International Union of Crystallography

Commission on Mathematical and Theoretical Crystallography

Symmetry Relationships between Crystal Structures with Applications to Structural and Magnetic Phase Transitions

Varanasi, India, 27-31 October 2014

international year of crystallography

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS II.

SPACE GROUPS

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Irreducible Representations of Space Groups

Method: Construct the irreps of the space group G starting from the irreps of one of its normal subgroups $H \triangleleft G$

1. Construct all irreps of H
2. Distribute the irreps of H into orbits under G and select a representative
3. Determine the little group for each representative
4. Find the small (allowed) irreps of the little group
5. Construct the irreps of G by induction from the the small (allowed) irreps of the little group

SPACE GROUPS

Crystal pattern: infinite, idealized crystal structure (without disorder, dislocations, impurities, etc.)

Space group G: The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup $T_G \triangleleft G$: The infinite set of all translations that are symmetry operations of the crystal pattern

Point group of the space groups P_G: The factor group of the space group G with respect to the translation subgroup T: $P_G \cong G/H$

Step 1. **TRANSLATION SUBGROUP IRREPS $T_G \lhd G$**

Born-von Karman boundary condition

$$(\mathbf{I},\, \mathbf{t}_i)^{N_i} = (\mathbf{I},\, \mathbf{N}_i) = (\mathbf{I},\, \mathbf{o})$$

$$(\mathbf{I},\, \mathbf{N\,t}); \quad \mathbf{N\,t} = (N_1 t_1,\, N_2 t_2,\, N_3 t_3)$$

infinite T_G:

{(I,0), (I,t}, (I,2t),...,(I,Nt),(I,(N+1)t), ...,(I,2Nt), ...}

finite T_G: {(I,0), (I,t}, (I,2t),...,(I,(N-1)t)}

Representations of finite Abelian groups

Finite Abelian groups $\left\{ \begin{array}{l} \text{cyclic groups} \\ \text{direct product of cyclic groups} \end{array} \right.$

A

$\{a, a^2, \ldots, a^s\}$

↓

$D^p(a^m)$, $p=0,1,\ldots,s-1$

$$exp(-i2\pi m)\frac{p}{s}$$

B

$\{b, b^2, \ldots, b^r\}$

↓

$D^q(b^n)$, $q=0,1,\ldots,r-1$

$$exp(-i2\pi n)\frac{q}{r}$$

→ $A \otimes B$

$\{(a^m, b^n)\}$ $m=1,\ldots,s;$ $n=1,\ldots,r$

↓

$D^p(a^m) \otimes D^q(b^n)$

↓

$$D^{p,q}(a^m, b^n) = exp(-i2\pi m)\frac{p}{s}\; exp(-i2\pi n)\frac{q}{r}$$

$p=0,1,\ldots,s-1 \quad q=0,1,\ldots,r-1$

IRREPS of Translational group

Translational subgroup: T

$$T = T_1 \otimes T_2 \otimes T_3 = \{(t_1^k, t_2^l, t_3^m)\}$$

$$D^{p,q,r}(t_1^k, t_2^l, t_3^m) =$$

$$exp(-i2\pi k)\frac{p}{N_1} \; exp(-i2\pi l)\frac{q}{N_2} \; exp(-i2\pi m)\frac{r}{N_3}$$

number of irreps:

$p = 0, 1, \ldots, N_1 - 1 \quad q = 0, 1, \ldots, N_2 - 1 \quad r = 0, 1, \ldots, N_3 - 1$

dim $D^{p,q,r}(t_1^k, t_2^l, t_3^m) = 1$

IRREPS of Translational group

reciprocal space

L: a_1, a_2, a_3 ⟷ L*: a^*_1, a^*_2, a^*_3

$a_i . a^*_j = 2\pi\delta_{ij}$

$$\Gamma^{(q_1\, q_2\, q_3)}[(\mathbf{I}, \mathbf{t})] = e^{-2\pi i (q_1 \frac{t_1}{N_1} + q_2 \frac{t_2}{N_2} + q_3 \frac{t_3}{N_3})}$$

$k_i = q_i / N_i$

$$\Gamma^{(q_1\, q_2\, q_3)}[(\mathbf{I}, \mathbf{t})] = \Gamma^{\mathbf{k}}[(\mathbf{I}, \mathbf{t})] = \exp -i(\mathbf{k}\, \mathbf{t})$$

ITA conventions:

$$(\mathbf{k}\ \mathbf{t}) = (k_1, k_2, k_3) \begin{vmatrix} \mathbf{a}^*_1 \\ \mathbf{a}^*_2 \\ \mathbf{a}^*_3 \end{vmatrix} (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \begin{vmatrix} t_1 \\ t_2 \\ t_3 \end{vmatrix} = 2\pi (k_1, k_2, k_3) \begin{vmatrix} t_1 \\ t_2 \\ t_3 \end{vmatrix}$$

IRREPS of Translational group

unit cell of reciprocal space (fundamental region)

$k' = k + K, \quad K = h_1 \mathbf{a_1}^* + h_2 \mathbf{a_2}^* + h_3 \mathbf{a_3}^*, \; K \in L^*$

$\Gamma^{k'} = \exp(-i(k+K)t) = \exp{-i(k.t)} = \Gamma^{k}$

first Brillouin zone (Wigner-Seitz cell)

