2019 年 2 月 8 日作成

Character Tables

HAMADA Noriaki

Tokyo University of Science

(reference)

柳瀬章「空間群のプログラム：TSPACE**」** (1995, **裳華房**).

犬井・田辺・小野寺「応用群論」 (1976, 2007, **裳華房**).

M. Lax, ”Symmetry Principles in Solid State and Molecular Physics”
(1974, Wiley, 2001, Dover).

Dresselhous, Dresselhous, Jorio, ”Group Theory” (2008, Springer).

P. Jacobs, ”Group Theory with Applications in Chemical Physics” (2005, Cambridge).

Bradley, Cracknell, ”The Mathematical Theory of Symmetry in Solids”
(1972, 2010, Oxford)

The group of $\boldsymbol{k}$

The point group of $\boldsymbol{k}$ ($\boldsymbol{k}$ point group):

$$P_{\boldsymbol{k}} = \left\{ \alpha \ : \ \ \alpha \boldsymbol{k} \doteq \boldsymbol{k} \right\}$$

The group of $\boldsymbol{k}$ ($\boldsymbol{k}$ group) :

$$\begin{aligned} G_{\boldsymbol{k}} &= \left\{ (\alpha | \boldsymbol{u}_\alpha + \boldsymbol{T}) \ : \ \ \alpha \in P_{\boldsymbol{k}} \right\} \\ &= \left\{ (\alpha | \boldsymbol{u}_\alpha + \boldsymbol{T}) \ : \ \ \alpha \boldsymbol{k} \doteq \boldsymbol{k} \right\} \end{aligned}$$

Irreducible representation of ”the group of $\boldsymbol{k}$”, $\Gamma^{(\lambda)}_{\boldsymbol{k}}\big((\alpha|\boldsymbol{u}_{\boldsymbol{\alpha}} + \boldsymbol{T})\big)$:

$$(\alpha|\boldsymbol{u}_{\boldsymbol{\alpha}} + \boldsymbol{T})\psi^{(\lambda)}_{\boldsymbol{k},i} = \sum_{j=1}^{d_\lambda} \psi^{(\lambda)}_{\boldsymbol{k},j} \, \Gamma^{(\lambda)}_{\boldsymbol{k}}\big((\alpha|\boldsymbol{u}_{\boldsymbol{\alpha}} + \boldsymbol{T})\big)_{ji}$$

where λ is the label of irreducible representation.

Irreducible representation of the group of $\boldsymbol{k}$

$$\Gamma_{\boldsymbol{k}}^{(\lambda)}\big((\alpha|\boldsymbol{u_\alpha}+\boldsymbol{T})\big) = \exp\big(-i\boldsymbol{k}\cdot\boldsymbol{T}\big)\ \exp\big(-i\boldsymbol{k}\cdot\boldsymbol{u_\alpha}\big)\ D_{\boldsymbol{k}}^{(\lambda)}\big((\alpha|\boldsymbol{u_\alpha})\big)\ ,$$

where the rotation α is restricted to leave $\boldsymbol{k}$ invariant ($\alpha \in P(\boldsymbol{k})$).

$$D_{\boldsymbol{k}}^{(\lambda)}\big((\alpha|\boldsymbol{u_\alpha})\big)D_{\boldsymbol{k}}^{(\lambda)}\big((\beta|\boldsymbol{u_\beta})\big) = \Phi(\alpha,\beta)D_{\boldsymbol{k}}^{(\lambda)}\big((\alpha\beta|\boldsymbol{u_{\alpha\beta}})\big)$$
$$\Phi(\alpha,\beta) = \exp\big(i\boldsymbol{G}_\alpha\cdot\boldsymbol{u_\beta}\big) \qquad \text{(factor system)}$$
$$\boldsymbol{G}_\alpha = \boldsymbol{k} - \alpha^{-1}\boldsymbol{k}$$

- On the Brillouin zone surface in nonsymmorphic space group,

  $\Phi(\alpha,\beta) \neq 1$: Ray representation (projective representation)
- Otherwise,

