

module II

Band Structure Models

Fredrik Karlsson

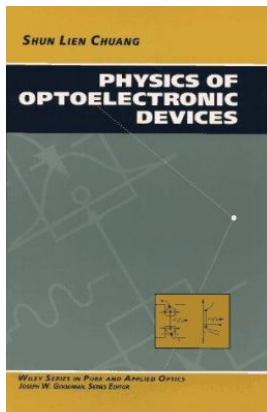
- Introduction
- Tight-binding approximation
- Pseudopotential
- **$\mathbf{k} \cdot \mathbf{p}$ approximation**

module II

Band Structure Models

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• $\mathbf{k} \cdot \mathbf{p}$ approximation

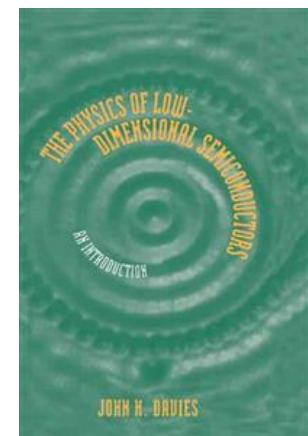


Physics of optoelectronic devices

Shun Lien Chuang

Chapter 3.6 (pages 114 - 116)

Chapter 4.1 – 4.4 (pages 124 - 144)



The physics of low-dimensional semiconductors

John H. Davies

Chapter 10.2 (pages 377 - 384)

Alternative books

Yu & Cardona: Fundamentals of Semiconductors, Chapter 2.6 (pages 68-82)

Enderlein & Horning: Fundamentals of Semiconductor Physics., Chapter 2.7 (179-200)

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• $\mathbf{k} \cdot \mathbf{p}$ approximation

Review articles

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APPLIED PHYSICS REVIEW

Band parameters for III–V compound semiconductors and their alloys

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Energy Band Theory

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band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

Single electron **Schrödinger equation** for the valence- or conduction band states.

$$H = \frac{\mathbf{p}^2}{2m_0} + V(\mathbf{r}), \text{ where } \mathbf{p}^2 = \mathbf{p} \cdot \mathbf{p} \text{ and } \mathbf{p} = -i\hbar\nabla$$

Bloch's theorem

$$\psi_{\mathbf{k}}^{(n)}(\mathbf{r}) = u_{\mathbf{k}}^{(n)}(\mathbf{r})e^{i\mathbf{k} \cdot \mathbf{r}}, \text{ where } u_{\mathbf{k}}^{(n)}(\mathbf{r} + \mathbf{a}) = u_{\mathbf{k}}^{(n)}(\mathbf{r})$$

$$\mathbf{p}^2 \psi_{\mathbf{k}}^{(n)}(\mathbf{r}) = \mathbf{p} \cdot \mathbf{p} \psi_{\mathbf{k}}^{(n)}(\mathbf{r}) = \mathbf{p} \cdot \left(\mathbf{p} u_{\mathbf{k}}^{(n)}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + u_{\mathbf{k}}^{(n)}(\mathbf{r}) \hbar \mathbf{k} e^{i\mathbf{k} \cdot \mathbf{r}} \right)$$

$$= p^2 u_{\mathbf{k}}^{(n)}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + \underbrace{\mathbf{p} \cdot u_{\mathbf{k}}^{(n)}(\mathbf{r}) \hbar \mathbf{k} e^{i\mathbf{k} \cdot \mathbf{r}} + \mathbf{p} \cdot u_{\mathbf{k}}^{(n)}(\mathbf{r}) \hbar \mathbf{k} e^{i\mathbf{k} \cdot \mathbf{r}}}_{\mathbf{k} \cdot \mathbf{p}} + u_{\mathbf{k}}^{(n)}(\mathbf{r}) \hbar^2 k^2 e^{i\mathbf{k} \cdot \mathbf{r}}$$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

Make the substitution $\psi_{\mathbf{k}}^{(n)}(\mathbf{r}) = u_{\mathbf{k}}^{(n)}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ in Schrödinger Equation and eliminate $e^{i\mathbf{k}\cdot\mathbf{r}}$ appearing on both sides.

$$\Rightarrow \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right] + \left[\frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \right] u_{\mathbf{k}}^{(n)}(\mathbf{r}) = \varepsilon_{\mathbf{k}}^{(n)} u_{\mathbf{k}}^{(n)}(\mathbf{r})$$

This is an exact result, no approximation has been made.

Suppose that we have solved this at $\mathbf{k} = \mathbf{0}$ and we know $u_{\mathbf{0}}^{(n)}(\mathbf{r})$ and $\varepsilon_{\mathbf{0}}^{(n)}$. Use the complete set of functions $u_{\mathbf{0}}^{(n)}(\mathbf{r})$ as a basis in which to expand the solutions at some other value of \mathbf{k} .

Approximation: Use a subset of $u_{\mathbf{0}}^{(n)}(\mathbf{r})$ $n \in \{i, j, k, l\}$

The minimal choice includes only those $u_{\mathbf{0}}^{(n)}(\mathbf{r})$ on either side of the band gap.

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

s-like conduction band

$$|u_0^{(S)}\rangle = |S\rangle \rightarrow s(r)$$

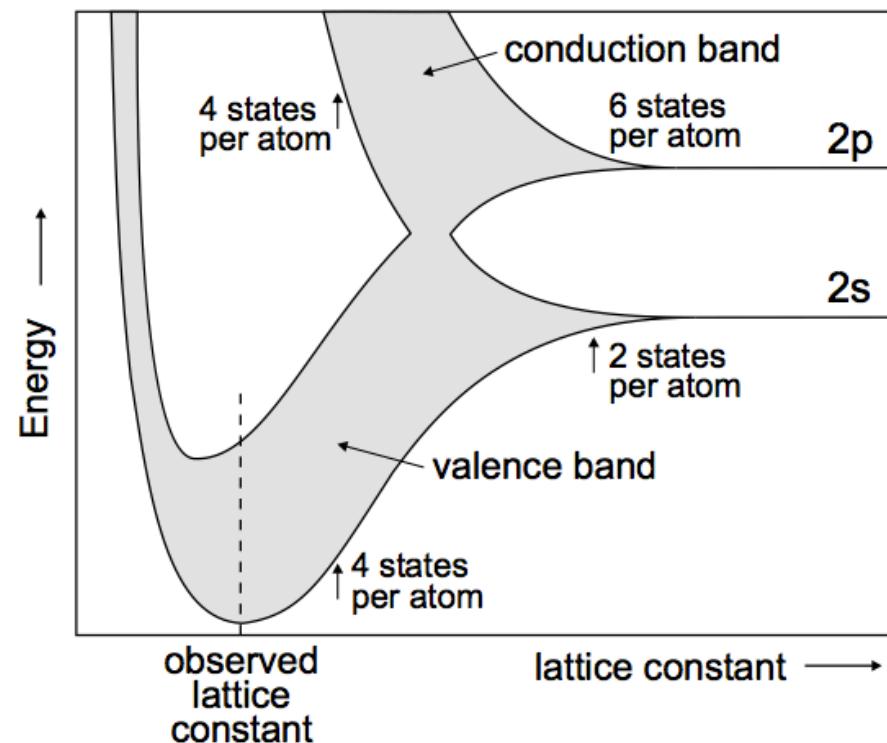
p-like valence band ($p_x p_y p_z$)

$$|u_0^{(X)}\rangle = |X\rangle \rightarrow f(r)x$$

$$|u_0^{(Y)}\rangle = |Y\rangle \rightarrow f(r)y$$

$$|u_0^{(Z)}\rangle = |Z\rangle \rightarrow f(r)z$$

$$H^{\mathbf{k}\cdot\mathbf{p}} = \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right] + \left[\frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \right]$$



Find the matrix elements in our restricted basis!

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

$$\mathbf{k=0} \Rightarrow H^{\mathbf{k}\cdot\mathbf{p}} = \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right]$$

$$\langle X | \frac{p^2}{2m_0} + V(\mathbf{r}) | X \rangle = \langle Y | \frac{p^2}{2m_0} + V(\mathbf{r}) | Y \rangle = \langle Z | \frac{p^2}{2m_0} + V(\mathbf{r}) | Z \rangle = E_V$$

$$\langle S | \frac{p^2}{2m_0} + V(\mathbf{r}) | S \rangle = E_C \quad |S\rangle \quad |X\rangle \quad |Y\rangle \quad |Z\rangle$$

All cross terms are zero

$$\begin{aligned} \langle S | & \quad \begin{pmatrix} E_C & 0 & 0 & 0 \\ 0 & E_V & 0 & 0 \\ 0 & 0 & E_V & 0 \\ 0 & 0 & 0 & E_V \end{pmatrix} \\ \langle X | \\ \langle Y | \\ \langle Z | \end{aligned}$$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

$$\mathbf{k} \neq \mathbf{0} \Rightarrow H^{\mathbf{k} \cdot \mathbf{p}} = \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right] + \left[\frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \right]$$

$$\varepsilon = \varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_0}$$

	$ S\rangle$	$ X\rangle$	$ Y\rangle$	$ Z\rangle$
$\langle S $	$E_C + \varepsilon$	0	0	0
$\langle X $	0	$E_V + \varepsilon$	0	0
$\langle Y $	0	0	$E_V + \varepsilon$	0
$\langle Z $	0	0	0	$E_V + \varepsilon$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

$$\mathbf{k} \neq \mathbf{0} \Rightarrow H^{\mathbf{k} \cdot \mathbf{p}} = \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right] + \left[\frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \right]$$

$$\frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | X \rangle = \frac{\hbar}{m_0} \langle S | k_x p_x + k_y p_y + k_z p_z | X \rangle$$

$$|S\rangle \rightarrow s(r) \quad \rightarrow k_x \int i x^2 d\mathbf{r} + k_y \cancel{\int i xy d\mathbf{r}} + k_z \cancel{\int i xz d\mathbf{r}} = ipk_x \neq 0$$

$$|X\rangle \rightarrow f(r)x \quad \Rightarrow \frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | X \rangle = iP_0 k_x$$

$$|Y\rangle \rightarrow f(r)y$$

$$|Z\rangle \rightarrow f(r)z$$

$$\mathbf{p} \rightarrow ix\hat{\mathbf{x}} + iy\hat{\mathbf{x}} + iz\hat{\mathbf{x}}$$

By symmetry arguments (cubic symmetry):

$$\frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | Y \rangle = iP_0 k_y \quad \frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | Z \rangle = iP_0 k_z$$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

$$|S\rangle \rightarrow s(r)$$

$$\Rightarrow \frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | X \rangle = iP_0 k_x$$

$$|X\rangle \rightarrow f(r)x$$

$$|Y\rangle \rightarrow f(r)y$$

$$|Z\rangle \rightarrow f(r)z$$

By symmetry arguments (cubic symmetry):

$$\frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | Y \rangle = iP_0 k_y \quad \frac{\hbar}{m_0} \langle S | \mathbf{k} \cdot \mathbf{p} | Z \rangle = iP_0 k_z$$

$$\mathbf{p} \rightarrow ix\hat{\mathbf{x}} + iy\hat{\mathbf{x}} + iz\hat{\mathbf{x}}$$

Exactly the same procedure yields: $\langle n | \mathbf{k} \cdot \mathbf{p} | n \rangle = 0$

$$\langle X | \mathbf{k} \cdot \mathbf{p} | Y \rangle = \langle X | \mathbf{k} \cdot \mathbf{p} | Z \rangle = \langle Y | \mathbf{k} \cdot \mathbf{p} | Z \rangle = 0$$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

$$\mathbf{k} \neq \mathbf{0} \Rightarrow H^{\mathbf{k} \cdot \mathbf{p}} = \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right] + \left[\frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \right]$$

$$|S\rangle \quad |X\rangle \quad |Y\rangle \quad |Z\rangle$$

$$\begin{array}{c} \langle S | \\ \langle X | \\ \langle Y | \\ \langle Z | \end{array} \left(\begin{array}{cccc} E_C + \varepsilon & iP_0 k_x & iP_0 k_y & iP_0 k_z \\ -iP_0 k_x & E_V + \varepsilon & 0 & 0 \\ -iP_0 k_y & 0 & E_V + \varepsilon & 0 \\ -iP_0 k_z & 0 & 0 & E_V + \varepsilon \end{array} \right)$$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

Set $E_V = 0$ and $E_C = E_g$

Analytical eigenvalues of the 4x4 matrix (solutions to the secular equation):

$$\varepsilon_{\mathbf{k}}^{(c)} = \frac{1}{2}E_g + \varepsilon(k) + \sqrt{\frac{1}{4}E_g^2 + P_0^2k^2} \quad \varepsilon(k) = \frac{\hbar^2 k^2}{2m_0}$$

$$\varepsilon_{\mathbf{k}}^{(lh)} = \frac{1}{2}E_g + \varepsilon(k) - \sqrt{\frac{1}{4}E_g^2 + P_0^2k^2}$$

$$\varepsilon_{\mathbf{k}}^{(hh)} = \varepsilon(k) \quad (\times 2)$$

Two material parameters: E_g and P

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

Taylor expand the square root $\sqrt{1+x} \approx 1 + \frac{1}{2}x$.

$$\sqrt{\frac{1}{4}E_g^2 + P_0^2 k^2} \approx \frac{E_g}{2} + \frac{P_0^2}{E_g} k^2 = \frac{E_g}{2} + \frac{\hbar^2}{2m_0} \frac{E_P}{E_g} k^2, \text{ where } E_P = 2m_0 \frac{P_0^2}{\hbar^2}$$

Effective electron mass

$$\varepsilon_{\mathbf{k}}^{(c)} = E_g + \frac{\hbar^2 k^2}{2m_0} \left(1 + \frac{E_P}{E_g} \right) = E_g + \frac{\hbar^2 k^2}{2m_0 m_e^*}$$

$$m_e^* = \left(1 + \frac{E_P}{E_g} \right)$$

Effective light-hole mass

$$\varepsilon_{\mathbf{k}}^{(lh)} = E_g + \frac{\hbar^2 k^2}{2m_0} \left(1 - \frac{E_P}{E_g} \right) = E_g - \frac{\hbar^2 k^2}{2m_0 m_{lh}^*}$$

$$m_{lh}^* = \left(\frac{E_P}{E_g} - 1 \right)$$

$$\varepsilon_k^{(hh)} = \frac{\hbar^2 k^2}{2m_0} \quad (\times 2) \quad \text{Free electron dispersion!!}$$

