Physics of Semiconductors (5)

Shingo Katsumoto
Institute for Solid State Physics,
University of Tokyo

2013/5/13

Presence of both drift and diffusion currents

$$\boldsymbol{v}\cdot\nabla f+\frac{\boldsymbol{F}}{m}\nabla_v f=-\frac{f-f_0}{\tau(E)} \qquad f=f_0-\tau(E)\boldsymbol{v}\cdot\left[-e\mathbf{E}+\frac{E_\mathrm{F}-E}{T}\nabla T\right]\frac{\partial f_0}{\partial E}$$

f_0

$$j_x=-e\langle nv_x\rangle=-e\int_0^\infty v_x f(E)\mathcal{D}(E)dE$$

$$=e\int_0^\infty v_x^2\tau\left[-e\mathcal{E}_x+\frac{E_\mathrm{F}-E}{T}\frac{\partial T}{\partial x}\right]\frac{\partial f_0}{\partial E}\mathcal{D}(E)dE$$

drift diffusion

$j_x = 0$: valance of drift and diffusion currents

$$S=\frac{\mathcal{E}_x}{\partial T/\partial x}=\int_0^\infty v_x^2\tau\frac{E_\mathrm{F}-E}{eT}\frac{\partial f_0}{\partial E}\mathcal{D}(E)dE\Big/\int_0^\infty v_x^2\tau\frac{\partial f_0}{\partial E}\mathcal{D}(E)dE$$

$$=-\frac{1}{eT}\left[\left(\frac{5}{2}+s\right)k_\mathrm{B}T-E_\mathrm{F}\right]$$

Absorption of electromagnetic radiation

Absorption coefficient

Electromagnetic wave propagating along z-axis

$\boldsymbol{A} = A_0 \boldsymbol{e} \exp[i(\boldsymbol{k}_p \cdot \boldsymbol{r} - \omega t)]$ $\boldsymbol{A}$: vector potential

polarization $\boldsymbol{e}$ = (1, 0, 0), wavenumber $\boldsymbol{k}_p$ = (0, 0, k_p)

Electric field $\mathbf{E} = -\dfrac{\partial \boldsymbol{A}}{\partial t}$, Magnetic flux density $\boldsymbol{B} = \mathrm{rot}\ \boldsymbol{A}$

Energy flux (Poynting vector) $\boldsymbol{I} = \langle \mathbf{E} \times \mathbf{H} \rangle = 2\epsilon_0 c \bar{n} \omega^2 A_0^2 \boldsymbol{e}_z$

refractive index

$$|\boldsymbol{I}| = I(z) = I_0 \exp(-\alpha z)$$

W: photon absorption number in unit time and volume

$$\alpha = \frac{\hbar\omega W}{I} = \frac{\hbar\omega W}{2\epsilon_0 c \bar{n} \omega^2 A_0^2}$$

Absorption of electromagnetic radiation

Hamiltonian

$$\hat{H} = \frac{(\boldsymbol{p} + e\boldsymbol{A})^2}{2m_0} + V(\boldsymbol{r}) \simeq \underbrace{\frac{\boldsymbol{p}^2}{2m_0} + V(\boldsymbol{r})}_{\hat{H}_0} + \underbrace{\frac{e\boldsymbol{p}\cdot\boldsymbol{A}}{m_0}}_{\hat{H}'}$$

dipole transition

Fermi's golden rule approximation

conduction valence

$$W_{\mathrm{vc}} = \frac{2\pi}{\hbar}\frac{e^2}{m_0^2}|\langle c\boldsymbol{k}|\boldsymbol{A}\cdot\boldsymbol{p}|v\boldsymbol{k}'\rangle|^2\delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

$$= \frac{2\pi e^2}{\hbar m_0^2}A_0^2|M|^2\delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

Absorption of electromagnetic radiation

$$M = \langle c\boldsymbol{k}|e^{i\boldsymbol{k}_p\boldsymbol{r}}\boldsymbol{e}\cdot\boldsymbol{p}|v\boldsymbol{k}'\rangle \qquad \text{Bloch function} \quad e^{i\boldsymbol{k}\boldsymbol{r}}u_{c\boldsymbol{k}}(\boldsymbol{r}),\ \ e^{i\boldsymbol{k}'\boldsymbol{r}}u_{v\boldsymbol{k}'}(\boldsymbol{r})$$

$$= \int_V \frac{d^3r}{V} e^{i(\boldsymbol{k}_p+\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot(\boldsymbol{p}+\hbar\boldsymbol{k}')u_{v\boldsymbol{k}'}(\boldsymbol{r})$$

$$u_{c\boldsymbol{k}}(\boldsymbol{r}) = u_{c\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}_l),\ \ u_{v\boldsymbol{k}'}(\boldsymbol{r}) = u_{v\boldsymbol{k}'}(\boldsymbol{r}+\boldsymbol{R}_l) \quad (\boldsymbol{R}_l : \text{lattice vector})$$

$$= \frac{\sum_l e^{i(\boldsymbol{k}_p+\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}_l}}{V} \int_\Omega d^3r u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot(\boldsymbol{p}+\hbar\boldsymbol{k}')u_{v\boldsymbol{k}'}(\boldsymbol{r})$$

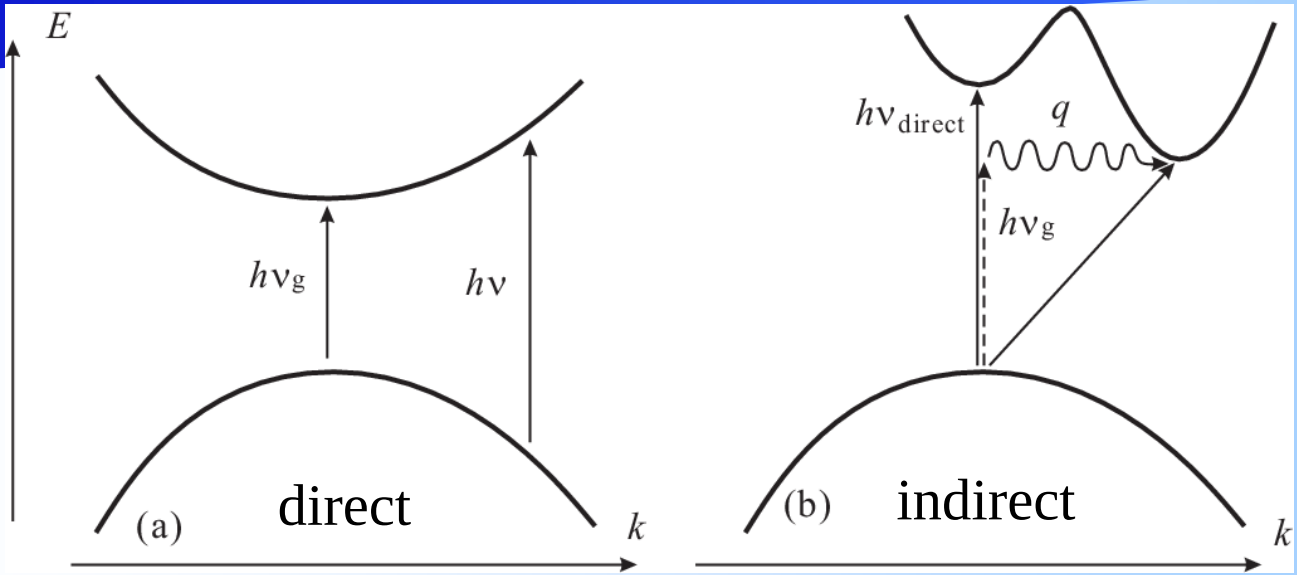
$$= \frac{N}{V}\delta_{\boldsymbol{k}_p+\boldsymbol{k}'-\boldsymbol{k},\boldsymbol{K}} \int_\Omega d^3r u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot\boldsymbol{p}u_{v\boldsymbol{k}'}(\boldsymbol{r}) = \int_\Omega \frac{d^3r}{\Omega} u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot\boldsymbol{p}u_{v\boldsymbol{k}}(\boldsymbol{r})$$

$\boldsymbol{k}_p + \boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{K}$ = 0 (no Umklapp)

$\simeq 0$

k' = k

Direct and indirect transitions



$$\alpha_{\mathrm{da}} = \frac{\pi e^2}{\bar{n}\epsilon_0 \omega c m_0^2} |M|^2 \sum_{\boldsymbol{k}} \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}) - \hbar\omega)$$

$E_{cv}(\boldsymbol{k})$

Joint density of states

$$J_{cv}(\hbar\omega) = \sum_{\boldsymbol{k}} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega) = 2\int \frac{d^3k}{(2\pi)^3} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega)$$

