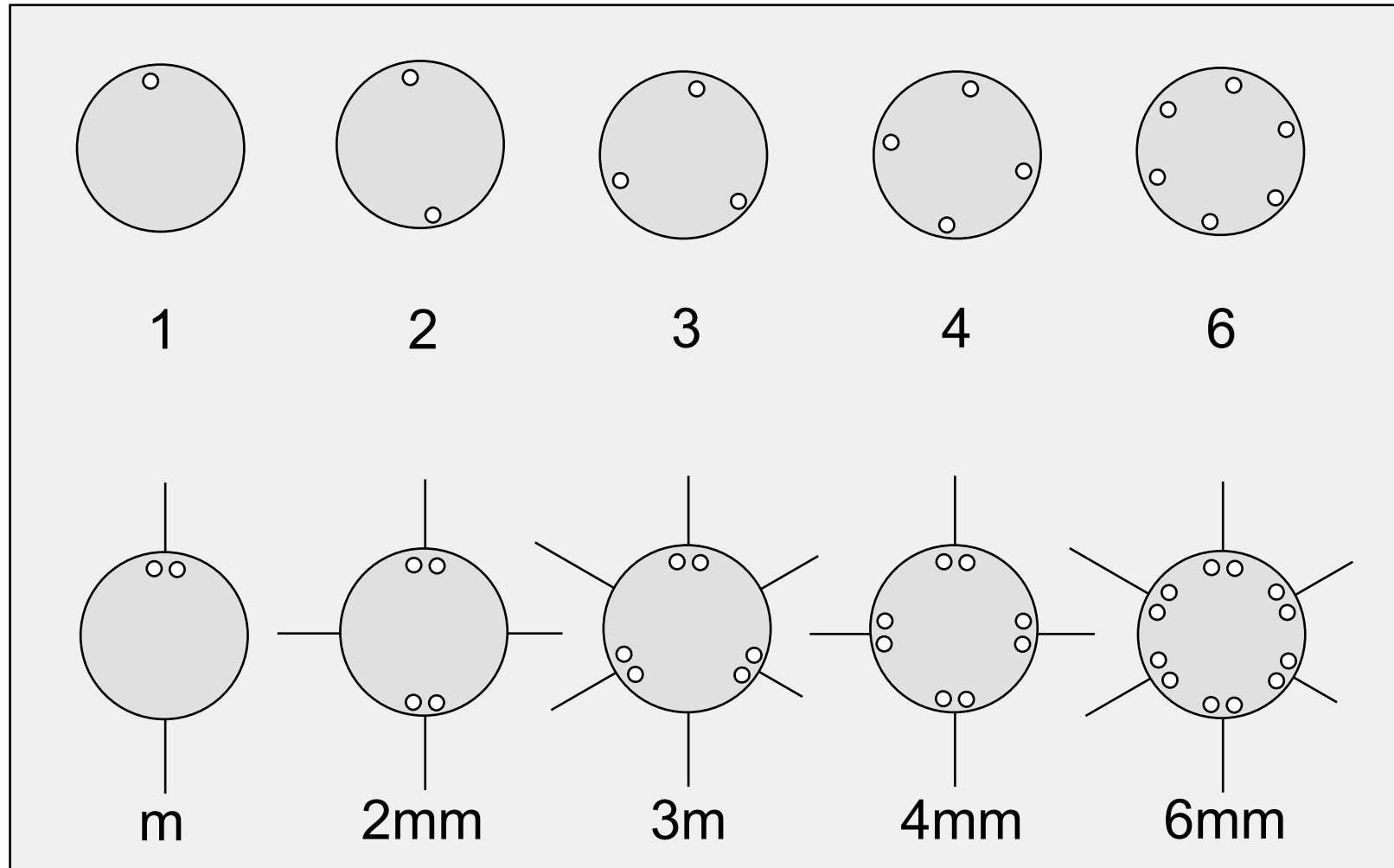
Bright Field (BF) symmetry

2D Information

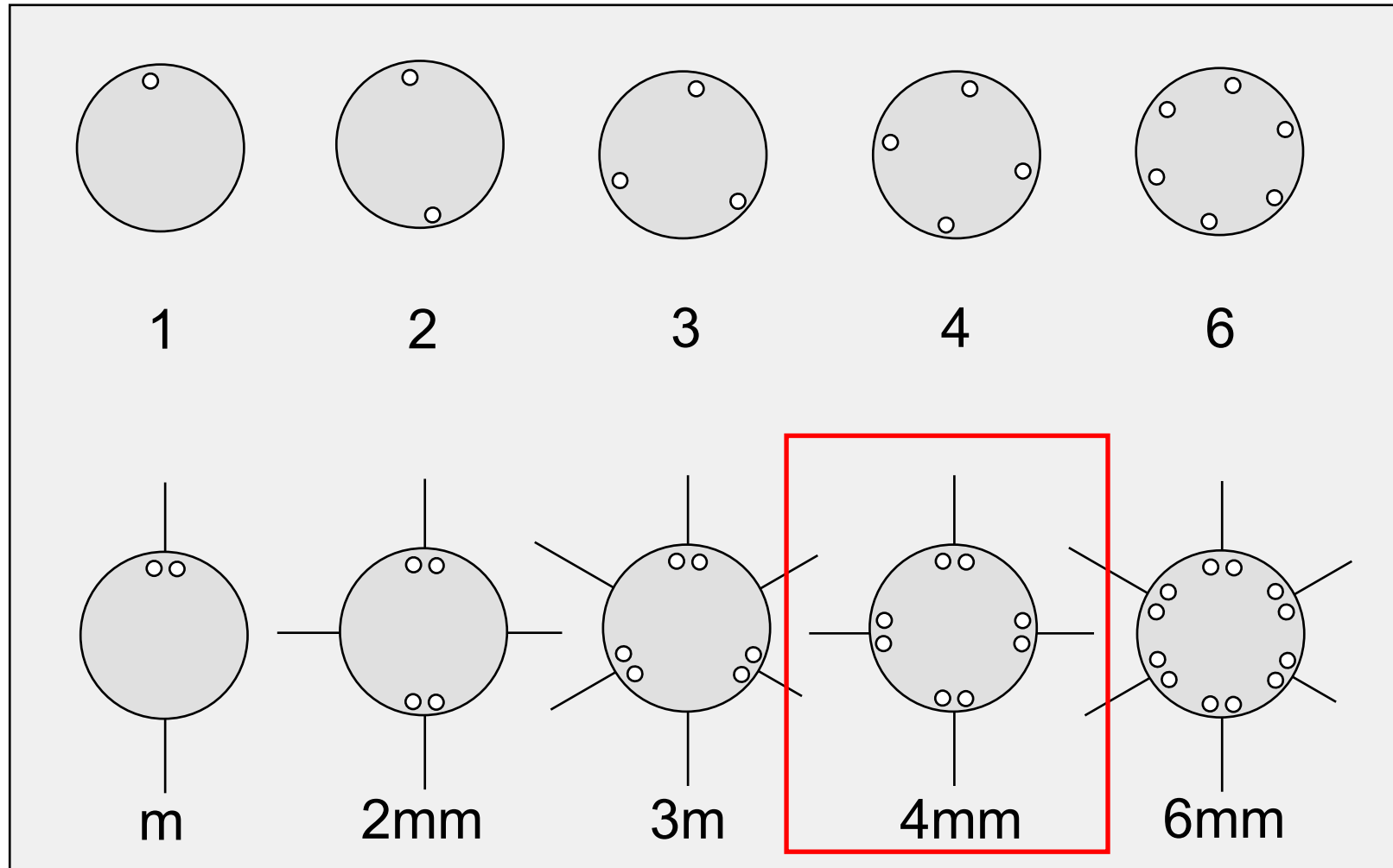


2D symmetry
4mm

Bright Field (BF) symmetry



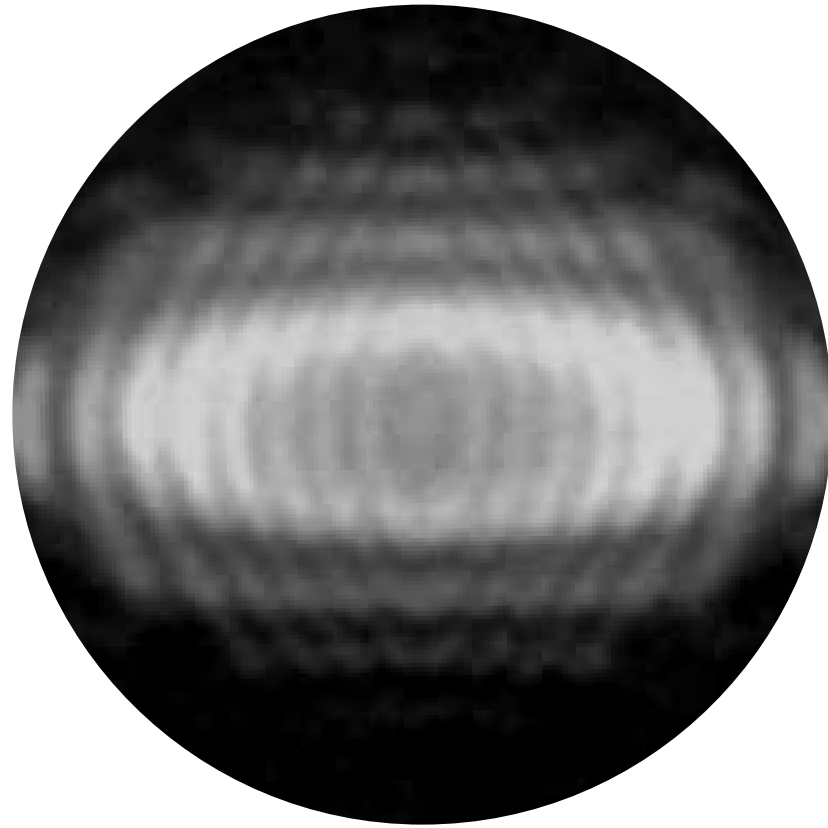
Bright Field (BF) symmetry



Dark Field (DF) symmetry ?