band structure models

Basics of $k \cdot p$ theory

For GaAs $E_g = 1.5$ eV

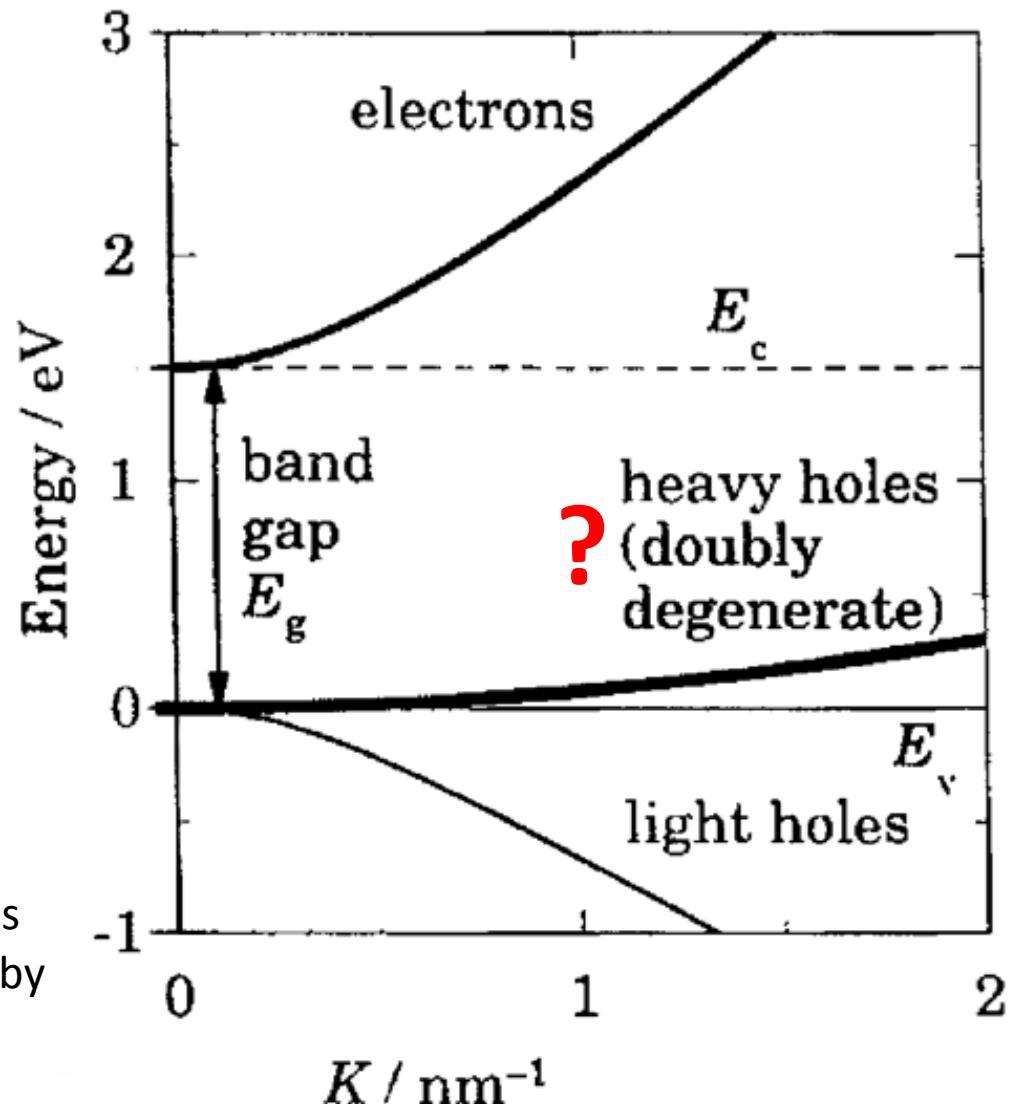
$E_P = 22$ eV

\Rightarrow

$m_e^* = 0.064$

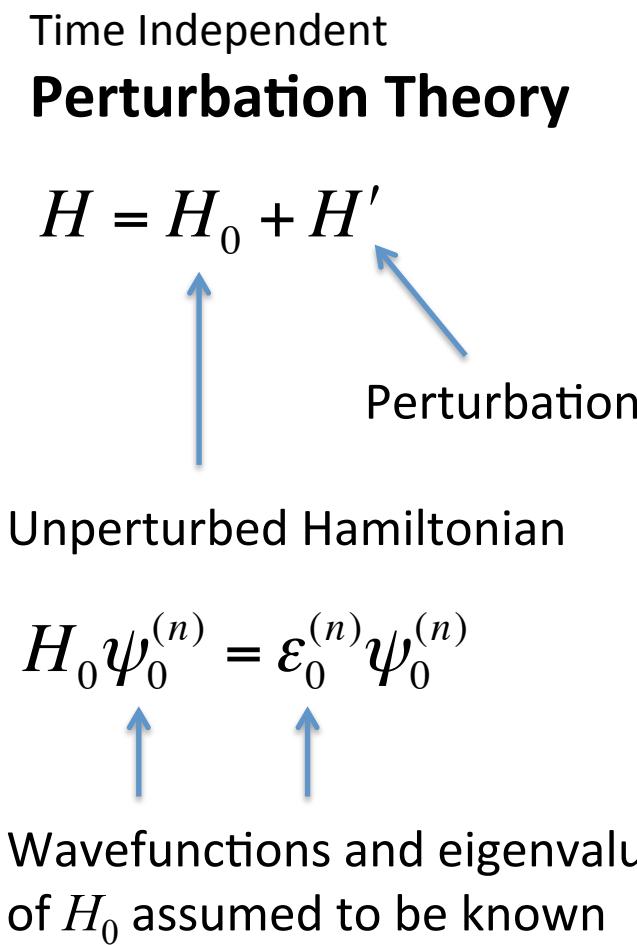
$m_{lh}^* = 0.073$

The $k \cdot p$ model with only 4 basis functions **insufficient**. Instead to including more basis functions, there influence can be included by perturbation theory.



band structure models

Basics of $k \cdot p$ theory



We want to solve $H\psi^{(n)} = \epsilon^{(n)}\psi^{(n)}$

Approximate values of $\epsilon^{(n)}$ are given by
perturbation theory

$$0^{\text{th}} \text{ order} \quad \epsilon^{(n)} \approx \epsilon_0^{(n)}$$

$$1^{\text{st}} \text{ order} \quad \epsilon^{(n)} \approx \epsilon_0^{(n)} + \left\langle \psi_0^{(n)} \middle| H' \middle| \psi_0^{(n)} \right\rangle$$

$$2^{\text{nd}} \text{ order} \quad \epsilon^{(n)} \approx \epsilon_0^{(n)} + \left\langle \psi_0^{(n)} \middle| H' \middle| \psi_0^{(n)} \right\rangle$$

$$+ \sum_{n \neq m} \frac{\left| \left\langle \psi_0^{(n)} \middle| H' \middle| \psi_0^{(m)} \right\rangle \right|^2}{E_0^{(n)} - E_0^{(m)}}$$

Even if we only are interested in state n , we have to take the influence of all other states into account.

band structure models

Basics of $k \cdot p$ theory

Matrix Form of

Schrödinger Equation $H\psi = \varepsilon\psi$

$$\begin{pmatrix} \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ H_{m,1} & \cdots & H_{m,n} & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} = \varepsilon \begin{pmatrix} a_1 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}$$

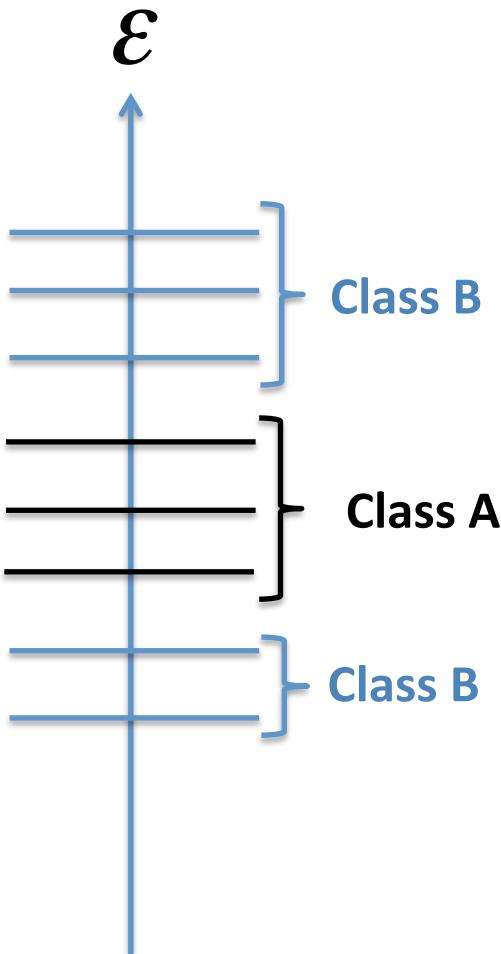
$$\Leftrightarrow \sum_n (H_{m,n} - \varepsilon \delta_{m,n}) a_n = 0$$

For row m $(\varepsilon - H_{m,m}) a_m = \sum_{n \neq m} H_{m,n} a_n$

band structure models

Basics of $k \cdot p$ theory

Löwdin's Perturbation



We are not interested in the states in B, but they have a non-negligible effect on the states in A, which can be treated by perturbation theory.

For row m

$$(\epsilon - H_{m,m})a_m = \sum_{n \neq m} H_{m,n} a_n$$

$$\Leftrightarrow (\epsilon - H_{m,m})a_m = \sum_{n \neq m}^A H_{m,n} a_n + \sum_{\alpha \neq m}^B H_{m,\alpha} a_\alpha$$

$$h_{m,n} \equiv \frac{H_{m,n}}{(\epsilon - H_{m,m})} \Rightarrow a_m = \sum_{n \neq m}^A h_{m,n} a_n + \sum_{\alpha \neq m}^B h_{m,\alpha} a_\alpha$$

$$\Rightarrow a_\alpha = \sum_{n \neq \alpha}^A h_{\alpha,n} a_n + \sum_{\beta \neq \alpha}^B h_{\alpha,\beta} a_\beta$$

band structure models

Basics of $k \cdot p$ theory

Löwdin's Perturbation

For row m

$$(\varepsilon - H_{m,m})a_m = \sum_{n \neq m} H_{m,n} a_n \quad h_{m,n} = \frac{H_{m,n}}{(\varepsilon - H_{m,m})} \quad (*)$$

$$a_m = \sum_{n \neq m}^A h_{m,n} a_n + \sum_{\alpha \neq m}^B h_{m,\alpha} \sum_{n \neq \alpha}^A h_{\alpha,n} a_n + \sum_{\alpha \neq m}^B h_{m,\alpha} \sum_{\beta \neq \alpha}^B h_{\alpha,\beta} a_\beta$$

$$\stackrel{(*)}{\Rightarrow} (\varepsilon - H_{m,m})a_m = \sum_{n \neq m}^A \left(H_{m,n} + \sum_{\alpha \neq m}^B \frac{H_{m,\alpha} H_{\alpha,n}}{\varepsilon - H_{\alpha,\alpha}} + \dots \right) a_n$$

Convergence
 $|H_{m,\alpha}| \ll |\varepsilon - H_{\alpha,\alpha}|$
 $m \in A, \alpha \in B$

$U_{m,n}^{(A)}$

Theorem

An eigenvalue problem with respect to a system of states belonging to two classes, A and B, can be reduced only to class A, if the matrix elements $H_{m,n}$ ($n \neq m$) are replaced by the elements $U_{m,n}^{(A)}$, where the influence of the class B states is taken into account by expansion.

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

Löwdin's Perturbation - Coupling with distant bands

The $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian for is modified according to Löwdin's Perturbation

$$H_{m,n} \rightarrow H_{m,n} + H'_{m,n}$$

where

$$H'_{m,n} = \sum_{\alpha \neq m}^B \frac{H_{m,\alpha} H_{\alpha,n}}{E_V - E_\alpha} \quad m, n \in \{S, X, Y, Z\}, \quad \alpha \in \text{Class } B$$

$$\text{But } H_{m,n} = \left\langle m \left| \frac{\hbar^2}{m_0^2} \mathbf{k} \cdot \mathbf{p} \right| n \right\rangle = \frac{\hbar^2}{m_0^2} \langle m | \mathbf{p} | n \rangle \cdot \mathbf{k}$$

$$\Rightarrow H'_{m,n} = \frac{\hbar^2}{m_0^2} \sum_{\alpha \neq m}^B \frac{\mathbf{k} \cdot \langle m | \mathbf{p} | \alpha \rangle \langle \alpha | \mathbf{p} | n \rangle \cdot \mathbf{k}}{E_V - E_\alpha}$$

band structure models

Basics of $\mathbf{k} \cdot \mathbf{p}$ theory

Löwdin's Perturbation - Coupling with distant bands

$$H'_{m,n} = \frac{\hbar^2}{m_0^2} \sum_{\alpha \neq m}^B \frac{\mathbf{k} \cdot \langle m | \mathbf{p} | \alpha \rangle \langle \alpha | \mathbf{p} | n \rangle \cdot \mathbf{k}}{E_V - E_\alpha}$$

These matrix elements can conveniently be determined by group theory, considering the finite set of symmetries available for the α states in a (e.g. cubic) crystal.

However, here we will show an explicit example for $\alpha \in d$ -symmetry basis in a cubic crystal.

$$|X\rangle \rightarrow f(r)x$$

$$|\alpha_1\rangle \rightarrow f_1(r)xy$$

$$|Y\rangle \rightarrow f(r)y$$

$$|\alpha_2\rangle \rightarrow f_2(r)xz$$

$$|Z\rangle \rightarrow f(r)z$$

$$|\alpha_3\rangle \rightarrow f_3(r)yz$$

$$|S\rangle \rightarrow s(r)$$

$$|\alpha_4\rangle \rightarrow f_4(r)(x^2 - y^2)$$

$$\mathbf{p} \rightarrow \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$|\alpha_5\rangle \rightarrow f_5(r)(2z^2 - x^2 - y^2)$$

Löwdin's perturbation

Coupling with distant bands

$$H'_{m,n} = \frac{\hbar^2}{m_0^2} \sum_{\alpha \neq m}^B \frac{\mathbf{k} \cdot \langle m | \mathbf{p} | \alpha \rangle \langle \alpha | \mathbf{p} | n \rangle \cdot \mathbf{k}}{E_V - E_\alpha}$$

Consider for example matrix element

$$H'_{X,Z}$$

The sum consists of five terms that has to be evaluated

$$\frac{\hbar^2}{m_0^2} \frac{\mathbf{k} \cdot \langle X | \mathbf{p} | \alpha_n \rangle \langle \alpha_n | \mathbf{p} | Z \rangle \cdot \mathbf{k}}{E_V - E_\alpha}, \quad n = 1, 2, \dots, 5$$

For the 1st term $n = 1$ $|\alpha_1\rangle \rightarrow f_1(r)xy$

$$\mathbf{k} \cdot \langle X | \mathbf{p} | \alpha_1 \rangle \langle \alpha_1 | \mathbf{p} | Z \rangle \cdot \mathbf{k} \propto \mathbf{k} \cdot \langle x | x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} | xy \rangle \langle xy | x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} | z \rangle \cdot \mathbf{k}$$

$$\begin{aligned} &= \left(k_x \cancel{\int x^3 y d\mathbf{r}} + k_y \cancel{\int x^2 y^2 d\mathbf{r}} + k_z \cancel{\int x^2 z y d\mathbf{r}} \right) \\ &\times \left(k_x \cancel{\int x^2 y z d\mathbf{r}} + k_y \cancel{\int x y^2 z d\mathbf{r}} + k_z \cancel{\int x^2 y z^2 d\mathbf{r}} \right) = 0 \end{aligned}$$

...also the 2nd and 3rd term are zero...

Löwdin's perturbation

Coupling with distant bands

$$H'_{m,n} = \frac{\hbar^2}{m_0^2} \sum_{\alpha \neq m}^B \frac{\mathbf{k} \cdot \langle m | \mathbf{p} | \alpha \rangle \langle \alpha | \mathbf{p} | n \rangle \cdot \mathbf{k}}{E_V - E_\alpha}$$

Consider for example matrix element

$$H'_{X,Z}$$

The sum consists of five terms that has to be evaluated

For the 4th term $n = 4$ $|\alpha_4\rangle \rightarrow f_4(r)(x^2 - y^2)$

$$\mathbf{k} \cdot \langle X | \mathbf{p} | \alpha_4 \rangle \langle \alpha_4 | \mathbf{p} | Z \rangle \cdot \mathbf{k}$$

$$\propto \mathbf{k} \cdot \langle x | x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} | x^2 - y^2 \rangle \langle x^2 - y^2 | x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} | z \rangle \cdot \mathbf{k}$$

$$= \left(k_x \int [x^4 - x^2 y^2] d\mathbf{r} + k_y \int [x^3 y - xy^3] d\mathbf{r} + k_z \int [x^3 z - xy^2 z] d\mathbf{r} \right)$$

$$\times \left(k_x \int [x^3 z - xy^2 z] d\mathbf{r} + k_y \int [x^2 yz - y^3 z] d\mathbf{r} + k_z \int [x^2 z^2 - y^2 z^2] d\mathbf{r} \right)$$

$$= 0$$

Löwdin's perturbation

Coupling with distant bands

$$H'_{m,n} = \frac{\hbar^2}{m_0^2} \sum_{\alpha \neq m}^B \frac{\mathbf{k} \cdot \langle m | \mathbf{p} | \alpha \rangle \langle \alpha | \mathbf{p} | n \rangle \cdot \mathbf{k}}{E_V - E_\alpha}$$

Consider for example matrix element

$$H'_{X,Z}$$

The sum consists of five terms that has to be evaluated

For the 5th term $n = 5$ $|\alpha_5\rangle \rightarrow f_5(r)(2z^2 - x^2 - y^2)$

$$\mathbf{k} \cdot \langle X | \mathbf{p} | \alpha_5 \rangle \langle \alpha_5 | \mathbf{p} | Z \rangle \cdot \mathbf{k}$$

$$\propto \mathbf{k} \cdot \langle x | x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} | 2z^2 - x^2 - y^2 \rangle \langle 2z^2 - x^2 - y^2 | x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} | z \rangle \cdot \mathbf{k}$$

$$= \left(k_x \int [2x^2z^2 - x^4 - x^2y^2] d\mathbf{r} + k_y \int [2xyz^2 - x^3y - xy^3] d\mathbf{r} + k_z \int [2xz^3 - x^3z - xzy^2] d\mathbf{r} \right) \\ \times \left(k_x \int [2xz^3 - x^3z - xy^2z] d\mathbf{r} + k_y \int [2yz^3 - x^2yz - y^3z] d\mathbf{r} + k_z \int [2z^4 - x^2z^2 - y^2z^2] d\mathbf{r} \right)$$

$$= nk_x k_z \neq 0$$

Löwdin's perturbation

Coupling with distant bands

$$H'_{m,n} = \frac{\hbar^2}{m_0^2} \sum_{\alpha \neq m}^B \frac{\mathbf{k} \cdot \langle m | \mathbf{p} | \alpha \rangle \langle \alpha | \mathbf{p} | n \rangle \cdot \mathbf{k}}{E_V - E_\alpha}$$

Thus, only the fifth term contribute to the X,Z matrix element:

$$H'_{X,Z} = \frac{\hbar^2}{m_0^2} \frac{n k_x k_z}{E_V - E_\alpha} = N' k_x k_z$$

By symmetry arguments (cubic symmetry): $H'_{X,Z} = H'_{Y,X} = H'_{Z,Y}$

Exactly the same procedure yields:

$$H'_{X,X} = L' k_x^2 + M k_y^2 + M k_z^2$$

$$H'_{Y,Y} = M k_x^2 + L' k_y^2 + M k_z^2$$

$$H'_{Z,Z} = M k_x^2 + M k_y^2 + L' k_z^2$$

$$H'_{S,S} = H'_{S,X} = H'_{S,Y} = H'_{S,Z} = 0$$

Löwdin's perturbation

Coupling with distant bands

The original $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian H_0 is modified by an extra term H'

$$H = H_0 + H'$$

$$H_0 = \begin{pmatrix} E_C + \varepsilon & iP_0 k_x & iP_0 k_y & iP_0 k_z \\ -iP_0 k_x & E_V + \varepsilon & 0 & 0 \\ -iP_0 k_y & 0 & E_V + \varepsilon & 0 \\ -iP_0 k_z & 0 & 0 & E_V + \varepsilon \end{pmatrix}, \text{ where } \varepsilon = \frac{\hbar^2 k^2}{2m_0}$$

$$H' = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & L'k_x^2 + Mk_y^2 + Mk_z^2 & N'k_x k_y & N'k_x k_z \\ 0 & N'k_y k_x & L'k_x^2 + Mk_y^2 + Mk_z^2 & N'k_y k_z \\ 0 & N'k_z k_x & N'k_z k_y & L'k_x^2 + Mk_y^2 + Mk_z^2 \end{pmatrix}$$

Löwdin's perturbation

Coupling with distant bands

H_0

$$H = \begin{pmatrix} E_C + \varepsilon & iP_0k_x & iP_0k_y & iP_0k_z \\ -iP_0k_x & E_V + \varepsilon & 0 & 0 \\ -iP_0k_y & 0 & E_V + \varepsilon & 0 \\ -iP_0k_z & 0 & 0 & E_V + \varepsilon \end{pmatrix}$$

Inclusion of other distant bands leads to further non-zero correction terms for matrix elements involving S -states.

$$\text{, where } \varepsilon = \frac{\hbar^2 k^2}{2m_0}$$

H'

$$+ \begin{pmatrix} A'k^2 & Bk_zk_y & Bk_xk_z & Bk_yk_x \\ Bk_yk_z & L'k_x^2 + Mk_y^2 + Mk_z^2 & N'k_xk_y & N'k_xk_z \\ Bk_zk_x & N'k_yk_x & Mk_x^2 + L'k_y^2 + Mk_z^2 & N'k_yk_z \\ Bk_xk_y & N'k_zk_x & N'k_zk_y & Mk_x^2 + Mk_y^2 + L'k_z^2 \end{pmatrix}$$

band structure models

Basics of $k \cdot p$ theory

The final Hamiltonian including coupling with distant bands has seven material parameters that have to be determined from experiments.