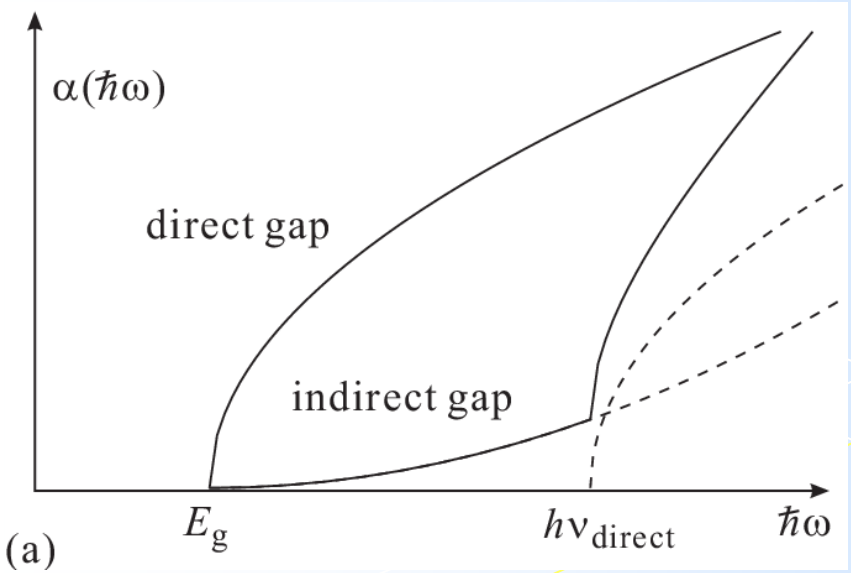
direct gap semicon. $= \dfrac{\sqrt{2}}{\pi^2} \dfrac{m_r^{3/2}}{\hbar^3} \sqrt{\hbar\omega - E_{\mathrm{g}}}$ $\qquad \dfrac{1}{m_r} = \dfrac{1}{m_e^*} + \dfrac{1}{m_h^*}$ (reduced mass)

Absorption coefficient

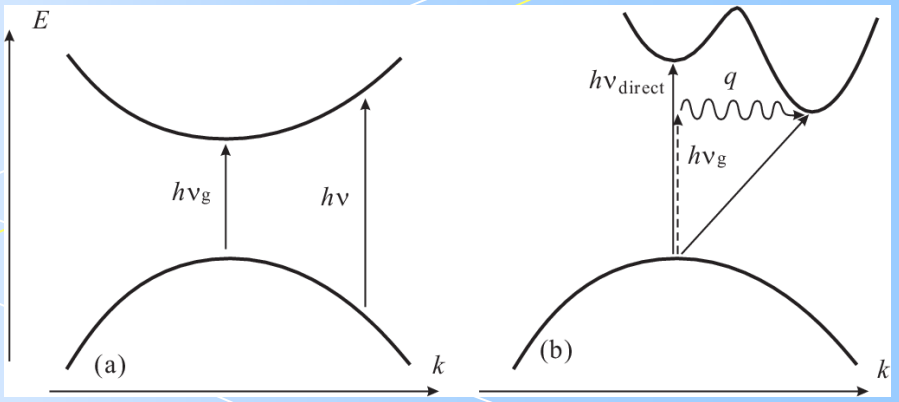
$$\alpha(\hbar\omega) = \frac{e^2(2m_r)^{3/2}|M|^2}{2\pi\epsilon_0 m_0^2 \bar{n}\omega c\hbar^3}\sqrt{\hbar\omega - E_g} = \frac{\pi}{\epsilon_0 c n_r}\frac{e^2|M|^2}{m_0^2}J_{cv}(\hbar\omega)$$

$$\alpha_{id}(\hbar\omega) \propto (\hbar\omega - E_g)^2$$

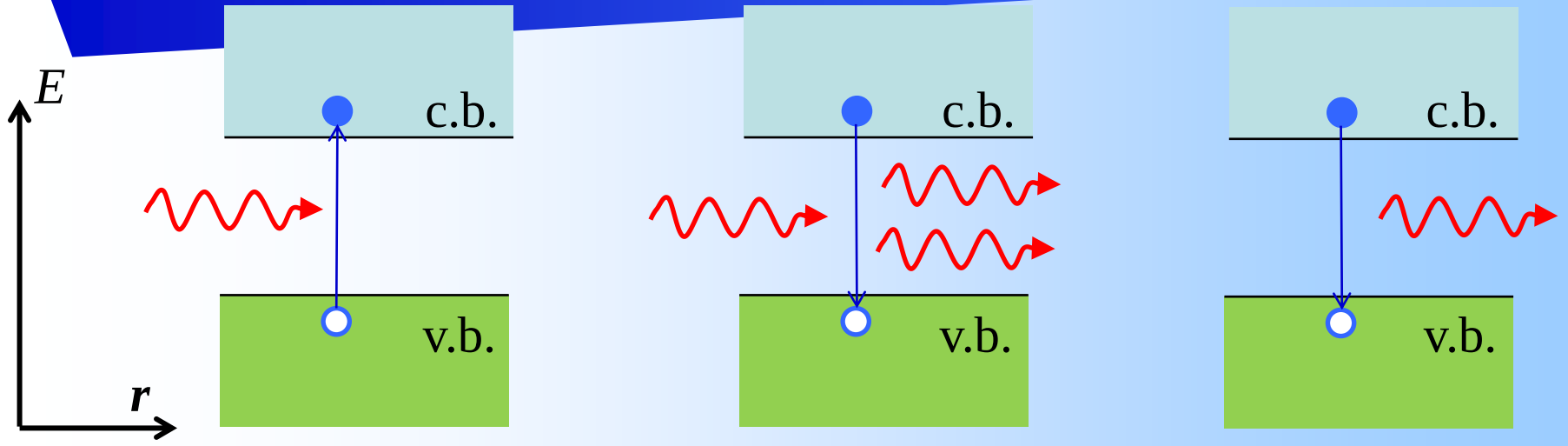
$$\frac{e^2}{m_0^2}|\langle 1|x|0\rangle|^2 \leftarrow \frac{e^2\hbar\omega}{2m_0}\frac{2|M|^2}{\hbar\omega m_0}$$



oscillator strength f_{vc}



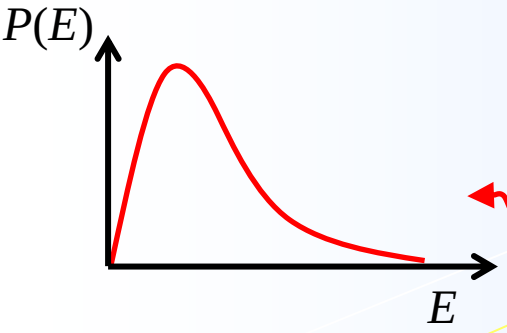
Photon emission

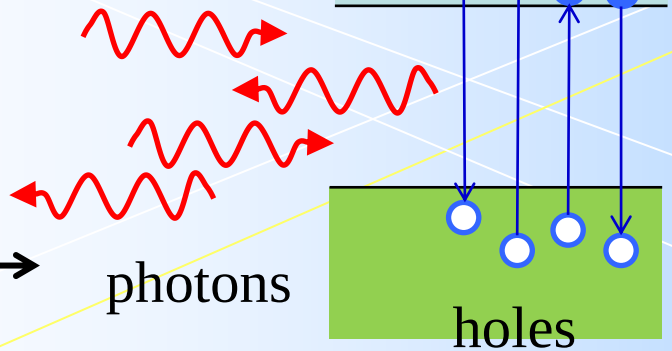


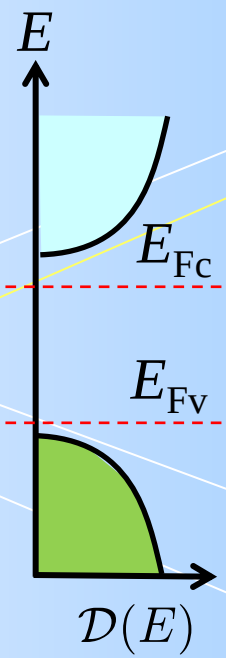
absorption = stimulated emission + spontaneous emission

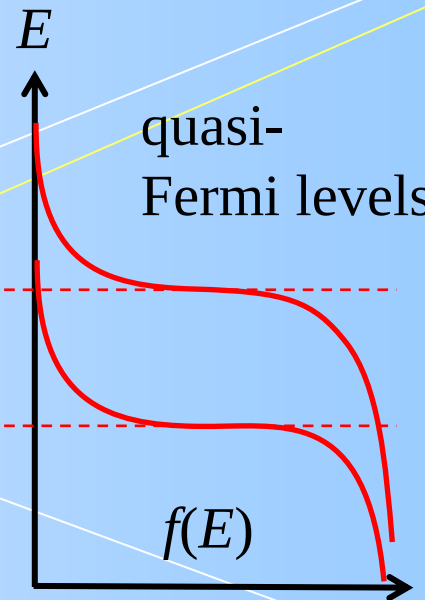
detailed balance

$$P(E) = \frac{8\pi\bar{n}^3 E^2}{h^3 c^3} \frac{1}{\exp(E/k_B T) - 1}$$



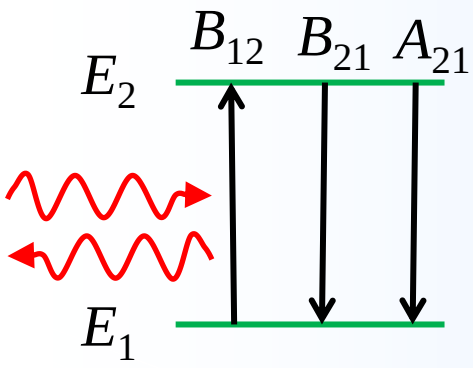






Einstein relation

$$f_c(E) = \left[\exp\left(\frac{E - E_{Fc}}{k_B T}\right) + 1\right]^{-1} \qquad f_v(E) = \left[\exp\left(\frac{E - E_{Fv}}{k_B T}\right) + 1\right]^{-1}$$



$$P(E) = \frac{8\pi\bar{n}^3 E^2}{h^3 c^3} \frac{1}{\exp(E/k_B T) - 1}$$

$$R(1 \to 2) = B_{12} f_v (1 - f_c) P(\hbar\omega)$$ absorption

$$R(\mathrm{st}, 2 \to 1) = B_{21} f_c(E_2)(1 - f_v(E_1)) P(\hbar\omega)$$ stimulated emission

$$R(\mathrm{sp}, 2 \to 1) = A_{21} f_c(E_2)(1 - f_v(E_1))$$ spontaneous emission

detailed balance $R(1 \to 2) = R(\mathrm{sp}, 2 \to 1) + R(\mathrm{st}, 2 \to 1)$