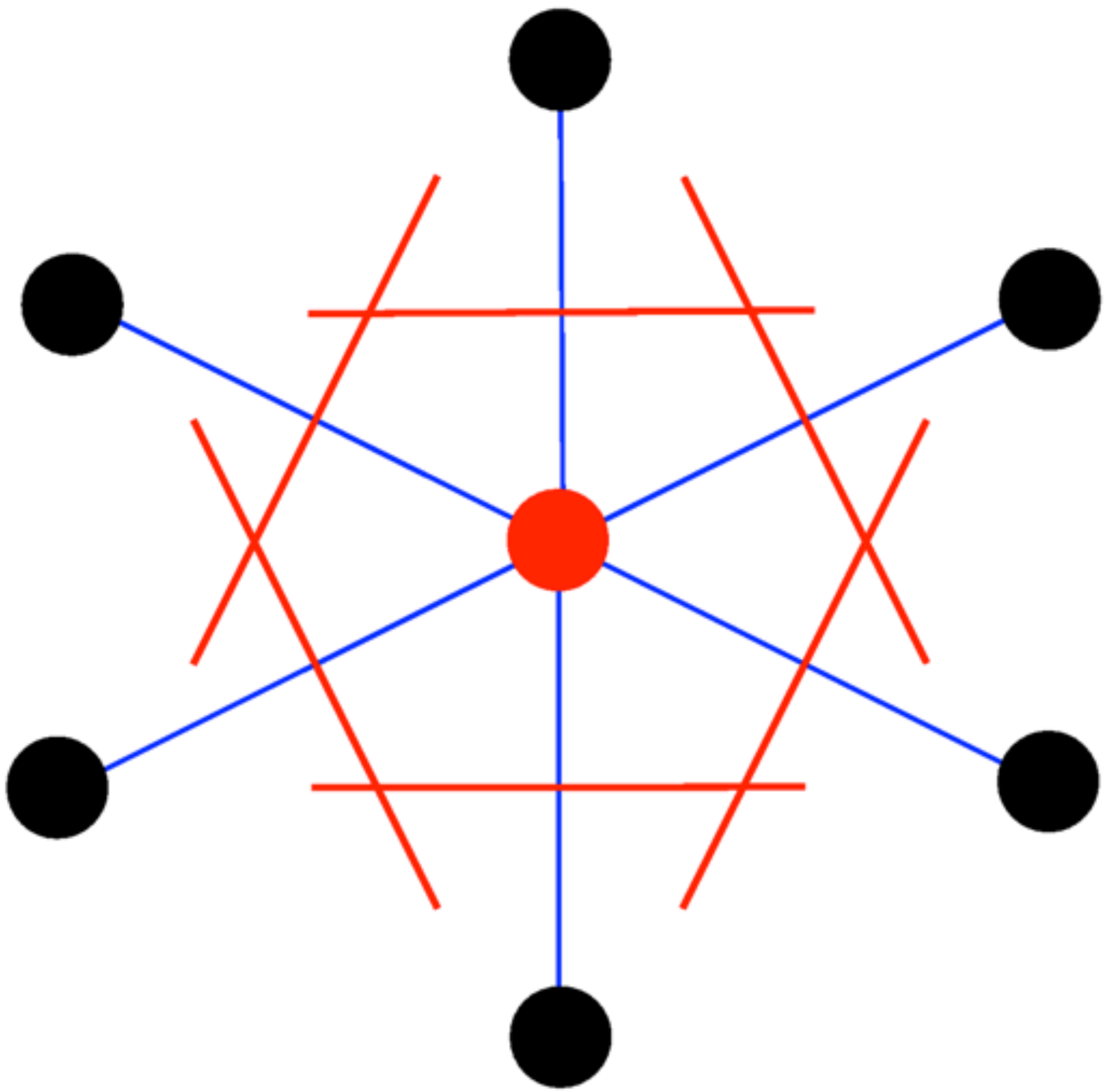
$|k| \leq |K-k|, \; \forall K \in L^*$

crystallographic unit cell

$0 \leq |k| < 1$

first Brillouin zone (Wigner-Seitz cell)