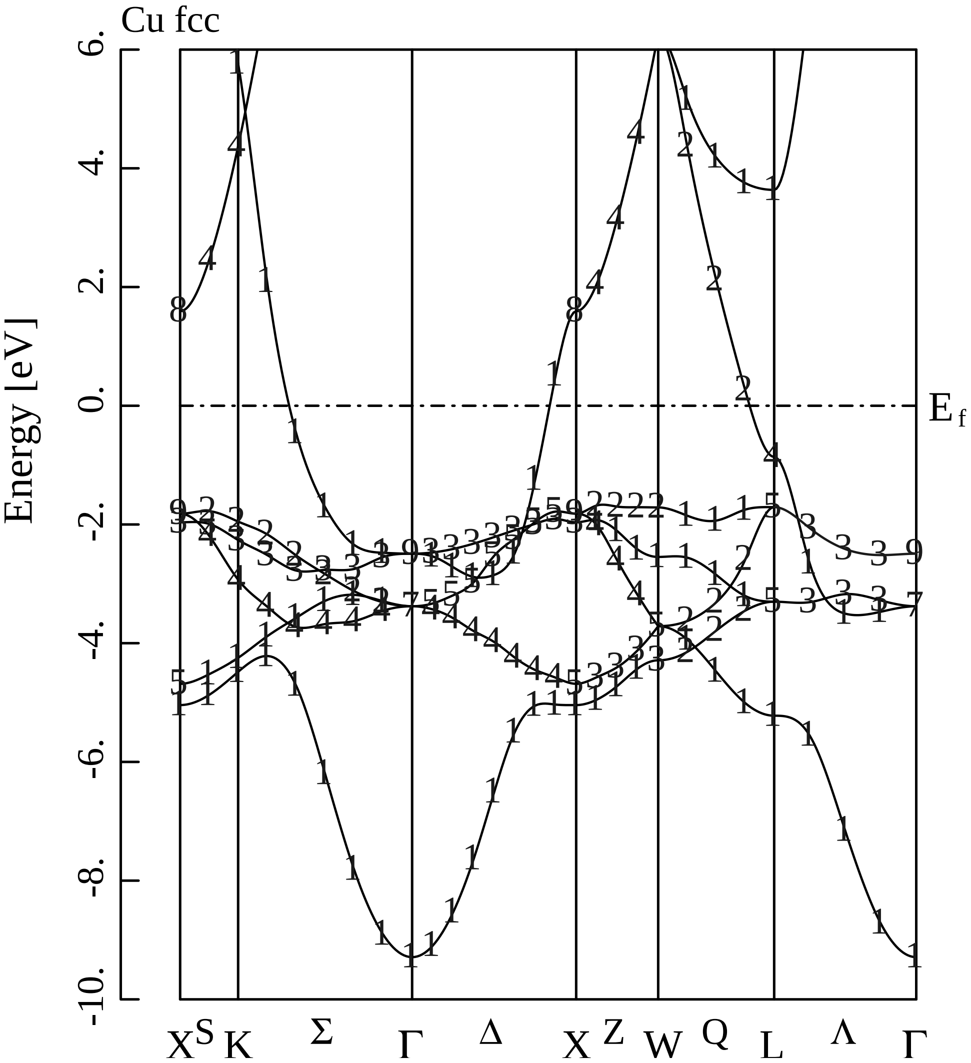
  $\Phi(\alpha,\beta) = 1$: usual point group representation

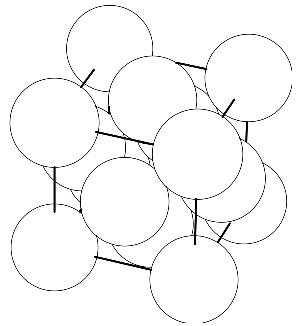
TSPACE gives the factor system in the form of