Comparison
in temperature dependence

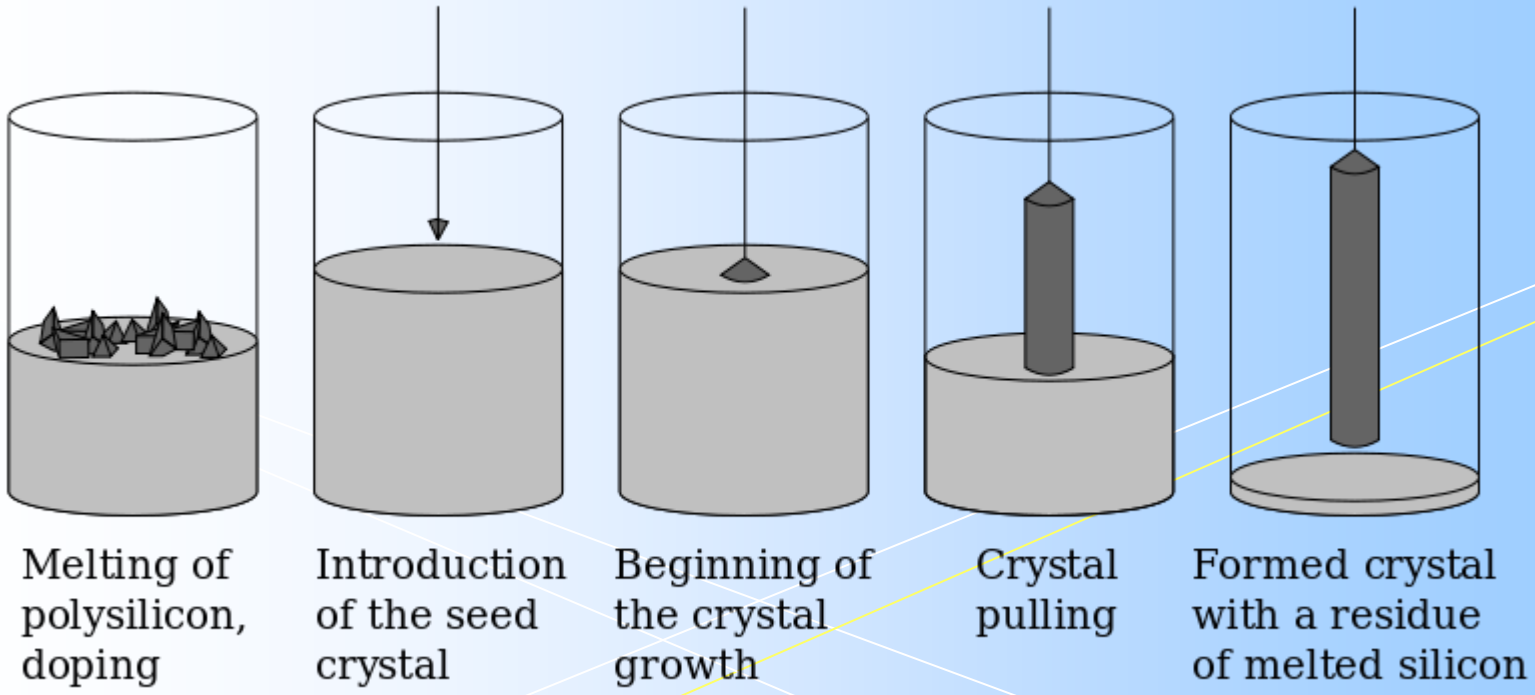
$$A_{21} = \frac{8\pi\bar{n}^3 E_{21}^2}{h^3 c^3} B_{21},$$
$$B_{12} = B_{21}.$$

Einstein relation

Ch.2 Crystal Growth and Band Structure

Bulk crystal growth

Czochralski growth process

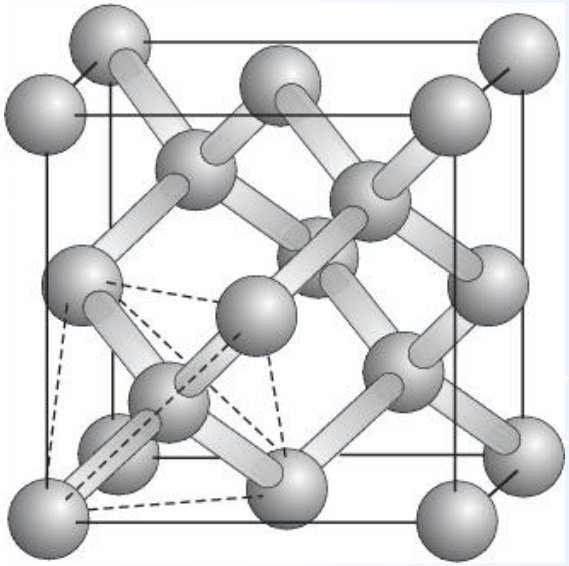


From Wikipedia

Inorganic semiconductor crystals

Carbon group (group 14)

diamond structure (fcc)



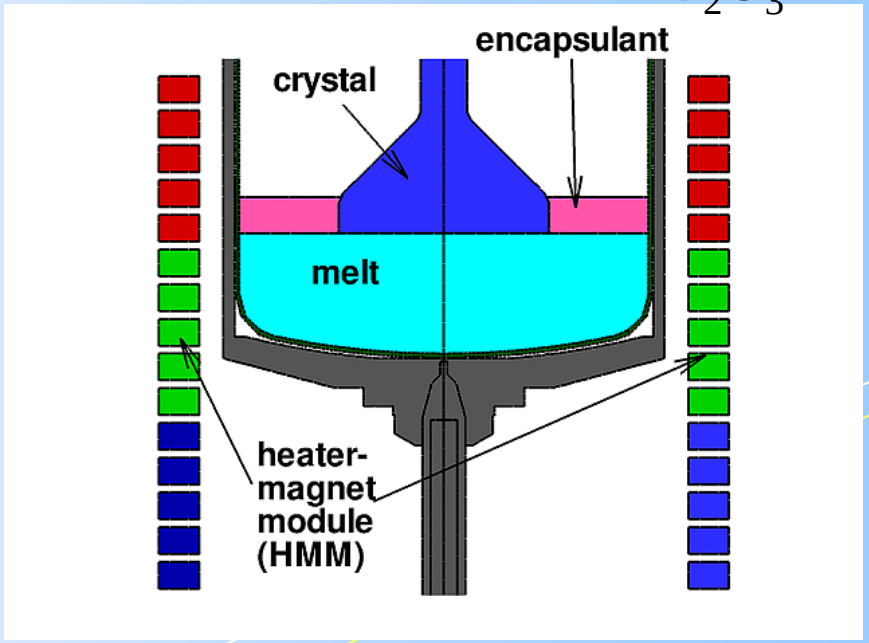
Diamonds

II	III	IV	V	VI
4 Be ベリリウム 9.012182	5 B ホウ素 10.811	6 C 炭素 12.0107	7 N 窒素 14.0067	8 O 酸素 15.9994
12 Mg マグネシウム 24.305	13 Al アルミニウム 26.98153...	14 Si ケイ素 28.0855	15 P リン 30.973762	16 S 硫黄 32.065
30 Zn 亜鉛 65.38	31 Ga ガリウム 69.723	32 Ge ゲルマニウム 72.63	33 As ヒ素 74.9216	34 Se セレン 78.96
48 Cd カドミウム 112.411	49 In インジウム 114.818	50 Sn スズ 118.71	51 Sb アンチモン 121.76	52 Te テルル 127.6

