CMS II-4: band theory, band structure, k-point sampling, and density of state

Horng-Tay Jeng
(鄭弘泰)
Institute of Physics, Academia Sinica
May 24, 2007

Band theory

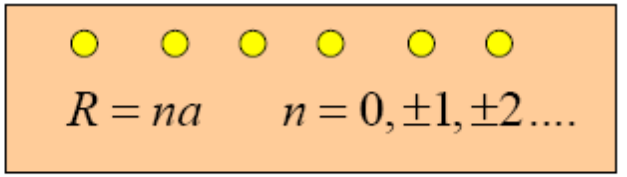
Bloch Theorem

In the presence of a periodic potential $\left(V(\vec{r}+\vec{R})=V(\vec{r})\right)$

$$\psi(\vec{r}+\vec{R})=\exp(i\vec{k}\cdot\vec{R})\psi(\vec{r})$$

where $\vec{R}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$

Proof: Bloch theorem in 1 D



if $V(x+R) = V(x)$

then $\psi(x+R) = \exp(ikR)\psi(x)$

Define T_R (translation operation)

$$T_R[H(x)\psi(x)] = H(x+R)\psi(x+R) = H(x)\psi(x+R) = H(x)T_R\psi(x)$$

$$\therefore [T_R, H] = 0 \quad \Rightarrow \quad \begin{cases} H\psi_n = E_n\psi_n \\ T_R\psi_n = C(R)\psi_n \end{cases}$$

$$\therefore T_R\psi(x) = \psi(x+R) = C(R)\psi(x)$$

☆ T_R and H commute: they have common eigen states

$$T_a T_a \psi(x) = \psi(x+2a) = T_{2a}\psi(x) \qquad \Rightarrow C(a)C(a) = C(2a)$$

$$C(a) = e^{ika}; \qquad C(2a) = C(a)C(a) = e^{i2ka} \qquad C(R) = e^{ikR}$$

Proof: Bloch theorem in 3 D $\quad \vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Define $T_{\vec{R}}$ (translation operation) : $T_{\vec{R}}\psi(\vec{r}) = \psi(\vec{r}+\vec{R})$

$$T_{\vec{R}}[H(\vec{r})\psi(\vec{r})] = H(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R}) = H(\vec{r})\psi(\vec{r}+\vec{R}) = H(\vec{r})T_{\vec{R}}\psi(\vec{r})$$

$$\therefore [T_{\vec{R}}, H] = 0 \Rightarrow \begin{cases} H\psi_n = E_n\psi_n \\ T_{\vec{R}}\psi_n = C(\vec{R})\psi_n \end{cases}$$

$$T_{\vec{R}}\psi(\vec{r}) = \psi(\vec{r}+\vec{R}) = C(\vec{R})\psi(\vec{r})$$

$$\int |\psi(\vec{r}+\vec{R})|^2 \, d^3r = \int |C(\vec{R})|^2 |\psi(\vec{r})|^2 \, d^3r = \int |\psi(\vec{r})|^2 d^3r$$

$$|C(\vec{R})|^2 = 1 \qquad \Rightarrow C(\vec{R}) = e^{i\theta(\vec{R})}$$

$$T_{\vec{R}}T_{\vec{R}'}\psi(\vec{r}) = T_{\vec{R}'}T_{\vec{R}}\psi(\vec{r}) = \psi(\vec{r}+\vec{R}+\vec{R}')$$

$$T_{\vec{R}}T_{\vec{R}'}\psi(\vec{r}) = T_{\vec{R}'}T_{\vec{R}}\psi(\vec{r}) = T_{\vec{R}+\vec{R}'}\psi(\vec{r})$$

$$C(\vec{R}')C(\vec{R}) = C(\vec{R})C(\vec{R}') = C(\vec{R}+\vec{R}') \Rightarrow C(\vec{R}) = \exp(i\vec{k}\cdot\vec{R})$$

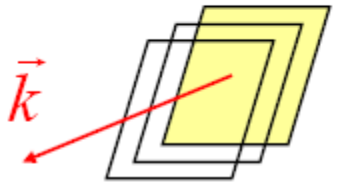
Another form of the Bloch function

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r}) \qquad where \quad u(\vec{r}+\vec{R}) = u(\vec{r})$$

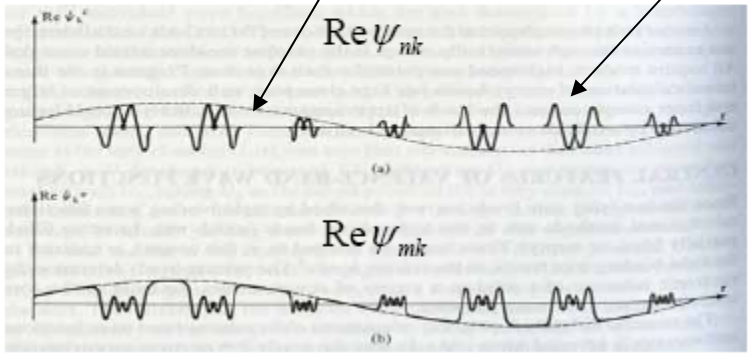
Proof:
$$\psi_k(\vec{r}+\vec{R}) = \exp[i\vec{k}\cdot(\vec{r}+\vec{R})]u(\vec{r}+\vec{R})$$
$$= \exp(i\vec{k}\cdot\vec{R})\exp(i\vec{k}\cdot\vec{r})u(\vec{r})$$
$$= \exp(i\vec{k}\cdot\vec{R})\psi_k(\vec{r})$$

What is the physical meaning of $\vec{k}$?

$$e^{i\vec{k}\cdot\vec{r}} = \cos(\vec{k}\cdot\vec{r}) + i\sin(\vec{k}\cdot\vec{r})$$



$$k = \frac{2\pi}{\lambda}$$



For a system with spherical symmetry $V(\vec{r}) = V(r)$

$$\left[H, L^2\right] = 0 \quad ; \quad \left[H, L_z\right] = 0$$

$$\begin{cases} H\psi_{nlm} = E_{nlm}\psi_{nlm} \\ L^2\psi_{nlm} = l(l+1)\hbar\psi_{nlm} \\ L_z\psi_{nlm} = m\hbar\psi_{nlm} \end{cases} \quad ; \quad \psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$$

Meaning of l,m ⟹ $Y_{lm}(\theta,\phi)$

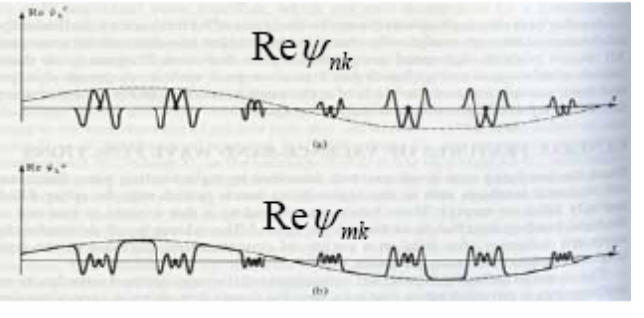
$$Y_{00} = \frac{1}{\sqrt{4\pi}}; \quad Y_{11} = -\sqrt{\frac{3}{8\pi}}e^{i\phi}\sin\theta; \quad Y_{1-1} = \sqrt{\frac{3}{8\pi}}e^{-i\phi}\sin\theta; \quad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

For a system with translational symmetry $V(\vec{r} + \vec{R}) = V(\vec{r})$

$$\left[H, T\right] = 0$$

$$\begin{cases} H\psi_{nk} = E_{nk}\psi_{nk} \\ T(\vec{R})\psi_{nk} = e^{i\vec{k}\cdot\vec{R}}\psi_{nk} \end{cases} \quad ; \quad \psi_{nk} = e^{i\vec{k}\cdot\vec{r}}u_{nk}(\vec{r})$$