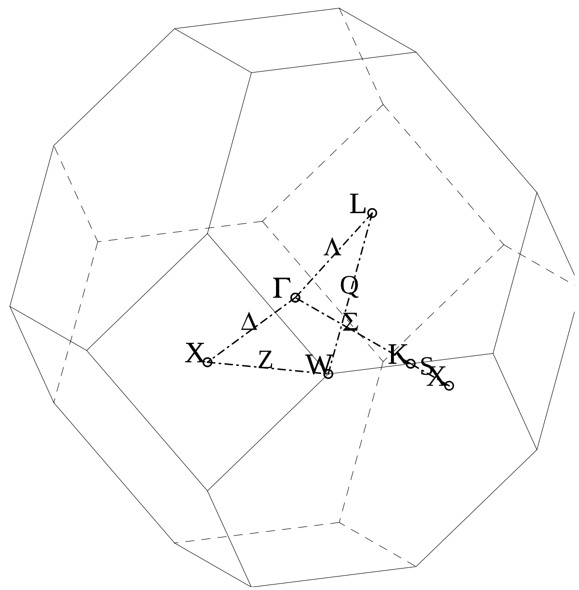
$$\Phi(\alpha,\beta) = \exp\left(2\pi i\frac{n}{m}\right) \qquad (n,m:\ \text{integer})$$

F$m\bar{3}m$ (225, O_h^5)

[Example] Cu fcc







Space group F$m\bar{3}m$ (fcc Ca, Ni, Cu, ...)

Γ point in F$m\bar{3}m$ (fcc Ca, Ni, Cu, ...)

O_h			E	$3C_2$	$8C_3$	$6C_2'$	$6C_4$	I	$3\sigma_h$	$8IC_3$	$6\sigma_d$	$6IC_4$
1	Γ_1	A_{1g}	1	1	1	1	1	1	1	1	1	1
3	Γ_2	A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
2	Γ_1'	A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
4	Γ_2'	A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
9	Γ_{12}	E_g	2	2	-1	0	0	2	2	-1	0	0
10	Γ_{12}'	E_u	2	2	-1	0	0	-2	-2	1	0	0
5	Γ_{15}'	T_{1g}	3	-1	0	-1	1	3	-1	0	-1	1
7	Γ_{25}'	T_{2g}	3	-1	0	1	-1	3	-1	0	1	-1
6	Γ_{15}	T_{1u}	3	-1	0	-1	1	-3	1	0	1	-1
8	Γ_{25}	T_{2u}	3	-1	0	1	-1	-3	1	0	-1	1
(T)	(B)	(M)										

(T): TSPACE code, (B): BSW notation at the Γ point, (M): Mulliken notation

Compatibility table in F$m\bar{3}m$ (fcc Ca, Ni, Cu, ...)

		1	3	2	4	9	10	5	7	6	8
		Γ_1	Γ_2	Γ'_1	Γ'_2	Γ_{12}	Γ'_{12}	Γ'_{15}	Γ'_{25}	Γ_{15}	Γ_{25}
1	Δ_1	1				1				1	
2	Δ'_1			1			1	1			
3	Δ_2		1			1					1
4	Δ'_2				1		1		1		
5	Δ_5							1	1	1	1

Δ axis in F$m\bar{3}m$ (fcc Ca, Ni, Cu, ...)

C_{4v}			E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_d$
1	Δ_1	A_1	1	1	1	1	1
2	Δ_1'	A_2	1	1	1	-1	-1
3	Δ_2	B_1	1	1	-1	1	-1
4	Δ_2'	B_2	1	1	-1	-1	1
5	Δ_5	E	2	-2	0	0	0
(T)	(B)	(M)					

(T): TSPACE code, (B): BSW notation at the Δ axis in F$m\bar{3}m$

(M): Mulliken notation

X point in F$m\bar{3}m$ (fcc Ca, Ni, Cu, ...)