Silicon

Czochralski process

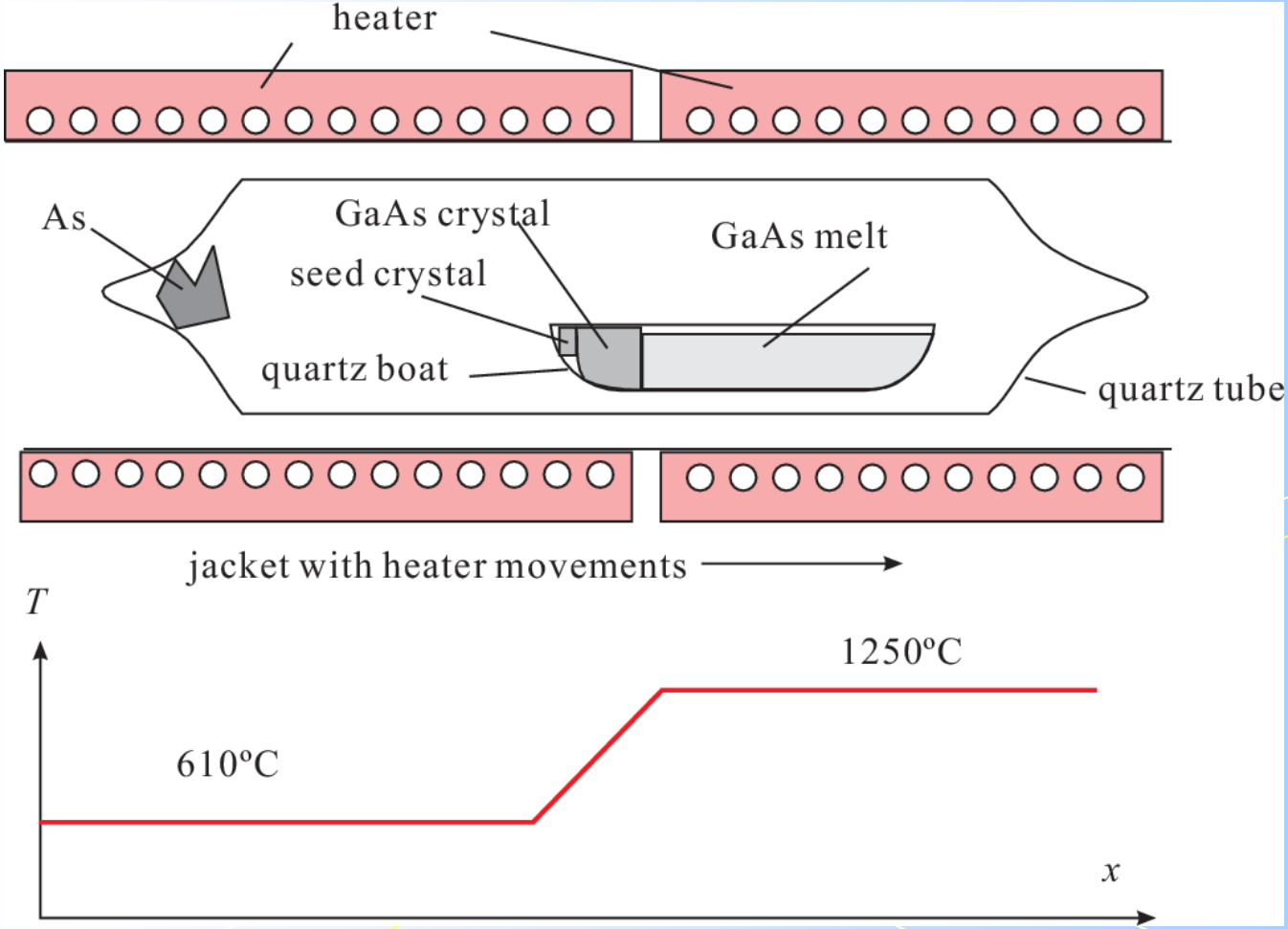
B_2O_3



liquid encapsulated Czochralski

Boat methods

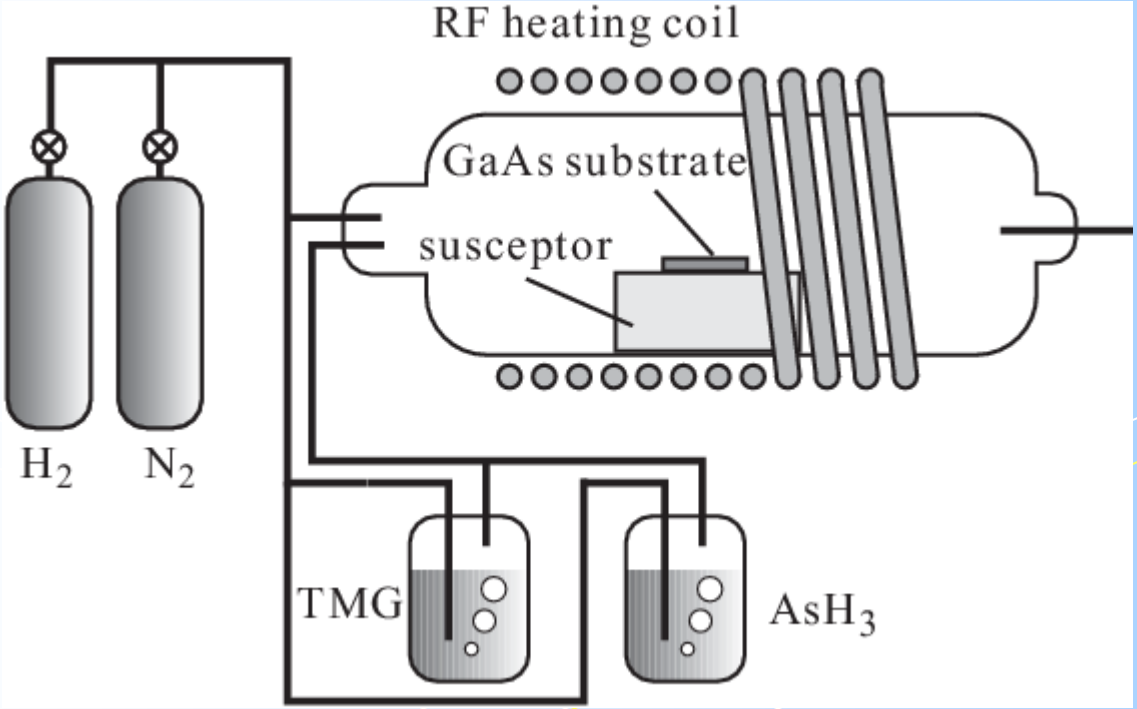
Horizontal Bridgeman (HB) process



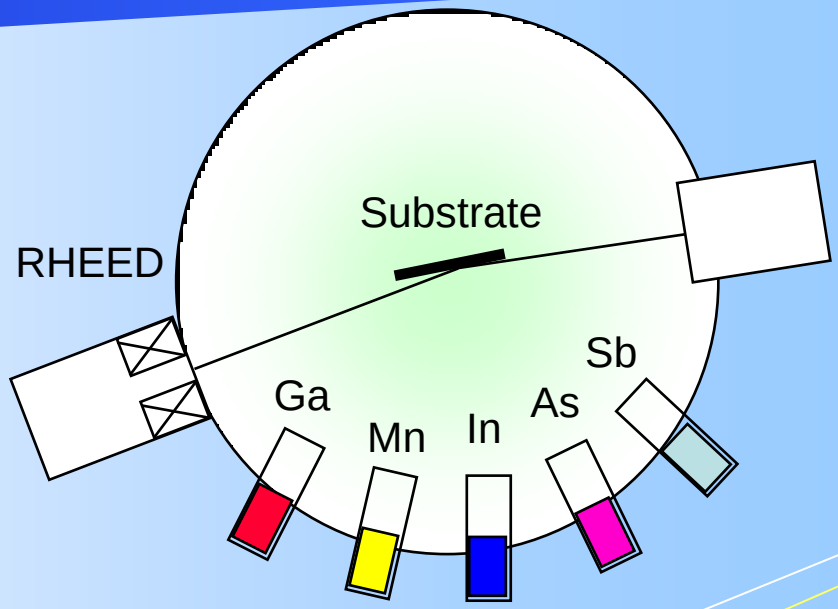
temperature gradient freezing method

Epitaxial growth of thin films

Metal-Organic Vapor Phase Epitaxy (MOVPE, MOCVD)

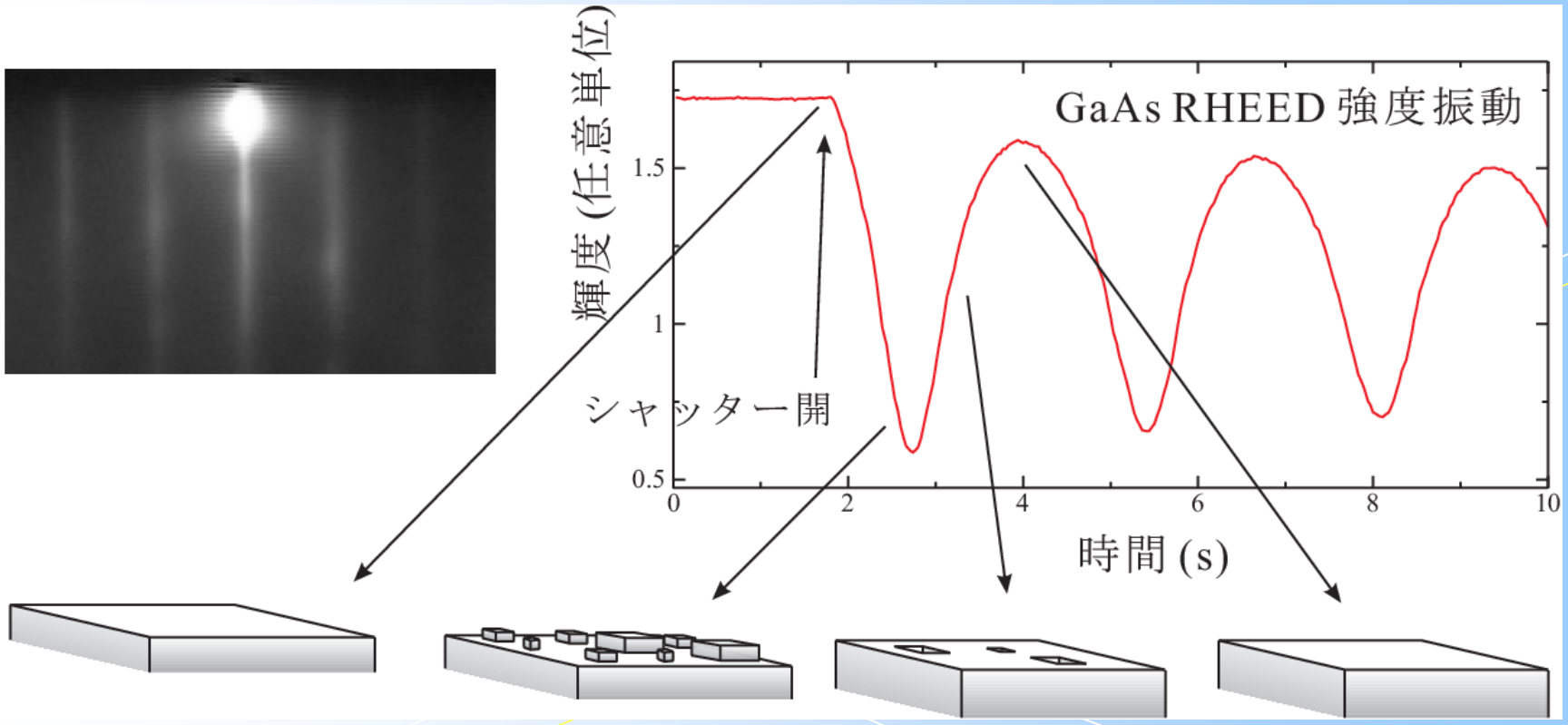


Molecular beam epitaxy (MBE)