$\vec{k}$ is continue ⟹ energy band



General remarks about Bloch's Theorem

(1) ψ_{nk} is not a momentum eigenstate, $\hbar\vec{k}$ is crystal momentum

$$\vec{p}\psi_{nk} = \frac{\hbar}{i}\vec{\nabla}\psi_{nk} = \frac{\hbar}{i}\vec{\nabla}[e^{i\vec{k}\cdot\vec{r}}u_{nk}(\vec{r})]$$

$$= \hbar\vec{k}\psi_{nk} + e^{i\vec{k}\cdot\vec{r}}\frac{\hbar}{i}\vec{\nabla}u_{nk}(\vec{r})$$

(2) $\vec{k}$ can always be confined to the first B.Z.

let $\vec{k}' = \vec{k} + \vec{G}$ (exp(i**G** · **R**)=1)

$$\because \exp(i\vec{k}'\cdot\vec{R}) = \exp[i(\vec{k}+\vec{G})\cdot\vec{R}] = \exp(i\vec{k}\cdot\vec{R})$$

$$\therefore \psi_{n\vec{k}'}(\vec{r}+\vec{R}) = \exp(i\vec{k}'\cdot\vec{R})\psi_{n\vec{k}'}(\vec{r}) = \exp(i\vec{k}\cdot\vec{R})\psi_{n\vec{k}'}(\vec{r})$$

=> $\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r})$

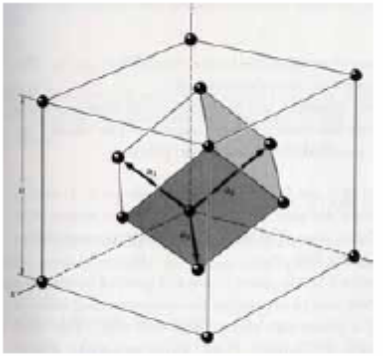
$E_{n,\vec{k}+\vec{G}} = E_{n,\vec{k}}$

Block theorem holds for Ψ_{nk}(**r**)

and also holds for Ψ_{nk}' (**r**)

(3) It can be reduced to a hermitian eigenvalue problem which is restricted to a single primitive cell of the crystal

$$H\psi_{nk} = E_{nk}\psi_{nk} \qquad where \quad H = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})$$



$$let \quad \psi_{nk}(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})u_{nk}(\vec{r})$$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_{nk}(\vec{r}) = -\frac{\hbar^2}{2m}\vec{\nabla}\cdot[\vec{\nabla}e^{i\vec{k}\cdot\vec{r}}u_{nk}(\vec{r})]$$

$$= -\frac{\hbar^2}{2m}\vec{\nabla}[e^{i\vec{k}\cdot\vec{r}}(i\vec{k}u_{nk} + \vec{\nabla}u_{nk})] = -\frac{\hbar^2}{2m}e^{i\vec{k}\cdot\vec{r}}(i\vec{k} + \vec{\nabla})^2 u_{nk}(\vec{r})$$

$$H_k u_{nk} = E_{nk}u_{nk}(\vec{r}) \qquad where \quad H_k = -\frac{\hbar^2}{2m}(i\vec{k} + \vec{\nabla})^2 + U(\vec{r})$$

$$with \quad B.C. \qquad u_{nk}(\vec{r}) = u_{nk}(\vec{r} + \vec{R})$$

Partial differential equation with complicate boundary condition

We can reduce this complicate boundary value problem to a simple matrix digonalization problem using variational principle.

$$H_k u_{nk} = E_{nk} u_{nk}(\vec{r}) \qquad where \quad H_k = -\frac{\hbar^2}{2m}(i\vec{k} + \vec{\nabla})^2 + U(\vec{r})$$

Choose a basis function $\chi_n(\vec{r})$ $\qquad$ *where* $\qquad \chi_n(\vec{r} + \vec{R}) = \chi_n(\vec{r})$

$$u_k(\vec{r}) = \sum_n C_n \chi_n(\vec{r})$$

Minimize $\quad \langle u_k \mid H_k \mid u_k \rangle$ with constraint $\langle u_k \mid u_k \rangle = 1$

$$\frac{\partial}{\partial C_l^*} \left\langle \sum_n C_n \chi_n \mid H_k \mid \sum_m C_m \chi_m \right\rangle - \lambda \frac{\partial}{\partial C_l^*} \left\langle \sum_n C_n \chi_n \mid \sum_m C_m \chi_m \right\rangle = 0$$

$$\frac{\partial}{\partial C_l^*}\left\langle \sum_n C_n \chi_n \mid H_k \mid \sum_m C_m \chi_m \right\rangle - \lambda \frac{\partial}{\partial C_l^*}\left\langle \sum_n C_n \chi_n \mid \sum_m C_m \chi_m \right\rangle = 0$$

$$\frac{\partial}{\partial C_l^*}\sum_n \sum_m C_n^* C_m H_{nm}(K) - \lambda \frac{\partial}{\partial C_l^*}\sum_n \sum_m C_n^* C_m S_{nm} = 0$$

$$\sum_m H_{lm}(k) C_m - \lambda \sum_m S_{lm} C_m = 0$$

$$\Rightarrow \boxed{\underset{\sim}{H}(\vec{k})\underset{\sim}{C} - \lambda \underset{\sim}{S}\underset{\sim}{C} = 0}$$

Matrix digonalization problem

where $H_{lm}(k) = \langle \chi_l \mid H_k \mid \chi_m \rangle \quad ; \quad S_{lm} = \langle \chi_l \mid \chi_m \rangle$

$$\Rightarrow \lambda_1; \underset{\sim}{C}^{(1)} \quad , \lambda_2; \underset{\sim}{C}^{(2)} \; \lambda_3; \underset{\sim}{C}^{(3)} \ldots\ldots\ldots \lambda_n; \underset{\sim}{C}^{(N)} \qquad (\varepsilon_{nk}, \psi_{nk})$$

Band structure:

k-dependence of eigenvalues (bands)

How many electrons can be occupied in a band ?

1-D Periodic b.c. $\psi(x+Na)=\psi(x)$ *where* $N\to\infty$

$$\psi(x+Na)=e^{ikNa}\psi(x)=\psi(x)$$

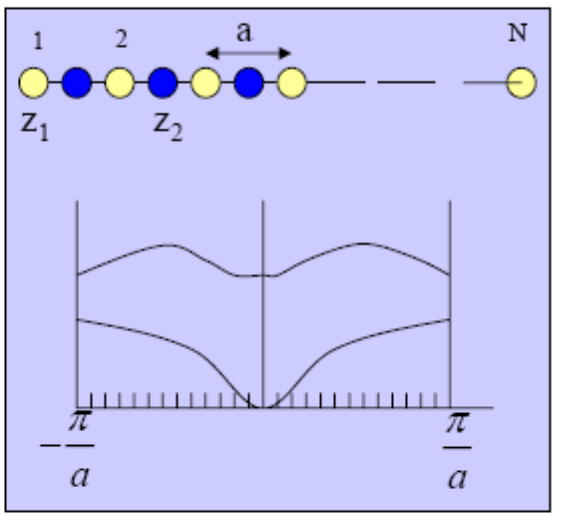
$$Nka = 2\pi m \qquad m = \text{integer}$$

k=2 π m/Na, b=2 π /a

So the allowed Bloch wave vector is $k=\frac{m}{N}b$

-b/2=- π /a<k< π /a=b/2

# of state in the 1BZ $= N$



$\frac{z_1+z_2}{2}$ bands are filled

Each band can occupy 2N electrons per supercell (2 electrons per unit cell).