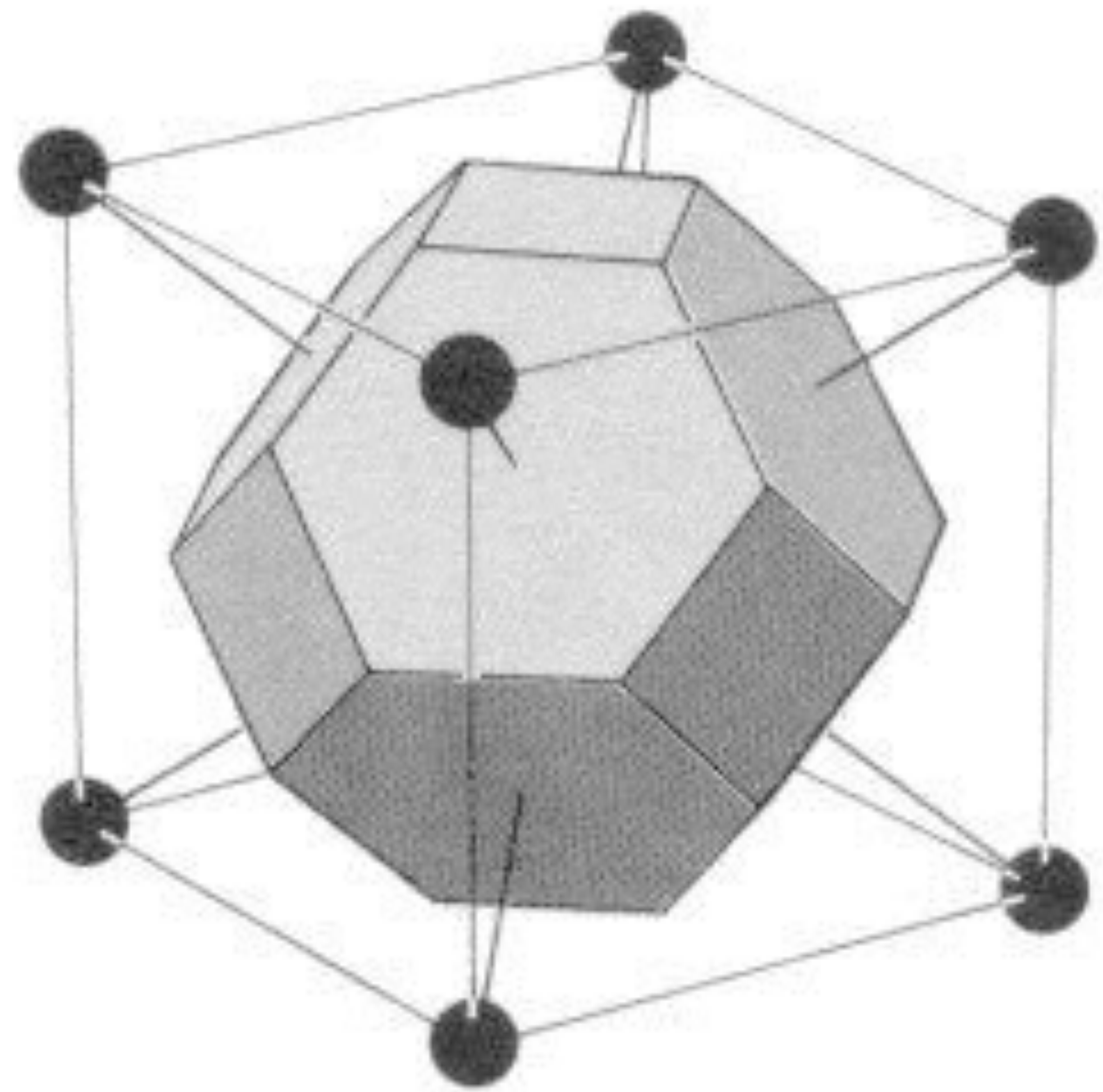
$|k| \leq |K-k|, \ \forall K \in L^*$



first Brillouin zone (Wigner-Seitz cell)

$|k| \leq |K-k|, \forall K \in L^*$

Wigner-Seitz construction for *bcc* lattice

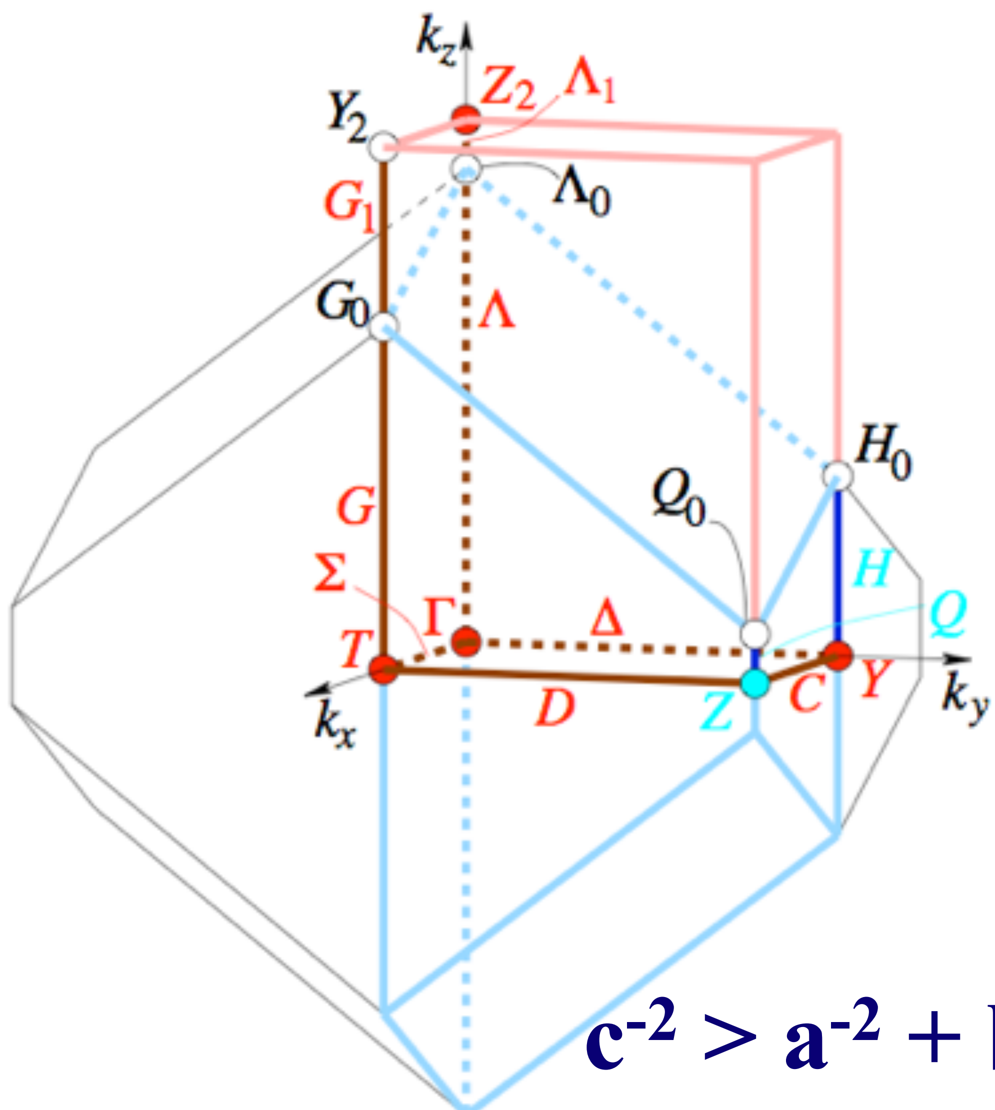


Brillouin Zone Database
Crystallographic Approach

Reciprocal space groups
- Brillouin zones
- Representation domain
- Wave-vector symmetry