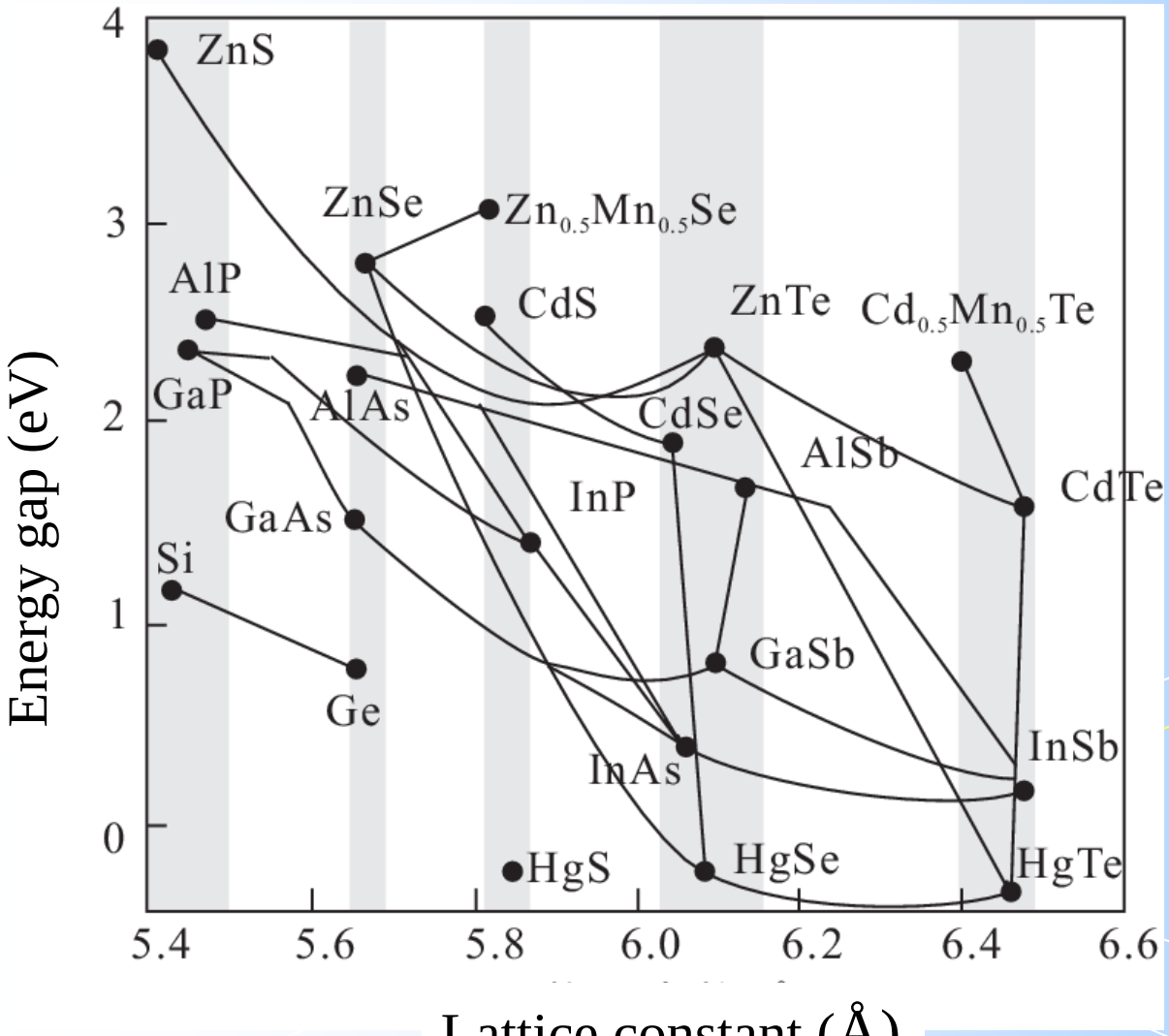


RHEED oscillation

Reflection high energy electron diffraction



Lattice constants and band gaps



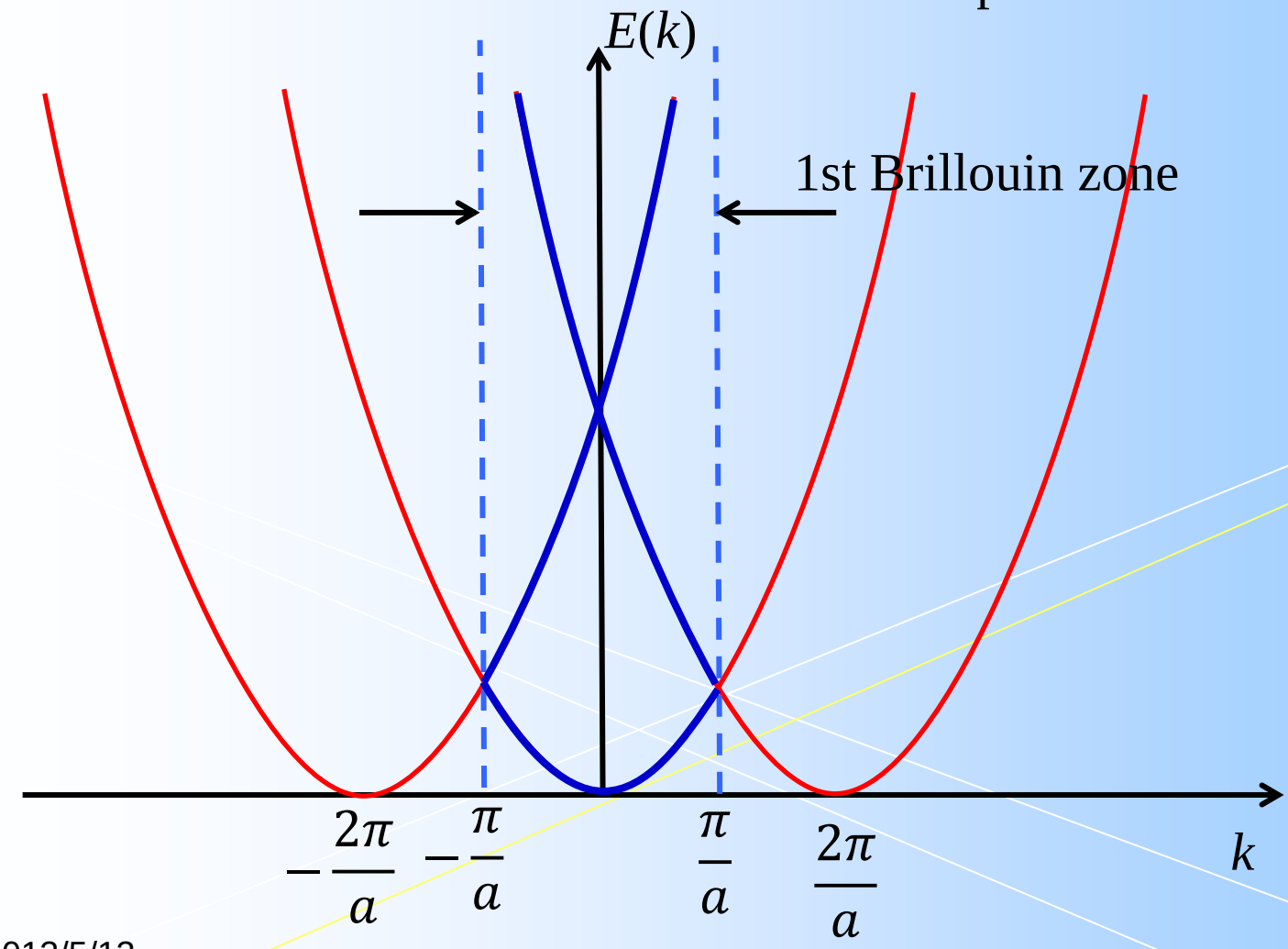
II	III	IV	V	VI
4 Be ベリリウム 9.012182	5 B ホウ素 10.811	6 C 炭素 12.0107	7 N 窒素 14.0067	8 O 酸素 15.9994
12 Mg マグネシウム 24.305	13 Al アルミニウム 26.98153...	14 Si ケイ素 28.0855	15 P リン 30.973762	16 S 硫黄 32.065
30 Zn 亜鉛 65.38	31 Ga ガリウム 69.723	32 Ge ゲルマニウム 72.63	33 As ヒ素 74.9216	34 Se セレン 78.96
48 Cd カドミウム 112.411	49 In インジウム 114.818	50 Sn スズ 118.71	51 Sb アンチモン 121.76	52 Te テルル 127.6