3-D

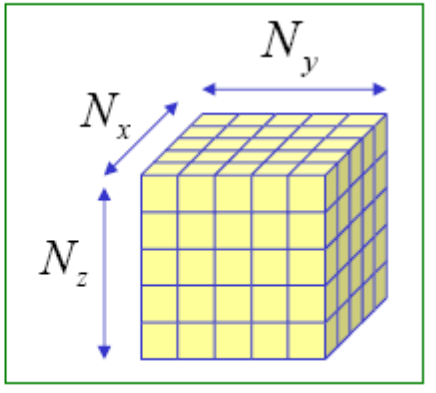
Periodic b.c. $\psi(\vec{r}+N_i\vec{a}_i)=\psi(\vec{r})$ $i=1,2,3$ *where* $N_i\to\infty$

$$\psi(\vec{r}+N_i\vec{a}_i)=e^{i\vec{k}\cdot N_i\vec{a}_i}\psi(\vec{r})=\psi(\vec{r}) \qquad \text{where} \quad \vec{k}=x_1\vec{b}_1+x_2\vec{b}_2+x_3\vec{b}_3$$

$$N_i\vec{k}\cdot\vec{a}_i=2\pi N_i x_i=2\pi m_i \qquad m_i=\text{integer}$$

$$\Rightarrow \quad x_i=\frac{m_i}{N_i} \qquad m_i=0,\pm1,\pm2,....$$

So the allowed Bloch wave vector is $\vec{k}=\sum_{i=1}^{3}\frac{m_i}{N_i}\vec{b}_i$



$$\Delta\vec{k}=\frac{\vec{b}_1}{N_1}\cdot\left(\frac{\vec{b}_2}{N_2}\times\frac{\vec{b}_3}{N_3}\right)=\frac{1}{N_1N_2N_3}\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)=\frac{1}{N}\frac{(2\pi)^3}{\Omega}=\frac{(2\pi)^3}{V}$$

$$\#\text{ of state in the 1BZ}=\frac{vol.\ \ of\ \ 1B.Z.}{\Delta\vec{k}}=\frac{\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}{\frac{1}{N}\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}=N$$

Each band can occupy 2N electrons per supercell (2 electrons per unit cell).

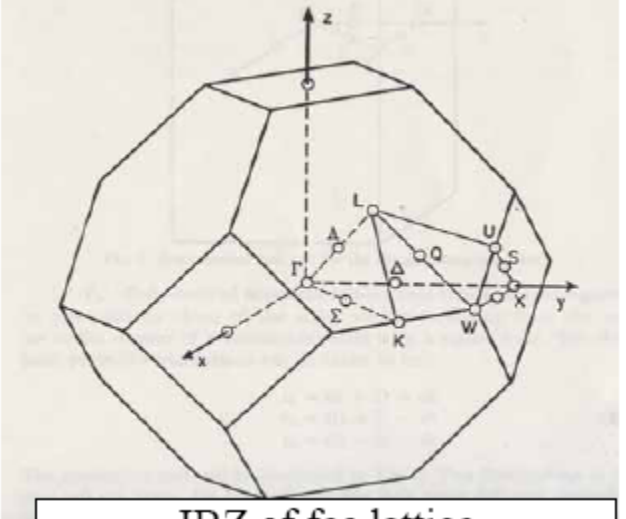
Example: 3 D

Copper (Cu) : fcc structure

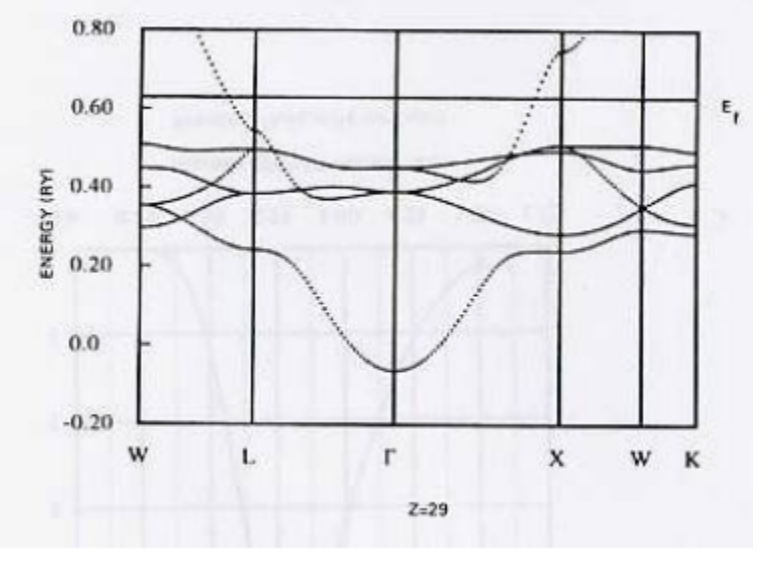
$$\vec{a}_1 = \frac{a}{2}\left(\vec{j} + \vec{k}\right) \qquad \vec{b}_1 = \frac{4\pi}{a}\frac{1}{2}\left(-\vec{i} + \vec{j} + \vec{k}\right)$$

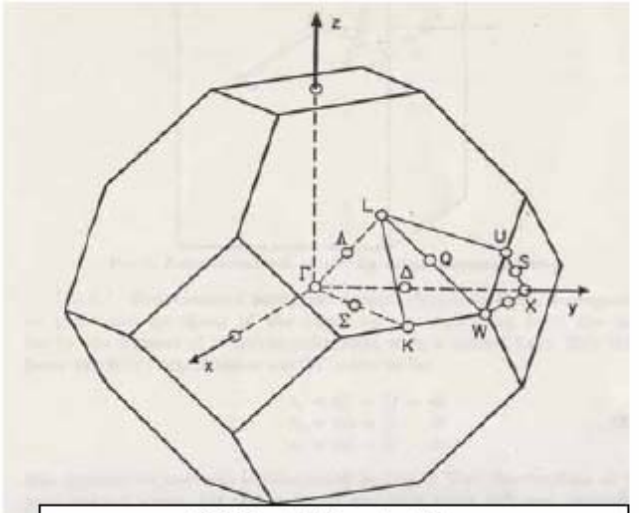
$$\vec{a}_2 = \frac{a}{2}\left(\vec{i} + \vec{k}\right) \qquad \vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}\left(\vec{i} - \vec{j} + \vec{k}\right)$$

$$\vec{a}_3 = \frac{a}{2}\left(\vec{i} + \vec{j}\right) \qquad \vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}\left(\vec{i} + \vec{j} - \vec{k}\right)$$



IBZ of fcc lattice





IBZ of fcc lattice

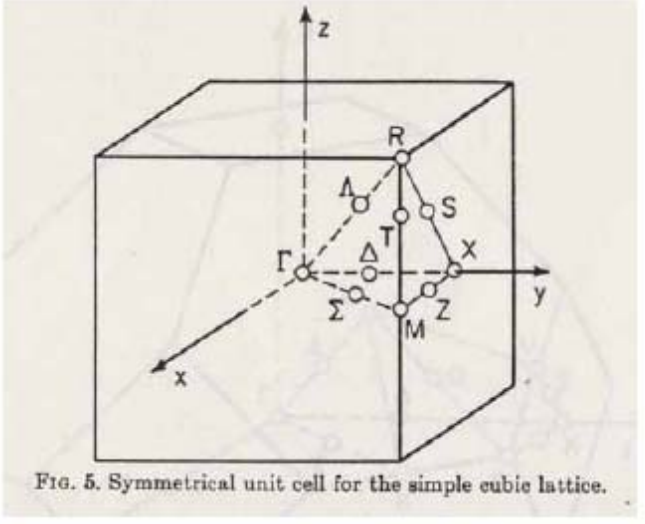
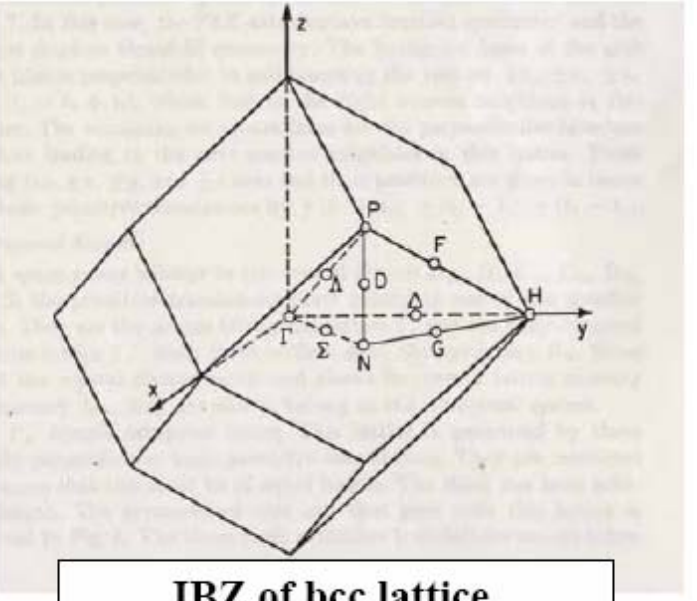


FIG. 5. Symmetrical unit cell for the simple cubic lattice.