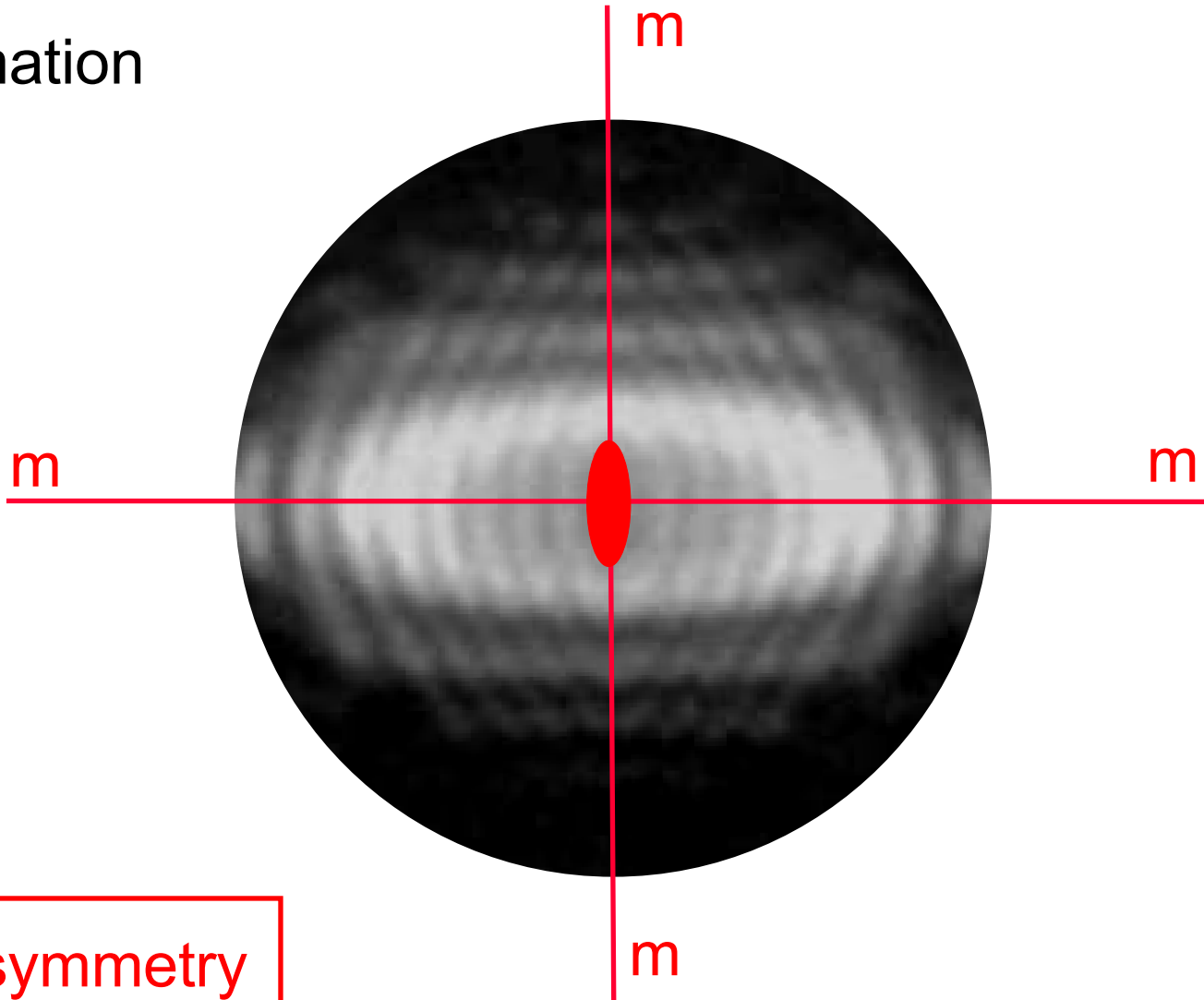
First pattern

2D Information



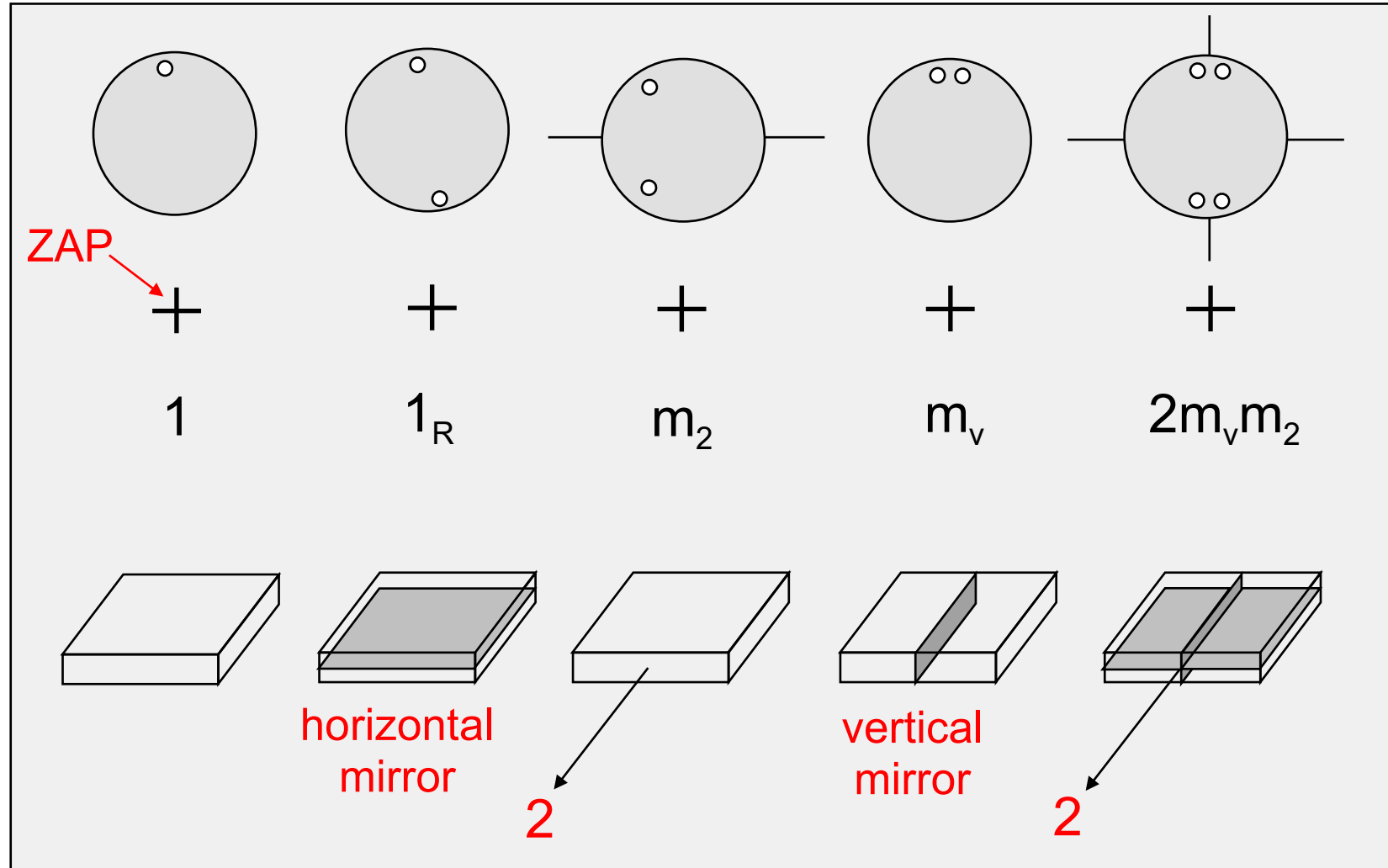
Dark Field (DF) symmetry
First pattern

2D Information

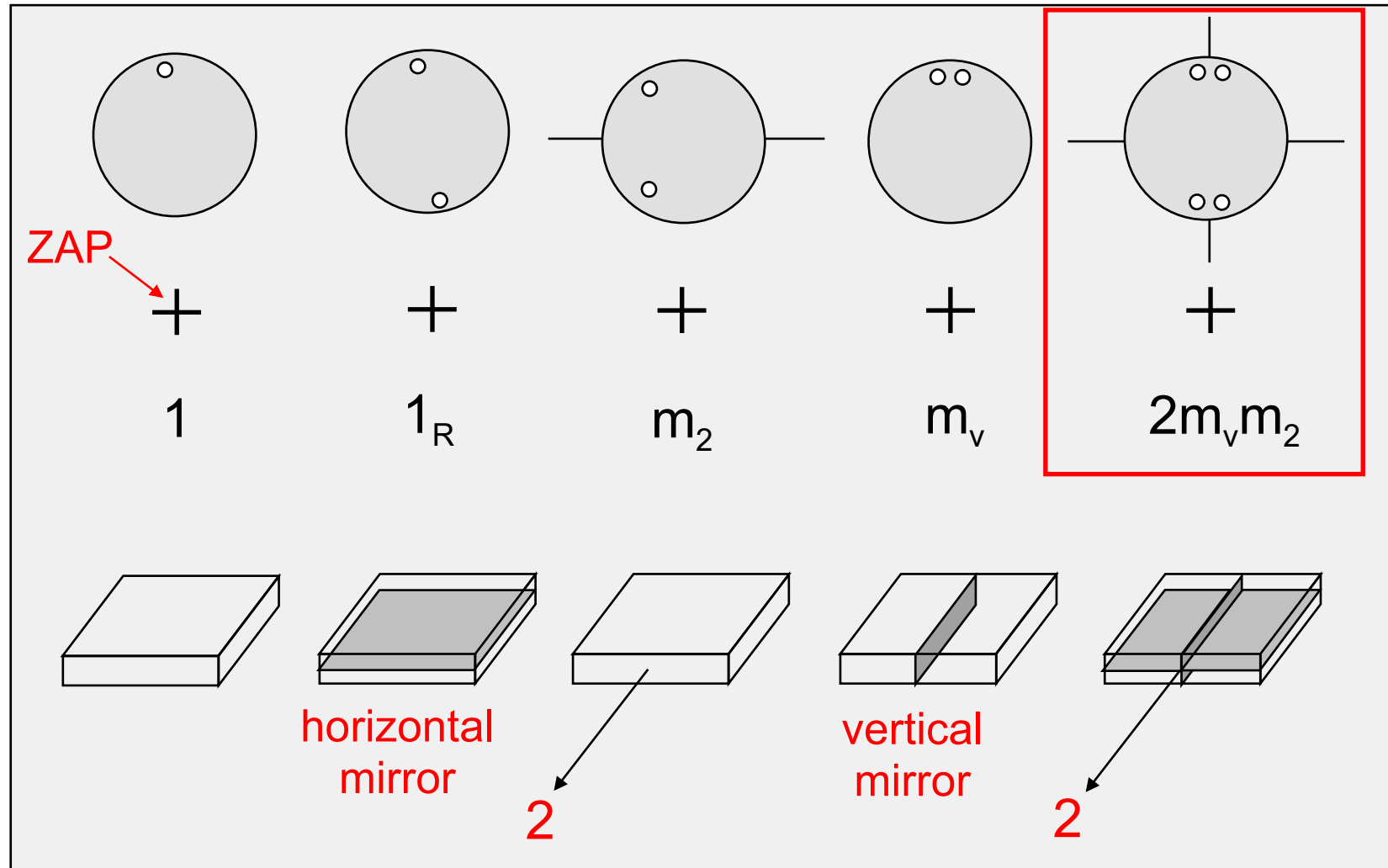


2D symmetry
2mm

Dark Field (DF) symmetry



Dark Field (DF) symmetry



Dark Field (DF) symmetry ?