Band structure

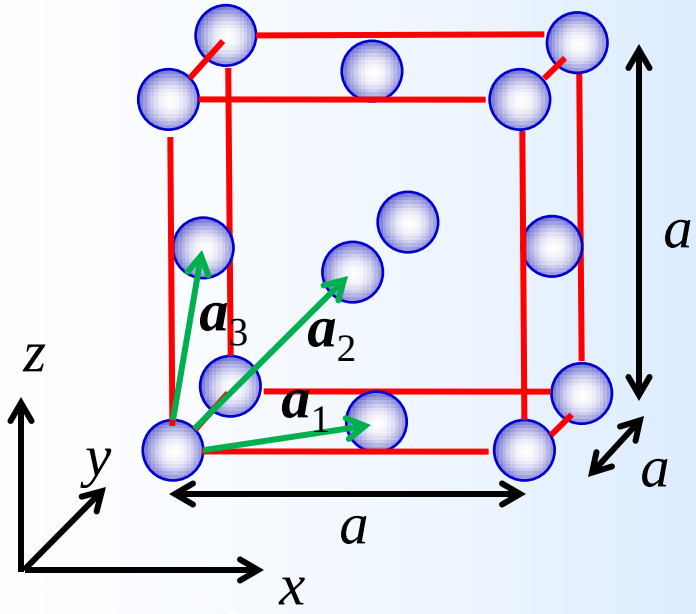
$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r})$$

Empty lattice approximation

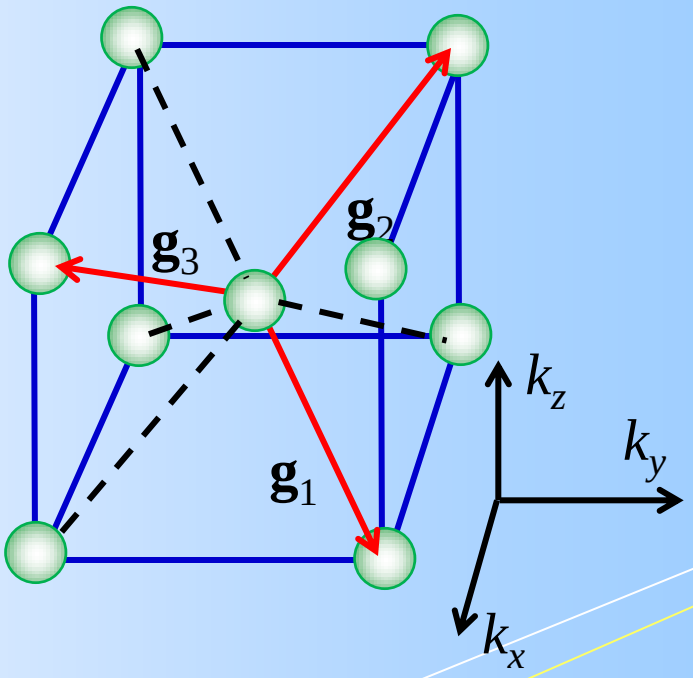
The free space has a lattice periodicity!



Face centered cubic (fcc) lattice



fcc lattice

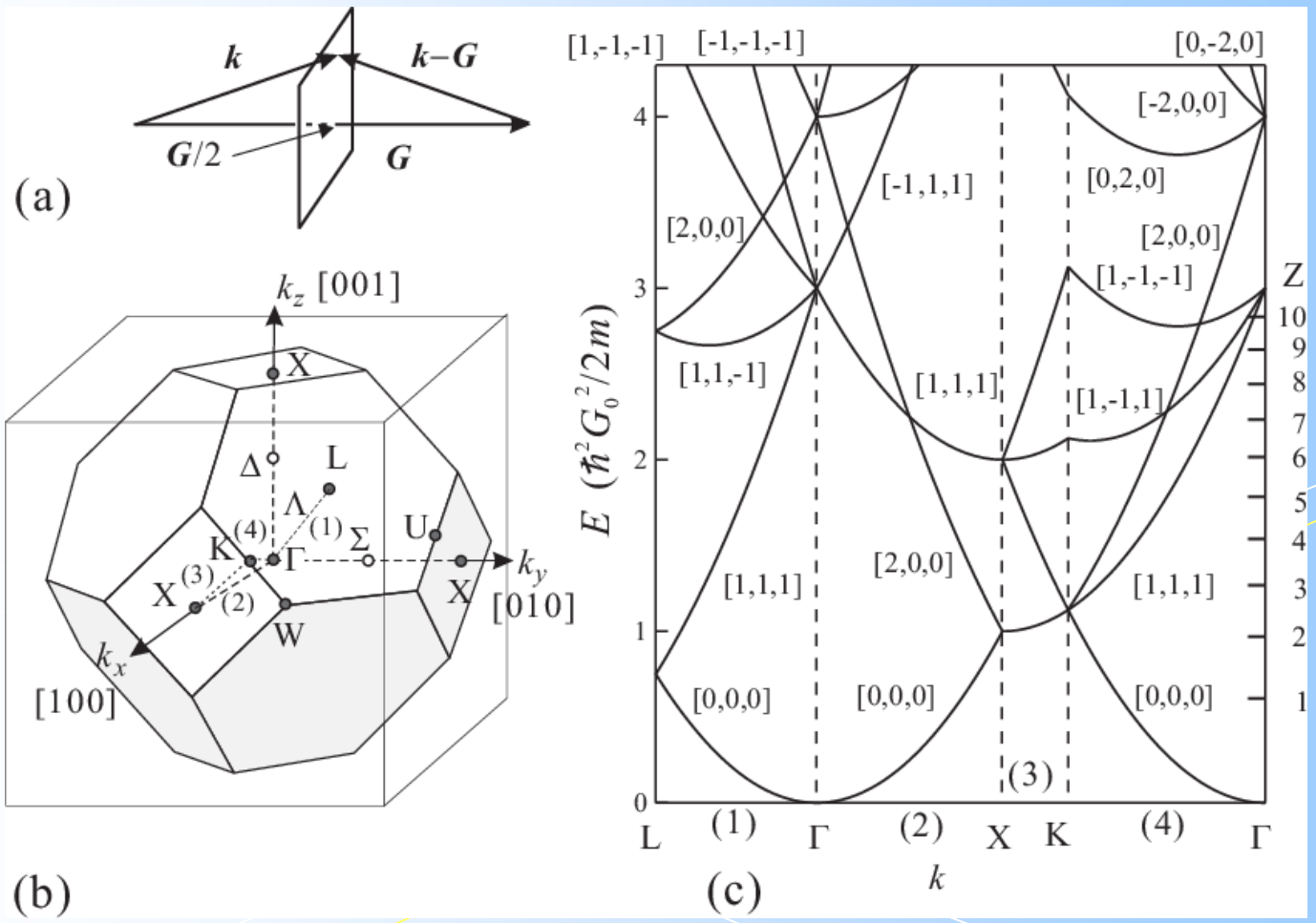


reciprocal lattice: body centered cubic (bcc)

$$\boldsymbol{g}_1 = \frac{2\pi \boldsymbol{a}_2 \times \boldsymbol{a}_3}{|A|}, \quad \boldsymbol{g}_2 = \frac{2\pi \boldsymbol{a}_3 \times \boldsymbol{a}_1}{|A|}, \quad \boldsymbol{g}_3 = \frac{2\pi \boldsymbol{a}_1 \times \boldsymbol{a}_2}{|A|}$$

$$|A| \equiv \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$$

Empty lattice approximation



Empirical band structure calculation

Plane wave expansion

$$\hat{H}\psi(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \qquad \psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r})$$

functions with lattice periodicity

$$V(\boldsymbol{r}) = \sum_{\boldsymbol{G}} V_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}, \quad u_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} C_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

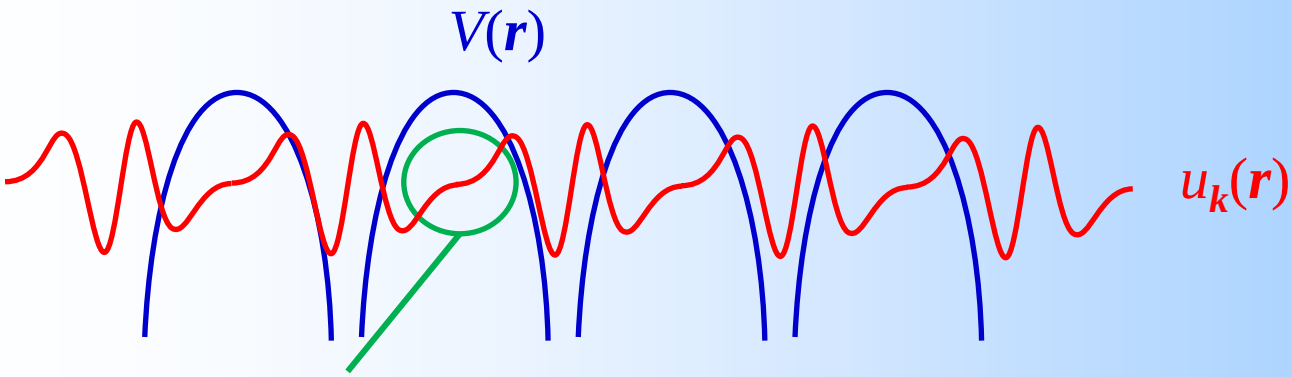
$\boldsymbol{G}$: reciprocal lattice vector

$$\sum_{\boldsymbol{G}} \left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E)\right\} C_{\boldsymbol{G}} + \sum_{\boldsymbol{G}'} V_{\boldsymbol{G}-\boldsymbol{G}'} C_{\boldsymbol{G}'}\right] e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}} = 0$$