IBZ of bcc lattice

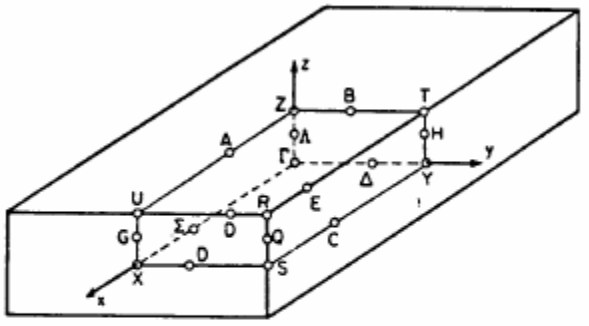


FIG. 10. Symmetrical unit cell for the simple orthorhombic lattice.

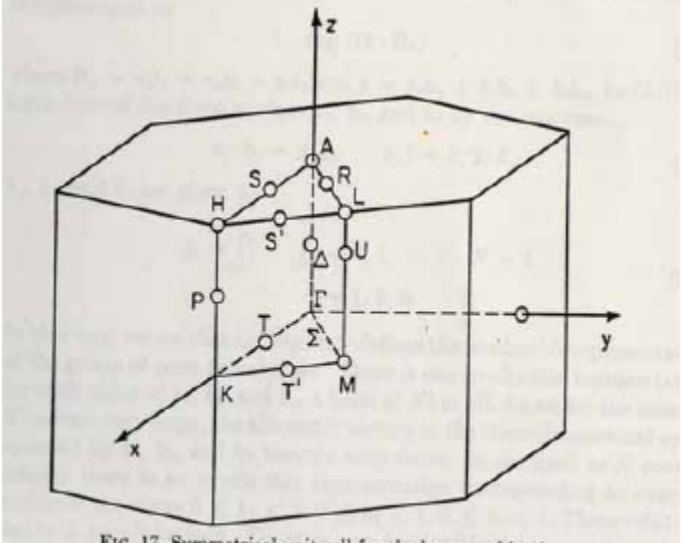


FIG. 17. Symmetrical unit cell for the hexagonal lattice.

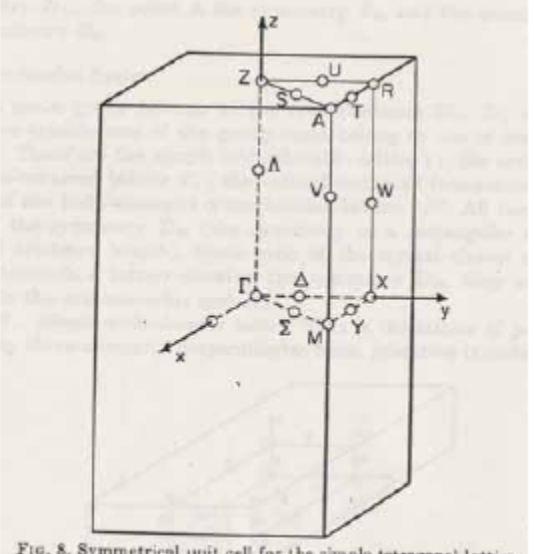


FIG. 8. Symmetrical unit cell for the simple tetragonal lattice.

K-point sampling

Monkhorst and Pack (1976):

Idea: equally spaced mesh in Brillouin-zone.

Construction-rule:

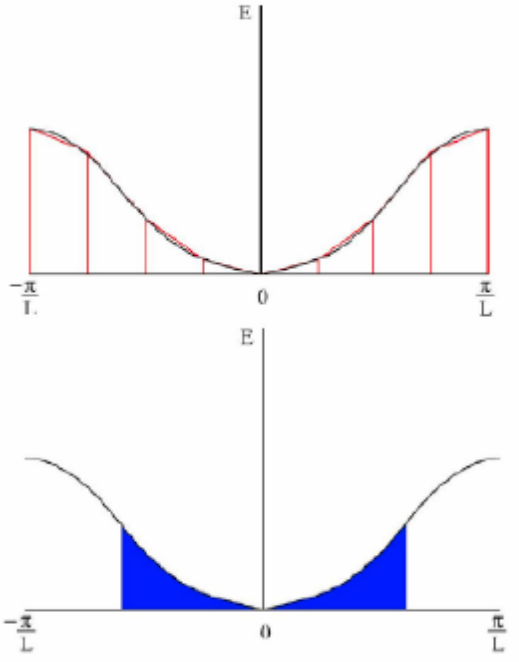
$$\mathbf{k}_{prs} = u_p \mathbf{b}_1 + u_r \mathbf{b}_2 + u_s \mathbf{b}_3$$

$$u_r = \frac{2r - q_r - 1}{2q_r} \qquad r = 1, 2, \ldots, q_r$$

$\mathbf{b}_i$ reciprocal lattice-vectors

q_r determines number of k-points in r-direction

Integrating Over The First Brillouin Zone



- Observables are calculated as integrals over all k-points within the first Brillouin zone:

$$E_{\text{tot}} = \frac{1}{V_{\text{BZ}}} \int_{1^{\text{st}}\text{BZ}} E(\mathbf{k}) d\mathbf{k}$$

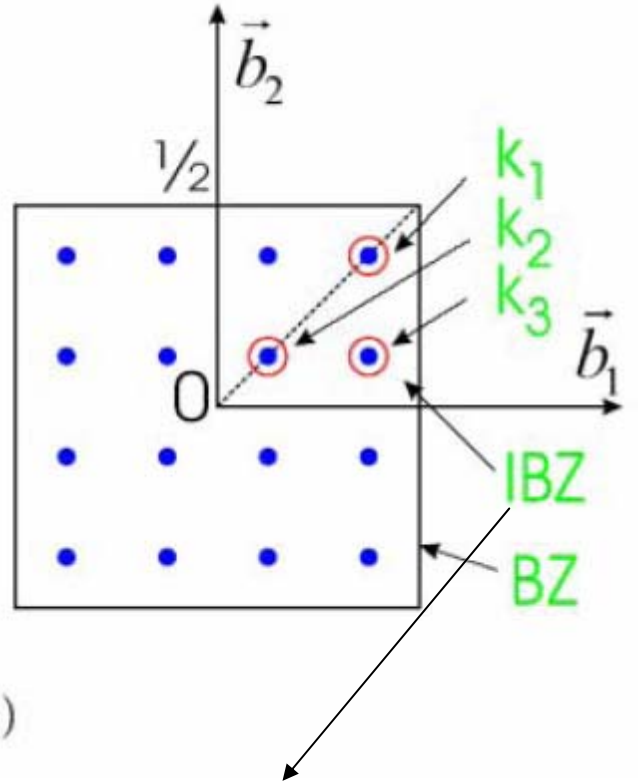
$$n(\mathbf{r}) = \frac{1}{V_{\text{BZ}}} \int_{1^{\text{st}}\text{BZ}} n_{\mathbf{k}}(\mathbf{r}) d\mathbf{k}$$