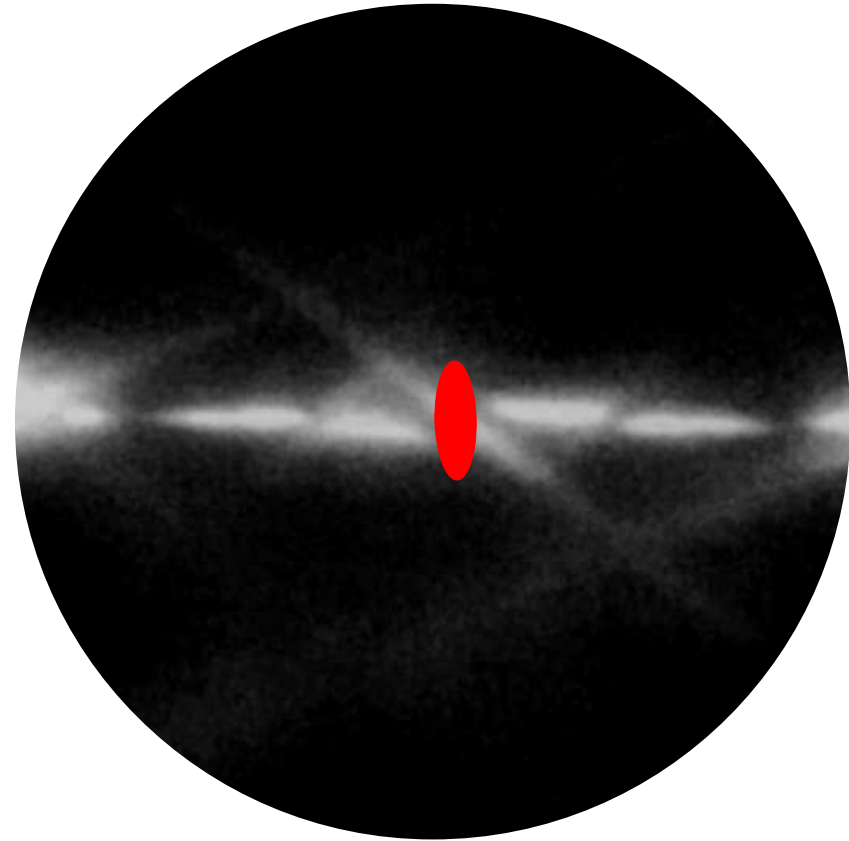
Second pattern

2D Information



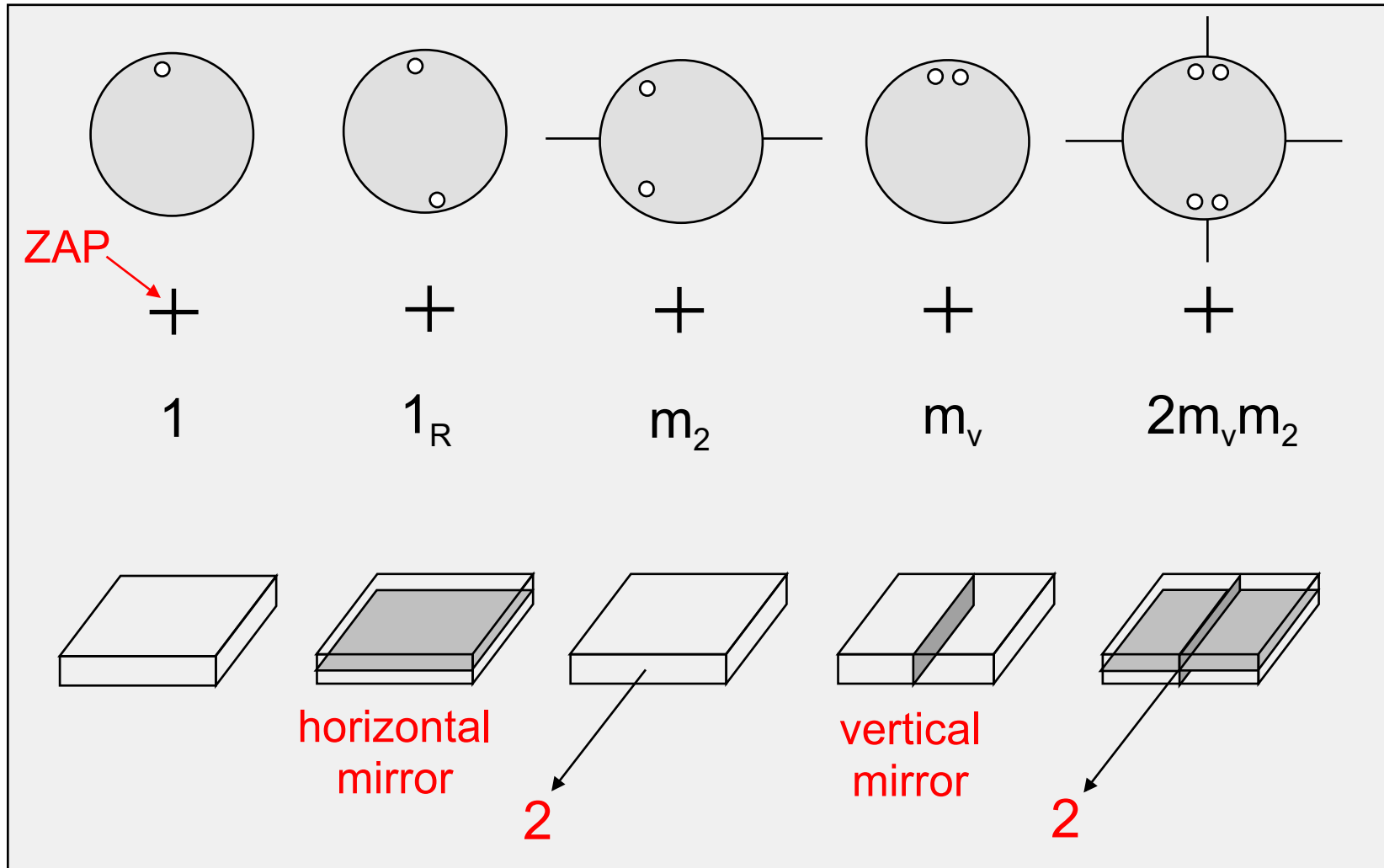
Dark Field (DF) symmetry
Second pattern

2D Information

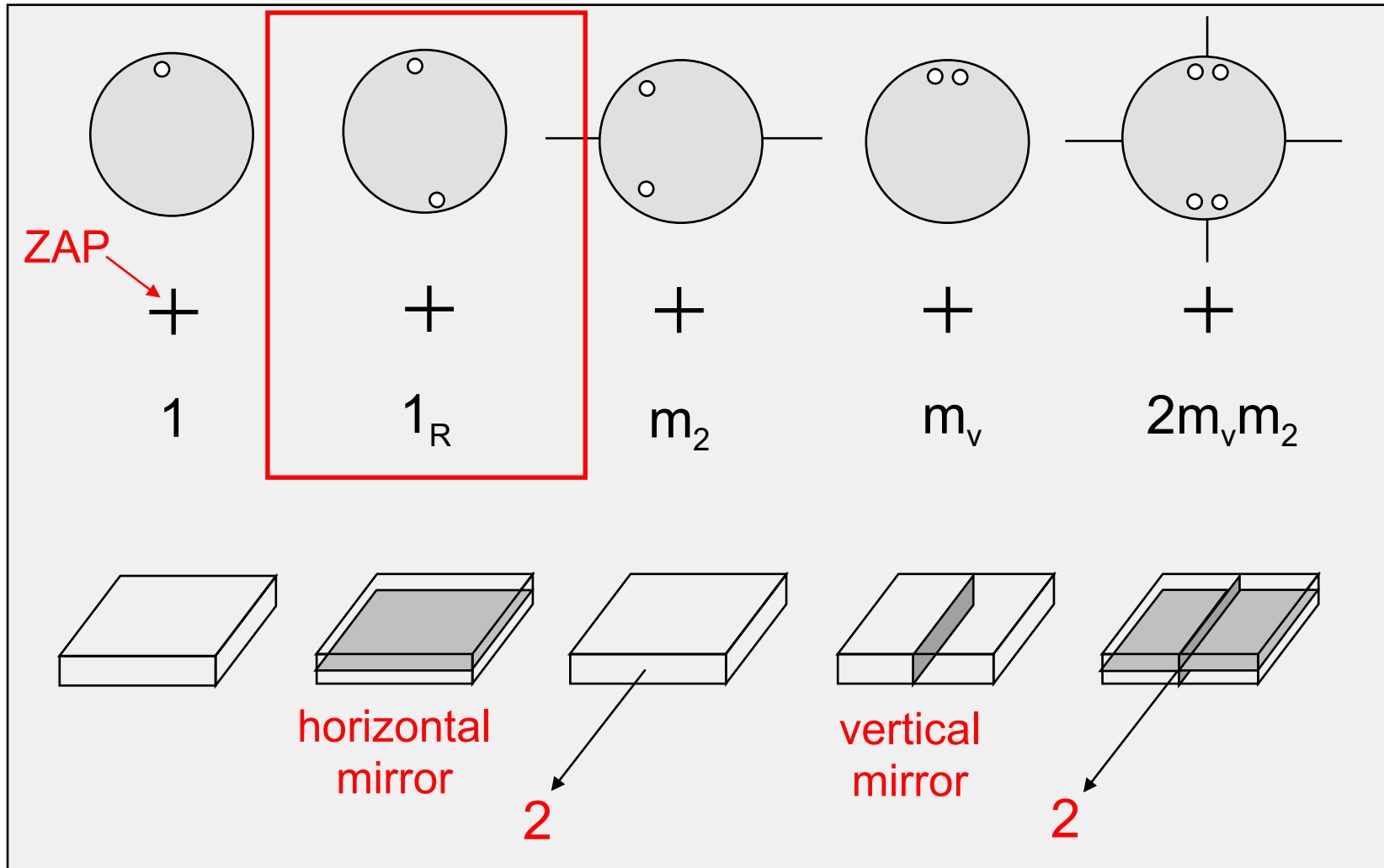


2D symmetry
 $2 = 1_R$

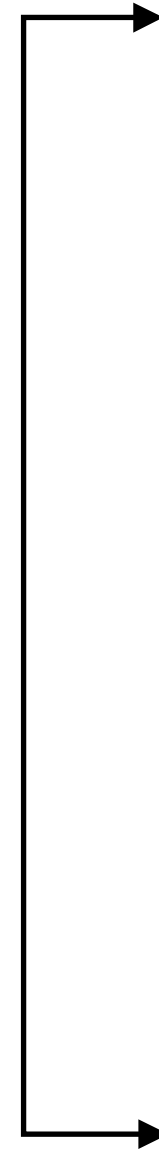
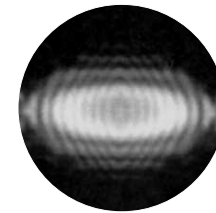
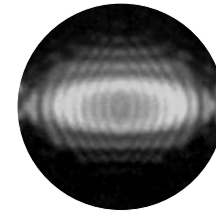
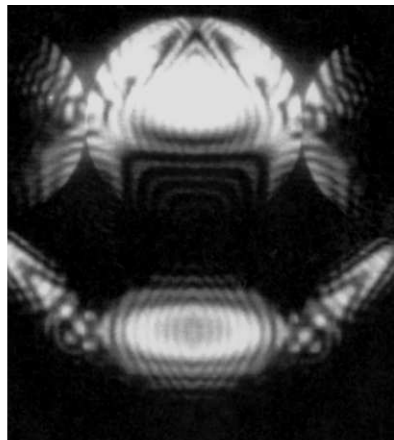
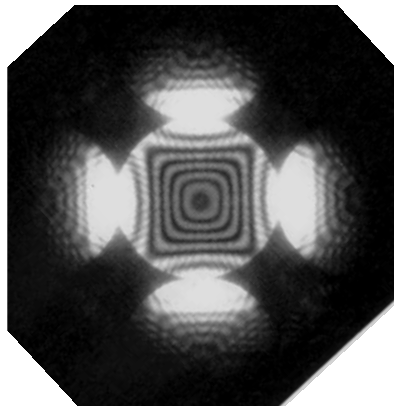
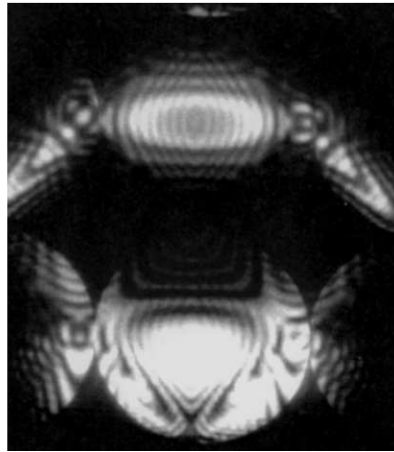
Dark Field (DF) symmetry