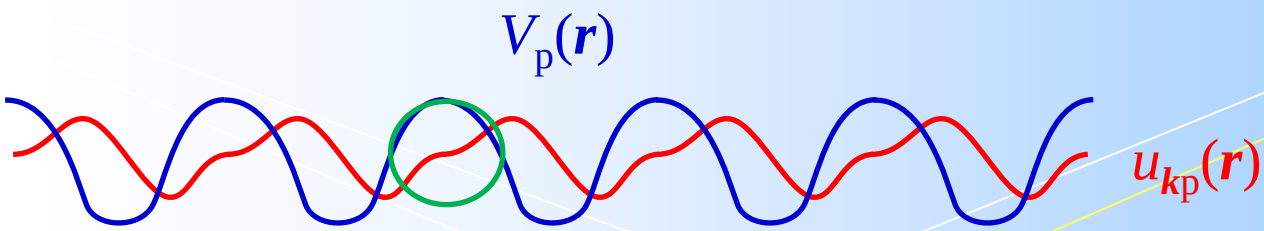
$$\sum_{\boldsymbol{G}'} \left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E\right\}\delta_{\boldsymbol{G}\boldsymbol{G}'} + V_{\boldsymbol{G}-\boldsymbol{G}'}\right] C_{\boldsymbol{G}'} = 0$$

$$\left|\left[\left\{\frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 - E\right\}\delta_{\boldsymbol{G}\boldsymbol{G}'} + V_{\boldsymbol{G}-\boldsymbol{G}'}\right]_{\boldsymbol{G}\boldsymbol{G}'}\right| = 0$$

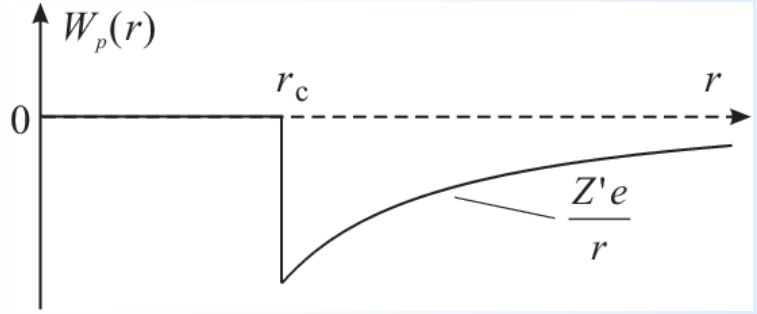
Pseudo potential method



band structure: almost determined in skirt characteristics



Pseudo potential method



$$V(r) = -\frac{Ze}{r}$$

$$W_p(r) = 0 \quad (r < r_c),$$

$$= -Z'e/r \quad (r \geq r_c)$$

$$V_p(\boldsymbol{r}) = \sum_{j,\alpha} W_p^{\alpha}(\boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{\tau}_{\alpha})$$

unit cell index → j,α ← atomic index in a unit cell

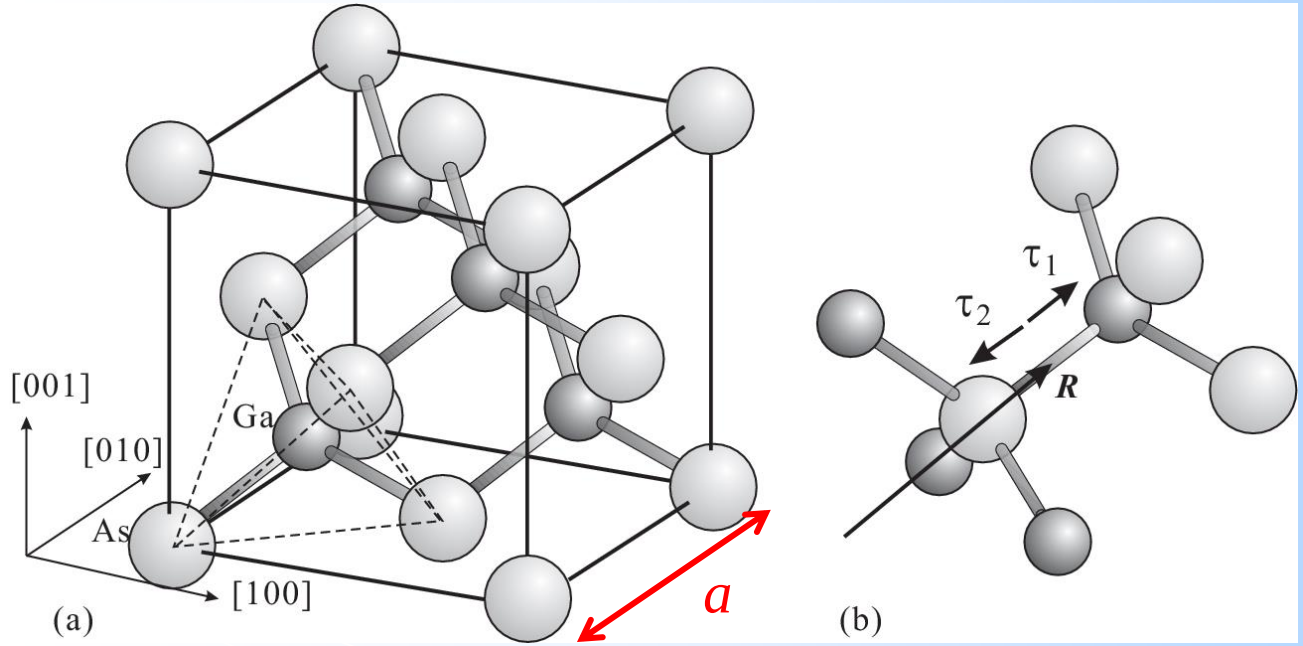
$$v_p(\boldsymbol{K}) = \int \sum_{j,\alpha} W_p^{\alpha}(\boldsymbol{r} - \boldsymbol{R}_j - \boldsymbol{\tau}_{\alpha}) e^{-i\boldsymbol{K}\cdot\boldsymbol{r}} \frac{d\boldsymbol{r}}{V}$$

$$= \frac{1}{N} \sum_{j} e^{-i\boldsymbol{K}\cdot\boldsymbol{R}_j} \sum_{\alpha} e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_{\alpha}} \frac{1}{\Omega} \int_{\Omega} W_p^{\alpha}(\boldsymbol{r}') e^{-i\boldsymbol{K}\cdot\boldsymbol{r}'} d\boldsymbol{r}$$

$$= \sum_{\alpha} e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_{\alpha}} \frac{1}{\Omega} \int_{\Omega} W_p^{\alpha}(\boldsymbol{r}') e^{-i\boldsymbol{K}\cdot\boldsymbol{r}'} d\boldsymbol{r}' \qquad \because e^{-i\boldsymbol{K}\cdot\boldsymbol{R}_j} = 1$$

$$= \sum_{\alpha} e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_{\alpha}} w_p^{\alpha}(\boldsymbol{K})$$

Empirical pseudo potential for fcc semiconductors



$$\mathrm{Ga}: \frac{a}{8}(1,1,1),$$

$$\mathrm{As}: \quad -\frac{a}{8}(1,1,1)$$

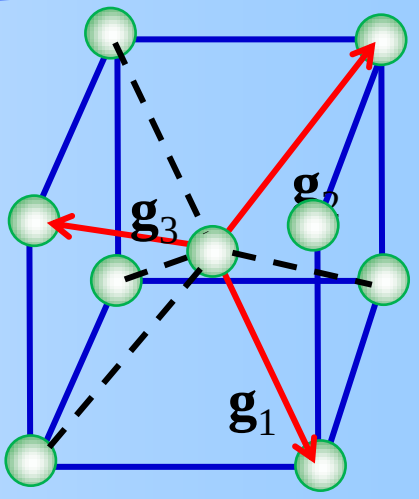
$$\begin{aligned} v_p(\boldsymbol{K}) &= e^{i\boldsymbol{K}\cdot\boldsymbol{\tau}_1} v_p^1(\boldsymbol{K}) + e^{-i\boldsymbol{K}\cdot\boldsymbol{\tau}_1} v_p^2(\boldsymbol{K}) \\ &= (v_p^1 + v_p^2)\cos\boldsymbol{K}\cdot\boldsymbol{\tau} + (v_p^1 - v_p^2)\sin\boldsymbol{K}\cdot\boldsymbol{\tau} \\ &= v_p^s(\boldsymbol{K})\cos\boldsymbol{K}\cdot\boldsymbol{\tau} + v_p^a(\boldsymbol{K})\sin\boldsymbol{K}\cdot\boldsymbol{\tau} \end{aligned}$$