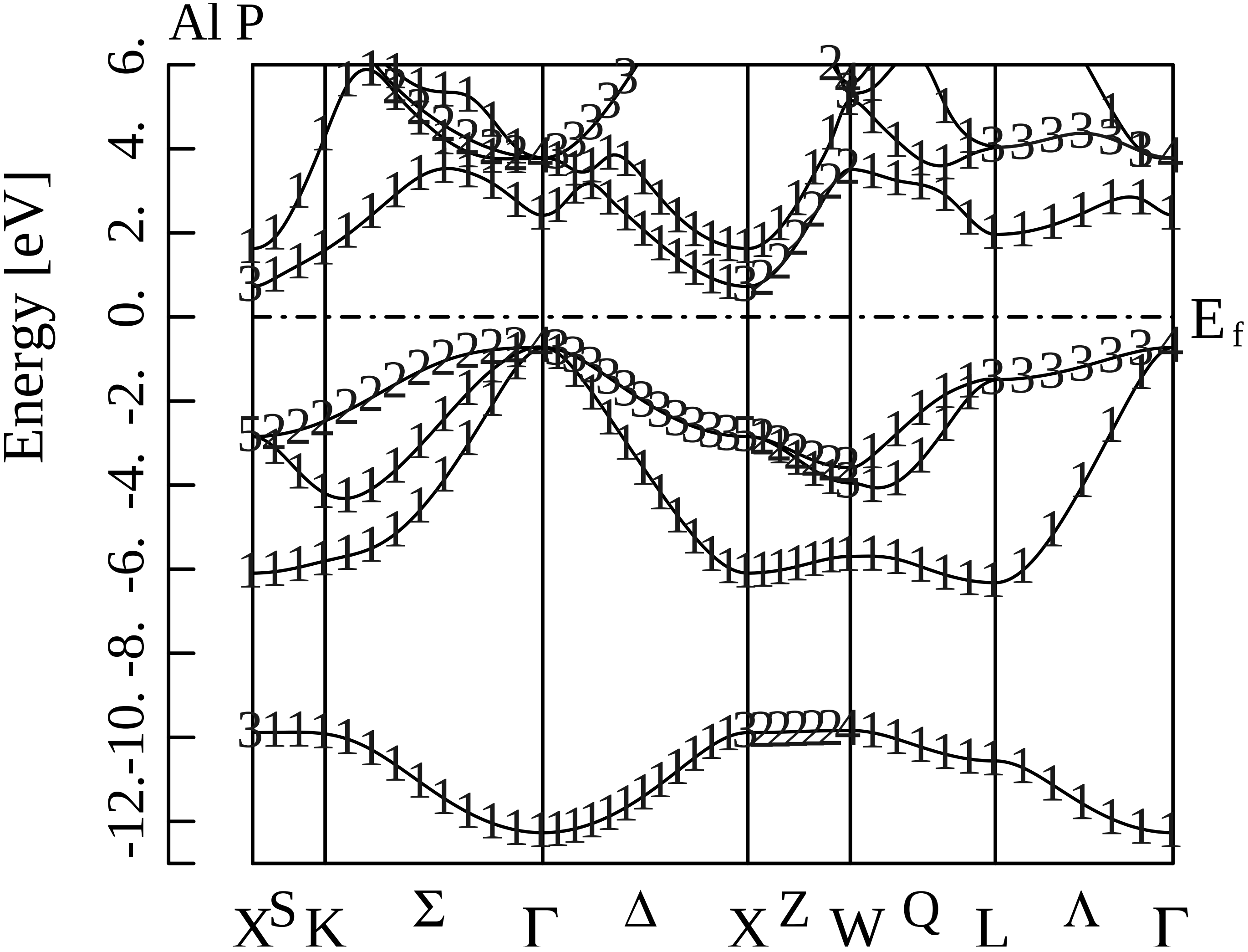
D_{4h}			E	C_2	$2C_2'$	$2C_2''$	$2C_4$	I	σ_h	$2\sigma_v$	$2\sigma_d$	$2IC_4$
1	X_1	A_{1g}	1	1	1	1	1	1	1	1	1	1
7	X_4	A_{2g}	1	1	-1	-1	1	1	1	-1	-1	1
2	X_1'	A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
8	X_4'	A_{2u}	1	1	-1	-1	1	-1	-1	1	1	-1
3	X_2	B_{1g}	1	1	1	-1	-1	1	1	1	-1	-1
5	X_3	B_{2g}	1	1	-1	1	-1	1	1	-1	1	-1
4	X_2'	B_{1u}	1	1	1	-1	-1	-1	-1	-1	1	1
6	X_3'	B_{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
9	X_5	E_g	2	-2	0	0	0	2	-2	0	0	0
10	X_5'	E_u	2	-2	0	0	0	-2	2	0	0	0
(T)	(B)	(M)										

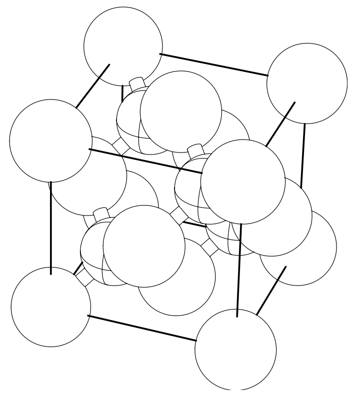
(T): TSPACE code, (B): BSW notation at the X point in cubic symmorphic