Dark Field (DF) symmetry

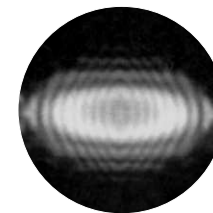
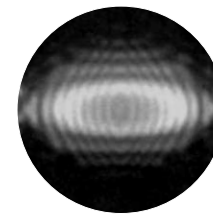
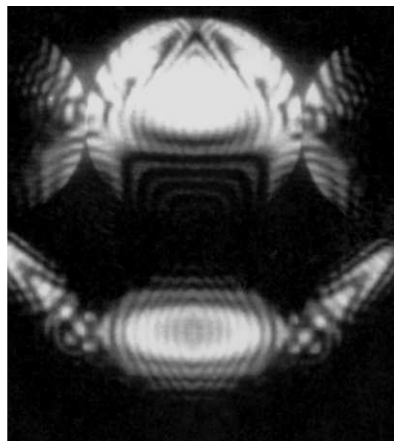
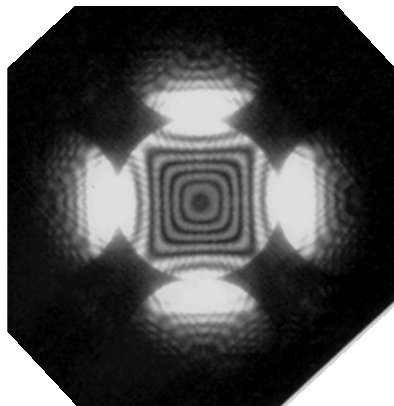
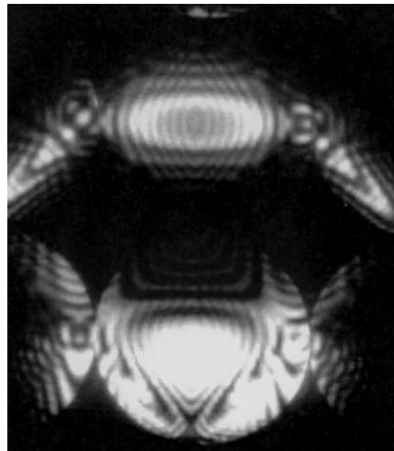


+g / -g symmetry ?
First patterns



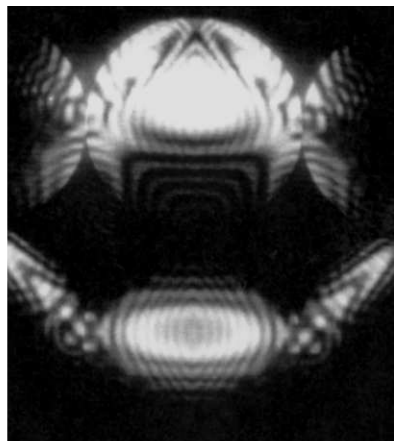
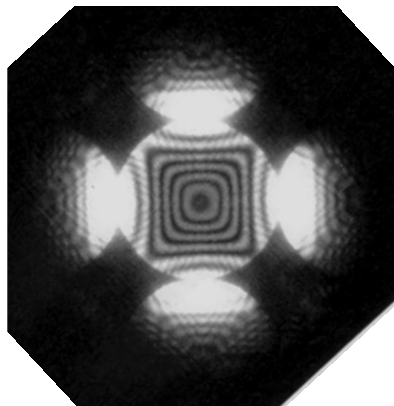
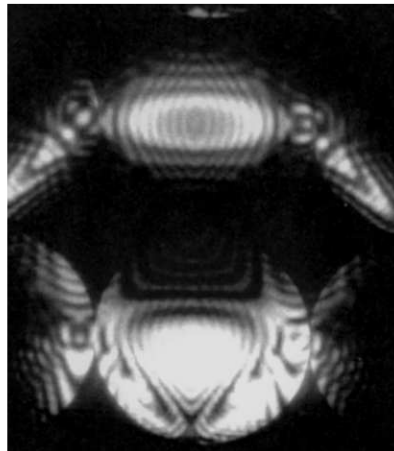
+g / -g symmetry
First patterns