↔

Symmorphic space groups
- IT unit cells
- Asymmetric unit
- Wyckoff positions



$$c^{-2} > a^{-2} + b^{-2}$$

The k-vector Types of Group 22 [*F*222]

k-vector description			Wyckoff Position			ITA description
CDML*		Conventional-ITA	ITA			Coordinates
Label	Primitive					
GM	0,0,0	0,0,0	a	2	222	0,0,0
T	1,1/2,1/2	0,1,1	b	2	222	0,1/2,1/2
T~T_2			b	2	222	1/2,0,0
Z	1/2,1/2,0	0,0,1	c	2	222	0,0,1/2
Y	1/2,0,1/2	0,1,0	d	2	222	0,1/2,0
Y~Y_2			d	2	222	1/2,0,1/2
SM	0,u,u ex	2u,0,0	e	4	2..	x,0,0 : 0 < x <= sm_0
U	1,1/2+u,1/2+u ex	2u,1,1	e	4	2..	x,1/2,1/2 : 0 < x < u_0
U~SM_1=[SM_0 T_2]			e	4	2..	x,0,0 : 1/2-u_0=sm_0 < x < 1/2
SM+SM_1=[GM T_2]			e	4	2..	x,0,0 : 0 < x < 1/2
A	1/2,1/2+u,u ex	2u,0,1	f	4	2..	x,0,1/2 : 0 < x <= a_0
C	1/2,u,1/2+u ex	2u,1,0	f	4	2..	x,1/2,0 : 0 < x < c_0

Step 2.

Classification of the irreps of the Translation subgroup.

orbits of irreps of T

$$\Gamma^{k'}(I,t) = \Gamma^{k}((W,w)^{-1}(I,t)(W,w)),\ (I,t)\in T,\quad (W,w)\in G$$

$$\Gamma^{k'}(I,t) = \Gamma^{k}(I,W^{-1}t) = \exp -i(k.(W^{-1}t)) = \exp -i((kW^{-1}).t)$$

$$k' = kW + K$$

little co-group of k: $\overline{G}^{k}$

$$k = kW + K,\ K\in L^{*}$$

special and general

$$\overline{G}^{k} = \{1\}\quad \overline{G}^{k} > \{1\}$$

Orbits of irreps of the Translation subgroup.

star of k: k*

$\overline{G}^{k} < \overline{G}$

$\overline{G} = \overline{G}^{k} + W_2 \overline{G}^{k} + \ldots + W_m \overline{G}^{k}$

$k^* = \{k' = kW_m + K, W_m \notin \overline{G}\}$

representation domain

exactly one k-vector from each star

Little group and Little-group irreps
(Allowed irreps of the little group)

Step 3.

Little group G^k

$$G^k=\{(W,w)\in G \mid W\in \overline{G}^k\}$$

Step 4.

Allowed irreps of G^k

$$(D^{k,i}\downarrow T) = \exp(-ikt)\boldsymbol{I}$$

special case: general k-vector

star of k
little group of k
allowed irreps

?

Little-group irreps
(Allowed irreps of the little group)

Step 4. Allowed irreps of G^k

1. $\mathbf{k}$ is a vector of the interior of the BZ
   OR
2. $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group.

Case 1.

allowed irreps $\mathbf{D}^{\mathbf{k},i}$:

$$\mathbf{D}^{\mathbf{k},i}(\mathbf{W},\mathbf{w}) = \exp-(i\mathbf{k}\mathbf{w})\,\overline{\mathbf{D}}^{\mathbf{k},i}(\mathbf{W})$$

Here $\mathbf{D}^{\mathbf{k},i}$ is an irrep of $\mathcal{G}^{\mathbf{k}}$,

Little-group irreps
(Allowed irreps of the little group)

CASE 2:

1. $\mathbf{k}$ is a vector on the surface of the BZ AND
2. $\mathcal{G}^{\mathbf{k}}$ is a nonsymmorphic space group.

allowed irreps $\mathbf{D}^{\mathbf{k},i}$:
induced from allowed irreps $\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}$ of $\mathcal{H}_0$ where
$\mathcal{H}_0$ is a symmorphic subgroup of $\mathcal{G}^{\mathbf{k}}$

$$\mathcal{G} \triangleright \mathcal{H}_1 \triangleright \mathcal{H}_2 \ \ldots \ \triangleright \mathcal{H}_0 \triangleright \ \ldots \ \triangleright \mathcal{T}$$

Step 5.

Induction procedure

Construction of the irreps of the space group G by induction from the the small (allowed) irreps of the little group $G^k < G$

PROCEDURE FOR THE CONSTRUCTION OF SPACE-GROUP REPRESENTATIONS

Procedure for the construction of the irreps of space groups.