- The integrals for metals are more difficult to converge

Example:

- quadratic 2-dimensional lattice
- $q_1 = q_2 = 4 \Rightarrow$ 16 k-points
- only 3 inequivalent k-points ($\Rightarrow$ IBZ)
  - $4 \times \mathbf{k}_1 = (\frac{1}{8}, \frac{1}{8}) \Rightarrow \omega_1 = \frac{1}{4}$
  - $4 \times \mathbf{k}_2 = (\frac{3}{8}, \frac{3}{8}) \Rightarrow \omega_2 = \frac{1}{4}$
  - $8 \times \mathbf{k}_3 = (\frac{3}{8}, \frac{1}{8}) \Rightarrow \omega_3 = \frac{1}{2}$

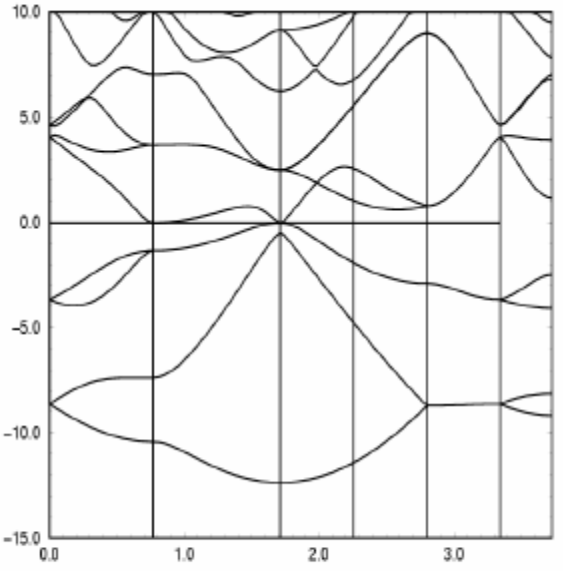
$$\frac{1}{\Omega_{BZ}} \int_{BZ} F(\mathbf{k}) d\mathbf{k} \Rightarrow \tfrac{1}{4} F(\mathbf{k}_1) + \tfrac{1}{4} F(\mathbf{k}_2) + \tfrac{1}{2} F(\mathbf{k}_3)$$

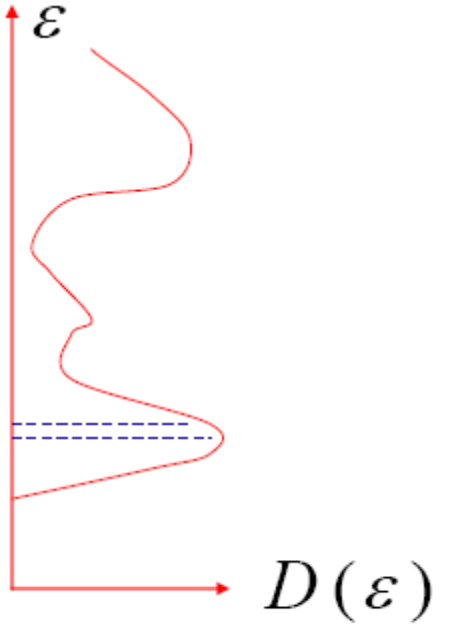


Algorithm:

- calculate equally spaced-mesh
- shift the mesh if desired
- apply all symmetry operations of Bravaislattice to all k-points
- extract the irreducible k-points ($\equiv$ IBZ)
- calculate the proper weighting

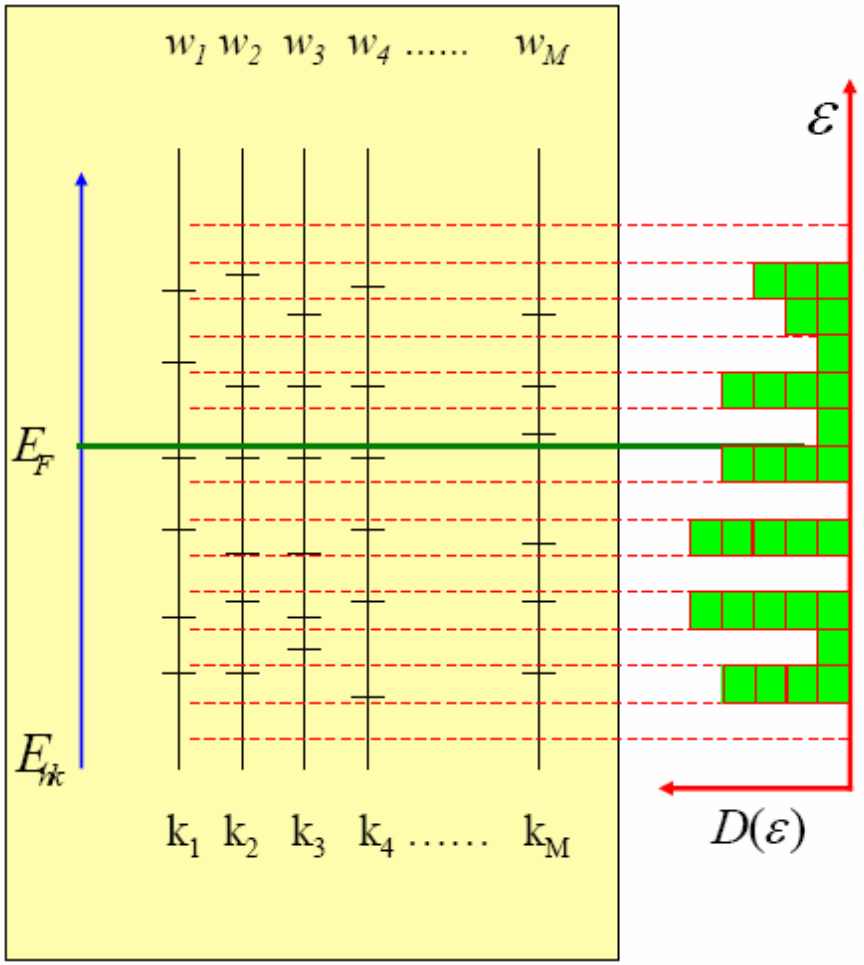
Density of state





$\Delta N = D(\varepsilon)\Delta\varepsilon$ *number of state from* ε *to* $\varepsilon + \Delta\varepsilon$