2D Information

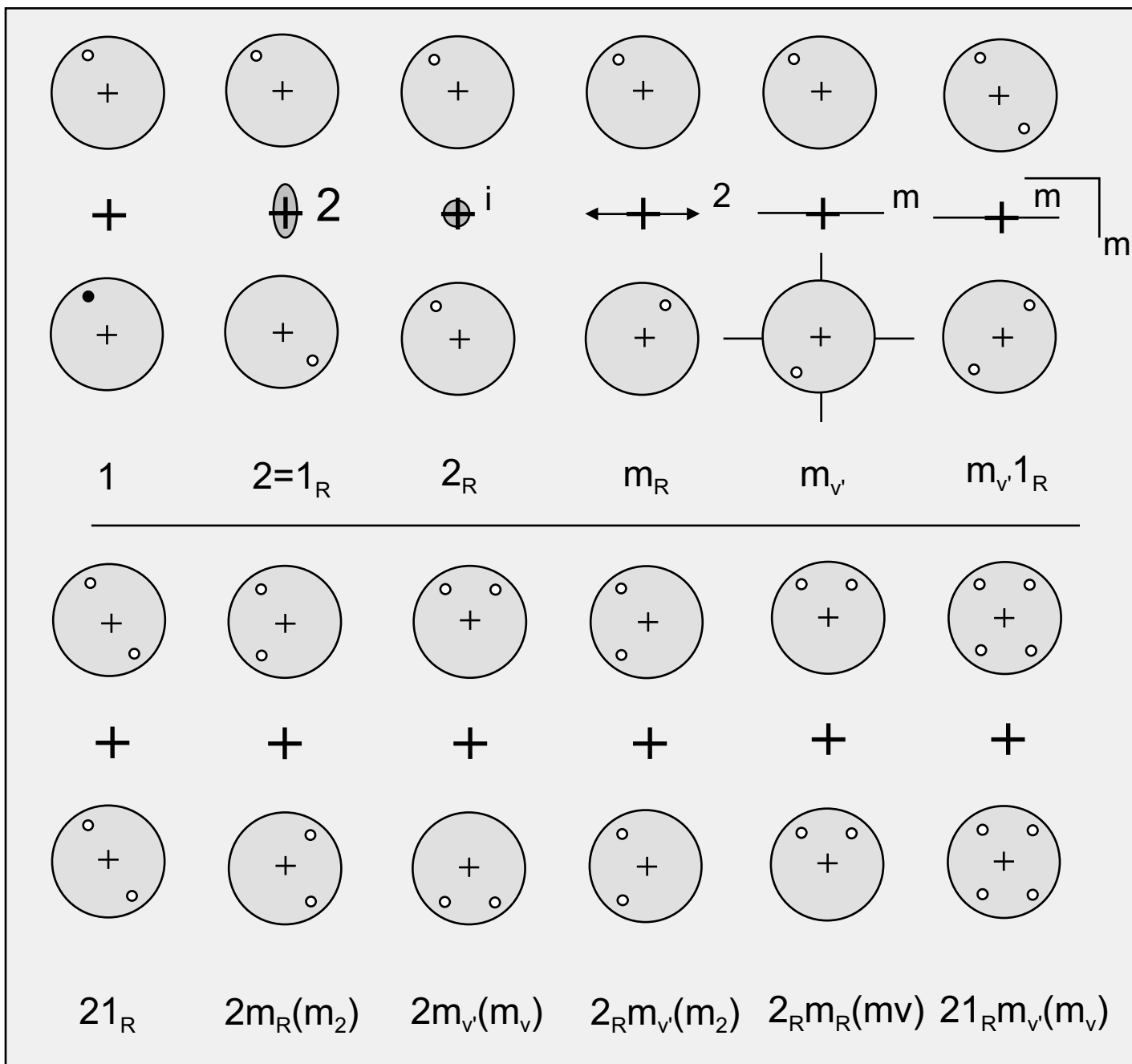


+g / -g symmetry
First patterns

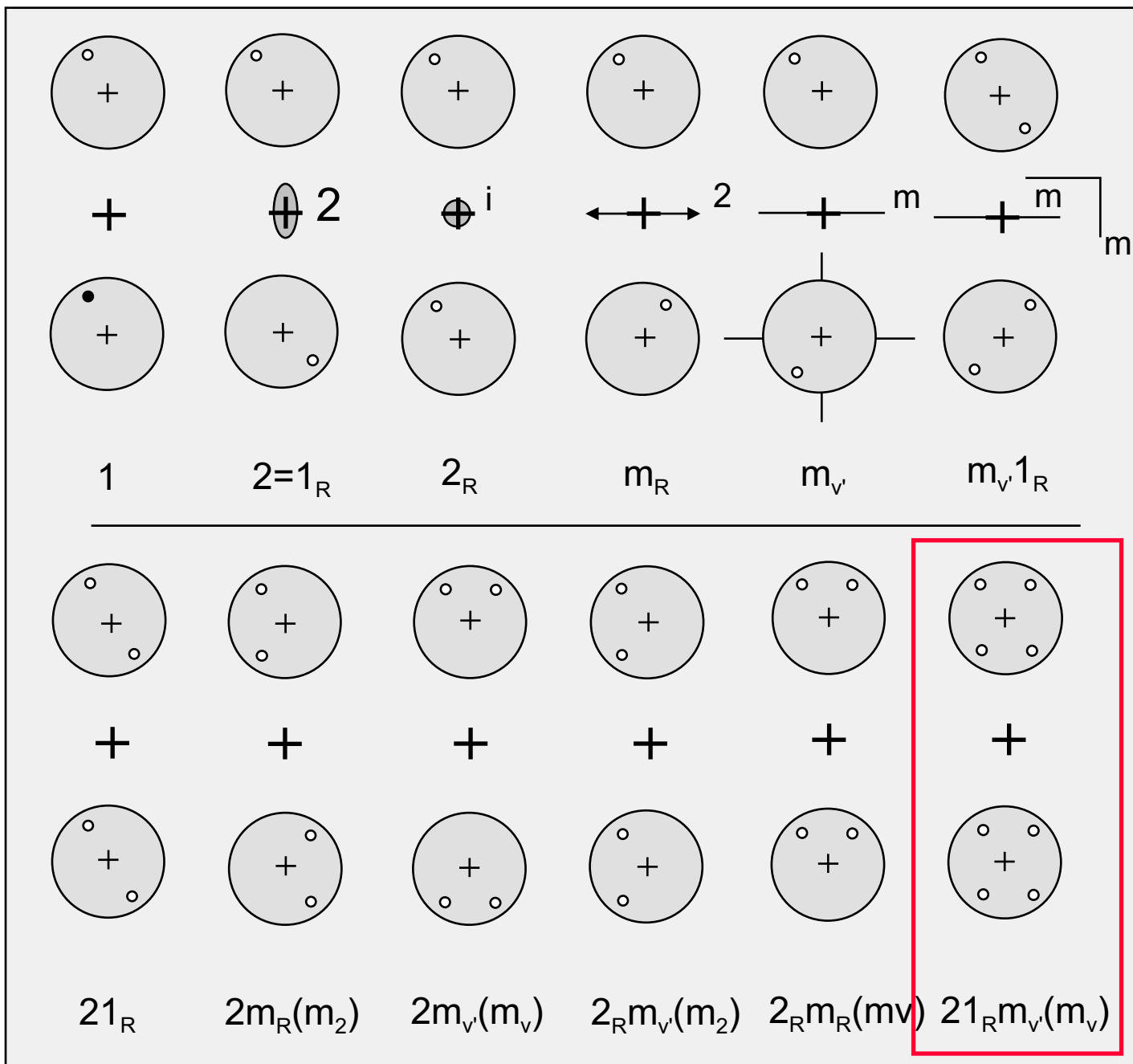
2D Information



+g / -g symmetry



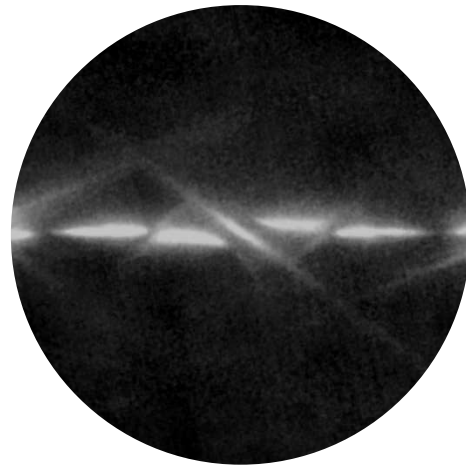
+g / -g symmetry



+g / -g symmetry ?

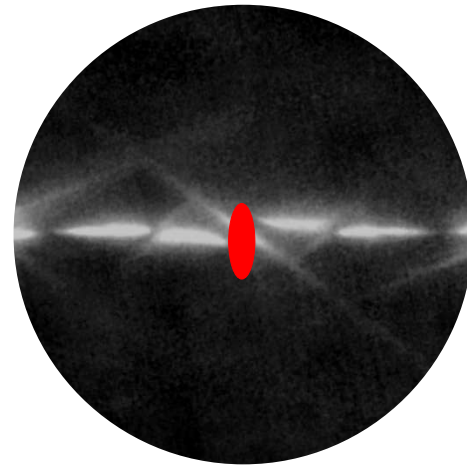
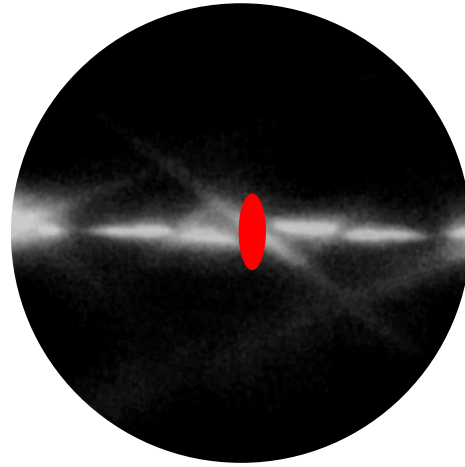
Second patterns

2D information

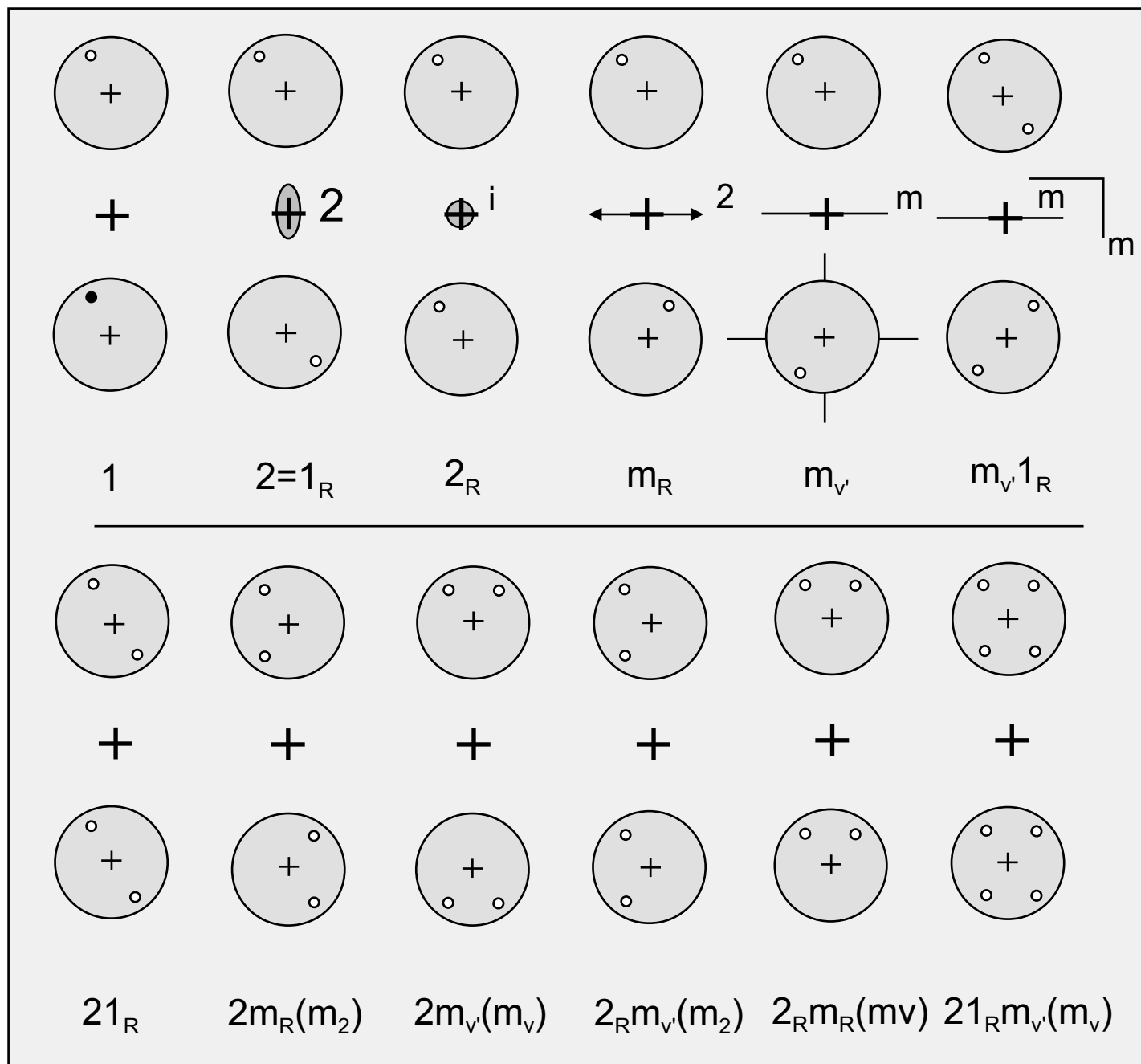


+g / -g symmetry
Second patterns

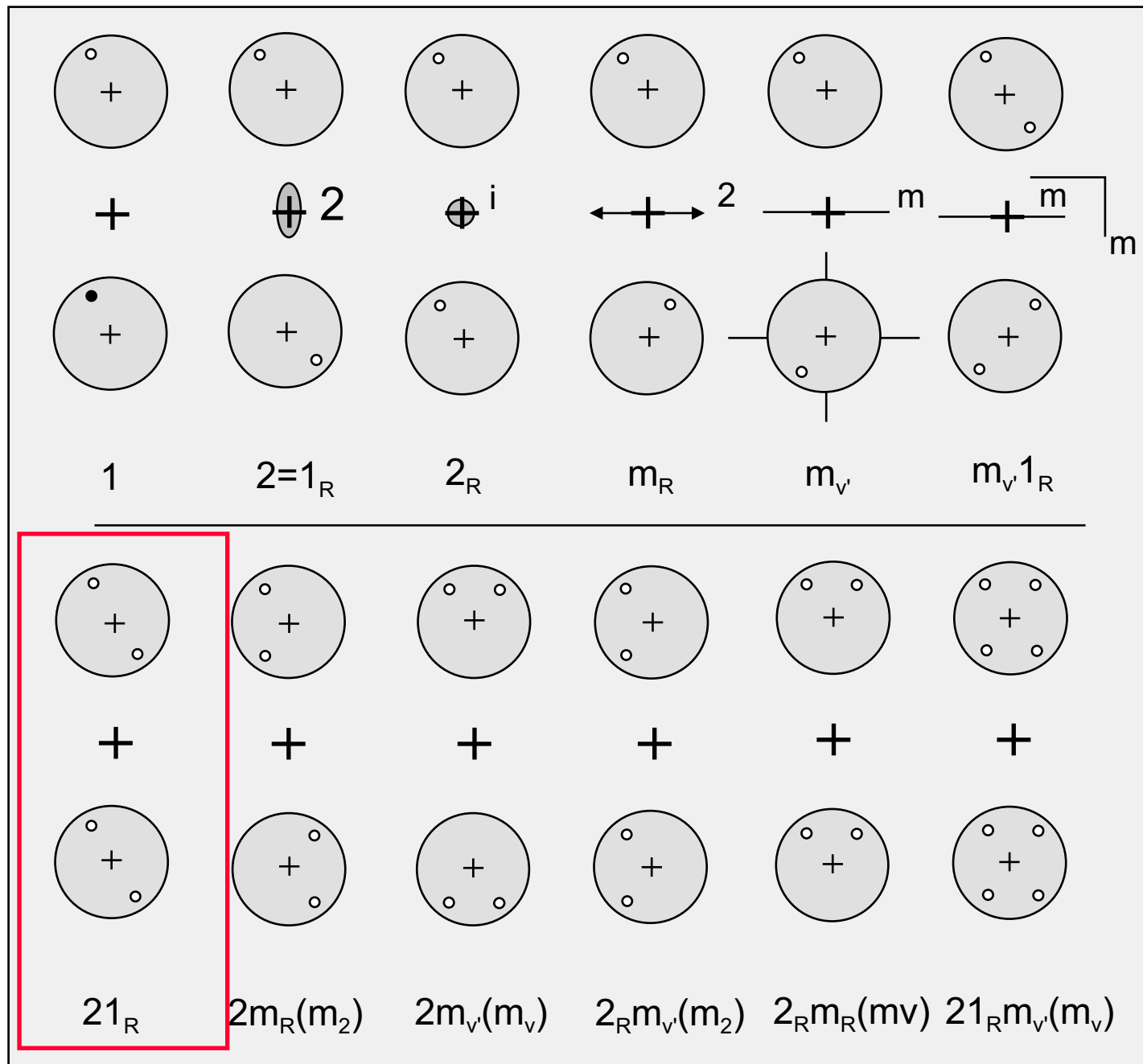
2D information



+g / -g symmetry



+g / -g symmetry



Recapitulation

Whole pattern

2D symmetry : 4mm

3D symmetry : 4mm

Bright Field

2D symmetry : 4mm

Dark field

2D symmetry : $2m_v m_2$ and $2 = 1_R$

+g / -g

2D symmetry : $21_R m_v (m'_v)$ and 21_R

2D Information

	WP	BF			Projection Diffraction group
	1	2			1_R
	2	2			21_R
	m_v	2mm			$m1_R$
	$2m_v m_v$	$2m_v m_v$			$2mm1_R$
	4	4			41_R
	$4m_v m_v$	$4m_v m_v$			$4mm1_R$
	3	6			31_R
	$3m_v$	6mm			$3m1_R$
	6	6			61_R
	$6m_v m_v$	$6m_v m_v$			$6mm1_R$