1. space-group information

(a) Decomposition of the space group $\mathcal{G}$ in cosets relative to its translation subgroup $\mathcal{T}$, see IT A (1996)

$$\mathcal{G} = \mathcal{T} \cup (\mathbf{W}_2, \mathbf{w}_2)\,\mathcal{T} \cup \ \ldots \ \cup (\mathbf{W}_p, \mathbf{w}_p)\,\mathcal{T}$$

(b) Choice of a convenient set of generators of $\mathcal{G}$, see IT A (1996)

2. k-vector information

(a) **k** vector from the representation domain of the BZ

(b) Little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of **k**:

$$\overline{\mathcal{G}}^{\mathbf{k}} = \{\widetilde{\mathbf{W}}_i \in \overline{\mathcal{G}} : \ \mathbf{k} = \mathbf{k}\,\widetilde{\mathbf{W}}_i + \mathbf{K}, \ \mathrm{k} \in \mathbf{L}^*\}$$

(c) **k**-vector star $\star(\mathbf{k})$

$\star(\mathbf{k}) = \{\mathbf{k}, \mathbf{k}_2, \ldots, \mathbf{k}_s\}$, with $\mathbf{k} = \mathbf{k}\,\overline{\mathbf{W}}_j$, $j = 1, \ldots s$, where $\overline{W}_j$ are the coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$.

(d) Determination of the little group $\mathcal{G}^{\mathbf{k}}$

$$\mathcal{G}^{\mathbf{k}} = \{(\widetilde{\mathbf{W}}_i, \widetilde{\mathbf{w}}_i) \in \mathcal{G} : \widetilde{\mathbf{W}}_i \in \overline{\mathcal{G}}\}$$

3. Allowed (small) irreps of $\mathcal{G}^{\mathbf{k}}$

(a) If $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group or $\mathbf{k}$ is inside the BZ, then the non-equivalent allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}^{\mathbf{k}}$ are related to the non-equivalent irreps $\overline{\mathbf{D}}^{\mathbf{k},i}$ of $\overline{\mathcal{G}}^{\mathbf{k}}$ in the following way:

$$\mathbf{D}^{\mathbf{k},i}(\widetilde{\mathbf{W}}_i, \widetilde{\mathbf{w}}_i) = \exp -(i\,\mathbf{k}\,\mathbf{w}_i)\,\overline{\mathbf{D}}^{\mathbf{k},i}(\widetilde{\mathbf{W}}_i)$$

(b) If $\mathcal{G}^{\mathbf{k}}$ is a non-symmorphic space group and $\mathbf{k}$ is on the surface of the BZ, then:

i. Look for a symmorphic subgroup $\mathcal{H}_0^{\mathbf{k}}$ (or an appropriate chain of normal subgroups) of index 2 or 3

ii. Find the allowed irreps $\mathbf{D}_{\mathcal{H}_0}^{\mathbf{k}\,i}$ of $\mathcal{H}_0^{\mathbf{k}}$, *i. e.* those for which is fulfilled $\mathbf{D}_{\mathcal{H}_0}^{\mathbf{k},i}(\mathbf{I}, \mathbf{t}) = \exp -(i\,\mathbf{k}, \mathbf{t})\,\mathbf{I}$ and distribute them into orbits relative to $\mathcal{G}^{\mathbf{k}}$

iii. Determine the allowed irrpes of $\mathcal{G}^{\mathbf{k}}$ using the results for the induction from the irreps of normal subgroups of index 2 or 3

Induction procedure

4. Induction procedure for the construction of the irreps $\mathbf{D}^{\star\mathbf{k},i}$ of $\mathcal{G}$ from the allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}$
The representation matrices of $\mathbf{D}^{\star\mathbf{k},i}(\mathcal{G})$ for any element of $\mathcal{G}$ can be obtained if the matrices for the generators $\{(\mathbf{W}_l, \mathbf{w}_l),\ l = 1, \ldots, k\}$ of $\mathcal{G}$ are available (step 1a).

$$\boldsymbol{D}^{Ind}(g) = \boldsymbol{M}(g) \otimes \boldsymbol{D}^{(j)}(h)$$

subgroup irrep matrix

induction matrix

Induction procedure

Decomposition of $\mathcal{G}$ relative to $\mathcal{G}^{\mathsf{k}}$

An obvious choice of coset representatives of $\mathcal{G}$ relative to $\mathcal{G}^{\mathsf{k}}$ is the set of of elements $\{q_i = (\overline{W}_i, \overline{w}_i),\ i = 1,\ \ldots,\ s\}$ where $\overline{W}_i$ are the coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathsf{k}}$

$$\mathcal{G} = \mathcal{G}^{\mathsf{k}} \cup (\overline{W}_2, \overline{w}_2)\,\mathcal{G}^{\mathsf{k}} \cup\ \ldots\ (\overline{W}_s, \overline{w}_s)\,\mathcal{G}^{\mathsf{k}}$$

a) Construction of the induction matrix

The elements of the little group $\mathcal{G}^{\mathbf{k}}$ and the coset representatives $\{q_1, q_2, \ldots, q_s\}$ of G relative to $\mathcal{G}^{\mathbf{k}}$ are necessary for the construction of the induction matrix

$$M(W,w)_{ij} = \begin{cases} 1 \text{ if } q_i^{-1}(W,w)q_j \in \mathcal{G}^{\mathbf{k}} \\ 0 \text{ if } q_i^{-1}(W,w)q_j \notin \mathcal{G}^{\mathbf{k}} \end{cases}$$

0	1	0	0
0	0	1	0
1	0	0	0
0	0	0	1

dim M=s x s

monomial matrix

$(\boldsymbol{W}_l, \boldsymbol{w}_l)$	q_i	q_i^{-1}	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)$	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)q_j$	$M(\boldsymbol{W}_l, \boldsymbol{w}_l$
…	…	…	…	…	