$D(\varepsilon)$: Density of states



$$D(\varepsilon_i)\Delta\varepsilon$$

Number of state within $\Delta\varepsilon$

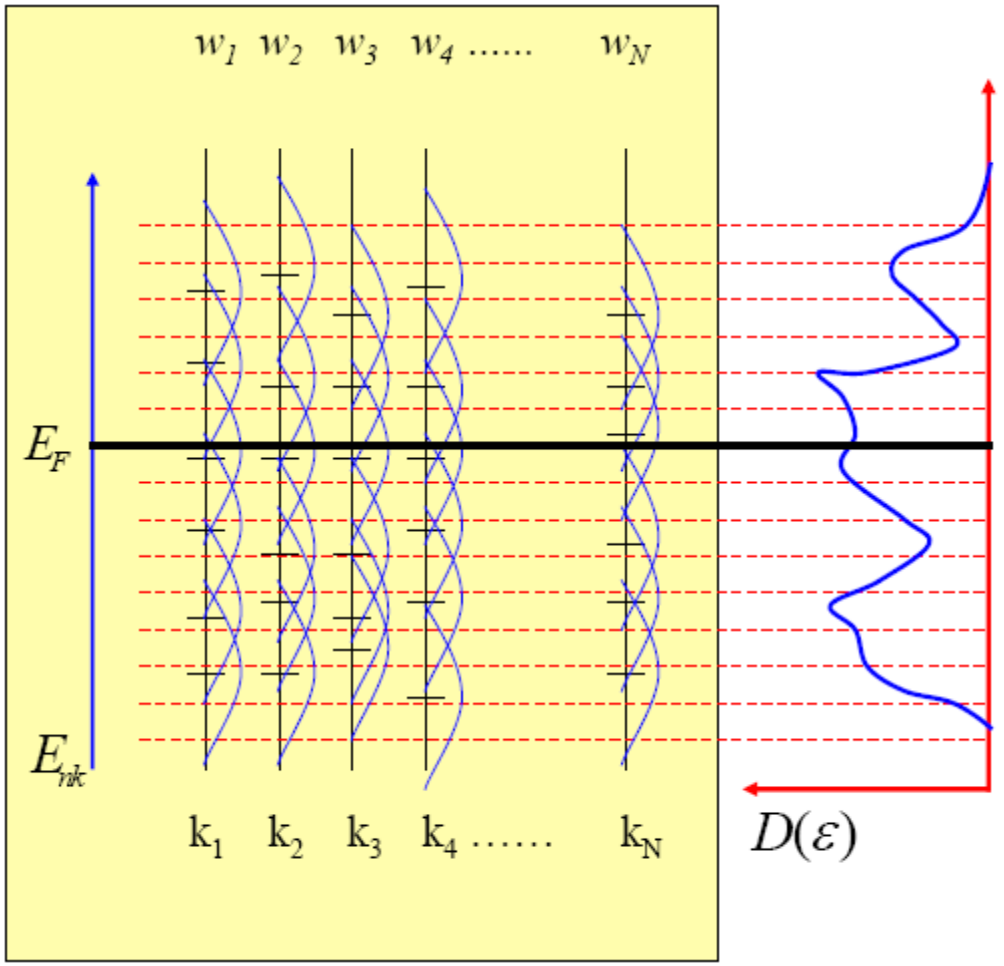
$$\omega_k = \frac{2A_k}{\sum_k A_k}$$

$$\sum_k \omega_k = 2$$

$$D(\varepsilon_i) = \frac{1}{\Delta\varepsilon}\sum_k \omega_k f_k$$

where

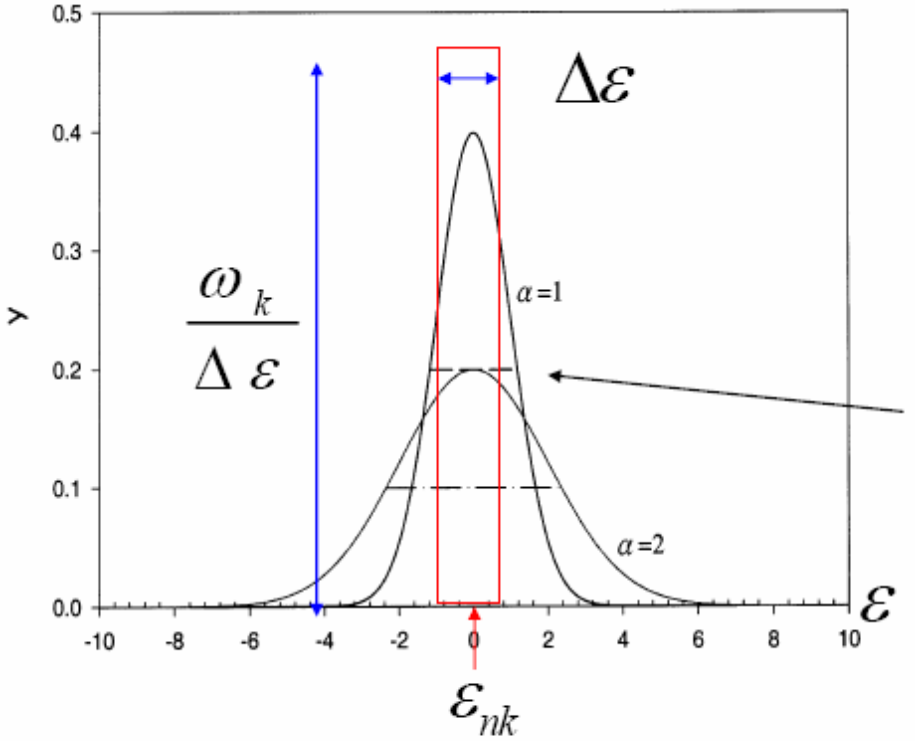
$$f_k = \begin{cases} 1 & \textit{occupied} \\ 0 & \textit{otherwise} \end{cases}$$



Smearing
(Gaussian)

$$A e^{-(\frac{\varepsilon-\varepsilon_i}{\sigma})^2}$$

$$\int_{\varepsilon<E_F} D(\varepsilon)d\varepsilon = N$$



They have the same area.

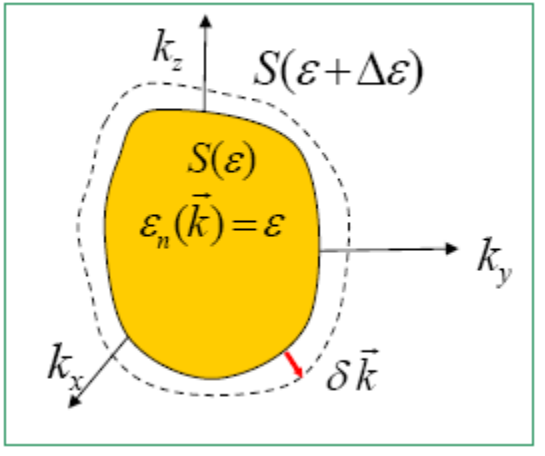
$$D_{nk}(\varepsilon) = \frac{\omega_k}{\sqrt{2\pi}\,\alpha} e^{-\frac{(\varepsilon-\varepsilon_{nk})^2}{2\alpha^2}}$$

Tetrahedrons method for Density of states

$$\varepsilon_n(\vec{k}+\delta\vec{k}) = \varepsilon + \Delta\varepsilon$$

$$\varepsilon_{nk} + \Delta\varepsilon = \varepsilon_{nk} + \left|\vec{\nabla}\varepsilon_{nk}\right| \delta\ k(\vec{k})$$

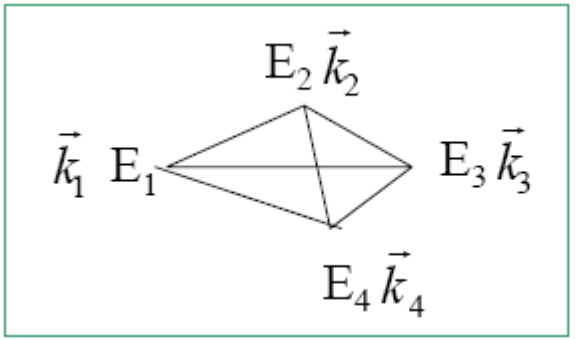
$$\delta\ k(\vec{k}) = \frac{d\varepsilon}{\left|\vec{\nabla}\varepsilon_{nk}\right|}$$



$$D_n(\varepsilon)d\varepsilon = \int\limits_{\substack{shell \\ \varepsilon<\varepsilon_{nk}<\varepsilon+\Delta\varepsilon}} \frac{d^3k}{\frac{(2\pi)^3}{V}} = \frac{\Omega}{(2\pi)^3} \int\limits_{\varepsilon<\varepsilon_{nk}<\varepsilon+\Delta\varepsilon} d^3k = \frac{\Omega}{(2\pi)^3} \int dS_\varepsilon(\delta\ k(\vec{k}))$$