2D Information

	WP	BF			Projection Diffraction group
	1	2			1_R
	2	2			21_R
	m_v	2mm			$m1_R$
	$2m_v m_v$	$2m_v m_v$			$2mm1_R$
	4	4			41_R
	$4m_v m_v$	$4m_v m_v$			$4mm1_R$
	3	6			31_R
	$3m_v$	6mm			$3m1_R$
	6	6			61_R
	$6m_v m_v$	$6m_v m_v$			$6mm1_R$

Projected
Diffraction group
 $4mm1_R$

3D Information

Diffraction group	WP	BF	DF	+/-g	Projection Diffraction group
1 1 _R	1 1	1 2	1 2=1 _R	1 1	1 _R 1 _R
2 2 _R 21 _R	2 1 2	2 1 2	1 1 2	2 2 _R 21 _R	21 _R 21 _R 21 _R
m _R m m1 _R	1 m _v m _v	m m _v 2mm	$\begin{bmatrix} 1 \\ m_2 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 1 \\ m_R \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v 1_R \\ 1 \end{bmatrix}$	m1 _R m1 _R m1 _R
2m _R m _R 2mm 2 _R mm _R 2mm1 _R	2 2m _v m _v m _v 2m _v m _v	2mm 2m _v m _v m _v 2m _v m _v	$\begin{bmatrix} 1 \\ m_2 \\ 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_2 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \\ 2m_R(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v(m_v) \\ 2 \\ 2m_R(m_2) \end{bmatrix}$	2mm1 _R 2mm1 _R 2mm1 _R 2mm1 _R
4 4 _R 41 _R	4 2 4	4 4 4	1 1 2	2 2 21 _R	41 _R 41 _R 41 _R
4m _R m _R 4mm 4 _R mm _R 4mm1 _R	4 4m _v m _v 2m _v m _v 4m _v m _v	4mm 4m _v m _v 4mm 4m _v m _v	$\begin{bmatrix} 1 \\ m_2 \\ 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_2 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_R(m_2) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \\ 2m_R(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_R(m_2) \end{bmatrix}$	4mm1 _R 4mm1 _R 4mm1 _R 4mm1 _R
3 31 _R	3 3	3 6	1 2	1 1	31 _R 31 _R
3m _R 3m 3m1 _R	3 3m _v 3m _v	3m 3m _v 6mm	$\begin{bmatrix} 1 \\ m_2 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 1 \\ m_R \\ 1 \\ 1 \\ m_v 1_R \\ 1 \end{bmatrix}$	3m1 _R 3m1 _R 3m1 _R
6 6 _R 61 _R	6 3 6	6 3 6	1 1 2	2 2 _R 21 _R	61 _R 61 _R 61 _R
6m _R m _R 6mm 6 _R mm _R 6mm1 _R	6 6m _v m _v 3m _v 6m _v m _v	6mm 6m _v m _v 3m _v 6m _v m _v	$\begin{bmatrix} 1 \\ m_2 \\ 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_2 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \\ 2m_R(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v(m_v) \\ 2 \\ 2m_R(m_2) \end{bmatrix}$	6mm1 _R 6mm1 _R 6mm1 _R 6mm1 _R

3D Information

Diffraction group	WP	BF	DF	+/-g	Projection Diffraction group
1 1 _R	1 1	1 2	1 2=1 _R	1 1	1 _R 1 _R
2 2 _R 21 _R	2 1 2	2 1 2	1 1 2	2 2 _R 21 _R	21 _R 21 _R 21 _R
m _R m m1 _R	1 m _v m _v	m m _v 2mm	$\begin{bmatrix} 1 \\ m_2 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 1 \\ m_R \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v 1_R \\ 1 \end{bmatrix}$	m1 _R m1 _R m1 _R
2m _R m _R 2mm 2 _R mm _R 2mm1 _R	2 2m _v m _v m _v 2m _v m _v	2mm 2m _v m _v m _v 2m _v m _v	$\begin{bmatrix} 1 \\ m_2 \\ 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_2 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$	2mm1 _R 2mm1 _R 2mm1 _R 2mm1 _R
4 4 _R 41 _R	4 2 4	4 4 4	1 1 2	2 2 21 _R	41 _R 41 _R 41 _R
4m _R m _R 4mm 4 _R mm _R 4mm1 _R	4 4m _v m _v 2m _v m _v 4m _v m _v	4mm 4m _v m _v 4mm 4m _v m _v	$\begin{bmatrix} 1 \\ m_2 \\ 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_2 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$	4mm1 _R 4mm1 _R 4mm1 _R 4mm1 _R
3 31 _R	3 3	3 6	1 2	1 1	31 _R 31 _R
3m _R 3m 3m1 _R	3 3m _v 3m _v	3m 3m _v 6mm	$\begin{bmatrix} 1 \\ m_2 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 1 \\ m_R \\ 1 \\ 1 \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v \\ 1 \\ 1 \\ 1 \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_v 1_R \\ 1 \end{bmatrix}$	3m1 _R 3m1 _R 3m1 _R
6 6 _R 61 _R	6 3 6	6 3 6	1 1 2	2 2 _R 21 _R	61 _R 61 _R 61 _R
6m _R m _R 6mm 6 _R mm _R 6mm1 _R	6 6m _v m _v 3m _v 6m _v m _v	6mm 6m _v m _v 3m _v 6m _v m _v	$\begin{bmatrix} 1 \\ m_2 \\ 1 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 1 \\ m_2 \\ m_v \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_v m_2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2 \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$ $\begin{bmatrix} 2 \\ 2m_R(m_2) \\ 2m_v(m_v) \end{bmatrix}$	6mm1 _R 6mm1 _R 6mm1 _R 6mm1 _R

4mm1_R
projected diffraction group



four possible diffraction groups

- 4m_Rm_R
- 4mm
- 4_Rmm_R
- 4mm1_R

2D Information

$2mm1_R$	$2m_v m_{v'}$	$2m_v m_{v'}$	$\left\{ \begin{array}{l} 2 \\ 2m_v m_2 \end{array} \right.$	$\left\{ \begin{array}{l} 21_R \\ 21_R m_{v'}(m_v) \end{array} \right.$	
4	4	4	1	2	
4_R	4	2	1	2	41_R
41_R	4	4	2	21_R	
$4m_R m_R$	$4mm$ $(4 + m_2)$	4	$\left\{ \begin{array}{l} 1 \\ m_2 \end{array} \right.$	$\left\{ \begin{array}{l} 2 \\ 2m_R(m_2) \end{array} \right.$	
$4mm$	$4m_v m_{v'}$	$4m_v m_{v'}$	$\left\{ \begin{array}{l} 1 \\ \bar{m}_v \end{array} \right.$	$\left\{ \begin{array}{l} 2 \\ 2m_{v'}(m_v) \end{array} \right.$	$4mm1_R$
$4_R mm_R$	$4mm$ $(2m_v m_{v'} + m_2)$	$2m_v m_{v'}$	$\left\{ \begin{array}{l} 1 \\ m_2 \\ m_v \end{array} \right.$	$\left\{ \begin{array}{l} 2 \\ 2m_R(m_2) \\ 2m_{v'}(m_v) \end{array} \right.$	
$4mm1_R$	$4m_v m_{v'}$	$4m_v m_{v'}$	$\left\{ \begin{array}{l} 2 \\ 2m_v m_2 \end{array} \right.$	$\left\{ \begin{array}{l} 21_R \\ 21_R m_{v'}(m_v) \end{array} \right.$	
3	3	3	1	1	

In 2D, the four diffraction groups give the same WP, BF, DF and +g / -g symmetries

3D Information

WP

$2mm1_R$	$2m_v m_{v'}$	$2m_v m_{v'}$	$\left\{ \begin{array}{l} 2 \\ 2m_v m_2 \end{array} \right.$	$\left\{ \begin{array}{l} 21_R \\ 21_R m_{v'}(m_v) \end{array} \right.$	
4	4	4	1	2	
4_R	4	2	1	2	41_R
41_R	4	4	2	21_R	
$4m_R m_R$	$4mm$ $(4 + m_2)$	4	$\left\{ \begin{array}{l} 1 \\ m_2 \end{array} \right.$	$\left\{ \begin{array}{l} 2 \\ 2m_R(m_2) \end{array} \right.$	
$4mm$	$4m_v m_{v'}$	$4m_v m_{v'}$	$\left\{ \begin{array}{l} 1 \\ m_v \end{array} \right.$	$\left\{ \begin{array}{l} 2 \\ 2m_{v'}(m_v) \end{array} \right.$	$4mm1_R$
$4_R mm_R$	$4mm$ $(2m_v m_{v'} + m_2)$	$2m_v m_{v'}$	$\left\{ \begin{array}{l} 1 \\ m_2 \\ m_v \end{array} \right.$	$\left\{ \begin{array}{l} 2 \\ 2m_R(m_2) \\ 2m_{v'}(m_v) \end{array} \right.$	
$4mm1_R$	$4m_v m_{v'}$	$4m_v m_{v'}$	$\left\{ \begin{array}{l} 2 \\ 2m_v m_2 \end{array} \right.$	$\left\{ \begin{array}{l} 21_R \\ 21_R m_{v'}(m_v) \end{array} \right.$	
3	3	3	1	1	