E_g, P_0 $E_g = E_C - E_V$...from direction interaction between s- and p-states.

A', B, L', M, N' ...second order interactions due to Löwdin renormalization involving states outside the s, p subspace.

$B = 0$ for diamond.

$B \approx 0$ for zincblende.

$A' \approx 0$ correction to the electron effective mass (GaAs $0.067m_0$ instead of $0.054m_0$).

band structure models

Basics of $k \cdot p$ theory

A different set of material parameters is frequently used:

$$E_g, E_P \quad P_0 = \sqrt{\frac{\hbar^2}{2m_0} E_P} \quad L' = \frac{P_0^2}{E_g} - \frac{\hbar^2}{2m_0} (1 + \gamma_1^{(0)} + 4\gamma_2^{(0)})$$

Luttinger Parameters

$$\gamma_1^{(0)}, \gamma_2^{(0)}, \gamma_3^{(0)} \quad N' = \frac{P^2}{E_g} - \frac{3\hbar^2}{m_0} \gamma_3^{(0)} \quad M = -\frac{\hbar^2}{2m_0} (1 + \gamma_1^{(0)} - 2\gamma_2^{(0)})$$

band structure models

Basics of $k \cdot p$ theory

TABLE I. Band structure parameters for GaAs.

Parameters	Recommended values	Range
a_{lc} (Å)	$5.65325 + 3.88 \times 10^{-5}(T - 300)$	
E_g^Γ (eV)	1.519	1.420–1.435 (300 K)
$\alpha(\Gamma)$ (meV/K)	0.5405	0.51–1.06
$\beta(\Gamma)$ (K)	204	190–671
E_g^X (eV)	1.981	...
$\alpha(X)$ (meV/K)	0.460	...
$\beta(X)$ (K)	204	...
E_g^L (eV)	1.815	...
$\alpha(L)$ (meV/K)	0.605	...
$\beta(L)$ (K)	204	...
Δ_{so} (eV)	0.341	0.32–0.36
$m_e^*(\Gamma)$	0.067	0.065–0.07 (0 K), 0.0635–0.067 (300 K)
$m_l^*(L)$	1.9	...
$m_i^*(L)$	0.0754	...
$m_{DOS}^*(L)$	0.56	...
$m_l^*(X)$	1.3	...
$m_i^*(X)$	0.23	...
$m_{DOS}^*(X)$	0.85	...
γ_1	6.98	6.79–7.20
γ_2	2.06	1.9–2.88
γ_3	2.93	2.681–3.05
m_{so}^*	0.172	0.133–0.388
E_p (eV)	28.8	25.5–29.0
F	-1.94	0.76–(-2)
VBO (eV)	-0.80	
a_c (eV)	-7.17	-6.3–(-18.3)
a_v (eV)	-1.16	-0.2–(-2.1)
b (eV)	-2.0	-1.66–(-3.9)
d (eV)	-4.8	-2.7–(-6.0)
c_{11} (GPa)	1221	...
c_{12} (GPa)	566	...
c_{44} (GPa)	600	...

Vurgaftman et al.
 J. Appl. Phys. **89** 5815, (2001)

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

Single electron **Schrödinger equation** for the valence- or conduction band states **with spin**.

$$H = \frac{p^2}{2m_0} + V(\mathbf{r}) + \boxed{\frac{\hbar}{4m^2c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}})}$$
$$\psi_{\mathbf{k}}^{(n)}(\mathbf{r}) = u_{\mathbf{k}}^{(n)}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\frac{\hbar}{4m^2c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}}) \psi_{\mathbf{k}}^{(n)}(\mathbf{r})$$

$$= \frac{\hbar}{4m^2c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}}) u_{\mathbf{k}}^{(n)}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + u_{\mathbf{k}}^{(n)}(\mathbf{r}) \frac{\hbar}{4m^2c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= \frac{\hbar}{4m^2c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}}) u_{\mathbf{k}}^{(n)}(\mathbf{r}) \cancel{e^{i\mathbf{k}\cdot\mathbf{r}}} + u_{\mathbf{k}}^{(n)}(\mathbf{r}) \frac{\hbar}{4m^2c^2} \bar{\sigma} \cdot (\nabla V \times \hbar\mathbf{k}) \cancel{e^{i\mathbf{k}\cdot\mathbf{r}}}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$\Rightarrow H^{\mathbf{k} \cdot \mathbf{p}} = \left[\frac{p^2}{2m_0} + V(\mathbf{r}) \right] + \left[\frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \right]$$

$$+ \frac{\hbar}{4m_0^2 c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}}) + \cancel{\frac{\hbar}{4m_0^2 c^2} \bar{\sigma} \cdot (\nabla V \times \hbar \mathbf{k})}$$

Crystal momentum much smaller than the atomic momentum $|\hbar \mathbf{k}| \ll \mathbf{p}$

$$H^{SO} = \frac{\hbar}{4m_0^2 c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}})$$

$$= \frac{\hbar}{4m_0^2 c^2} \begin{bmatrix} \sigma_x & \sigma_y & \sigma_z \end{bmatrix} \begin{pmatrix} \nabla V \times \hat{\mathbf{p}} \\ \left[\begin{array}{c} \partial V / \partial x \\ \partial V / \partial y \\ \partial V / \partial z \end{array} \right] \times \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$H^{SO} = \frac{\hbar}{4m_0^2 c^2} \left[\begin{array}{ccc} \bar{\sigma}^t & & \\ \sigma_x & \sigma_y & \sigma_z \end{array} \right] \left(\begin{bmatrix} \partial V / \partial x \\ \partial V / \partial y \\ \partial V / \partial z \end{bmatrix} \times \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} \right)$$

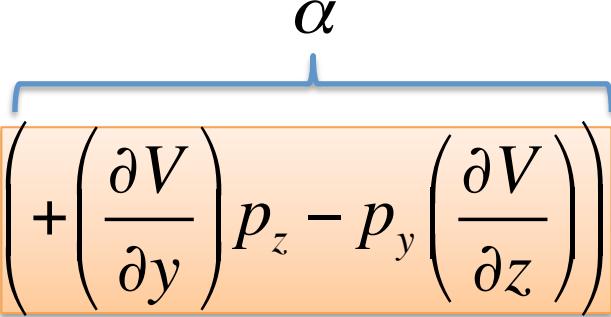
$$\nabla V \times \hat{\mathbf{p}} = \begin{bmatrix} \partial V / \partial x \\ \partial V / \partial y \\ \partial V / \partial z \end{bmatrix} \times \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} = \begin{bmatrix} +(\partial V / \partial y)p_z - p_y(\partial V / \partial z) \\ -(\partial V / \partial x)p_z + p_x(\partial V / \partial z) \\ +(\partial V / \partial x)p_y - p_x(\partial V / \partial y) \end{bmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$\Rightarrow \frac{\hbar}{4m_0^2 c^2} \bar{\sigma} \cdot (\nabla V \times \hat{\mathbf{p}}) = \frac{\hbar}{4m_0^2 c^2} \left[\left(+ \left(\frac{\partial V}{\partial y} \right) p_z - p_y \left(\frac{\partial V}{\partial z} \right) \right) \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right. \\ \left. + \left(- \left(\frac{\partial V}{\partial x} \right) p_z + p_x \left(\frac{\partial V}{\partial z} \right) \right) \cdot \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \right. \\ \left. + \left(+ \left(\frac{\partial V}{\partial x} \right) p_y - p_x \left(\frac{\partial V}{\partial y} \right) \right) \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right]$$

α



band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$\alpha = + \left(\frac{\partial V}{\partial y} \right) p_z - p_y \left(\frac{\partial V}{\partial z} \right)$$

Determine the Matrix elements

$$\alpha_{m,n} = \langle m | \alpha | n \rangle$$

$$\mathbf{p} \rightarrow \begin{bmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{bmatrix}$$

$$\alpha \rightarrow \tilde{y}\hat{z} - \hat{y}\tilde{z} \rightarrow yz$$

$$\alpha_{X,X} \propto \int x^2 yz d\mathbf{r} = 0$$

$$\alpha_{X,Y} \propto \int xy^2 z d\mathbf{r} = 0$$

$$\alpha_{X,Z} \propto \int xyz^2 d\mathbf{r} = 0$$

$$\alpha_{Y,Z} \propto \int y^2 z^2 d\mathbf{r} \neq 0$$

$$\frac{\partial V}{\partial x} \rightarrow \tilde{x}$$

$$\frac{\partial V}{\partial x}$$

$$\frac{\partial V}{\partial y} \rightarrow \tilde{y}$$

$$\frac{\partial V}{\partial y}$$

$$\frac{\partial V}{\partial z} \rightarrow \tilde{z}$$

All other elements zero except $\alpha_{Z,Y} = -\alpha_{Y,Z}$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$H^{SO} = \alpha \left[\frac{\hbar}{4m_0^2 c^2} \left[\left(+ \left(\frac{\partial V}{\partial y} \right) p_z - p_y \left(\frac{\partial V}{\partial z} \right) \right) \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right] \right]$$

$\rightarrow \alpha_{Z,Y} = -\alpha_{Y,Z} \neq 0$

$$+ \beta \left[\left(- \left(\frac{\partial V}{\partial x} \right) p_z + p_x \left(\frac{\partial V}{\partial z} \right) \right) \cdot \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \right]$$

$\rightarrow \beta_{Z,X} = -\beta_{X,Z} \neq 0$

$$+ \gamma \left[\left(+ \left(\frac{\partial V}{\partial x} \right) p_y - p_x \left(\frac{\partial V}{\partial y} \right) \right) \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right]$$

$\rightarrow \gamma_{X,Y} = -\gamma_{Y,X} \neq 0$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

Spin basis neglected:

$$H^{SO} = \begin{pmatrix} \langle S | & |S\rangle & |X\rangle & |Y\rangle & |Z\rangle \\ \langle X | & 0 & 0 & 0 & 0 \\ \langle Y | & 0 & 0 & -\gamma_{Y,Z} & -\beta_{Z,Y} \\ \langle Z | & 0 & +\gamma_{Y,Z} & 0 & -\alpha_{Z,Y} \\ & 0 & +\beta_{Z,X} & +\alpha_{Z,Y} & 0 \end{pmatrix}$$

From symmetry:

$$\frac{\hbar}{4m_0^2c^2}\langle Y|\alpha|Z\rangle = \frac{\hbar}{4m_0^2c^2}\langle X|\beta|Z\rangle = \frac{\hbar}{4m_0^2c^2}\langle X|\gamma|Y\rangle = +\frac{\Delta_0}{3}i$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$H^{\mathbf{k} \cdot \mathbf{p}} = H + H^{SO} \Rightarrow H_{ms',ns}^{\mathbf{k} \cdot \mathbf{p}} = H_{m,n} \delta_{s',s} + H_{ms',ns}^{SO}$$

$$s, s' \in \{\uparrow, \downarrow\} \quad |\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\left(\begin{array}{c|c} \text{Block 1} & \text{Block 2} \\ \hline s = +\frac{1}{2}, s' = +\frac{1}{2} & s = +\frac{1}{2}, s' = -\frac{1}{2} \\ \hline \text{Block 3} & \text{Block 4} \\ \hline s = -\frac{1}{2}, s' = +\frac{1}{2} & s = -\frac{1}{2}, s' = -\frac{1}{2} \end{array} \right)$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$\begin{aligned}
 & \frac{\hbar}{4m_0^2 c^2} \left[\left(+ \left(\frac{\partial V}{\partial y} \right) p_z - p_y \left(\frac{\partial V}{\partial z} \right) \right) \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right] \sigma_x \quad \langle \uparrow | \sigma_x | \uparrow \rangle = \langle \downarrow | \sigma_x | \downarrow \rangle = 0 \\
 & \qquad \qquad \qquad \langle \uparrow | \sigma_x | \downarrow \rangle = \langle \downarrow | \sigma_x | \uparrow \rangle = 1 \\
 & + \left(- \left(\frac{\partial V}{\partial x} \right) p_z + p_x \left(\frac{\partial V}{\partial z} \right) \right) \cdot \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \sigma_y \quad \langle \uparrow | \sigma_y | \uparrow \rangle = \langle \downarrow | \sigma_y | \downarrow \rangle = 0 \\
 & \qquad \qquad \qquad \langle \uparrow | \sigma_y | \downarrow \rangle = - \langle \downarrow | \sigma_y | \uparrow \rangle = i \\
 & + \left(+ \left(\frac{\partial V}{\partial x} \right) p_y - p_x \left(\frac{\partial V}{\partial y} \right) \right) \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \sigma_z \quad \langle \uparrow | \sigma_z | \uparrow \rangle = - \langle \downarrow | \sigma_z | \downarrow \rangle = 1 \\
 & \qquad \qquad \qquad \langle \uparrow | \sigma_z | \downarrow \rangle = \langle \downarrow | \sigma_z | \uparrow \rangle = 0
 \end{aligned}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

Spin basis neglected:

$$H^{SO} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\gamma_{Y,Z} & -\beta_{Z,Y} \\ 0 & +\gamma_{Y,Z} & 0 & -\alpha_{Z,Y} \\ 0 & +\beta_{Z,X} & +\alpha_{Z,Y} & 0 \end{pmatrix}$$

Spin basis:

$$\begin{aligned} |\uparrow\rangle &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\ |\downarrow\rangle &= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \end{aligned}$$

Spin included:

$$H_{SO} = \left(\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\gamma_{Y,Z} & 0 & 0 & 0 & 0 & -i\beta_{Z,Y} \\ 0 & +\gamma_{Y,Z} & 0 & 0 & 0 & 0 & 0 & -\alpha_{Z,Y} \\ 0 & 0 & 0 & 0 & 0 & +i\beta_{Z,X} & +\alpha_{Z,Y} & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +i\beta_{Z,Y} & 0 & 0 & 0 & +\gamma_{Y,Z} \\ 0 & 0 & 0 & -\alpha_{Z,Y} & 0 & -\gamma_{Y,Z} & 0 & 0 \\ 0 & -i\beta_{Z,X} & +\alpha_{Z,Y} & 0 & 0 & 0 & 0 & 0 \end{array} \right)$$

$$+ \frac{\Delta_0}{3} i$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – spin orbit interaction

$$H^{SO} = \frac{\Delta_0}{3} \begin{pmatrix} \langle S \uparrow | & |S \uparrow\rangle & |X \uparrow\rangle & |Y \uparrow\rangle & |Z \uparrow\rangle & |S \downarrow\rangle & |X \downarrow\rangle & |Y \downarrow\rangle & |Z \downarrow\rangle \\ \langle X \uparrow | & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \langle Y \uparrow | & 0 & 0 & -i & 0 & 0 & 0 & 0 & +1 \\ \langle Z \uparrow | & 0 & +i & 0 & 0 & 0 & 0 & 0 & -i \\ \hline \langle S \downarrow | & 0 & 0 & 0 & 0 & 0 & -1 & +i & 0 \\ \langle X \downarrow | & 0 & 0 & 0 & -1 & 0 & 0 & +i & 0 \\ \langle Y \downarrow | & 0 & 0 & 0 & -i & 0 & -i & 0 & 0 \\ \langle Z \downarrow | & 0 & +1 & +i & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ Hamiltonian

$$H^{\mathbf{k} \cdot \mathbf{p}} = H_0 + H' + H^{SO}$$

$$H_0 = \begin{pmatrix} E_C + \varepsilon & iP_0 k_x & iP_0 k_y & iP_0 k_z & 0 & 0 & 0 & 0 \\ -iP_0 k_x & E_V + \varepsilon & 0 & 0 & 0 & 0 & 0 & 0 \\ -iP_0 k_y & 0 & E_V + \varepsilon & 0 & 0 & 0 & 0 & 0 \\ -iP_0 k_z & 0 & 0 & E_V + \varepsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_C + \varepsilon & iP_0 k_x & iP_0 k_y & iP_0 k_z \\ 0 & 0 & 0 & 0 & -iP_0 k_x & E_V + \varepsilon & 0 & 0 \\ 0 & 0 & 0 & 0 & -iP_0 k_y & 0 & E_V + \varepsilon & 0 \\ 0 & 0 & 0 & 0 & -iP_0 k_z & 0 & 0 & E_V + \varepsilon \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ Hamiltonian – diamond & zincblende

$$H^{\mathbf{k} \cdot \mathbf{p}} = H_0 + H' + H^{SO}$$

$$H_0 = \begin{pmatrix} E_C + \varepsilon & iP_0k_x & iP_0k_y & iP_0k_z & 0 & 0 & 0 & 0 \\ -iP_0k_x & E_V + \varepsilon & 0 & 0 & 0 & 0 & 0 & 0 \\ -iP_0k_y & 0 & E_V + \varepsilon & 0 & 0 & 0 & 0 & 0 \\ -iP_0k_z & 0 & 0 & E_V + \varepsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_C + \varepsilon & iP_0k_x & iP_0k_y & iP_0k_z \\ 0 & 0 & 0 & 0 & -iP_0k_x & E_V + \varepsilon & 0 & 0 \\ 0 & 0 & 0 & 0 & -iP_0k_y & 0 & E_V + \varepsilon & 0 \\ 0 & 0 & 0 & 0 & -iP_0k_z & 0 & 0 & E_V + \varepsilon \end{pmatrix} \quad H^{SO} = \frac{\Delta_0}{3} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & +i & 0 & 0 & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & +i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & +i & 0 \\ 0 & 0 & 0 & -i & 0 & -i & 0 & 0 & 0 \\ 0 & +1 & +i & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\varepsilon = \frac{\hbar^2 k^2}{2m_0}$$