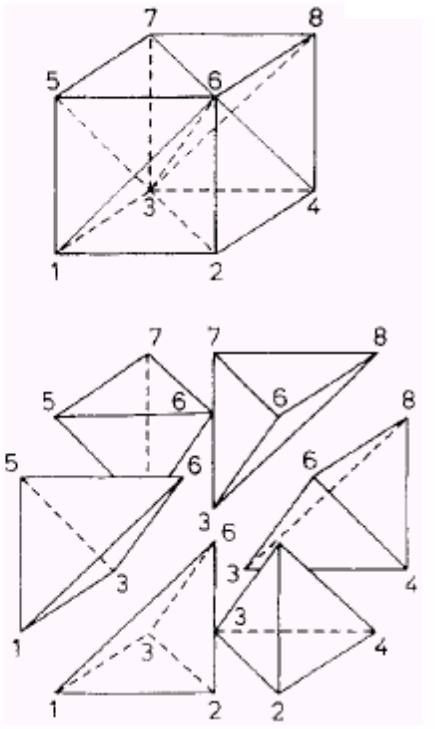
$$D(\varepsilon) = \frac{\Omega}{4\pi^3} \int \frac{dS_\varepsilon}{\left|\vec{\nabla}_k \varepsilon_{nk}\right|} \quad \Rightarrow \quad D(\varepsilon) = \frac{\Omega}{(2\pi)^3} \sum_{n,l} \frac{S_n(\varepsilon,\vec{k}_l)}{\left|\vec{\nabla}_k \varepsilon_n(\vec{k}_l)\right|}$$

The irreducible Brillouin zone is divided into a large number of tetrahedrons. In the small tetrahedrons, we assume that the energy varies linearly inside the cube.



$$E_4 \le E_3 \le E_2 \le E_1$$

Energy varies linearly



$$E_n(\vec{k}) = E_n(\vec{k}_l) + \nabla_{\vec{k}} E_n(\vec{k})\Big|_{\vec{k}=\vec{k}_l} \cdot (\vec{k} - \vec{k}_l)$$

$$E(\vec{k}) = E(\vec{k}_4) + \vec{b} \cdot (\vec{k} - \vec{k}_4)$$

$$\vec{b} = \sum_{i=1}^{3} \left[E(\vec{k}_i) - E(\vec{k}_4) \right] \cdot \vec{r}_i$$

where

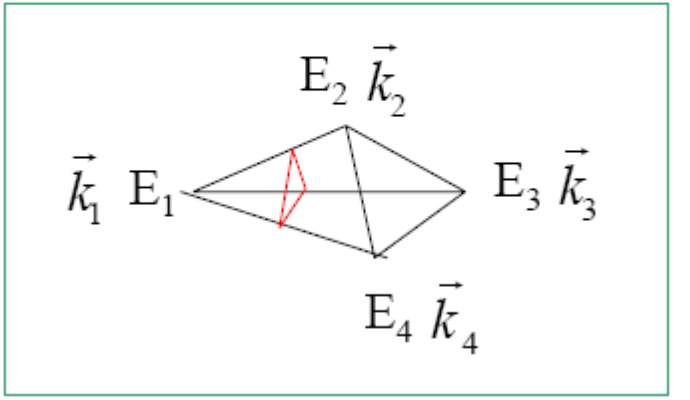
$$\vec{r}_1 = \frac{\vec{k}'_2 \times \vec{k}'_3}{\mathrm{V}} \; ; \vec{r}_2 = \frac{\vec{k}'_3 \times \vec{k}'_1}{\mathrm{V}} \; ; \vec{r}_3 = \frac{\vec{k}'_1 \times \vec{k}'_2}{\mathrm{V}}$$

$$\vec{r}_i \times \vec{k}_j = \delta_{ij} ; \vec{k}_j' = \vec{k}_j - \vec{k}_4, \quad \mathrm{j} = 1,2,3$$

$$\mathrm{V} = \vec{k}'_1 \times \vec{k}'_2 \times \vec{k}'_3$$

$$D_{nl}(E) = \frac{2\Omega}{(2\pi)^3} \frac{dS(E)}{|\vec{b}|} \quad \text{,where } \vec{b} = \vec{\nabla}_k E(\vec{k}) = \vec{b}$$

$$dS = \begin{cases} f_0 & E_4 \le E \le E_3 \\ f_0 - f_1 & E_3 \le E \le E_4 \\ f_3 & E_2 \le E \le E_1 \\ 0 & E \le E_4 \text{ or } E_1 \le E \end{cases}$$



$$\frac{f_0}{|\vec{b}|} = \frac{V}{2} \frac{(E - E_4)^2}{(E_3 - E_4)(E_2 - E_4)(E_1 - E_4)}$$

$$\frac{f_1}{|\vec{b}|} = \frac{V}{2} \frac{(E - E_3)^2}{(E_3 - E_4)(E_2 - E_3)(E_1 - E_3)}$$

$$\frac{f_3}{|\vec{b}|} = \frac{V}{2} \frac{(E - E_1)^2}{(E_1 - E_4)(E_1 - E_3)(E_1 - E_2)}$$

CMS II-4 Hands-on: calculate and plot band structure

Horng-Tay Jeng
(鄭弘泰)
Institute of Physics, Academia Sinica
May 24, 2007

Work list

- Perform self-consistent field (SCF) bulk calculation for Si(Dia) first, and make sure of the convergence (neglect this step if done)
- Setup band structure calculation for Si(Dia)
- Extract BS data using tool: bndacenm
- Plot BS using xmgrace

Setup band structure calculation for Si(Dia)

- Make a working subdirectory for bnd in directory si
  %cd si
  %mkdir bnd
- Copy the three input files: INCAR, POSCAR, and POTCAR and the convergent CHGCAR into bnd
  %cp INCAR POSCAR POTCAR CHGCAR bnd
- Go to bnd, revise INCAR, and setup KPOINTS
  %cd bnd
  …
- Run the VASP code
  %vasp4620s&

INCAR(SCF):

SYSTEM = Si Diamond

DOS related values
ISMEAR = -5
RWIGS = 1.3

INCAR(BS):

SYSTEM = Si Diamond

DOS related values
ISMEAR = 0
ICHARG = 11
RWIGS = 1.3

KPOINTS(SCF):

Si
0
Monkhorst-Pack
16 16 16
0 0 0

KPOINTS(BS):

Si(FCC)
11
Line-mode
Cartesian
0.5 0.5 0.5 ! L
0.0 0.0 0.0 ! G
0.0 0.0 0.0 ! G
0.0 0.0 1.0 ! X
0.0 0.0 1.0 ! X
0.5 0.0 1.0 ! W
0.5 0.0 1.0 ! W
0.75 0.0 0.75 ! K
0.75 0.0 0.75 ! K
0.0 0.0 0.0 ! G

High symmetry points in BZ

KPOINTS:

Si(FCC)
11
Line-mode
Cartesian
0.5 0.5 0.5 ! L
0.0 0.0 0.0 ! G
0.0 0.0 0.0 ! G
0.0 0.0 1.0 ! X
0.0 0.0 1.0 ! X
0.5 0.0 1.0 ! W
0.5 0.0 1.0 ! W
0.75 0.0 0.75 ! K
0.75 0.0 0.75 ! K
0.0 0.0 0.0 ! G

KPOINTS:

Fe(BCC)
11
Line-mode
Cartesian
0.0 0.0 0.0 ! G
0.0 1.0 0.0 ! H

0.0 1.0 0.0 ! H
0.5 0.5 0.0 ! N

0.5 0.5 0.0 ! N
0.0 0.0 0.0 ! G

0.0 0.0 0.0 ! G
0.5 0.5 0.5 ! P

KPOINTS:

ZnO(HCP)
11
Line-mode
Reciprocal
0.0 0.0 0.0 ! G
0.0 0.0 0.5 ! A
0.0 0.0 0.5 ! A
0.33333 0.33333 0.5 ! H
0.33333 0.33333 0.5 ! H
0.33333 0.33333 0.0 ! K
0.33333 0.33333 0.0 ! K
0.0 0.0 0.0 ! G
0.0 0.0 0.0 ! G
0.0 0.5 0.0 ! M
0.0 0.5 0.0 ! M
0.0 0.5 0.5 ! L
0.0 0.5 0.5 ! L