in 3D, two possible Diffraction groups : $4mm$ and $4mm1_R$

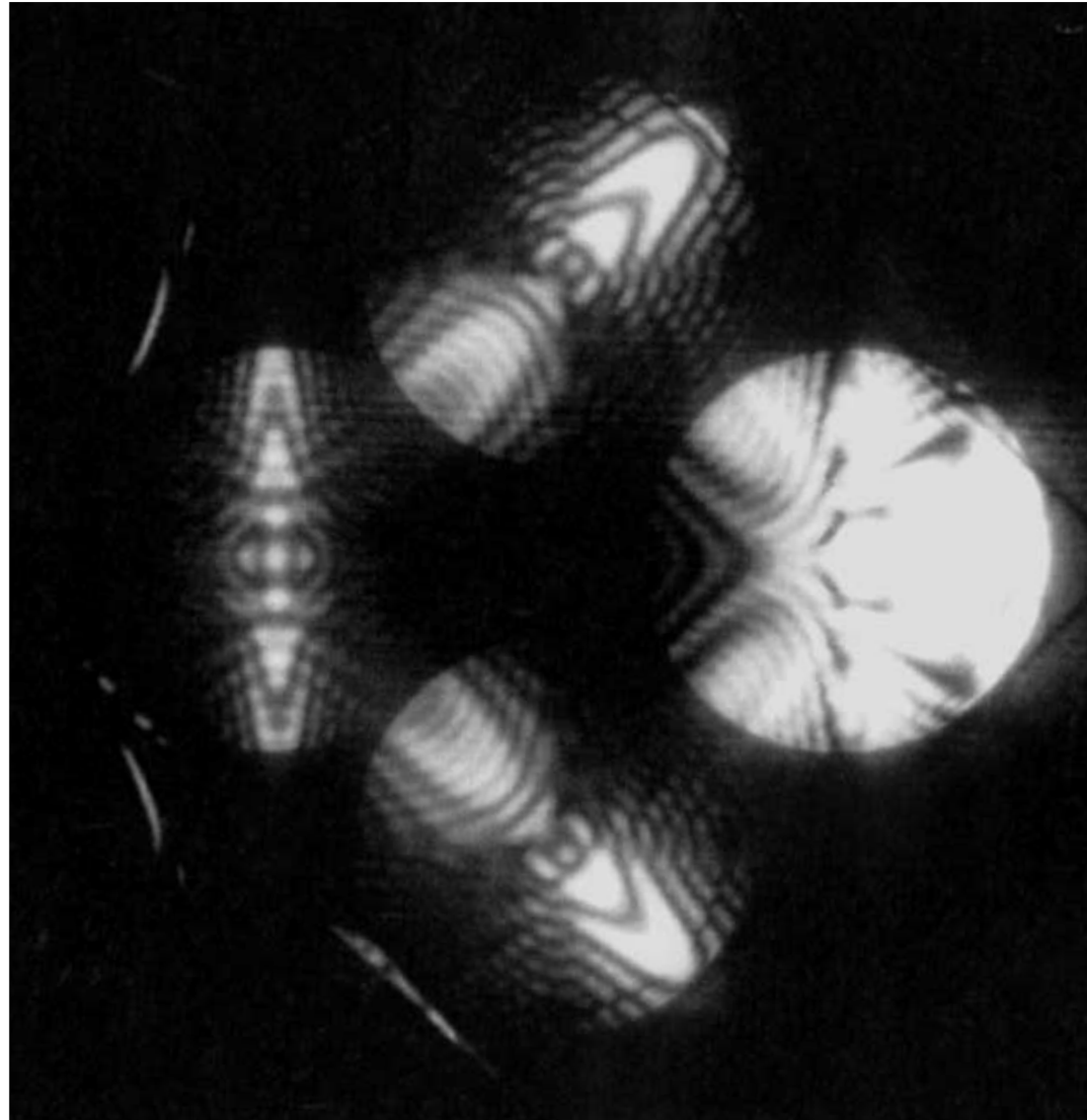
Identification of the POINT GROUP

Diffraction groups

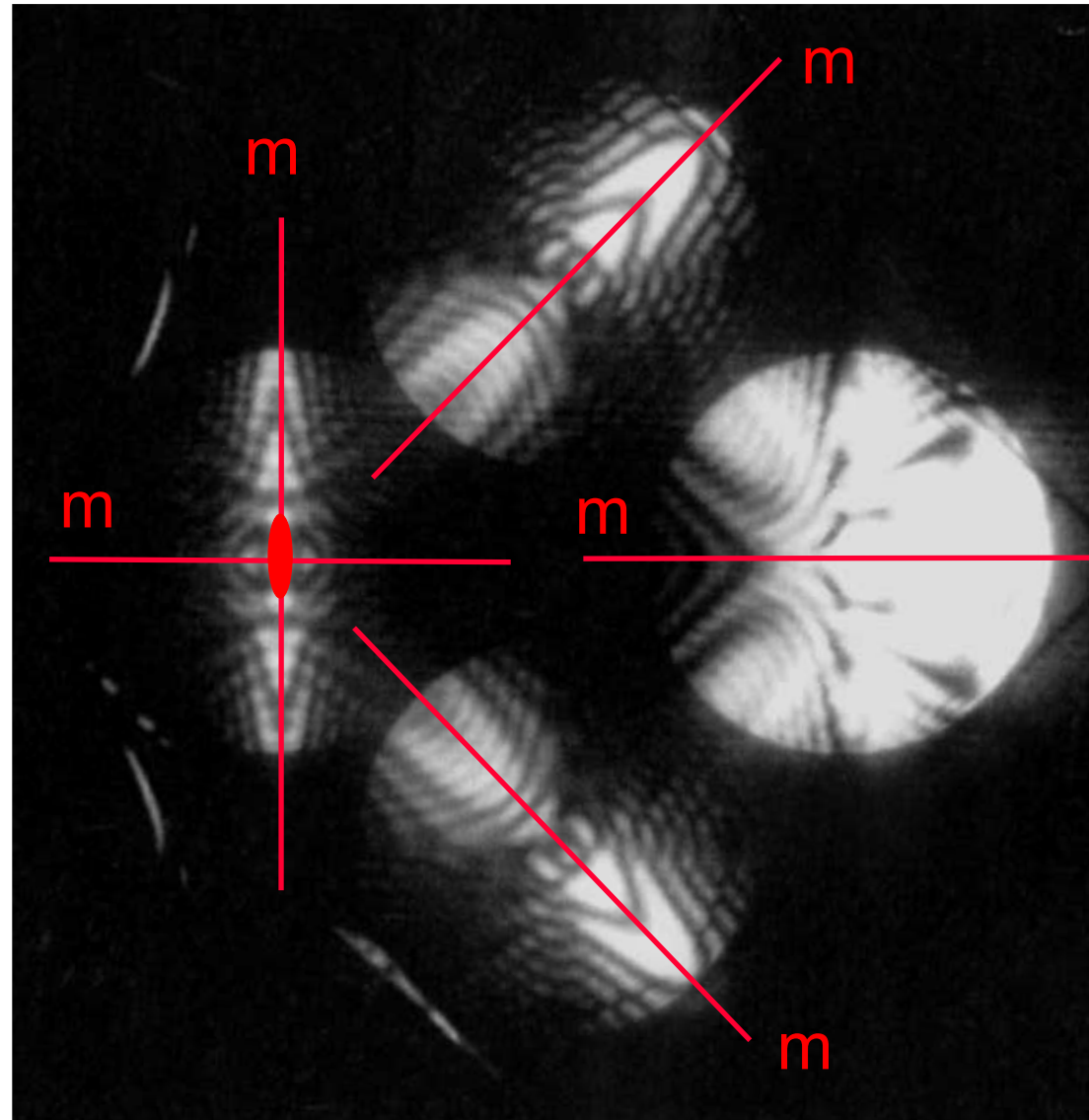
DIFFRACTION GROUPS		RELATION BETWEEN THE DIFFRACTION GROUPS AND THE CRYSTAL POINT GROUPS																														
N																																
6m1 _R																																
3m1 _R																																
6mm																																
6m _R m _R																																
61 _R																																
31 _R																																
6																																
6 _R mm _R																																
3m																																
3m _R																																
6 _R																																
3																																
4m1 _R																																
4Rmm _R																																
4mm																																
4m _R m _R																																
41 _R																																
4 _R																																
4																																
2mm1 _R																																
2 _R mm _R																																
2mm																																
2m _R m _R																																
m1 _R																																
m																																
m _R																																
21 _R																																
2 _R																																
2																																
1 _R																																
1																																
	1	1	2	m	2/m	222	mm2	mmm	4	4	4/m	422	4mm	42m	4/mmm	8 ₃	3	32	3m	3m	6	6	6/m	622	6mm	6m2	6/mmm	23	m3	432	43m	m3m

POINT GROUP

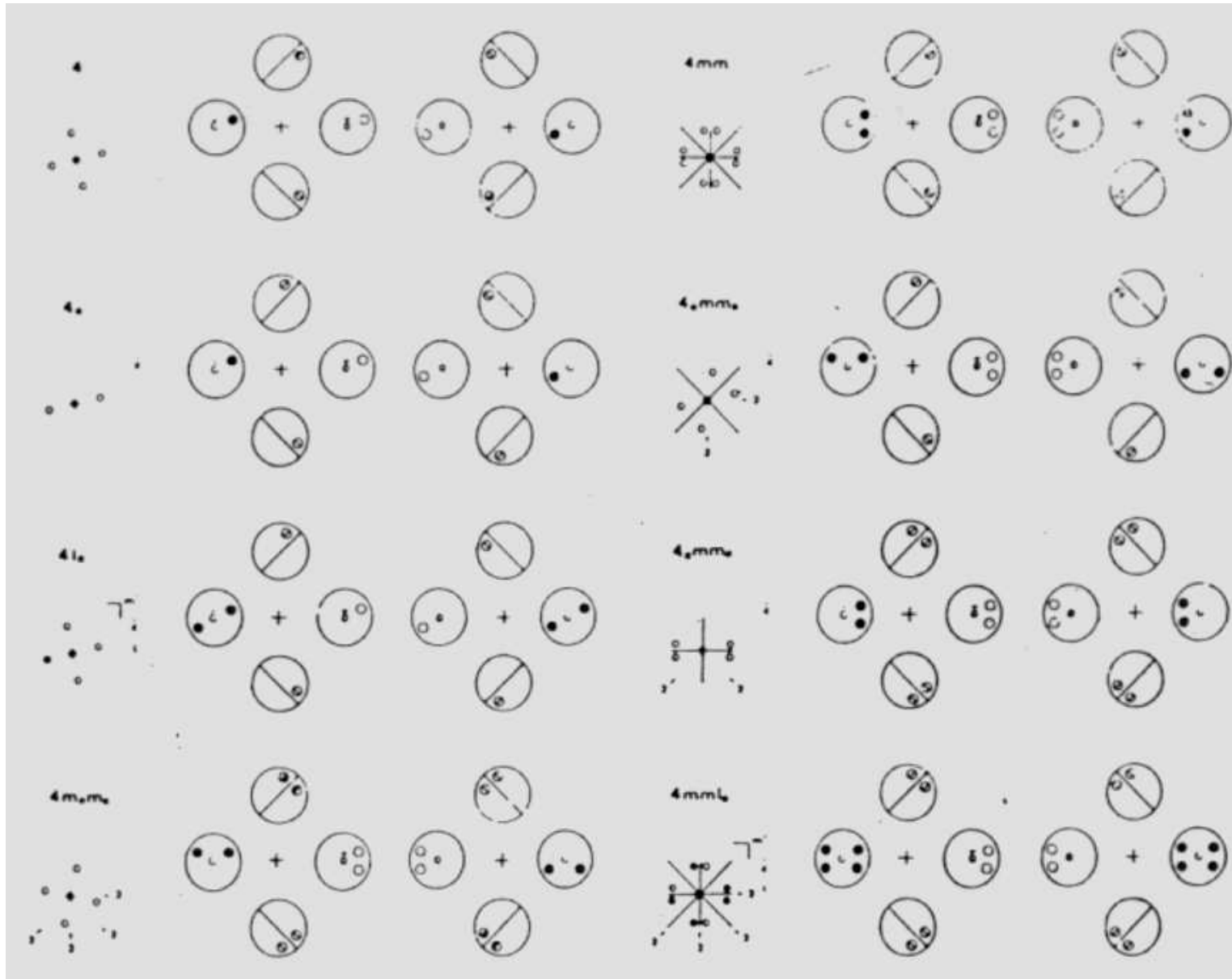
- Tanaka "multibeam" method
2D Information