(b) Matrices of the irreps $\mathbf{D}^{\star\mathbf{k},m}$ of $\mathcal{G}$:

$$\mathbf{D}^{\star\mathbf{k},m}(\boldsymbol{W}_l, \boldsymbol{w}_l)_{i\mu,j\nu} = M(\boldsymbol{W}_l, \boldsymbol{w}_l)_{ij}\, \mathbf{D}^{\mathbf{k},m}(\widetilde{\boldsymbol{W}}_p, \tilde{\boldsymbol{w}}_p)_{\mu\,\nu},$$

where $(\widetilde{\boldsymbol{W}}_p, \tilde{\boldsymbol{w}}_p) = q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)\, q_j$.

0	I	0	0
0	0	I	0
I	0	0	0
0	0	0	I

All irreps of the space group $\mathcal{G}$ for a given **k** vector are obtained considering all allowed irreps of the little group $\mathcal{G}^{\mathbf{k}}$ $\mathbf{D}^{\mathbf{k},m}$ obtained in step 3.

EXERCISES

Problem 1.

Consider the **k**-vectors Γ(000) and **X** (0½0) of the group ***P4mm***

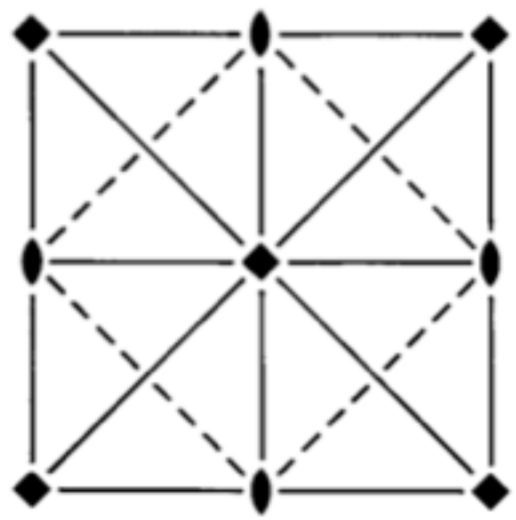
(i) Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group ***P4mm***

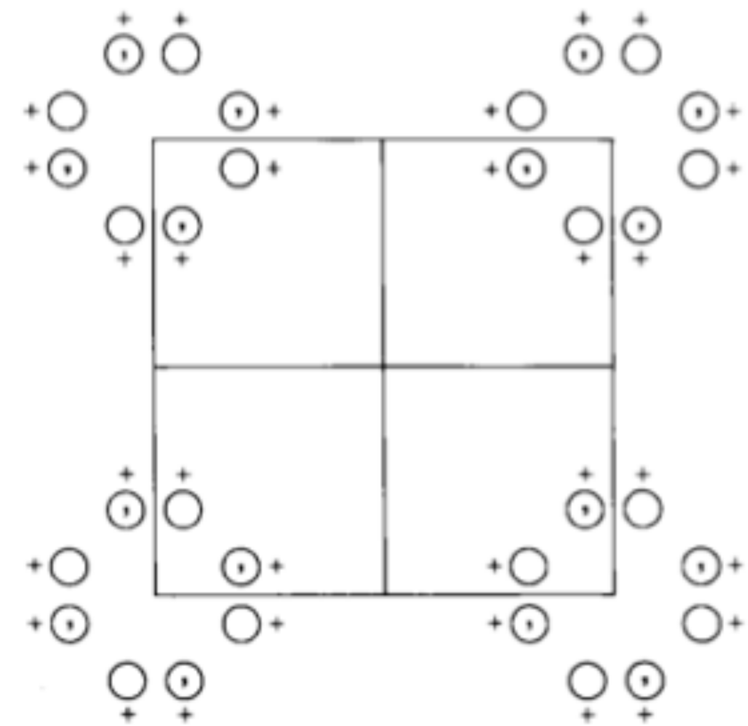
(ii) Calculate a set of coset representatives of the decomposition of the group ***P4mm*** with respect to the little group of the **k**-vectors Γ(000) and **X**, and construct the corresponding full space group irreps of ***P4mm***

International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

$P4mm$	C_{4v}^{1}	$4mm$	Tetragonal
No. 99	$P4mm$		Patterson symmetry $P4/mmm$

ITA space-group data (selection)





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1	(2) $2 \quad 0,0,z$	(3) $4^{+} \quad 0,0,z$	(4) $4^{-} \quad 0,0,z$
(5) $m \quad x,0,z$	(6) $m \quad 0,y,z$	(7) $m \quad x,\bar{x},z$	(8) $m \quad x,x,z$

General position

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Brillouin Zone Database BilbaoCrystServer