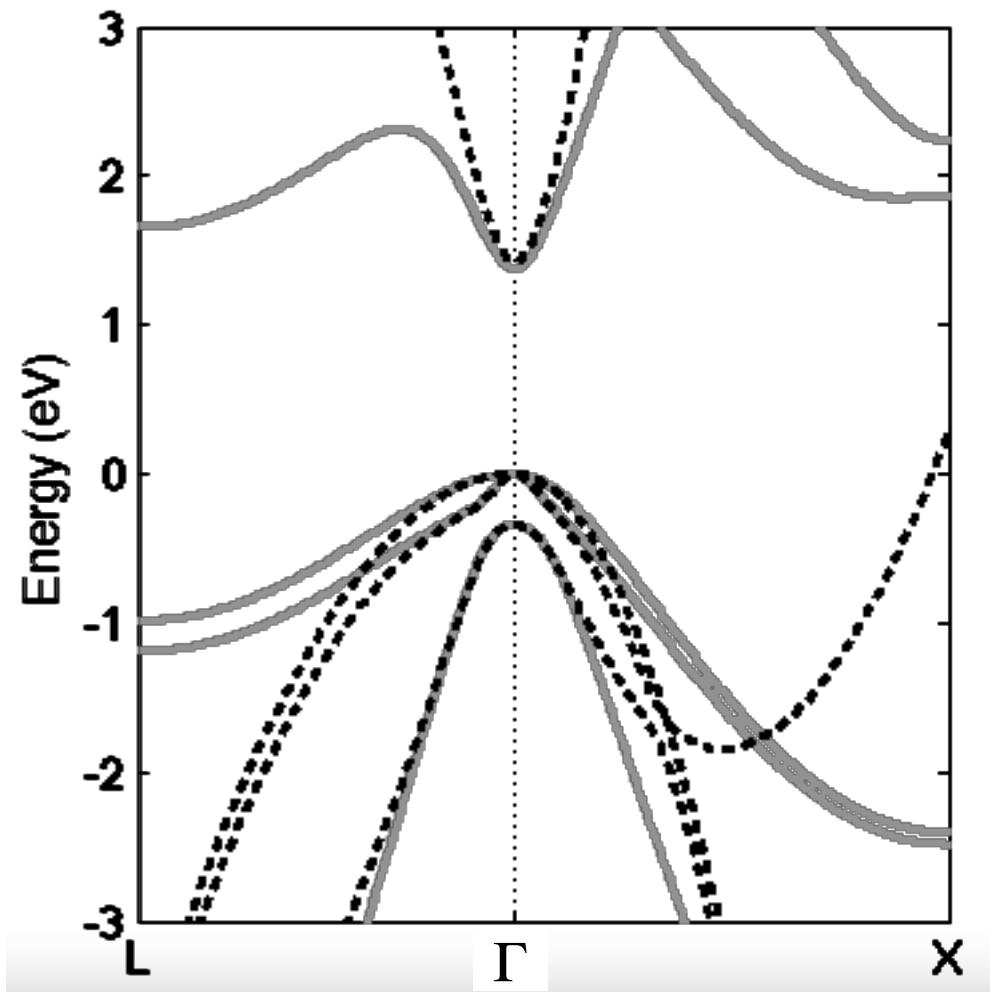
$$H' = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +L'k_x^2 + Mk_y^2 + Mk_z^2 & N'k_xk_y & N'k_xk_z & 0 & 0 & 0 & 0 \\ 0 & N'k_yk_x & Mk_x^2 + L'k_y^2 + Mk_z^2 & N'k_yk_z & 0 & 0 & 0 & 0 \\ 0 & N'k_zk_x & N'k_zk_y & Mk_x^2 + Mk_y^2 + L'k_z^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +L'k_x^2 + Mk_y^2 + Mk_z^2 & N'k_xk_y & N'k_xk_z \\ 0 & 0 & 0 & 0 & 0 & N'k_yk_x & Mk_x^2 + L'k_y^2 + Mk_z^2 & N'k_yk_z \\ 0 & 0 & 0 & 0 & 0 & N'k_zk_x & N'k_zk_y & Mk_x^2 + Mk_y^2 + L'k_z^2 \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – diamond & zincblende

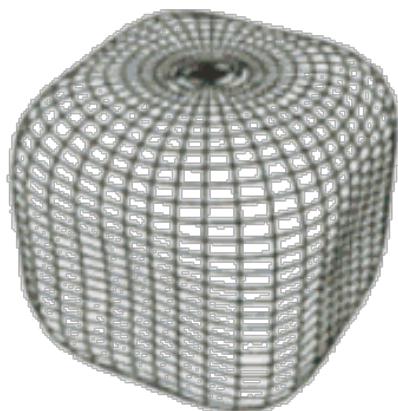
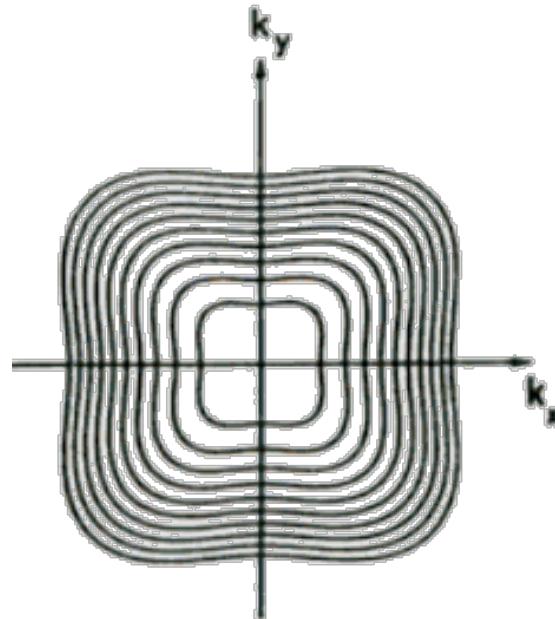
Band structure parameters:

$$E_g, P_0, L', M, N', \Delta_0$$

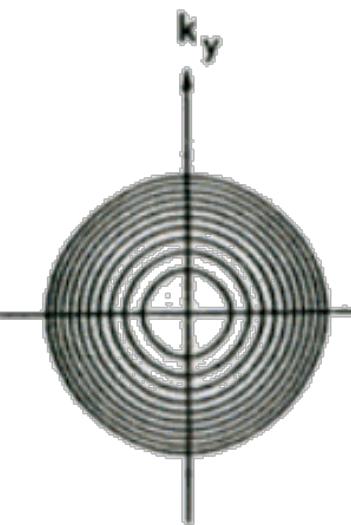


Black dotted – $\mathbf{k} \cdot \mathbf{p}$
Gray solid – pseudo pot.

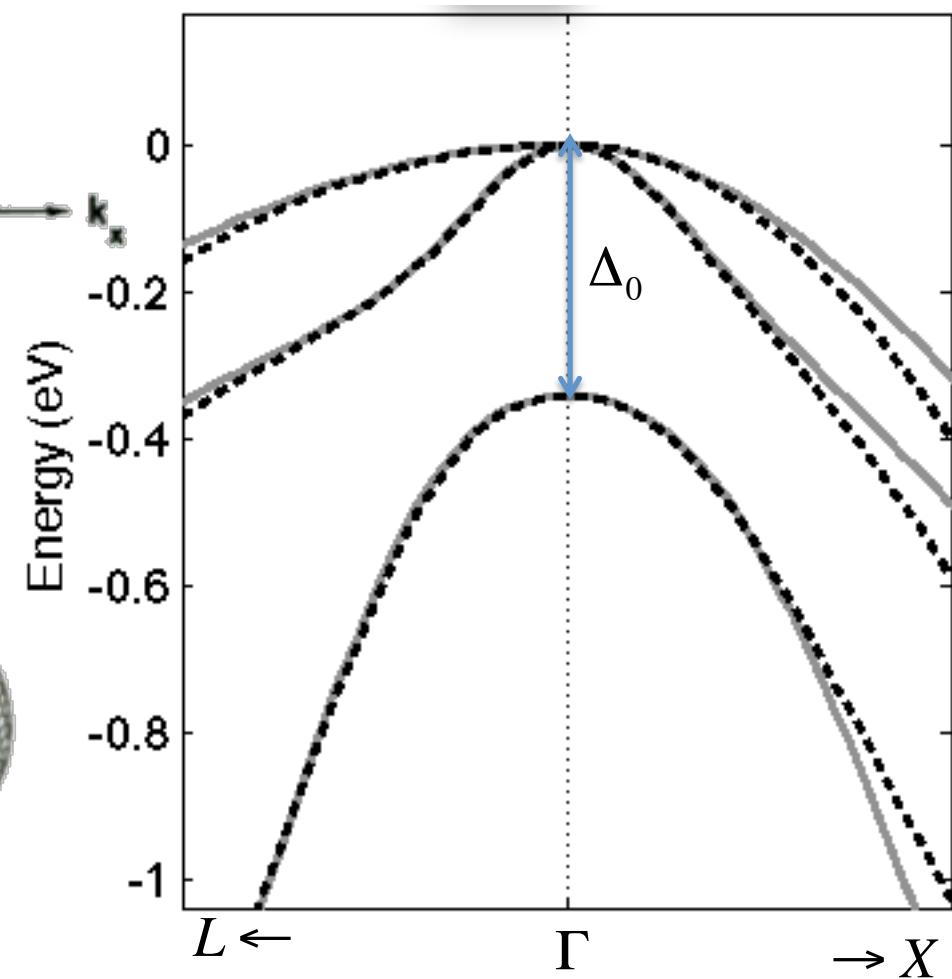
band structure models $k \cdot p$ theory



Heavy Hole

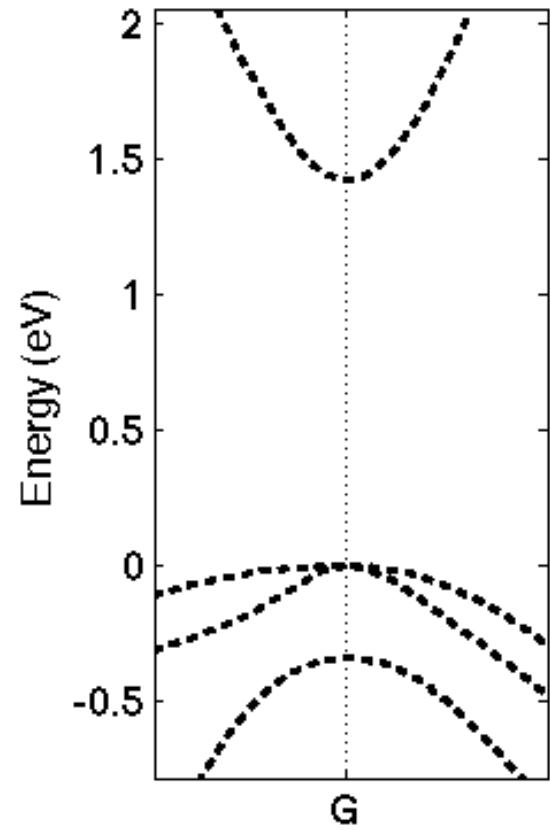


Light Hole



band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory



Eigenvectors of the 8x8 Kane Hamiltonian

Eigenvalues and corresponding eigenstates at $\mathbf{k} = 0$.

Energy	First Kramers Set	Second Kramers Set	Name
E_c	$\left \frac{1}{2}, -\frac{1}{2} \right\rangle = S \downarrow\rangle$	$\left \frac{1}{2}, \frac{1}{2} \right\rangle = S \uparrow\rangle$	Electron
$E_v + \frac{1}{3}\Delta_0$	$\left \frac{3}{2}, \frac{3}{2} \right\rangle = \frac{i}{\sqrt{2}} (X + iY) \uparrow\rangle$	$\left \frac{3}{2}, -\frac{3}{2} \right\rangle = \frac{-i}{\sqrt{2}} (X - iY) \downarrow\rangle$	Heavy Hole
$E_v + \frac{1}{3}\Delta_0$	$\left \frac{3}{2}, \frac{1}{2} \right\rangle = \frac{-i}{\sqrt{6}} (X + iY) \downarrow - 2Z \uparrow\rangle$	$\left \frac{3}{2}, -\frac{1}{2} \right\rangle = \frac{i}{\sqrt{6}} (X - iY) \uparrow + 2Z \downarrow\rangle$	Light Hole
$E_v - \frac{2}{3}\Delta_0$	$\left \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{-i}{\sqrt{3}} (X + iY) \downarrow + Z \uparrow\rangle$	$\left \frac{1}{2}, -\frac{1}{2} \right\rangle = \frac{-i}{\sqrt{3}} (X - iY) \uparrow - Z \downarrow\rangle$	SO Hole

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Uniform strain – potential has new periodicity with lattice constants c_x , c_y and c_z along new axes \mathbf{x}' , \mathbf{y}' and \mathbf{z}' related to the original orthogonal basis vectors \mathbf{x} , \mathbf{y} and \mathbf{z} by

$$\mathbf{x}' = \sum_{j=x,y,z} (\delta_{x,j} + \varepsilon_{xj}) \mathbf{x} \quad c_i = \sum_{j=x,y,z} (\delta_{i,j} + \varepsilon_{ij}) a_0$$

$$\mathbf{y}' = \sum_{j=x,y,z} (\delta_{y,j} + \varepsilon_{yj}) \mathbf{y} \quad i = x, y, z$$

$$\mathbf{z}' = \sum_{j=x,y,z} (\delta_{z,j} + \varepsilon_{zj}) \mathbf{z}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Uniform strain

Original position without strain $\mathbf{r} = \begin{bmatrix} r_x \\ r_y \\ r_z \end{bmatrix}$

The displaced position \mathbf{r}' is given by

$$\mathbf{r}' = \begin{bmatrix} r'_x \\ r'_y \\ r'_z \end{bmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{r} + \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} \mathbf{r} = (\mathbf{1} + \tilde{\varepsilon}) \mathbf{r}$$

$$r'_i = r_i + \sum_{j=x,y,z} \varepsilon_{ij} r_j$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- **p operator is modified by strain**
- potential is modified by strain

The strain is assumed to be small (a few %)

$$r'_i = r_i + \sum_{j=x,y,z} \varepsilon_{ij} r_j \Rightarrow r_i = r'_i - \sum_{j=x,y,z} \varepsilon_{ij} r_j \approx r'_i - \sum_{j=x,y,z} \varepsilon_{ij} r'_j$$

$$\frac{\partial}{\partial r'_i} = \sum_{j=x,y,z} \frac{\partial r_j}{\partial r'_i} \frac{\partial}{\partial r_j} \approx \frac{\partial}{\partial r_i} - \sum_{j=x,y,z} \varepsilon_{ij} \frac{\partial}{\partial r_j} \quad \varepsilon_{ij} = \frac{\partial r'_i}{\partial r_j}$$

$$\Rightarrow \mathbf{p}' = (1 - \tilde{\varepsilon}) \mathbf{p}$$
$$\mathbf{k}' = (1 - \tilde{\varepsilon}) \mathbf{k}$$
$$k'_i = k_i - \sum_{j=x,y,z} \varepsilon_{ij} k_i$$

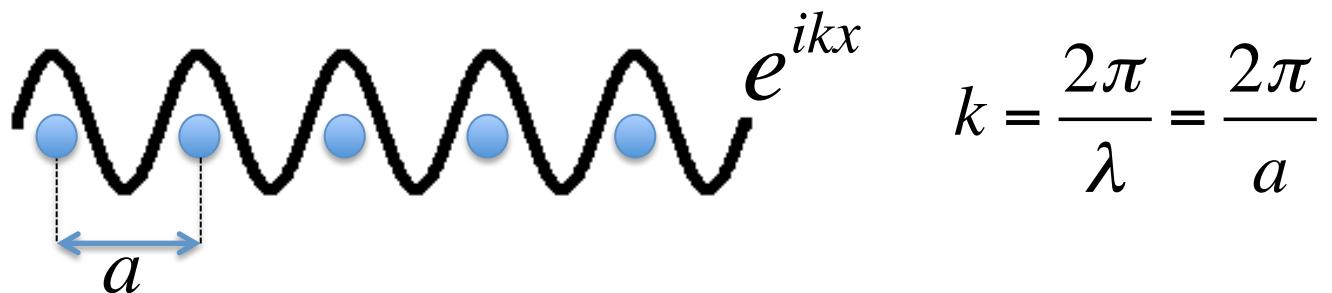
band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