Extract BS data using tool: bndacenm

EIGENVAL:

```
2    2    1    1
  0.2001288E+02  0.3839590E-09  0.3839590E-09  0.3839590E-09  0.5000000E-15
  1.000000000000000E-004
  CAR
 Si Diamond
    8   55    8
```

55 k-points, 8bands(eigenvalues)

```
  0.5000000E+00  0.5000000E+00  0.5000000E+00  0.1818182E-01
  1        -3.8463
  2        -1.2175
  3         4.5852
  4         4.5852
  5         7.2185
  6         9.0933
  7         9.0933
  8        13.2997
```

coordinates of the 1st k-point

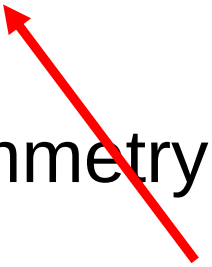
the 8 eigenvalues of the 1st k-point

```
  0.4500000E+00  0.4500000E+00  0.4500000E+00  0.1818182E-01
  1        -3.9826
  2        -1.0202
  3         4.6023
……………………………………………
```

the 2nd k-point …

How to use bndacenm

- Execute bndacenm and input Ef
  %~/tool/bndacenm
  Input Fermi level 5.77032221
- Output: bnd.kp and bnd.dat
- bnd.kp: distances of high symmetry points
  0.0000: L
  0.2165: G
  0.4665: X
  0.5915: W
  0.6799: K
  0.9451: G



Note!!!
Ef should be from SCF calculation!!!

bnd.dat (for xmgrace):

	k length	eig1	eig2	eig3	…				
L	0.0000	-9.6166	-6.9878	-1.1851	-1.1851	1.4482	3.3230	3.3230	7.5294
	0.0217	-9.7529	-6.7905	-1.1680	-1.1680	1.4686	3.3425	3.3425	7.5615
	0.0433	-10.0726	-6.2859	-1.1143	-1.1143	1.5322	3.3980	3.3980	7.6466
	0.0650	-10.4514	-5.6012	-1.0254	-1.0254	1.6344	3.4684	3.4684	7.7146
	0.0866	-10.8223	-4.8049	-0.9021	-0.9021	1.7751	3.5157	3.5157	7.4806
	0.1083	-11.1561	-3.9355	-0.7474	-0.7474	1.9483	3.4873	3.4873	6.7833
	0.1299	-11.4388	-3.0156	-0.5665	-0.5665	2.1420	3.3449	3.3449	5.9249
	0.1516	-11.6632	-2.0703	-0.3702	-0.3702	2.3453	3.1055	3.1055	5.0360
	0.1732	-11.8255	-1.1433	-0.1824	-0.1824	2.5202	2.8370	2.8370	4.1705
	0.1949	-11.9237	-0.3471	-0.0380	-0.0380	2.5933	2.6249	2.6249	3.4702
G	0.2165	-11.9566	0.0167	0.0167	0.0167	2.5430	2.5431	2.5431	3.2173
G	0.2165	-11.9566	0.0167	0.0167	0.0167	2.5430	2.5431	2.5431	3.2173
	0.2415	-11.9128	-0.2694	-0.1601	-0.1601	2.4321	2.7747	2.7748	3.4948
	0.2665	-11.7816	-0.9364	-0.5643	-0.5642	2.1460	3.3377	3.3378	4.0623

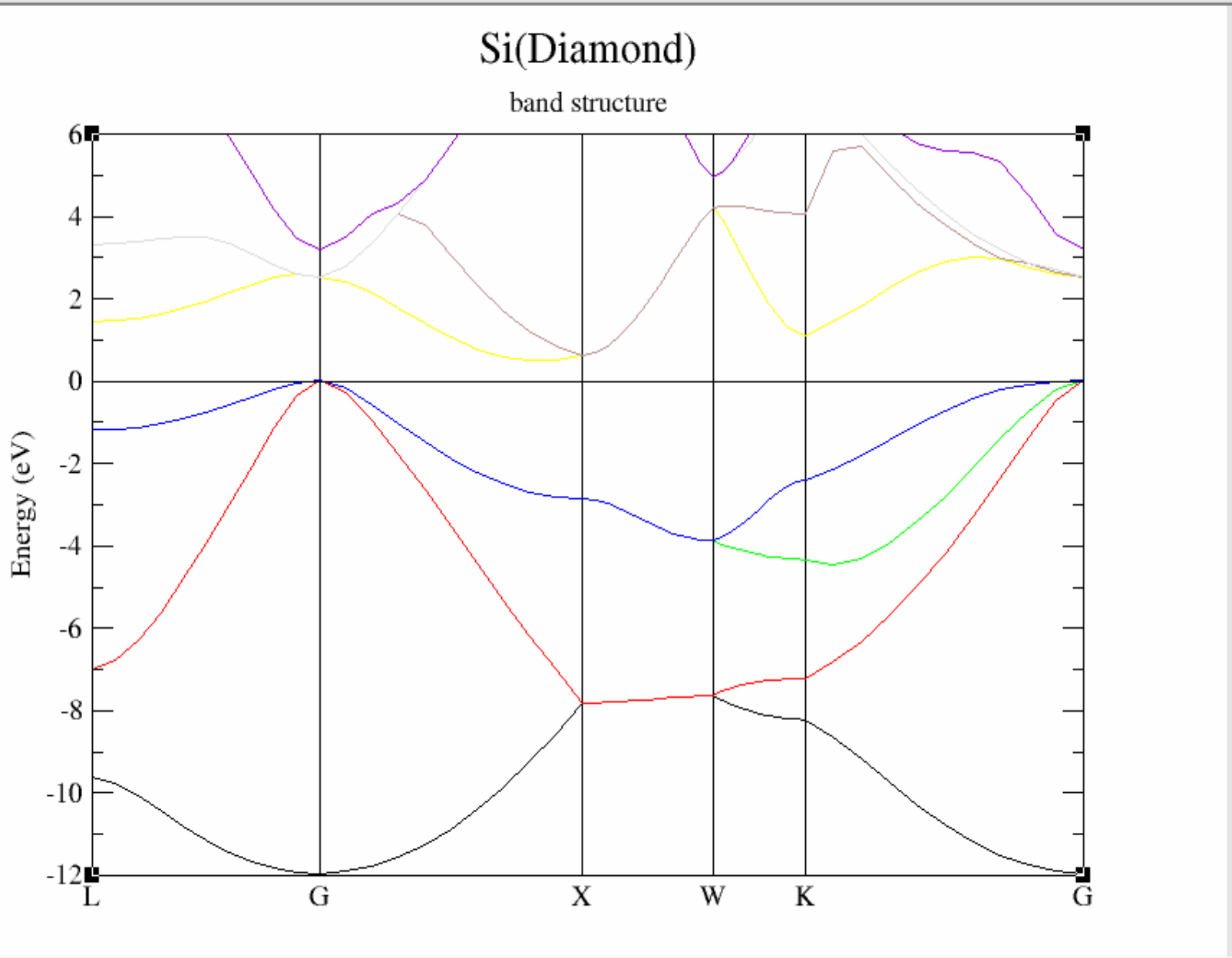
……

X

…

Edit Data Plot View Window

X, Y = [0.459912, -7.29817]



Homework

please Email to jeng@phys.sinica.edu.tw

- Calculate and plot LDA band structure along high symmetry lines LGXWKG for Si(Dia) and C(Dia) using exprimental lattice constants
- Calculate and plot GGA band structure along high symmetry lines LGXWKG, GHNGP, GMKGA, for Cu(FCC), V(BCC), and Ti(HCP), respectively, using experimental lattice constants