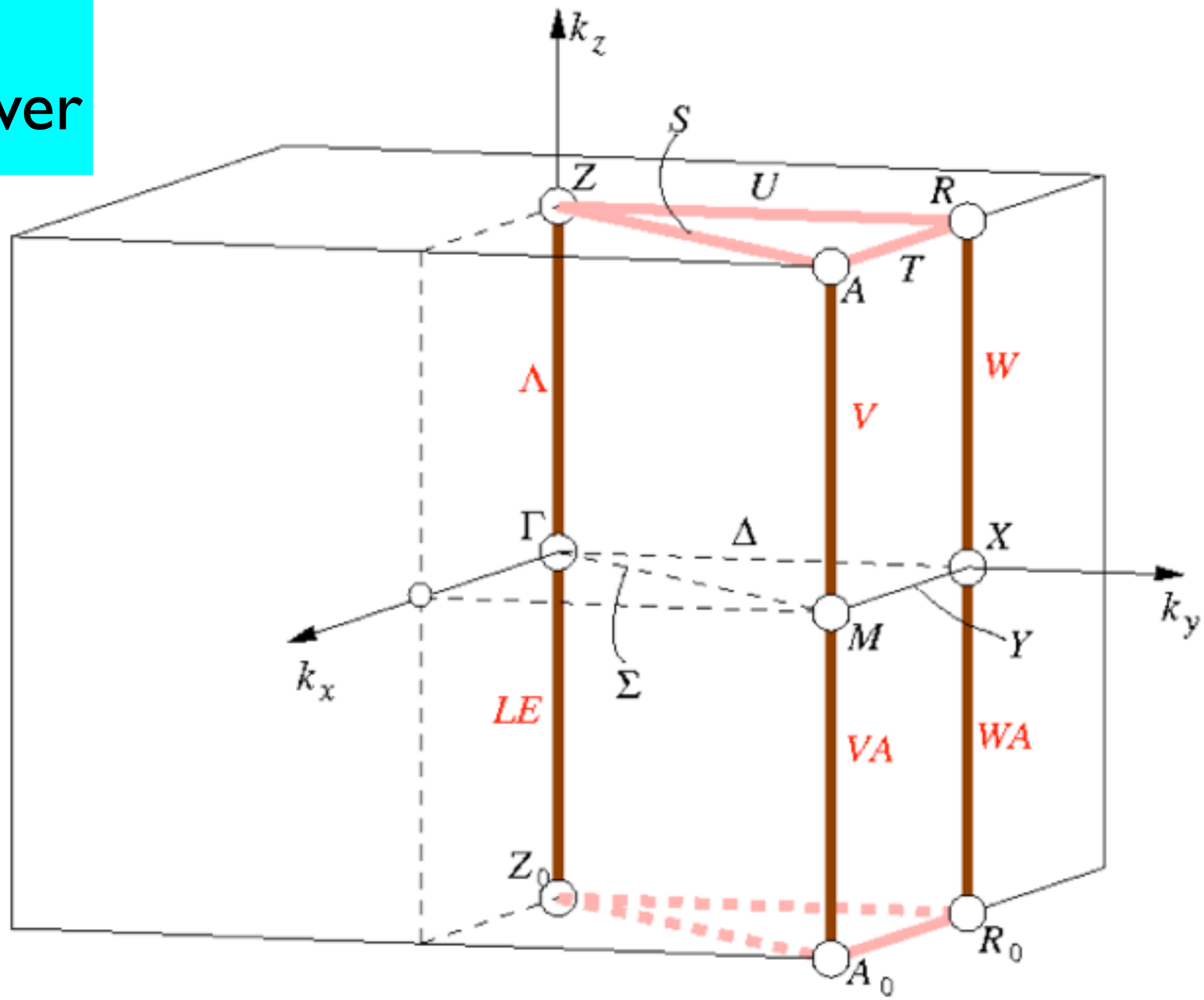
5.5 Crystal class $4mm$

5.5.1 Arithmetic crystal class $4mmP$

Fig. 5.5.1.1 Diagram for arithmetic crystal class $4mmP$

$P4mm - C_{4v}^{1}$ (99) to $P4_2bc - C_{4v}^{8}$ (106)

Reciprocal-space group $(P4mm)^*$, No. 99 see Tab. 5.5.1.1



SOLUTION

Problem 1

Irreps of P4mm, Γ(000) and X(01/20)

1. Space-group information

(a) Decomposition of *P4mm* relative to its translation subgroup;

coset representatives from IT A (1996):

$(\mathbf{1},\mathbf{o}),(\mathbf{2}_z,\mathbf{o}),(\mathbf{4},\mathbf{o}),(\mathbf{4}^{-1},\mathbf{o}),$
$(\mathbf{m}_{yz},\mathbf{o}),(\mathbf{m}_{xz},\mathbf{o}),(\mathbf{m}_{x\bar{x}},\mathbf{o}),(\mathbf{m}_{xx},\mathbf{o})$

(b) generators of *P4mm* from IT A (1996)
$\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3,(\mathbf{2}_z,\mathbf{o}),(\mathbf{4},\mathbf{o}),\ (\mathbf{m}_{yz},\mathbf{o})$

2. $\vec{k}$-vector information

(a) X (0, 1/2, 0)

(b) little co-group $\overline{\mathcal{G}}^X = \{\mathbf{1},\ \mathbf{2}_z,\ \mathbf{m}_{yz},\ \mathbf{m}_{xz}\} =$ $2_z m_{yz} m_{xz}$

$$e.g.,\ X\,2_z = (0,\,1/2,\,0)\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} =$$

$$(0,\,-1/2,\,0) = (0,\,1/2,\,0) + (0,\,\bar{1},\,0)$$

And the little co-group of Γ(000)?

(c) $\vec{k}$-vector star: $\star X = \{(0, 1/2, 0), (1/2, 0, 0)\}$ coset representative of $\overline{G} = 4mm$ relative to $\overline{G}^{\mathbf{k}} = 2_z m_{yz} m_{xz}$, HM symbol $mm2$

$4mm = 2_z m_{yz} m_{xz} \cup \mathbf{m}_{xx}\, 2_z m_{yz} m_{xz}$

(d) little group $\mathcal{G}^X = P2_z m_{yz} m_{xz}$, HM symbol $Pmm2$

(e) decomposition of $P4mm$ relative to $P2_z m_{yz} m_{xz}$

$P4mm = P2_z m_{yz} m_{xz} \cup (\mathbf{m}_{xx}, \mathbf{o}) P2_z m_{yz} m_{xz}$

And for the point Γ(000)?