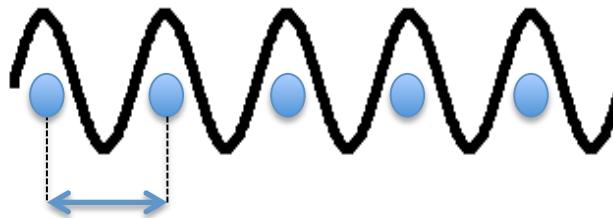
- **\mathbf{p} operator is modified by strain** $\mathbf{p}' = (1 - \tilde{\varepsilon})\mathbf{p} \Rightarrow \mathbf{k}' = (1 - \tilde{\varepsilon})\mathbf{k}$
- potential is modified by strain

1D example



Compressive strain

$$\varepsilon < 0$$



$$k' = \frac{2\pi}{a(1 + \varepsilon)} \approx \frac{2\pi}{a}(1 - \varepsilon)$$

$$k' = (1 - \varepsilon)k$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- **p operator is modified by strain** $\mathbf{p}' = (\mathbf{1} - \tilde{\boldsymbol{\varepsilon}}) \mathbf{p} \Rightarrow \mathbf{k}' = (\mathbf{1} - \tilde{\boldsymbol{\varepsilon}}) \mathbf{k}$
- potential is modified by strain

$$\begin{aligned}
 & \text{extra term for strain correction } H_0^\varepsilon \\
 & \text{without strain } H_0 \\
 & \left(\begin{array}{cccc}
 E'_C + \varepsilon & iP_0 k_x & iP_0 k_y & iP_0 k_z \\
 -iP_0 k_x & E'_V + \varepsilon & 0 & 0 \\
 -iP_0 k_y & 0 & E'_V + \varepsilon & 0 \\
 -iP_0 k_z & 0 & 0 & E'_V + \varepsilon
 \end{array} \right) + \left(\begin{array}{cccc}
 0 & -iP_0 \sum_j \varepsilon_{xj} k_{xj} & -iP_0 \sum_j \varepsilon_{yj} k_{yj} & -iP_0 \sum_j \varepsilon_{zj} k_{zj} \\
 +iP_0 \sum_j \varepsilon_{xj} k_{xj} & 0 & 0 & 0 \\
 +iP_0 \sum_j \varepsilon_{yj} k_{yj} & 0 & 0 & 0 \\
 +iP_0 \sum_j \varepsilon_{zj} k_{zj} & 0 & 0 & 0
 \end{array} \right)
 \end{aligned}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- **\mathbf{p} operator is modified by strain** $\mathbf{p}' = (1 - \tilde{\varepsilon})\mathbf{p} \Rightarrow \mathbf{k}' = (1 - \tilde{\varepsilon})\mathbf{k}$
- potential is modified by strain

with strain & without strain

$$H' = \begin{pmatrix} k^2 & Bk_z k_y & Bk_x k_z & Bk_y k_x \\ Bk_y k_z & L'k_x^2 + M k_y^2 + M k_z^2 & N'k_x k_y & N'k_x k_z \\ Bk_z k_x & N'k_y k_x & M k_x^2 + L'k_y^2 + M k_z^2 & N'k_y k_z \\ Bk_x k_y & N'k_z k_x & N'k_z k_y & M k_x^2 + M k_y^2 + L'k_z^2 \end{pmatrix}$$

The strain correction to H' contains elements like $k_i k_j \varepsilon_{kl}$, which are small and can be **neglected**.

We also neglect the modification of H^{SO} .

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- \mathbf{p} operator is modified by strain
- potential is modified by strain

For small strain components the change $H_V^\varepsilon = \sum_{i,j} D_{ij} \varepsilon_{ij}$ can be considered as a perturbation.

We should find the matrix elements $\langle m | H_V^\varepsilon | n \rangle \quad m, n \in \{S, X, Y, Z\}$

Consider term by term

$$\langle S | D_{xx} | S \rangle \approx \langle S | XX | S \rangle = \langle S | YY | S \rangle = \langle S | ZZ | S \rangle = a_c$$

$$\langle S | D_{xy} | S \rangle = \langle S | XY | S \rangle = \langle S | YZ | S \rangle = \langle S | ZX | S \rangle = 0$$

$$\Rightarrow \langle S | H_V^\varepsilon | S \rangle = a_c (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- \mathbf{p} operator is modified by strain
- potential is modified by strain

$$\langle S | H_V^\varepsilon | S \rangle = a_c (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

Consider term by term

$$\langle X | D_{xx} | X \rangle \approx \langle X | XX | X \rangle = l$$

$$\langle X | D_{yy} | X \rangle \approx \langle X | YY | X \rangle = \langle X | ZZ | X \rangle = m$$

$$\langle X | D_{xy} | X \rangle \approx \langle X | XY | X \rangle = \langle X | XZ | X \rangle = \langle X | ZY | X \rangle = 0$$

$$\Rightarrow \langle X | H_V^\varepsilon | X \rangle = l\varepsilon_{xx} + m(\varepsilon_{yy} + \varepsilon_{zz})$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- \mathbf{p} operator is modified by strain
- potential is modified by strain

$$\langle S | H_V^\varepsilon | S \rangle = a_c (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$
$$\langle X | H_V^\varepsilon | X \rangle = l\varepsilon_{xx} + m(\varepsilon_{yy} + \varepsilon_{zz})$$

Consider term by term

$$\langle X | D_{xz} | Y \rangle \approx \langle X | XZ | Y \rangle = \langle X | YZ | Y \rangle = \langle X | ZZ | Y \rangle = \langle X | XX | Y \rangle = \langle X | YY | Y \rangle = 0$$

$$\langle X | D_{xy} | Y \rangle = \langle X | XY | Y \rangle = n$$

$$\Rightarrow \langle X | H_V^\varepsilon | Y \rangle = n\varepsilon_{xy}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Investigate

- \mathbf{p} operator is modified by strain
- potential is modified by strain

$$\langle S | H_V^\varepsilon | S \rangle = a_c (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$\langle X | H_V^\varepsilon | X \rangle = l\varepsilon_{xx} + m(\varepsilon_{yy} + \varepsilon_{zz})$$

$$\langle X | H_V^\varepsilon | Y \rangle = n\varepsilon_{xy}$$

$$H_V^\varepsilon = \begin{pmatrix} a_c (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) & 0 & 0 & 0 \\ 0 & l\varepsilon_{xx} + m\varepsilon_{yy} + m\varepsilon_{zz} & n\varepsilon_{xy} & n\varepsilon_{xz} \\ 0 & n\varepsilon_{xy} & m\varepsilon_{xx} + l\varepsilon_{yy} + m\varepsilon_{zz} & n\varepsilon_{zy} \\ 0 & n\varepsilon_{xz} & n\varepsilon_{zy} & m\varepsilon_{xx} + m\varepsilon_{yy} + l\varepsilon_{zz} \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

Total strain correction: $H^\varepsilon = H_0^\varepsilon + H_V^\varepsilon$

$$H^\varepsilon = \begin{pmatrix} a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) & -iP_0 \sum_j \varepsilon_{xj} k_{xj} & -iP_0 \sum_j \varepsilon_{yj} k_{yj} & -iP_0 \sum_j \varepsilon_{zj} k_{zj} \\ +iP_0 \sum_j \varepsilon_{xj} k_{xj} & l\varepsilon_{xx} + m\varepsilon_{yy} + m\varepsilon_{zz} & n\varepsilon_{xy} & n\varepsilon_{xz} \\ +iP_0 \sum_j \varepsilon_{yj} k_{yj} & n\varepsilon_{xy} & m\varepsilon_{xx} + l\varepsilon_{yy} + m\varepsilon_{zz} & n\varepsilon_{zy} \\ +iP_0 \sum_j \varepsilon_{zj} k_{zj} & n\varepsilon_{xz} & n\varepsilon_{zy} & m\varepsilon_{xx} + m\varepsilon_{yy} + l\varepsilon_{zz} \end{pmatrix}$$

A different set of deformation potentials is frequently used: a_v , b_v and d_v

$m = a_v - b_v$ **Bir-Pikus deformation potential constants**

$l = a_v + 2b_v$ a_c hydrostatic CB deformation potential

$n = \sqrt{3}d_v$ a_v hydrostatic VB deformation potential

b_v uniaxial VB deformation potential [100]

d_v uniaxial VB deformation potential [111]

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

A different set of deformation potentials is frequently used:

$$m = a_v - b_v \quad \text{Bir-Pikus deformation potential constants}$$

$$l = a_v + 2b_v \quad a_c \text{ hydrostatic CB deformation potential} \quad b_v \text{ uniaxial VB deformation potential [100]}$$

$$n = \sqrt{3}d_v \quad a_v \text{ hydrostatic VB deformation potential} \quad d_v \text{ uniaxial VB deformation potential [111]}$$

For GaAs:

$$a_c = -7.17 \text{ eV} \quad b_v = -2.0 \text{ eV}$$

$$a_v = 1.16 \text{ eV} \quad d_v = -4.8 \text{ eV}$$

$$a = a_c - a_v = -8.33 \text{ eV}$$

Note! I. Vurgaftman *et al.*, uses different sign convention for a_v (in his table $a_v = -1.16$):

Under positive hydrostatic pressure, i.e., negative strain, the change in energy $\Delta E_g = a(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$ must be positive. This implies a negative value for $a \equiv a_c + a_v$. Note that our sign convention for a_v is different from many other works found in the literature. It is generally believed that the conduction band edge moves upward in energy while the valence band moves downward, with most of the change being in the conduction band edge, although Wei and Zunger recently argued that this is not always the case.⁴² The distribution J. Appl. Phys. **89** 5815, (2001)

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal

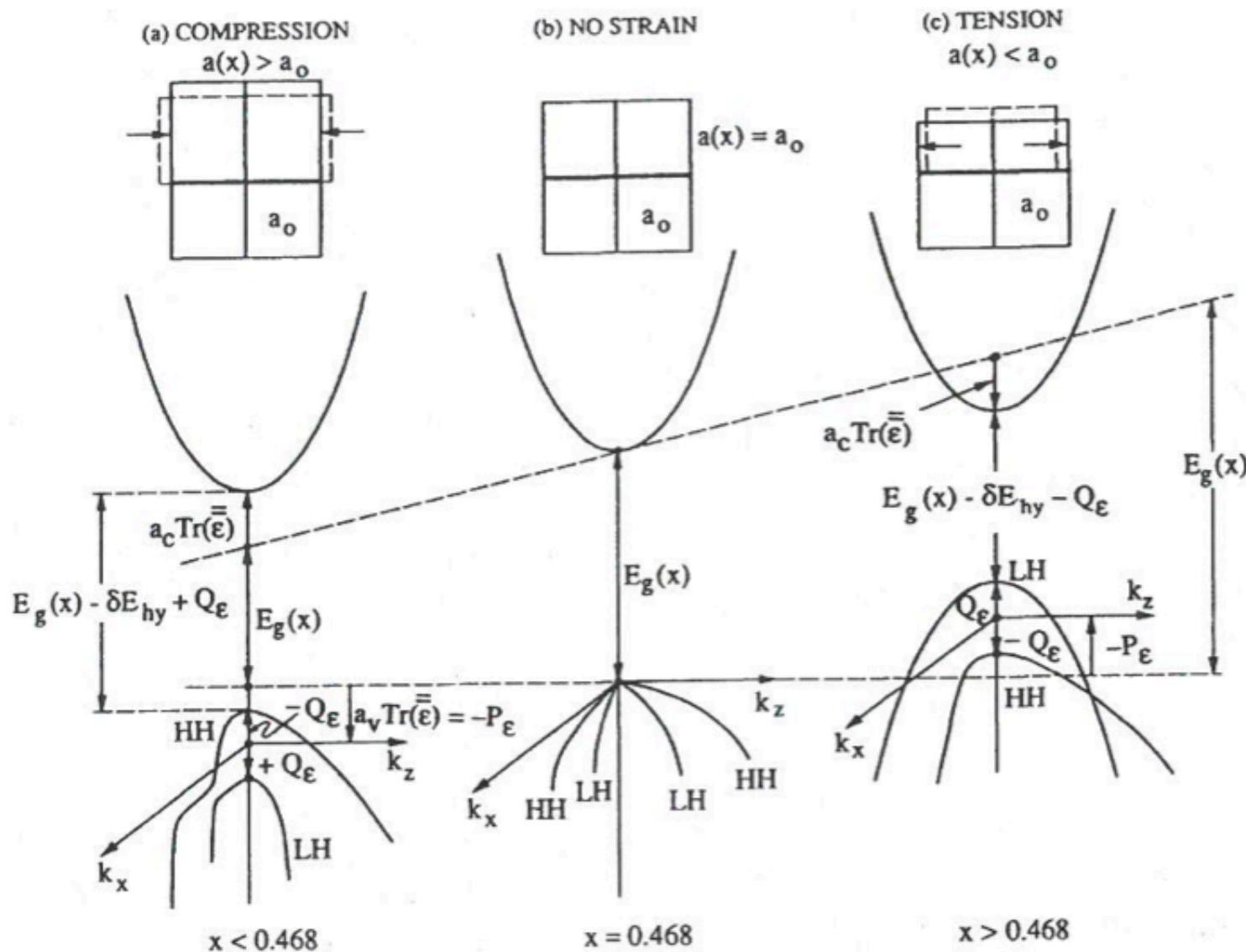
TABLE I. Band structure parameters for GaAs.

Parameters	Recommended values	Range
a_{lc} (Å)	$5.65325 + 3.88 \times 10^{-5}(T - 300)$	
E_g^Γ (eV)	1.519	1.420–1.435 (300 K)
$\alpha(\Gamma)$ (meV/K)	0.5405	0.51–1.06
$\beta(\Gamma)$ (K)	204	190–671
E_g^X (eV)	1.981	...
$\alpha(X)$ (meV/K)	0.460	...
$\beta(X)$ (K)	204	...
E_g^L (eV)	1.815	...
$\alpha(L)$ (meV/K)	0.605	...
$\beta(L)$ (K)	204	...
Δ_{so} (eV)	0.341	0.32–0.36
$m_e^*(\Gamma)$	0.067	0.065–0.07 (0 K), 0.0635–0.067 (300 K)
$m_l^*(L)$	1.9	...
$m_i^*(L)$	0.0754	...
$m_{bos}^*(L)$	0.56	...
$m_l^*(X)$	1.3	...
$m_i^*(X)$	0.23	...
$m_{bos}^*(X)$	0.85	...
γ_1	6.98	6.79–7.20
γ_2	2.06	1.9–2.88
γ_3	2.93	2.681–3.05
m_{so}^*	0.172	0.133–0.388
E_p (eV)	28.8	25.5–29.0
F	-1.94	0.76–(-2)
VBO (eV)	-0.80	
a_c (eV)	-7.17	-6.3–(-18.3)
a_v (eV)	-1.16	-0.2–(-2.1)
b (eV)	-2.0	-1.66–(-3.9)
d (eV)	-4.8	-2.7–(-6.0)
c_{11} (GPa)	1221	...
c_{12} (GPa)	566	...
c_{44} (GPa)	600	...

Vurgaftman et al.
J. Appl. Phys. **89** 5815, (2001)

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – strained crystal



band structure models

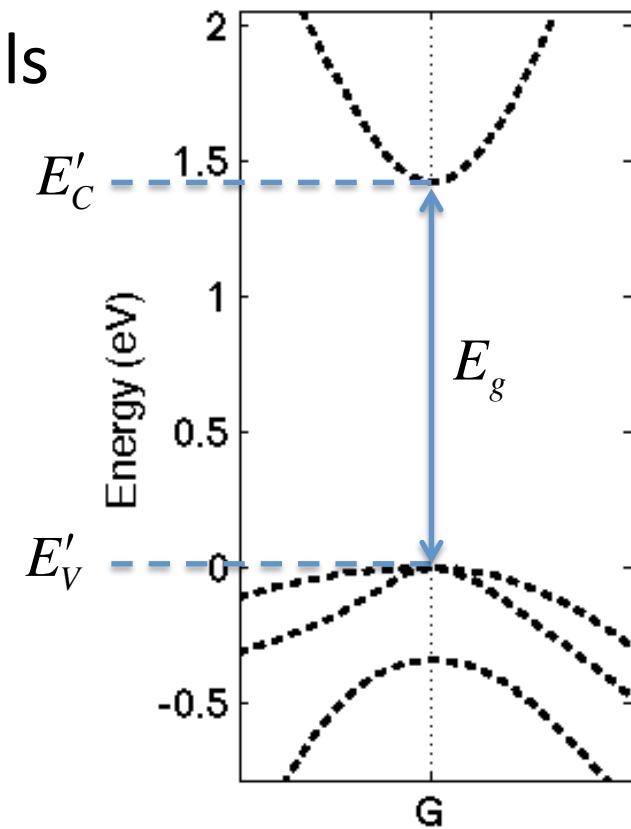
$\mathbf{k} \cdot \mathbf{p}$ theory

Band structure parameters:

$$E_g, P_0, L', M, N', \Delta_0$$

$$E'_V = E_V - \frac{1}{3}\Delta_0$$

$$E'_C = E'_V + E_g$$



Eigenvectors of the 8x8 Kane Hamiltonian

Eigenvalues and corresponding eigenstates at $\mathbf{k} = 0$.