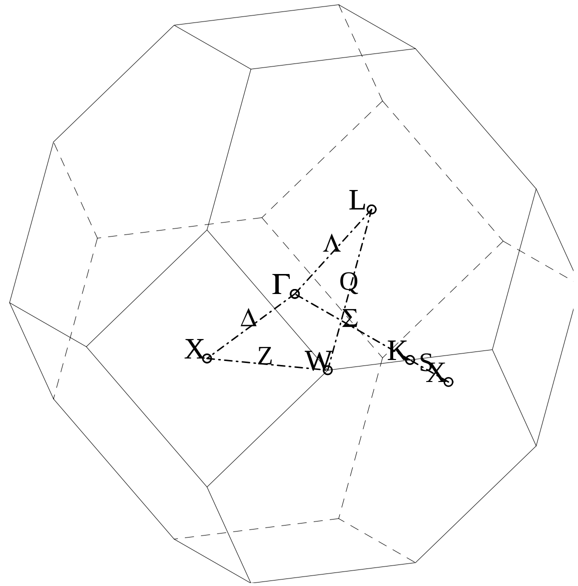
(M): Mulliken notation

F$\bar{4}3m$ (216, T_d^2)

[Example] AlP zinc blende







Space group F$\bar{4}3m$ (Zinc blende structure, AlP, GaAs, ...)

Γ point in F$\bar{4}3m$

T_d			E	$3C_2$	$8C_3$	$6\sigma_d$	$6IC_4$
1	Γ_1	A_1	1	1	1	1	1
2	Γ_2	A_2	1	1	1	-1	-1
5	Γ_{12}	E	2	2	-1	0	0
3	Γ_{25}	T_1	3	-1	0	-1	1
4	Γ_{15}	T_2	3	-1	0	1	-1
(T)	(B)	(M)					

(T): TSPACE code

(B): BSW notation at the Γ point in the zinc blende structure

R.H.Parmenter, Phys. Rev. 100, 573-579 (1955).

(M): Mulliken notation

Δ axis in F$\bar{4}3m$

C_{2v}			E	C_2	σ_v	σ'_v	T.R.sum
1	Δ_1	A_1	1	1	1	1	4
2	Δ_2	A_2	1	1	-1	-1	4
3	Δ_3	B_1	1	-1	1	-1	0
4	Δ_4	B_2	1	-1	-1	1	0
(T)	(B)	(M)					

(T): TSPACE code

(B): BSW notation at the Γ point in the zinc blende structure

R.H.Parmenter, Phys. Rev. 100, 573-579 (1955).

(M): Mulliken notation

TSPACE gives the degeneracy by the time-reversal symmetry. (Herring's rule)

Time reversal elements: c_{2y}, c_{2z}, ic_{4x}, ic_{4x}^{-1}

$\rightarrow$ Time Reversal Sum (T.R.sum) = 0 $\rightarrow$ Irreps. 3 and 4 degenerates.

X point (D_{2d}) in F$\bar{4}3m$

D_{2d}			E	C_2	$2C_2$	$2\sigma_d$	$2IC_4$
1	X_1	A_1	1	1	1	1	1
4	X_4	A_2	1	1	-1	-1	1
2	X_2	B_1	1	1	1	-1	-1
3	X_3	B_2	1	1	-1	1	-1
5	X_5	E	2	-2	0	0	0
(T)	(B)	(M)					