3. Allowed irreps of $\mathcal{G}^X$

Because $\mathcal{G}^X$ is a symmorphic group,

$$\mathbf{D}^{X,i}(\widetilde{W}_i, \tilde{w}_i) = \exp -(i\,\mathbf{X}\,\tilde{\mathbf{w}}_i)\,\overline{\mathbf{D}}^{X,i}(\widetilde{W}_i)$$

$P2_zmm$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{2}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$
$\boldsymbol{D}^{X,1}$	1	1	1	1	$\exp -(i\,\mathbf{X}\,\mathbf{t})$
$\boldsymbol{D}^{X,2}$	1	1	-1	-1	$= \exp -(i\pi n_2)$
$\boldsymbol{D}^{X,3}$	1	-1	1	-1	$= (-1)^{n_2}$
$\boldsymbol{D}^{X,4}$	1	-1	-1	1	

$\boldsymbol{t}$ is the column of integer coefficients (n_1, n_2, n_3)

And for the point Γ(000)?

4. Induction procedure

Generators of $P4mm$: $\langle(\boldsymbol{W}_l,\ \boldsymbol{w}_l)\rangle = \langle(\boldsymbol{1}, \boldsymbol{t}_i),\ (\boldsymbol{4}, \boldsymbol{o}),\ (\boldsymbol{m}_{yz}, \boldsymbol{o})\rangle$

Representatives of $P2_z m_{yz} m_{xz}$ relative to $\mathcal{T}$:

$\{(\widetilde{W}_j,\ \tilde{w}_j)\} = \{(\boldsymbol{1}, \boldsymbol{o}),\ (\boldsymbol{2}_z, \boldsymbol{o}), (\boldsymbol{m}_{yz}, \boldsymbol{o}),\ (\boldsymbol{m}_{xz}, \boldsymbol{o})\}$

Coset representatives of $P4mm$ relative to $P2_z m_{yz} m_{xz}$:

$\{q_1,\ q_2\} = \{(\boldsymbol{1}, \boldsymbol{o}),\ (\boldsymbol{m}_{xx}, \boldsymbol{o})\}$.

Induction matrix

$(\boldsymbol{W}_l, \boldsymbol{w}_l)$	q_i	q_i^{-1}	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)$	q_j	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)\, q_j = (\widetilde{W}_j, \tilde{w}_j)$	$M_{ij} \neq 0$
$(\boldsymbol{1}, \boldsymbol{t})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$	11
	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{m}_{xx}\boldsymbol{t})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{m}_{xx}\boldsymbol{t})$	22
$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	11
	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{4}^{-1}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	22
$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	12
	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	21

(b) Matrices of the irreps $\mathbf{D}^{*X,\,i}$ of $\mathcal{G}$

$$\mathbf{D}^{*X,\,i}(\mathbf{1},\,\mathbf{t}) = \left(\begin{array}{c|c} \mathbf{D}^{X,\,i}(\mathbf{1},\,\mathbf{t}) & \mathbf{O} \\ \hline \mathbf{O} & \mathbf{D}^{X,\,i}(\mathbf{1},\,\mathbf{m}_{xx}\mathbf{t}) \end{array}\right);$$

$$\mathbf{D}^{*X,\,i}(\mathbf{m}_{yz},\,\mathbf{o}) = \left(\begin{array}{c|c} \mathbf{D}^{X,\,i}(\mathbf{m}_{yz},\,\mathbf{o}) & \mathbf{O} \\ \hline \mathbf{O} & \mathbf{D}^{X,\,i}(\mathbf{m}_{xz},\,\mathbf{o}) \end{array}\right)$$

$$\mathbf{D}^{*X,\,i}(\mathbf{4},\,\mathbf{o}) = \left(\begin{array}{c|c} \mathbf{O} & \mathbf{D}^{X,\,i}(\mathbf{m}_{yz},\,\mathbf{o}) \\ \hline \mathbf{D}^{X,\,i}(\mathbf{m}_{xz},\,\mathbf{o}) & \mathbf{O} \end{array}\right)$$

Table of irreps $\mathbf{D}^{*X,i}$ for the generators of $P4mm$ $\quad t =$

	(m_{yz}, o)	$(4, o)$	$(1, t)$
$\mathbf{D}^{*X,1}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,2}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,3}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,4}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$

EXERCISES

Problem 2

Consider a general ***k***-vector of a space group G. Determine its little co-group, the ***k***-vector star. How many arms has its star? How many full-group irreps will be induced and of what dimension? Write down the matrix of the full-group irrep of a general ***k***-vector of a translation.

SOLUTION

Problem 2

general k-vector k

irrep of T: Γ^k

little co-group $\overline{G}^k = \{1\}$

little group $G^k = T$

star of k, $k^* = \{kW_i, W_i \in \overline{G}\}$

allowed irrep: Γ^k

induction procedure

(W,w)	q_j	$(W,w)q_j$	q_i	$q_i^{-1}(W,w)q_j$	M_{ij}
(I,t)	(W_j,w_j)				

SOLUTION

Problem 2

$k^* = \{k, k', k'', \ldots, k^n\}$

$D^{k^*}(l,t) =$

exp-ikt					
	exp-ik't			0	
		exp-ik''t			
	0		...		
				...	
					exp-ik^{n}t