Energy	First Kramers Set	Second Kramers Set	Name
E_c	$\left \frac{1}{2}, -\frac{1}{2} \right\rangle = S \downarrow\rangle$	$\left \frac{1}{2}, \frac{1}{2} \right\rangle = S \uparrow\rangle$	Electron
E'_v	$\left \frac{3}{2}, \frac{3}{2} \right\rangle = \frac{i}{\sqrt{2}} (X + iY) \uparrow\rangle$	$\left \frac{3}{2}, -\frac{3}{2} \right\rangle = \frac{-i}{\sqrt{2}} (X - iY) \downarrow\rangle$	Heavy Hole
E'_v	$\left \frac{3}{2}, \frac{1}{2} \right\rangle = \frac{-i}{\sqrt{6}} (X + iY) \downarrow - 2Z \uparrow\rangle$	$\left \frac{3}{2}, -\frac{1}{2} \right\rangle = \frac{i}{\sqrt{6}} (X - iY) \uparrow + 2Z \downarrow\rangle$	Light Hole
$E'_v - \Delta_0$	$\left \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{-i}{\sqrt{3}} (X + iY) \downarrow + Z \uparrow\rangle$	$\left \frac{1}{2}, -\frac{1}{2} \right\rangle = \frac{-i}{\sqrt{3}} (X - iY) \uparrow - Z \downarrow\rangle$	SO Hole

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

We change the basis to:

$$\begin{aligned}
 & \text{conduction band} \quad \text{valence band} \\
 |j, j_z\rangle \in \{ & |1/2, -1/2\rangle, |1/2, +1/2\rangle, |3/2, +1/2\rangle, |3/2, +3/2\rangle, |3/2, -3/2\rangle, |3/2, -1/2\rangle, |1/2, -1/2\rangle, |1/2, +1/2\rangle \} \\
 & \frac{i}{\sqrt{2}}|X \uparrow\rangle - \frac{1}{\sqrt{2}}|Y \uparrow\rangle \\
 \left\langle \frac{3}{2}, +\frac{3}{2} \right| H \left| \frac{3}{2}, +\frac{3}{2} \right\rangle &= \left\langle \frac{i}{\sqrt{2}}(X + iY) \uparrow \right| H \left| \frac{i}{\sqrt{2}}(X + iY) \uparrow \right\rangle \\
 &= \left(-\frac{i}{\sqrt{2}}\langle X \uparrow | - \frac{1}{\sqrt{2}}\langle Y \uparrow | \right) H \left(\frac{i}{\sqrt{2}}|X \uparrow\rangle - \frac{1}{\sqrt{2}}|Y \uparrow\rangle \right) \\
 &= \frac{1}{2}\langle X \uparrow | H | X \uparrow \rangle + \frac{i}{2}\langle X \uparrow | H | Y \uparrow \rangle - \frac{i}{2}\langle Y \uparrow | H | X \uparrow \rangle + \frac{1}{2}\langle Y \uparrow | H | Y \uparrow \rangle \\
 &\quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \\
 &\quad \frac{1}{2}(E_V + \varepsilon + L'k_x^2 + M k_y^2 + M k_z^2) \\
 &\quad + \frac{i}{2}\left(-i \frac{\Delta_0}{3} + N'k_x k_y\right) \\
 &\quad - \frac{i}{2}\left(+i \frac{\Delta_0}{3} + N'k_y k_x\right) \\
 &\quad + \frac{1}{2}(E_V + \varepsilon + M k_x^2 + L'k_y^2 + M k_z^2)
 \end{aligned}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

$$\left\langle \frac{3}{2}, +\frac{3}{2} \middle| H \middle| \frac{3}{2}, +\frac{3}{2} \right\rangle = E'_V + \varepsilon + \frac{1}{2} [(L' + M)k_x^2 + (L' + M)k_y^2 + 2Mk_z^2]$$

$$\left\langle \frac{3}{2}, +\frac{1}{2} \middle| H \middle| \frac{3}{2}, +\frac{1}{2} \right\rangle = E'_V + \varepsilon + \frac{1}{6} [(L' + 5M)k_x^2 + (L' + 5M)k_y^2 + (4L' + 2M)k_z^2]$$

$$\left\langle \frac{1}{2}, +\frac{1}{2} \middle| H \middle| \frac{3}{2}, +\frac{3}{2} \right\rangle = -P_0 \frac{1}{\sqrt{2}} (k_x + ik_y)$$

$$\left\langle \frac{1}{2}, +\frac{1}{2} \middle| H \middle| \frac{3}{2}, +\frac{1}{2} \right\rangle = \frac{-i}{\sqrt{6}} \langle S \uparrow | H | (X + iY) \downarrow - 2Z \uparrow \rangle = \frac{2i}{\sqrt{6}} \langle S \uparrow | H | Z \uparrow \rangle = -\frac{2}{\sqrt{6}} P_0 k_z$$

:

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

$$H_0 = \begin{pmatrix} E_C + \varepsilon & 0 & V & 0 & \sqrt{3}V^* & -\sqrt{2}U & -U & \sqrt{2}V \\ 0 & E_C + \varepsilon & -\sqrt{2}U & -\sqrt{3}V & 0 & -V^* & \sqrt{2}V^* & U \\ V^* & -\sqrt{2}U^* & E_V & 0 & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{3}V^* & 0 & E_V & 0 & 0 & 0 & 0 \\ \sqrt{3}V & 0 & 0 & 0 & E_V & 0 & 0 & 0 \\ -\sqrt{2}U^* & -V & 0 & 0 & 0 & E_V & 0 & 0 \\ -U^* & \sqrt{2}V & 0 & 0 & 0 & 0 & E_V & 0 \\ \sqrt{2}V^* & U^* & 0 & 0 & 0 & 0 & 0 & E_V \end{pmatrix}, \quad \varepsilon = \frac{\hbar^2 k^2}{2m_0}$$

$$U = \frac{P_0}{\sqrt{3}} k_z$$

$$V = \frac{P_0}{\sqrt{6}} (k_x + ik_z)$$

ε removed from H^D and inserted in H .

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

$$H^{so} = \frac{\Delta_0}{3} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

$$H' = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -P+Q & -S^* & R & 0 & \sqrt{3/2}S & -\sqrt{2}Q \\ 0 & 0 & -S & -P-Q & 0 & R & -\sqrt{2}R & \sqrt{1/2}S \\ 0 & 0 & R^* & 0 & -P-Q & S^* & \sqrt{1/2}S^* & \sqrt{2}R^* \\ 0 & 0 & 0 & R^* & S & -P+Q & \sqrt{2}Q & \sqrt{3/2}S^* \\ 0 & 0 & \sqrt{3/2}S^* & -\sqrt{2}R^* & \sqrt{1/2}S & \sqrt{2}Q & -P & 0 \\ 0 & 0 & -\sqrt{2}Q & \sqrt{1/2}S^* & \sqrt{2}R & \sqrt{3/2}S & 0 & -P \end{pmatrix}$$

re-introduces
 $\varepsilon = \frac{\hbar^2 k^2}{2m_0}$



$$P = -\frac{1}{3}(L' + 2M)(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m_0} \gamma_1 (k_x^2 + k_y^2 + k_z^2)$$

$$Q = -\frac{1}{6}(L' - M)(k_x^2 + k_y^2 - 2k_z^2) = \frac{\hbar^2}{2m_0} \gamma_2 (k_x^2 + k_y^2 - 2k_z^2)$$

$$S = -\frac{1}{\sqrt{3}}N'(k_x k_z - i k_y k_z) = 2\sqrt{3} \frac{\hbar^2}{2m_0} \gamma_3 (k_x k_z - i k_y k_z)$$

$$R = \frac{\sqrt{3}}{6}[(L' - M)(k_x^2 - k_y^2) - 2iN' k_x k_y] = -\sqrt{3} \frac{\hbar^2}{2m_0} [\gamma_2 (k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y]$$

$$\gamma_1 = -\frac{2}{3} \frac{m_0}{\hbar^2} (L' + 2M) - 1 = \gamma_1^{(0)} - \frac{E_p}{3E_g}$$

$$\gamma_2 = -\frac{1}{3} \frac{m_0}{\hbar^2} (L' - M) = \gamma_2^{(0)} - \frac{1}{2} \frac{E_p}{3E_g}$$

$$\gamma_3 = -\frac{1}{3} \frac{m_0}{\hbar^2} N' = \gamma_3^{(0)} - \frac{1}{2} \frac{E_p}{3E_g}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

$$H^{\mathbf{k} \cdot \mathbf{p}} = H_0 + H' + H^{SO}$$

Kane Hamiltonian (8x8)

$$H_0 = \begin{pmatrix} E_c + \varepsilon & 0 & V & 0 & \sqrt{3}V^* & -\sqrt{2}U & -U & \sqrt{2}V \\ 0 & E_c + \varepsilon & -\sqrt{2}U & -\sqrt{3}V & 0 & -V^* & \sqrt{2}V^* & U \\ V^* & -\sqrt{2}U^* & E_v & 0 & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{3}V^* & 0 & E_v & 0 & 0 & 0 & 0 \\ \sqrt{3}V & 0 & 0 & 0 & E_v & 0 & 0 & 0 \\ -\sqrt{2}U^* & -V & 0 & 0 & 0 & E_v & 0 & 0 \\ -U^* & \sqrt{2}V & 0 & 0 & 0 & 0 & E_v & 0 \\ \sqrt{2}V^* & U^* & 0 & 0 & 0 & 0 & 0 & E_v \end{pmatrix}$$

$$H' = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -P+Q & -S^* & R & 0 & \sqrt{3/2}S & -\sqrt{2}Q \\ 0 & 0 & -S & -P-Q & 0 & R & -\sqrt{2}R & \sqrt{1/2}S \\ 0 & 0 & R^* & 0 & -P-Q & S^* & \sqrt{1/2}S^* & \sqrt{2}R^* \\ 0 & 0 & 0 & R^* & S & -P+Q & \sqrt{2}Q & \sqrt{3/2}S^* \\ 0 & 0 & \sqrt{3/2}S^* & -\sqrt{2}R^* & \sqrt{1/2}S & \sqrt{2}Q & -P & 0 \\ 0 & 0 & -\sqrt{2}Q & \sqrt{1/2}S^* & \sqrt{2}R & \sqrt{3/2}S & 0 & -P \end{pmatrix}$$

$$H^{SO} = \frac{\Delta_0}{3} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

$$U = \frac{P_0}{\sqrt{3}} k_z$$

$$V = \frac{P_0}{\sqrt{6}} (k_x + ik_z)$$

$$P = \frac{\hbar^2}{2m_0} \gamma_1 (k_x^2 + k_y^2 + k_z^2)$$

$$Q = \frac{\hbar^2}{2m_0} \gamma_2 (k_x^2 + k_y^2 - 2k_z^2)$$

$$S = 2\sqrt{3} \frac{\hbar^2}{2m_0} \gamma_3 (k_x k_z - ik_y k_z)$$

$$R = -\sqrt{3} \frac{\hbar^2}{2m_0} [\gamma_2 (k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y]$$

$$\gamma_1 = \gamma_1^{(0)} - \frac{E_p}{3E_g}$$

$$\gamma_2 = \gamma_2^{(0)} - \frac{1}{2} \frac{E_p}{3E_g}$$

$$\gamma_3 = \gamma_3^{(0)} - \frac{1}{2} \frac{E_p}{3E_g}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

Approximation: Neglect coupling between conduction band and valence band

$P_0 \rightarrow 0 \quad E_P \rightarrow 0 \quad \text{Top of valence band: Luttinger-Kohn Hamiltonian (6x6)}$

$$H_{6 \times 6}^{\mathbf{k} \cdot \mathbf{p}} = \begin{pmatrix} -P+Q & -S^* & R & 0 & \sqrt{3/2}S & -\sqrt{2}Q \\ -S & -P-Q & 0 & R & -\sqrt{2}R & \sqrt{1/2}S \\ R^* & 0 & -P-Q & S^* & \sqrt{1/2}S^* & \sqrt{2}R^* \\ 0 & R^* & S & -P+Q & \sqrt{2}Q & \sqrt{3/2}S^* \\ \sqrt{3/2}S^* & -\sqrt{2}R^* & \sqrt{1/2}S & \sqrt{2}Q & -P-\Delta_0 & 0 \\ -\sqrt{2}Q & \sqrt{1/2}S^* & \sqrt{2}R & \sqrt{3/2}S & 0 & -P-\Delta_0 \end{pmatrix} \quad \text{Bottom of conduction band (1x1)}$$

$$H_{CB} = \frac{\hbar^2 k^2}{2m_e}$$

$$P = \frac{\hbar^2}{2m_0} \gamma_1^{(0)} (k_x^2 + k_y^2 + k_z^2)$$

$$S = 2\sqrt{3} \frac{\hbar^2}{2m_0} \gamma_3^{(0)} (k_x k_z - i k_y k_z)$$

$$Q = \frac{\hbar^2}{2m_0} \gamma_2^{(0)} (k_x^2 + k_y^2 - 2k_z^2)$$

$$R = -\sqrt{3} \frac{\hbar^2}{2m_0} \left[\gamma_2^{(0)} (k_x^2 - k_y^2) - 2i \gamma_3^{(0)} k_x k_y \right]$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis

Approximation: Neglect coupling between HH & LH bands with SO band

$\Delta \rightarrow \infty$ **Top of valence band: Luttinger Hamiltonian (4x4)**

$$H_{4 \times 4}^{\mathbf{k} \cdot \mathbf{p}} = \begin{pmatrix} -P+Q & -S^* & R & 0 \\ -S & -P-Q & 0 & R \\ R^* & 0 & -P-Q & S^* \\ 0 & R^* & S & -P+Q \end{pmatrix} \quad \text{Bottom of conduction band (1x1)}$$

$$H_{CB} = \frac{\hbar^2 k^2}{2m_e}$$

$$P = \frac{\hbar^2}{2m_0} \gamma_1^{(0)} (k_x^2 + k_y^2 + k_z^2) \quad S = 2\sqrt{3} \frac{\hbar^2}{2m_0} \gamma_3^{(0)} (k_x k_z - i k_y k_z)$$

$$Q = \frac{\hbar^2}{2m_0} \gamma_2^{(0)} (k_x^2 + k_y^2 - 2k_z^2) \quad R = -\sqrt{3} \frac{\hbar^2}{2m_0} \left[\gamma_2^{(0)} (k_x^2 - k_y^2) - 2i \gamma_3^{(0)} k_x k_y \right]$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – change of basis – strain

$$H^\varepsilon = \begin{pmatrix} a_c \varepsilon & 0 & v & 0 & \sqrt{3}v^* & -\sqrt{2}u & -u & \sqrt{2}v \\ 0 & a_c \varepsilon & -\sqrt{2}u & -\sqrt{3}v & 0 & -v^* & \sqrt{2}v^* & u \\ v^* & -\sqrt{2}u^* & -p+q & -s^* & r & 0 & \sqrt{3/2}s & -\sqrt{2}q \\ 0 & -\sqrt{3}v^* & -s & -p-q & 0 & r & -\sqrt{2}r & \sqrt{1/2}s \\ \sqrt{3}v & 0 & r^* & 0 & -p-q & s^* & \sqrt{1/2}s^* & \sqrt{2}r^* \\ -\sqrt{2}u^* & -v & 0 & r^* & s & -p+q & \sqrt{2}q & \sqrt{3/2}s^* \\ -u^* & \sqrt{2}v & \sqrt{3/2}s^* & -\sqrt{2}r^* & \sqrt{1/2}s & \sqrt{2}q & -p & 0 \\ \sqrt{2}v^* & u^* & -\sqrt{2}q & \sqrt{1/2}s^* & \sqrt{2}r & \sqrt{3/2}s & 0 & -p \end{pmatrix}$$

$$a_c \varepsilon = a_c (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$p = a_v (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$q = -\frac{1}{2} b_v (\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

$$s = -d_v (\varepsilon_{xz} - i\varepsilon_{yz})$$

$$r = +\frac{\sqrt{3}}{2} b_v (\varepsilon_{xx} - \varepsilon_{yy}) - id_v \varepsilon_{xy}$$

$$u = -i \frac{P_0}{\sqrt{3}} \sum_{j=x,y,z} \varepsilon_{zj} k_j$$

$$v = -\frac{P_0}{\sqrt{6}} \sum_{j=x,y,z} (i\varepsilon_{xj} - \varepsilon_{yj}) k_j$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory

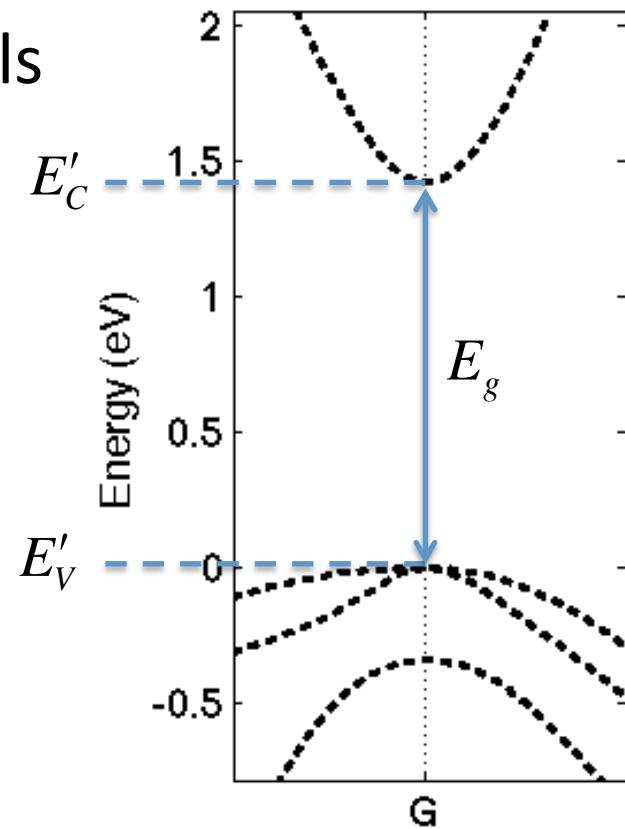
Band structure parameters:

$$E_g, P_0, L', M, N', \Delta_0 \rightarrow E_g, E_P, \gamma_1^{(0)}, \gamma_2^{(0)}, \gamma_3^{(0)}, \Delta_0$$

$$E'_V = E_V - \frac{1}{3}\Delta_0$$

$$E'_C = E'_V + E_g$$

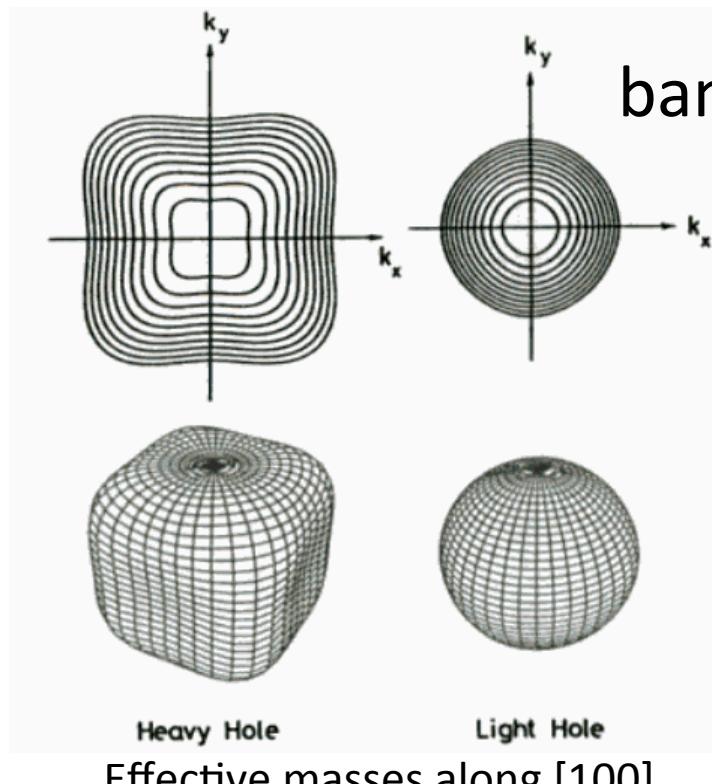
For GaAs $\gamma_1^{(0)} = 6.85$
 $\gamma_2^{(0)} = 2.1$
 $\gamma_3^{(0)} = 2.9$



Eigenvectors of the 8x8 Kane Hamiltonian

Eigenvalues and corresponding eigenstates at $\mathbf{k} = 0$.

Energy	First Kramers Set	Second Kramers Set	Name
E_c	$\left \frac{1}{2}, -\frac{1}{2} \right\rangle = S \downarrow\rangle$	$\left \frac{1}{2}, \frac{1}{2} \right\rangle = S \uparrow\rangle$	Electron
E'_v	$\left \frac{3}{2}, \frac{3}{2} \right\rangle = \frac{i}{\sqrt{2}} (X + iY) \uparrow\rangle$	$\left \frac{3}{2}, -\frac{3}{2} \right\rangle = \frac{-i}{\sqrt{2}} (X - iY) \downarrow\rangle$	Heavy Hole
E'_v	$\left \frac{3}{2}, \frac{1}{2} \right\rangle = \frac{-i}{\sqrt{6}} (X + iY) \downarrow - 2Z \uparrow\rangle$	$\left \frac{3}{2}, -\frac{1}{2} \right\rangle = \frac{i}{\sqrt{6}} (X - iY) \uparrow + 2Z \downarrow\rangle$	Light Hole
$E'_v - \Delta_0$	$\left \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{-i}{\sqrt{3}} (X + iY) \downarrow + Z \uparrow\rangle$	$\left \frac{1}{2}, -\frac{1}{2} \right\rangle = \frac{-i}{\sqrt{3}} (X - iY) \uparrow - Z \downarrow\rangle$	SO Hole



Effective masses along [100]

$$m_{hh} = \frac{1}{\gamma_1^{(0)} - 2\gamma_2^{(0)}}$$

$$m_{lh} = \frac{1}{\gamma_1^{(0)} + 2\gamma_2^{(0)}}$$

Effective masses along [110]

$$m_{hh} = \frac{2}{2\gamma_1^{(0)} - \gamma_2^{(0)} - 3\gamma_3^{(0)}}$$

$$m_{lh} = \frac{2}{2\gamma_1^{(0)} + \gamma_2^{(0)} + 3\gamma_3^{(0)}}$$

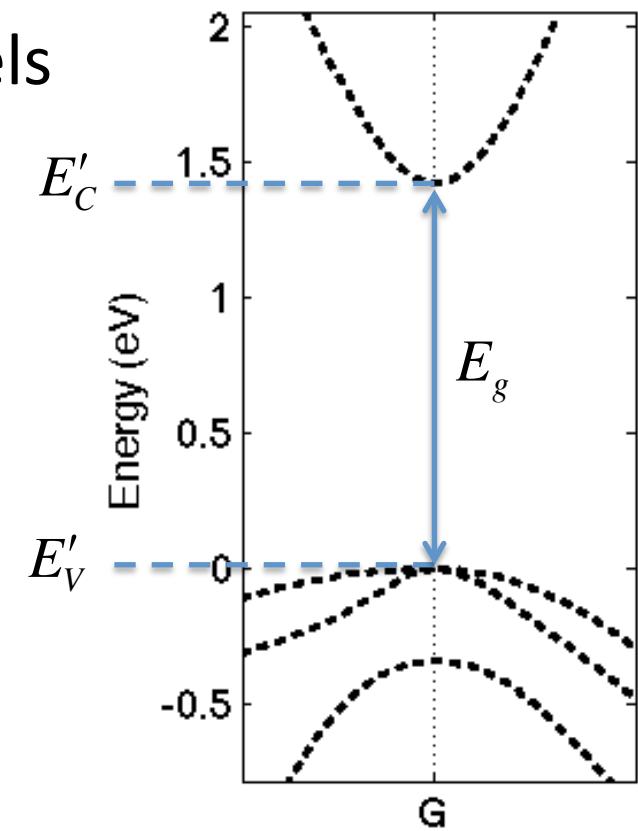
Effective masses along [111]

$$m_{hh} = \frac{1}{\gamma_1^{(0)} - 2\gamma_3^{(0)}}$$

$$m_{lh} = \frac{1}{\gamma_1^{(0)} + 2\gamma_3^{(0)}}$$

band structure models $\mathbf{k} \cdot \mathbf{p}$ theory

For GaAs $\gamma_1^{(0)} = 6.85$
 $\gamma_2^{(0)} = 2.1$
 $\gamma_3^{(0)} = 2.9$



band structure models

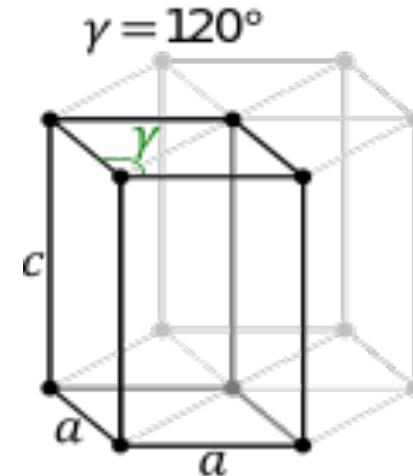
$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

In a wurtzite crystal the z -axis is unique, different from x - and y -directions.
It has lower symmetry with two lattice constants a & c

The electron effective masses different for
different directions:

m_e^{\parallel} along z

m_e^{\perp} in the x - y -plane



$$i \frac{m_0 P_2}{\hbar} \equiv \langle S | p_x | X \rangle = \langle S | p_y | Y \rangle \neq \langle S | p_z | Z \rangle \equiv i \frac{m_0 P_1}{\hbar}$$

Crystal field splitting:

$$\langle Z | p_z | Z \rangle = E_V$$
$$\langle X | p_x | X \rangle = \langle Y | p_z | Y \rangle = E_V + \Delta_1$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

Crystal field splitting: $\langle Z | p_z | Z \rangle = E_V$

$$\langle X | p_x | X \rangle = \langle Y | p_z | Y \rangle = E_V + \Delta_1$$

Spin orbit interaction: $\langle X | H_Z^{SO} | Y \rangle = -i\Delta_2$

$$\langle Y | H_X^{SO} | Z \rangle = \langle Z | H_Y^{SO} | X \rangle = -i\Delta_3$$

Common approximation: $\Delta_2 = \Delta_3 = \Delta_{SO}$
 $\Delta_1 = \Delta_{CR}$

$$\begin{pmatrix} E_C & iP_2 k_x & iP_2 k_y & iP_1 k_z \\ -iP_2 k_x & E_V + \Delta_{CR} & 0 & 0 \\ -iP_2 k_y & 0 & E_V + \Delta_{CR} & 0 \\ -iP_1 k_z & 0 & 0 & E_V \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

$$H' \quad L' \rightarrow \left\{ \begin{array}{l} L'_1 \\ L'_2 \end{array} \right.$$
$$M' \rightarrow \left\{ \begin{array}{l} M'_1 \\ M'_2 \\ M'_3 \end{array} \right. \quad \begin{array}{l} 4 \text{ parameters} \rightarrow 10 \text{ parameters} \\ \\ \end{array}$$
$$N' \rightarrow \left\{ \begin{array}{l} N'_1 \\ N'_2 \\ N'_3 \end{array} \right. \quad \begin{array}{l} 3 \text{ Luttinger parameters } \gamma_{1-3}^{(0)} \\ \rightarrow 7 \text{ parameters Luttinger-like} \\ \text{parameters } A_{1-7} \end{array}$$
$$A' \rightarrow \left\{ \begin{array}{l} A'_1 \\ A'_2 \end{array} \right.$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

$$H^\varepsilon \quad l \rightarrow \begin{cases} l_1 \\ l_2 \end{cases}$$
$$m \rightarrow \begin{cases} m_1 \\ m_2 \\ m_3 \end{cases}$$

4 parameters \rightarrow 9parameters

3 valence band deformation potentials a_v, b_v and d_v
 \rightarrow 6 deformation potentials D_{1-6}

$$n \rightarrow \begin{cases} n_1 \\ n_2 \\ n_3 \end{cases}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

$$H = \begin{bmatrix} H_0 & 0 \\ 0 & H_0 \end{bmatrix} + \begin{bmatrix} H' & 0 \\ 0 & H' \end{bmatrix} + H^{SO} + H^{CR}$$

$$H_0 = \begin{pmatrix} E_c & iP_2k_x & iP_2k_y & iP_1k_z \\ -iP_2k_x & E_v & 0 & 0 \\ -iP_2k_y & 0 & E_v & 0 \\ -iP_1k_z & 0 & 0 & E_v \end{pmatrix}$$

$$H' = \begin{pmatrix} A_2(k_x^2 + k_y^2) + A_1k_z^2 & 0 & 0 & 0 \\ 0 & L_1k_x^2 + M_1k_y^2 + M_2k_z^2 & N_1k_xk_y & N_2k_xk_z - N_3k_x \\ 0 & N_1k_yk_x & M_1k_x^2 + L_1k_y^2 + M_2k_z^2 & N_2k_yk_z - N_3k_y \\ 0 & N_2k_zk_x + N_3k_x & N_2k_zk_y + N_3k_y & M_3k_x^2 + M_3k_y^2 + L_2k_z^2 \end{pmatrix}$$

$$H_{CR} = \Delta_{CR} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$H^{SO} = \frac{\Delta}{3} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & +i & 0 & 0 & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 & -1 & +i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +i & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & -i & 0 & 0 & 0 \\ 0 & +1 & +i & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

where

$$E_c = E_v + E_g + \Delta_{CR} + \frac{\Delta_{SO}}{3}$$

$$P_1^2 = \frac{\hbar^2}{2m_0} \left(\frac{m_0}{m_e^{\parallel}} - 1 \right) \frac{3E_g(\Delta_{SO} + E_g) + \Delta_{CR}(2\Delta_{SO} + 3E_g)}{2\Delta_{SO} + 3E_g}$$

$$P_2^2 = \frac{\hbar^2}{2m_0} \left(\frac{m_0}{m_e^{\perp}} - 1 \right) E_g \left(\frac{3E_g(\Delta_{SO} + E_g) + \Delta_{CR}(2\Delta_{SO} + 3E_g)}{\Delta_{CR}\Delta_{SO} + 3\Delta_{CR}E_g + 2\Delta_{SO}E_g + 3E_g^2} \right)$$

$$A_1 = \frac{\hbar^2}{2m_e^{\parallel}} - \frac{P_1^2}{E_g}$$

$$L_1 = \frac{P_1^2}{E_g} + \frac{\hbar^2}{2m_0} (A_2 + A_4 + A_5)$$

$$A_2 = \frac{\hbar^2}{2m_e^{\perp}} - \frac{P_2^2}{E_g}$$

$$L_2 = \frac{P_2^2}{E_g} + \frac{\hbar^2}{2m_0} A_1$$

$$M_1 = \frac{\hbar^2}{2m_0} (A_2 + A_4 + A_5)$$

$$M_2 = \frac{\hbar^2}{2m_0} (A_1 + A_3)$$

$$M_3 = \frac{\hbar^2}{2m_0} A_2$$

$$N_1 = \frac{P_1^2}{E_g} + \frac{\hbar^2}{2m_0} 2A_5$$

$$N_2 = \frac{P_1 P_2}{E_g} + \frac{\hbar^2}{2m_0} \sqrt{2} A_6$$

$$N_3 = i\sqrt{2} A_7$$

E_g fundamental band gap

Δ_{SO} split off (SO) energy

Δ_{CR} crystal-field splitting energy

E_v valence band edge

$m_e^{\parallel}, m_e^{\perp}$ electron effective masses times m_0

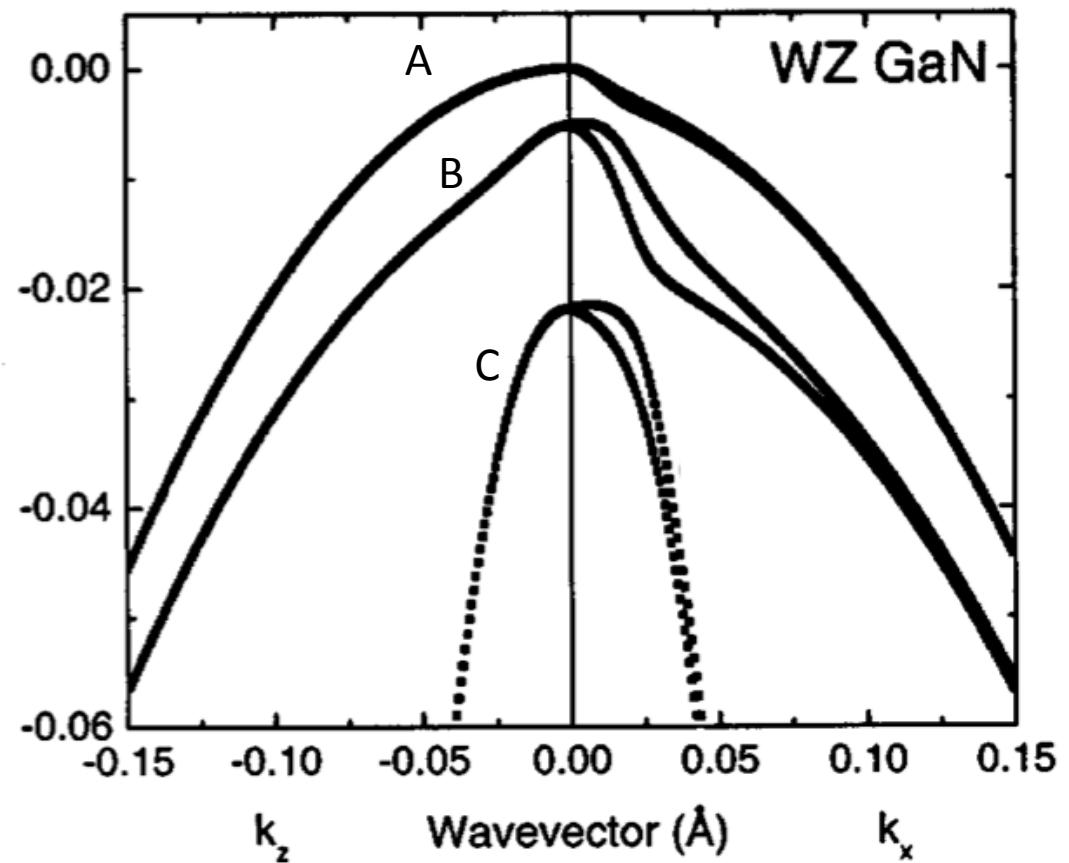
A_{1-7} Luttinger-like parameters

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

See I. Vurgaftman *et al.*, J. Appl. Phys. **94** 3675. (2003) for III-Nitride material parameters.