structure factor

form factor

Empirical pseudo potential for fcc semiconductors

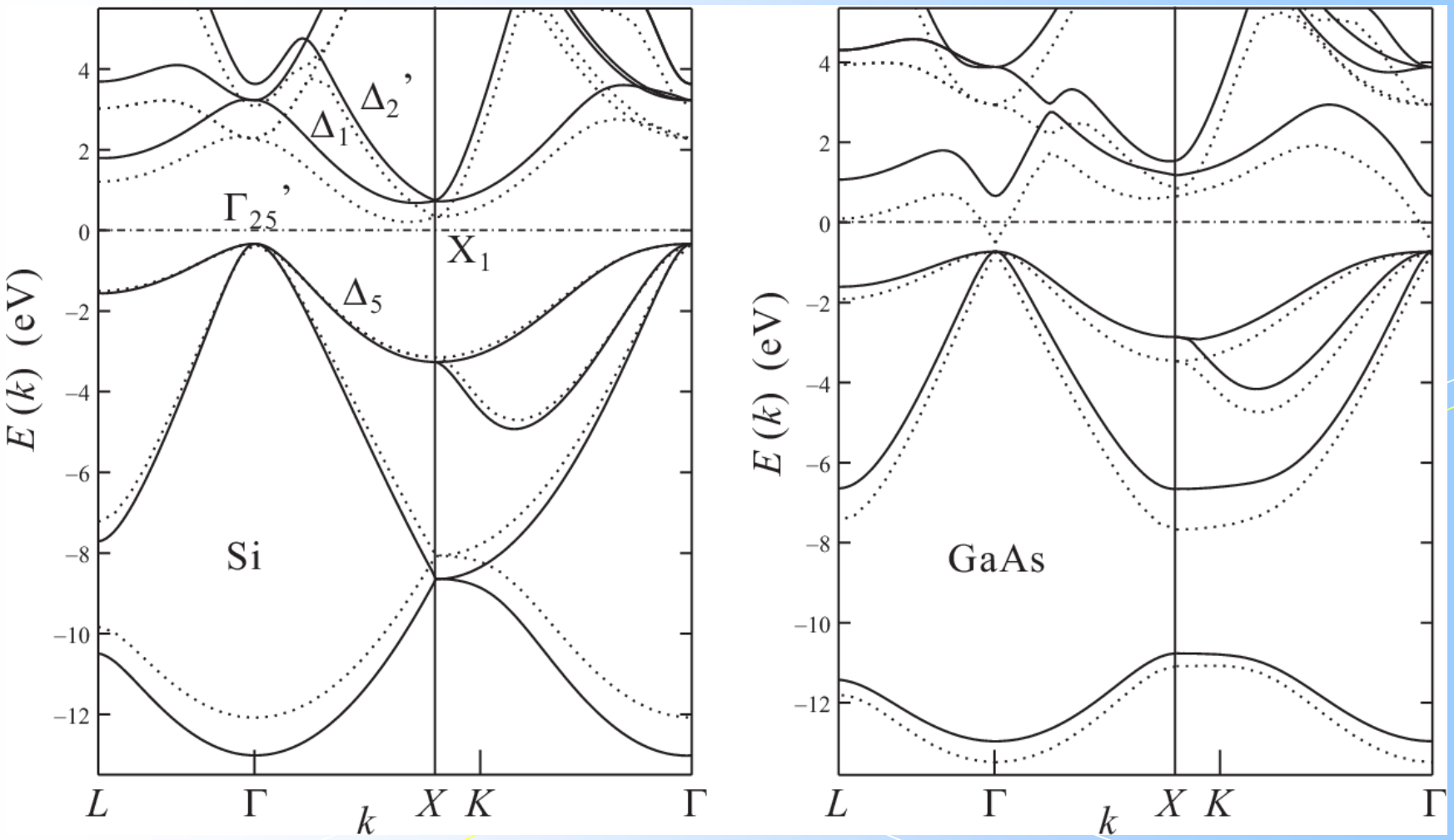
distance :	reciprocal lattice point	number
0 :	(0,0,0)	1
$\sqrt{3}$:	(1,1,1), (1,1,-1), (1,-1,1), $\cdots$	8
2 :	(2,0,0), (0,2,0), (0,0,2), (-2,0,0),$\cdots$	6
$\sqrt{8}$:	(2,2,0), (2,0,2), (0,2,2), (-2,2,0), $\cdots$	12
$\sqrt{11}$:	(3,1,1), (1,3,1), (1,1,3), (-3,1,1), $\cdots$	24



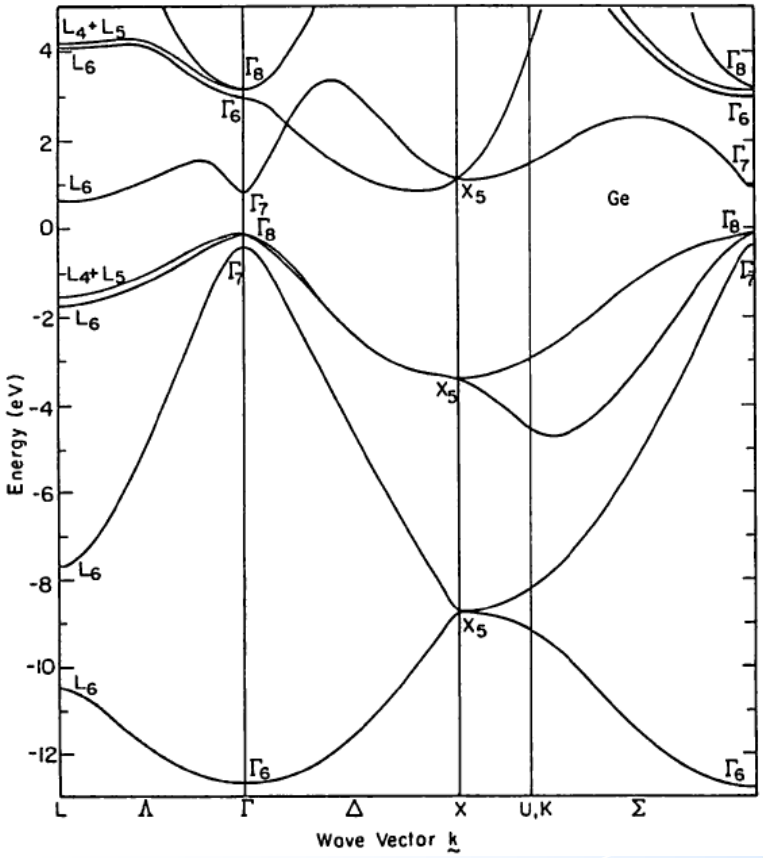
empirical structure factors

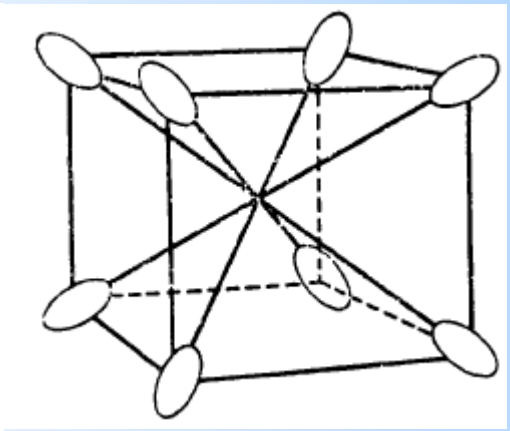
	$v_p^s(111)$	$v_p^s(220)$	$v_p^s(311)$	$v_p^a(111)$	$v_p^a(200)$	$v_p^a(311)$
Si	-2.856	0.544	1.088	0	0	0
Ge	-3.128	0.136	0.816	0	0	0
GaAs	-3.128	0.136	0.816	0.952	0.68	0.136
CdTe	-2.72	0	0.544	2.04	1.224	0.544

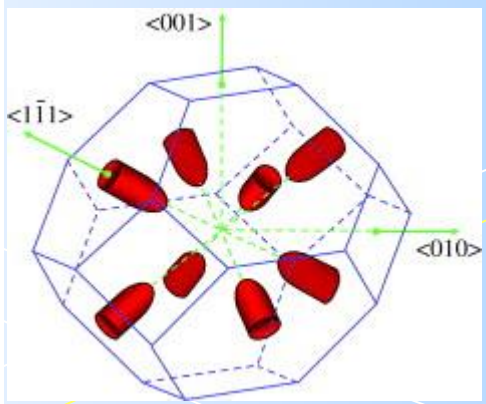
Band structure of Si and GaAs



Conduction valley structures

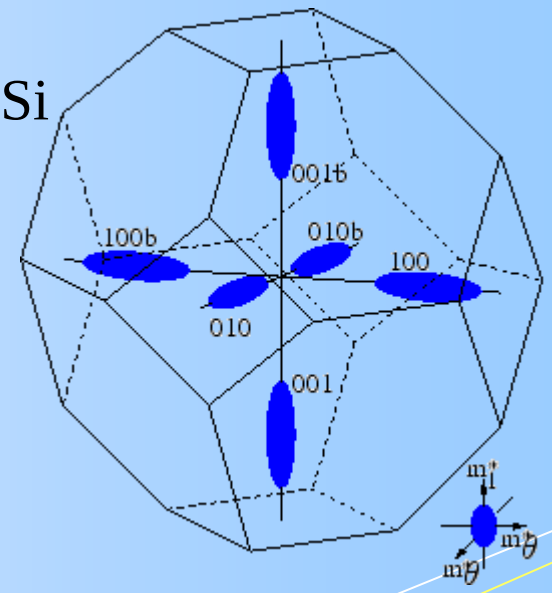


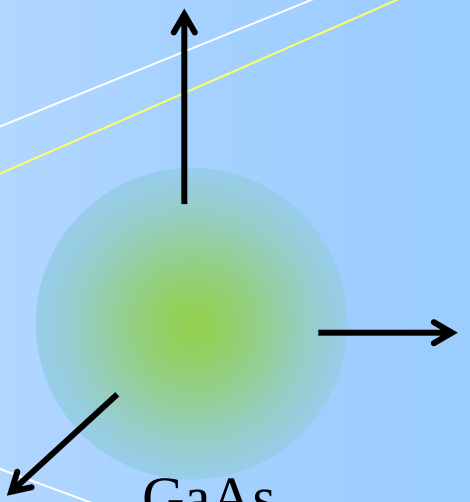




Ge

Si





GaAs