(T): TSPACE code

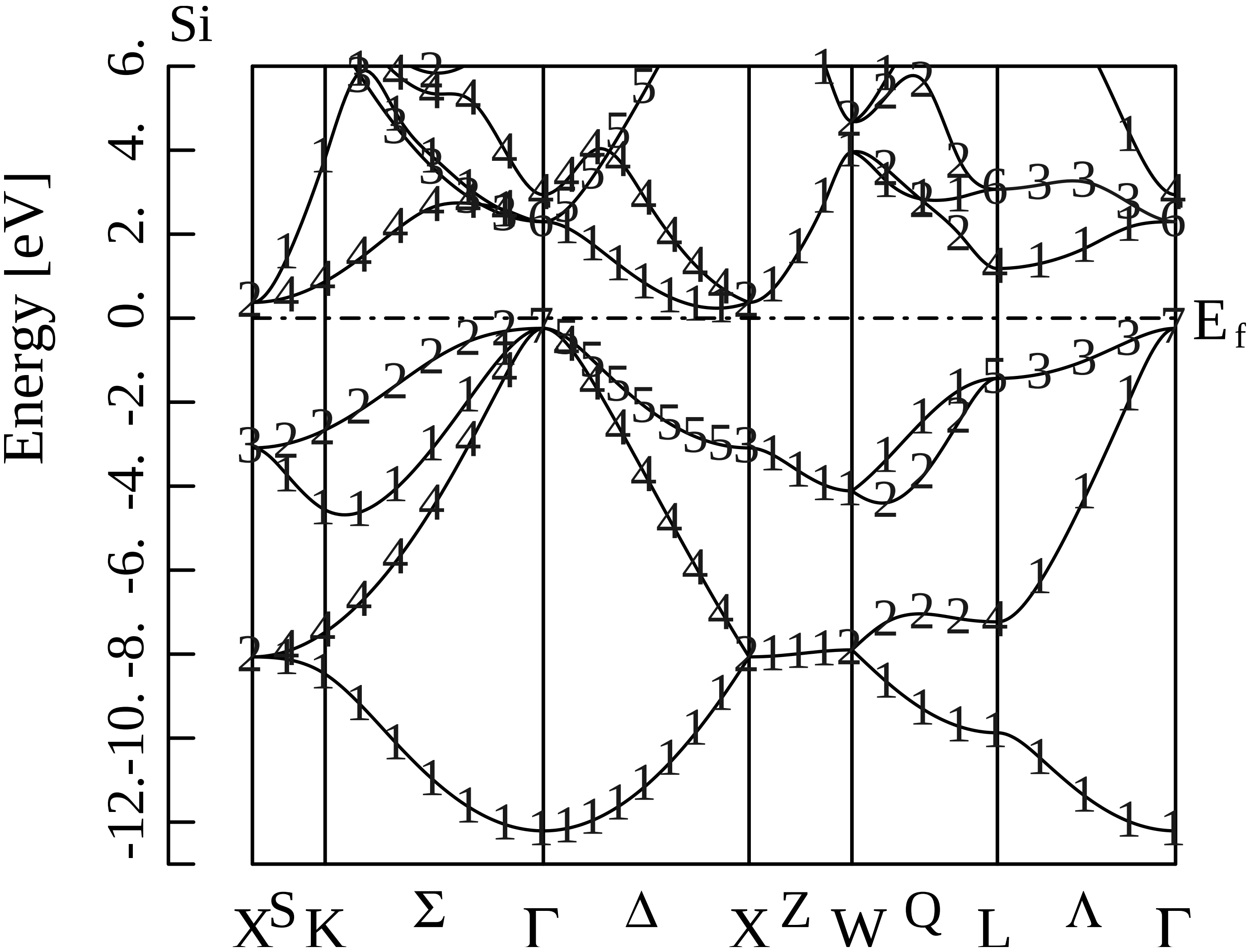
(B): BSW notation at the X point

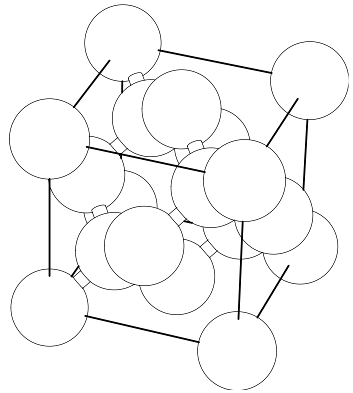
R.H.Parmenter, Phys. Rev. 100, 573-579 (1955).