- Tanaka "multibeam" method
2D Information

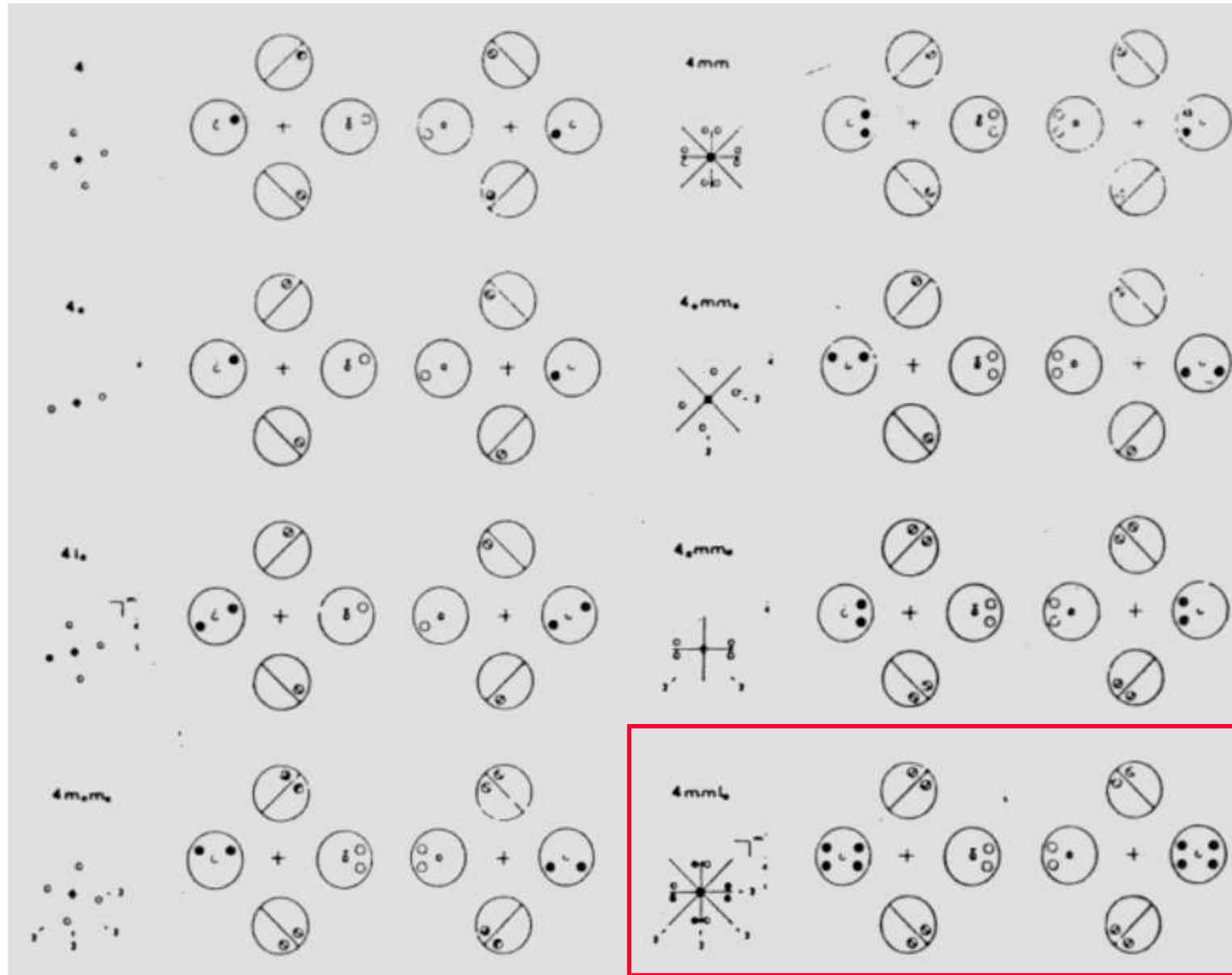


- Multibeam method



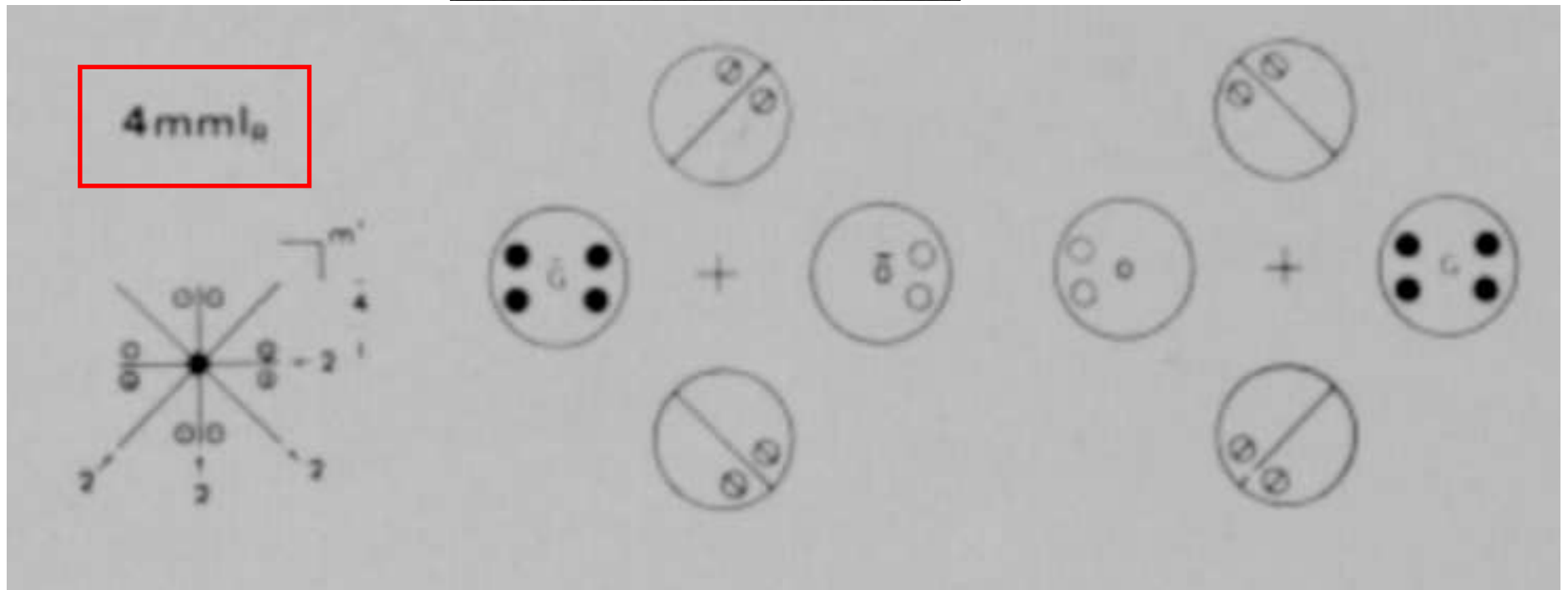
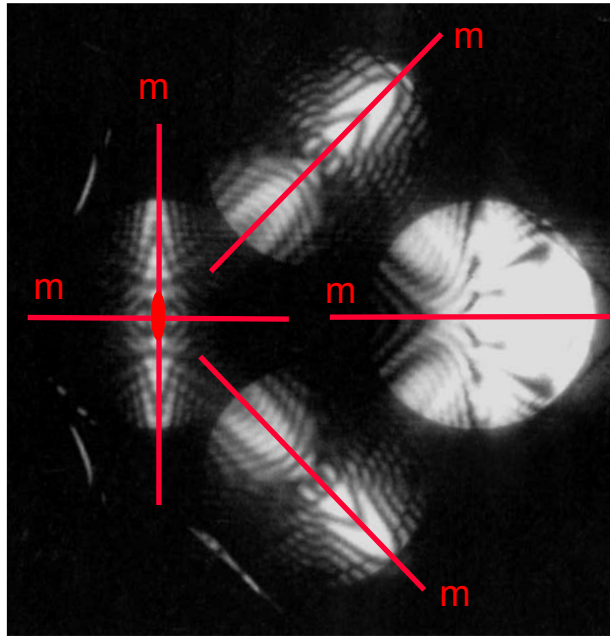
Tanaka Table for 4mm patterns

- Multibeam method



Tanaka Table for 4mm patterns

- Tanaka
"multibeam" method
2D Information



Projected diffraction group $4mm1_R$

2D Information

$2mm1_R$	$2m_v m_{v'}$	$2m_v m_{v'}$	$\begin{cases} 2 \\ 2m_v m_2 \end{cases}$	$\begin{cases} 21_R \\ 21_R m_{v'}(m_v) \end{cases}$	
4	4	4	1	2	
4_R	4	2	1	2	41_R
41_R	4	4	2	21_R	
$4m_R m_R$	$4mm$ $(4 + m_2)$	4	$\begin{cases} 1 \\ m_2 \end{cases}$	$\begin{cases} 2 \\ 2m_R(m_2) \end{cases}$	
$4mm$	$4m_v m_{v'}$	$4m_v m_{v'}$	$\begin{cases} 1 \\ \bar{m}_v \end{cases}$	$\begin{cases} 2 \\ 2m_{v'}(m_v) \end{cases}$	$4mm1_R$
$4_R mm_R$	$4mm$ $(2m_v m_{v'} + m_2)$	$2m_v m_{v'}$	$\begin{cases} 1 \\ m_2 \\ m_v \end{cases}$	$\begin{cases} 2 \\ 2m_R(m_2) \\ 2m_{v'}(m_v) \end{cases}$	
$4mm1_R$	$4m_v m_{v'}$	$4m_v m_{v'}$	$\begin{cases} 2 \\ 2m_v m_2 \end{cases}$	$\begin{cases} 21_R \\ 21_R m_{v'}(m_v) \end{cases}$	
3	3	3	1	1	

2D ; Four possible Diffraction groups

Conclusion

3D information very important

In 2D, DF and +g / -g not useful