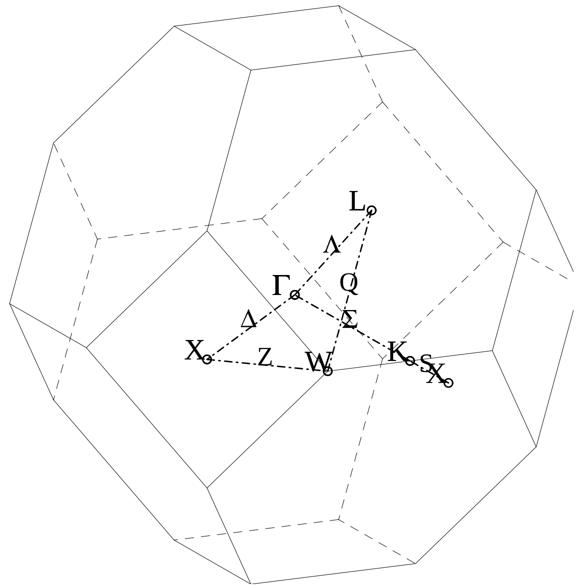
(M): Mulliken notation

F$d\bar{3}m$ (227, O_h^7)

[Example] Si diamond







Space group F$d\bar{3}m$ (diamond)

Γ point in F$d\bar{3}m$

O_h			E	$3C_2$	$8C_3$	$6C_2'$	$6C_4$	I	$3\sigma_h$	$8IC_3$	$6\sigma_d$	$6IC_4$
1	Γ_1	A_{1g}	1	1	1	1	1	1	1	1	1	1
3	Γ_2	A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
2	Γ_1'	A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
4	Γ_2'	A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
9	Γ_{12}	E_g	2	2	-1	0	0	2	2	-1	0	0
10	Γ_{12}'	E_u	2	2	-1	0	0	-2	-2	1	0	0
5	Γ_{15}'	T_{1g}	3	-1	0	-1	1	3	-1	0	-1	1
7	Γ_{25}'	T_{2g}	3	-1	0	1	-1	3	-1	0	1	-1
6	Γ_{15}	T_{1u}	3	-1	0	-1	1	-3	1	0	1	-1
8	Γ_{25}	T_{2u}	3	-1	0	1	-1	-3	1	0	-1	1
(T)	(B)	(M)										

(T): TSPACE code, (B): BSW notation at the Γ point, (M): Mulliken notation

X point in F$d\bar{3}m$ (diamond)

		(E,0)	(C$_2$,0)	(C$'_2$,$\boldsymbol{u}_d$)	(C$''_2$,$\boldsymbol{u}_d$)	2(σ_d,0)
2	X_1	2	2	0	0	2
1	X_2	2	2	0	0	-2
3	X_3	2	-2	-2	2	0
4	X_4	2	2	2	-2	0
(T)	(B)			(T): i	(T): i	

$\boldsymbol{u}_d = (1/4, 1/4, 1/4)a$

Factor system is needed for the ray representation.

(T): TSPACE code

(B): BSW notation at the X point in diamond (nonsymmorphic)

(See Lax's book!)

X point in F$d\bar{3}m$ (diamond)

$$\chi_{\boldsymbol{k}}^{(\lambda)}\big((\alpha|\boldsymbol{u_\alpha})\big) = \exp\big(-i\boldsymbol{k}\cdot\boldsymbol{u_\alpha}\big)\ Tr\ D_{\boldsymbol{k}}^{(\lambda)}\big((\alpha|\boldsymbol{u_\alpha})\big)$$

		E	C_2	$2C_2$	$(C_2'\|\boldsymbol{u})$	$(C_2''\|\boldsymbol{u})$	$2(C_4\|\boldsymbol{u})$	$(I\|\boldsymbol{u})$	$(\sigma_h\|\boldsymbol{u})$	$2(\sigma_v\|\boldsymbol{u})$	$2\sigma_d$	$2IC_4$
2	X_1	2	2	0	0	0	0	0	0	0	2	0
1	X_2	2	2	0	0	0	0	0	0	0	-2	0
3	X_3	2	-2	0	-2	2	0	0	0	0	0	0
4	X_4	2	-2	0	2	-2	0	0	0	0	0	0
(T)	(B)				(T): i	(T): i						

$\boldsymbol{u} = (1/4, 1/4, 1/4)a$, TSPACE code gives $D_{\boldsymbol{k}}^{(\lambda)}\big((\alpha|\boldsymbol{u_\alpha})\big)$.

Factor system is needed for the ray representation. (See TSPACE output!)

(T): TSPACE code

(B): BSW notation at the X point in diamond (nonsymmorphic)

(See Lax's book!)