Parameters	GaN	AlN	InN
a_{lc} (Å) at $T=300$ K	3.189	3.112	3.545
c_{lc} (Å) at $T=300$ K	5.185	4.982	5.703
E_g (eV)	3.510	6.25	0.78
α (meV/K)	0.909	1.799	0.245
β (K)	830	1462	624
Δ_{cr} (eV)	0.010	-0.169	0.040
Δ_{so} (eV)	0.017	0.019	0.005
m_e^{\parallel}	0.20	0.32	0.07
m_e^{\perp}	0.20	0.30	0.07
A_1	-7.21	-3.86	-8.21
A_2	-0.44	-0.25	-0.68
A_3	6.68	3.58	7.57
A_4	-3.46	-1.32	-5.23
A_5	-3.40	-1.47	-5.11
A_6	-4.90	-1.64	-5.96
A_7 (eV Å)	0.0937	0	0
a_1 (eV)	-4.9	-3.4	-3.5
a_2 (eV)	-11.3	-11.8	-3.5
D_1 (eV)	-3.7	-17.1	-3.7
D_2 (eV)	4.5	7.9	4.5
D_3 (eV)	8.2	8.8	8.2
D_4 (eV)	-4.1	-3.9	-4.1
D_5 (eV)	-4.0	-3.4	-4.0
D_6 (eV)	-5.5	-3.4	-5.5
c_{11} (GPa)	390	396	223
c_{12} (GPa)	145	137	115
c_{13} (GPa)	106	108	92
c_{33} (GPa)	398	373	224
c_{44} (GPa)	105	116	48
d_{13} (pm/V)	-1.6	-2.1	-3.5
d_{33} (pm/V)	3.1	5.4	7.6
d_{15} (pm/V)	3.1	3.6	5.5
P_{sp} (C/m ²)	-0.034	-0.090	-0.042



band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite – strain

$$H = \begin{bmatrix} H_0 & 0 \\ 0 & H_0 \end{bmatrix} + \begin{bmatrix} H' & 0 \\ 0 & H' \end{bmatrix} + \boxed{\begin{bmatrix} H^\varepsilon & 0 \\ 0 & H^\varepsilon \end{bmatrix}} + H^{SO} + H^{CR}$$

$$H^\varepsilon = \begin{pmatrix} a_2(\varepsilon_{xx} + \varepsilon_{yy}) + a_1\varepsilon_{zz} & 0 & 0 & 0 \\ 0 & l_1\varepsilon_{xx} + m_1\varepsilon_{yy} + m_2\varepsilon_{zz} & n_1\varepsilon_{xy} & n_2\varepsilon_{xz} \\ 0 & n_1\varepsilon_{xy} & m_1\varepsilon_{xx} + l_1\varepsilon_{yy} + m_2\varepsilon_{zz} & n_2\varepsilon_{yz} \\ 0 & n_2\varepsilon_{xz} & n_2\varepsilon_{yz} & m_3\varepsilon_{xx} + m_3\varepsilon_{yy} + l_2\varepsilon_{zz} \end{pmatrix}$$

where

$$l_1 = D_2 + D_4 + D_5 \quad l_2 = D_1$$

$$m_1 = D_2 + D_4 - D_5 \quad m_2 = D_1 + D_3 \quad m_3 = D_2$$

$$n_1 = 2D_5 \quad n_2 = \sqrt{2}D_6$$

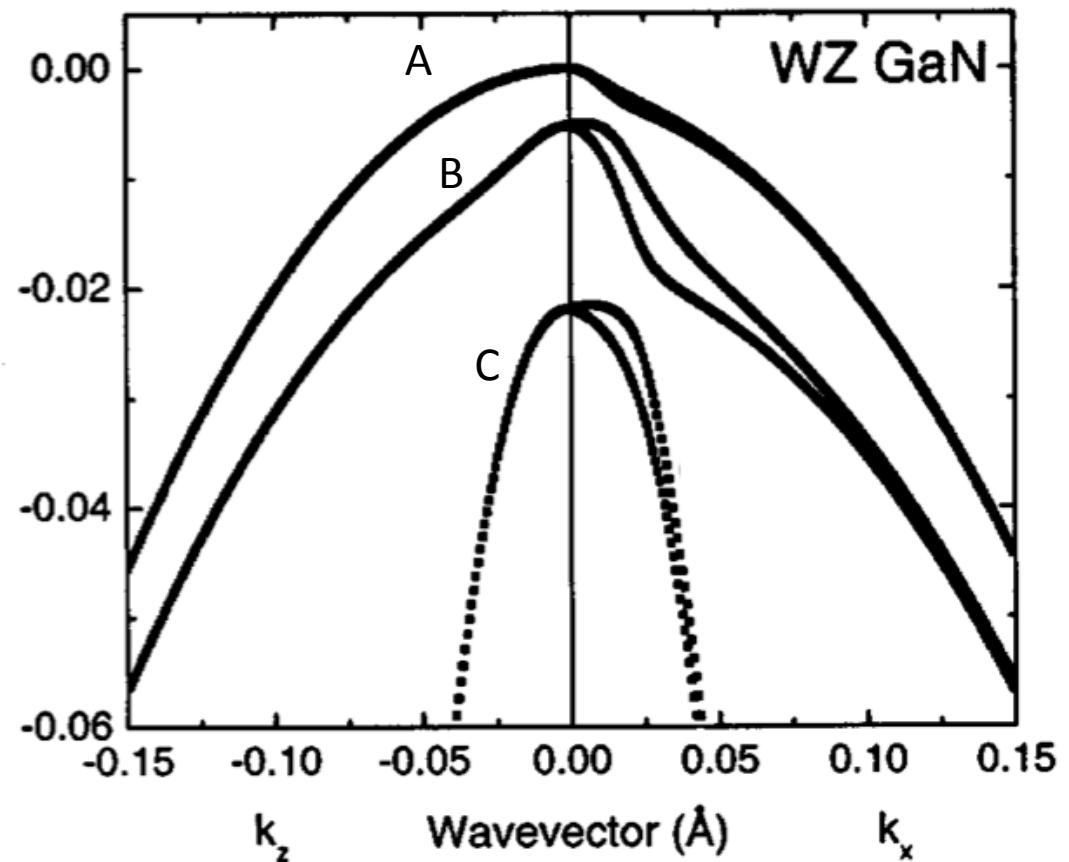
a_{1-2} conduction band deformation potentials D_{1-6} valence band deformation potentials
 Vurgaftman uses the same sign convention as above for the deformation potentials.

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – wurtzite

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A_6	-4.90	-1.64	-5.96
A_7 (eV \AA)	0.0937	0	0
a_1 (eV)	-4.9	-3.4	-3.5
a_2 (eV)	-11.3	-11.8	-3.5
D_1 (eV)	-3.7	-17.1	-3.7
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c_{13} (GPa)	106	108	92
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P_{sp} (C/m ²)	-0.034	-0.090	-0.042



band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – more bands

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Energy-band structure in strained silicon: A 20-band $\mathbf{k} \cdot \mathbf{p}$ and Bir–Pikus Hamiltonian model

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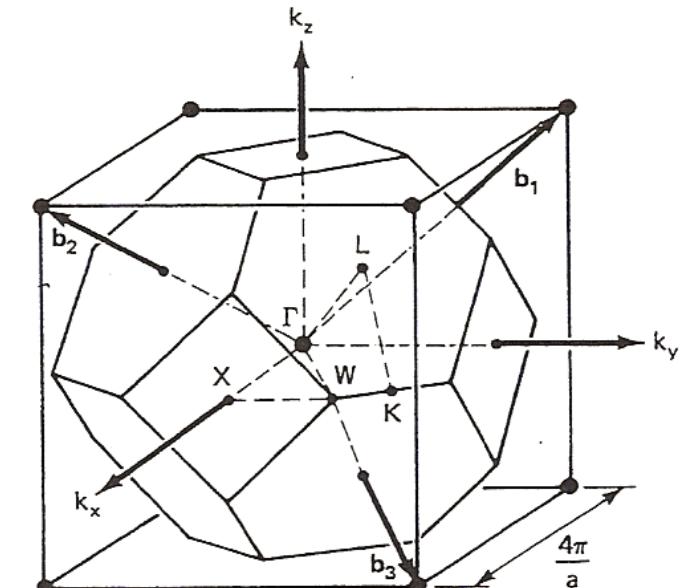
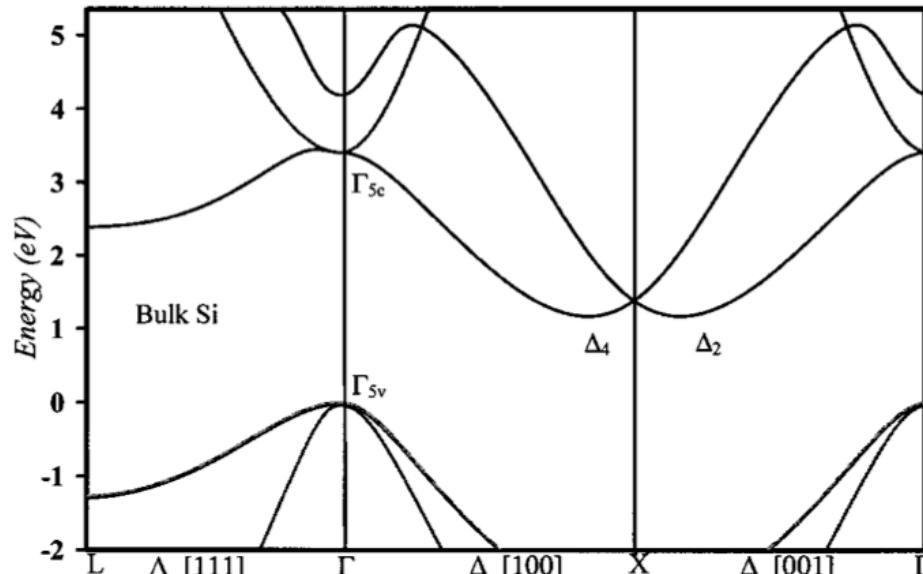
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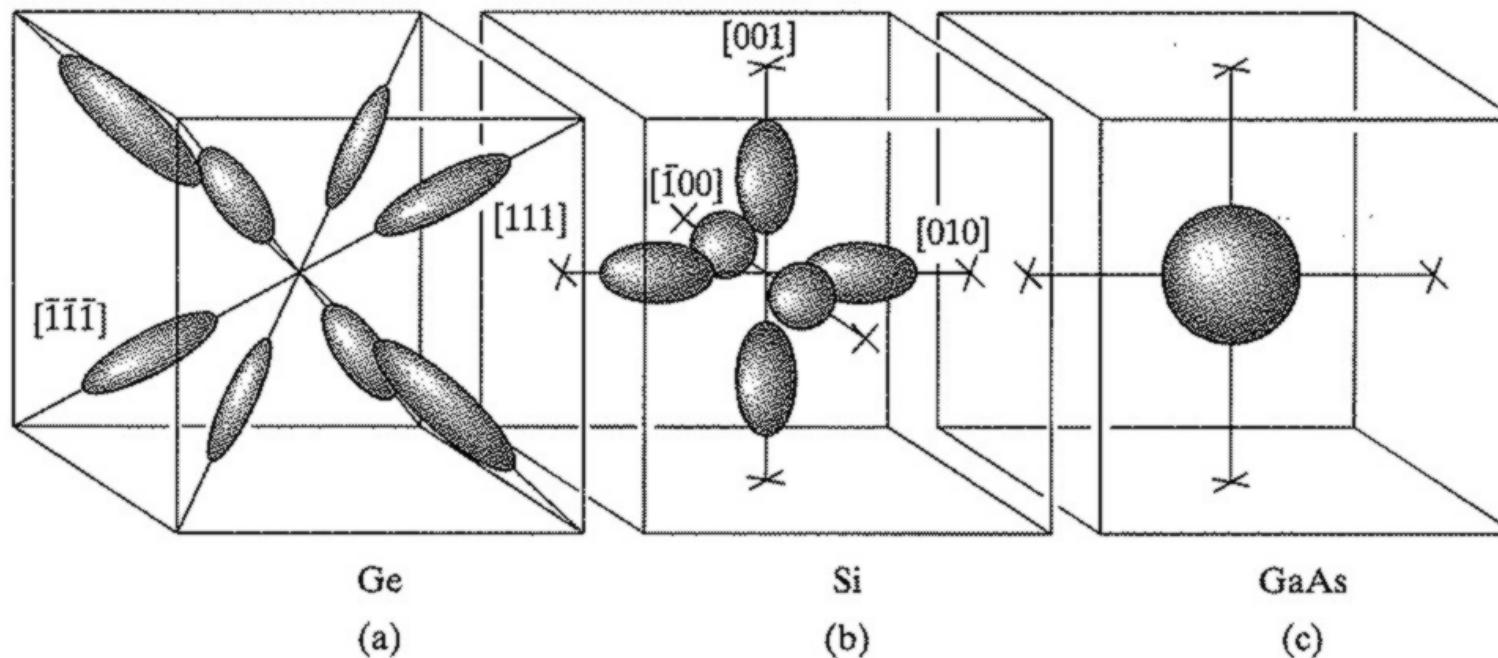
(Received 2 April 2002; accepted 1 May 2003)

A strain Bir–Pikus Hamiltonian H_{st} , associated with a 20-band $sp^3s^* \mathbf{k} \cdot \mathbf{p}$ Hamiltonian H_{kp} , is used to describe the valence band and the first two conduction bands all over the Brillouin zone.



band structure models $k \cdot p$ theory – more bands

Conduction band minima



band structure models $k \cdot p$ theory – more bands

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Band structures of GaAs, InAs, and Ge: A 24-k.p model

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band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – other directions

For the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians discussed so far, the x , y and z directions correspond to the principal crystallographic directions. For computing the effect of strain on the bandstructure of a film grown, for example, on a (111) plane, the coordinate system has to be rotated accordingly, e.g. $z \rightarrow [111]$.

$$\begin{bmatrix} \uparrow' \\ \downarrow' \end{bmatrix} = \begin{bmatrix} e^{-i\phi/2} \cos \frac{\theta}{2} & e^{i\phi/2} \sin \frac{\theta}{2} \\ -e^{-i\phi/2} \sin \frac{\theta}{2} & e^{i\phi/2} \cos \frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \uparrow \\ \downarrow \end{bmatrix} \quad \text{Spin coordinates}$$

$$\begin{bmatrix} X' \\ Y' \\ Z' \end{bmatrix} = \begin{bmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \quad \text{Spatial coordinates}$$

band structure models

$\mathbf{k} \cdot \mathbf{p}$ theory – other directions

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6×6 effective mass Hamiltonian for heterostructures grown on (11N)-oriented substrates

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(Received 17 January 2003; published 27 August 2003)

$$H = \frac{\hbar^2}{2m_0} \begin{pmatrix} P+Q & S & R & 0 & \frac{1}{\sqrt{2}}S & \sqrt{2}R \\ S^\dagger & P-Q & 0 & R & -\sqrt{2}Q & -\sqrt{\frac{3}{2}}S \\ R^\dagger & 0 & P-Q & -S & -\sqrt{\frac{3}{2}}S^\dagger & \sqrt{2}Q \\ 0 & R^\dagger & -S^\dagger & P+Q & -\sqrt{2}R^\dagger & \frac{1}{\sqrt{2}}S^\dagger \\ \frac{1}{\sqrt{2}}S^\dagger & -\sqrt{2}Q & -\sqrt{\frac{3}{2}}S & -\sqrt{2}R & P-\Delta & 0 \\ \sqrt{2}R^\dagger & -\sqrt{\frac{3}{2}}S^\dagger & \sqrt{2}Q & \frac{1}{\sqrt{2}}S & 0 & P-\Delta \end{pmatrix} .$$

$N=0$	$P = -\gamma_1 k^2$
	$Q = -\frac{\gamma_2}{2}(2k_1^2 - k_2^2 - k_3^2) - \frac{3}{2}\gamma_3(k_2^2 - k_3^2)$
	$S = 2\sqrt{3}(\gamma_3 k_1 k_3 - i\gamma_2 k_2 k_3)$
	$R = \frac{\sqrt{3}}{2}\{\gamma_2(2k_1^2 - k_2^2 - k_3^2) - \gamma_3[(k_2^2 - k_3^2) + i4k_1 k_2]\}$
$N=1$	$P = -\gamma_1 k^2$
	$Q = -\gamma_3(k_1^2 + k_2^2 - 2k_3^2)$
	$S = -\frac{\sqrt{6}}{3}(\gamma_2 - \gamma_3)(k_1 + ik_2)^2 + \frac{2\sqrt{3}}{3}(2\gamma_2 + \gamma_3)(k_1 - ik_2)k_3$
	$R = \frac{\sqrt{3}}{3}(\gamma_2 + 2\gamma_3)(k_1 - ik_2)^2 - \frac{2\sqrt{6}}{3}(\gamma_2 - \gamma_3)(k_1 + ik_2)k_3$

band structure models

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N=2

$P = -\gamma_1 k^2$
 $Q = -\frac{\gamma_2}{2}(k_2^2 - k_3^2 + 2\sqrt{2}k_1k_3) - \frac{\gamma_3}{2}(2k_1^2 + k_2^2 - 3k_3^2 - 2\sqrt{2}k_1k_3)$
 $S = \frac{\sqrt{6}}{3}\gamma_2[(k_2^2 - k_3^2 + 2\sqrt{2}k_1k_3) - i(2k_1k_2 + \sqrt{2}k_2k_3)]$
 $- \frac{\sqrt{6}}{3}\gamma_3[(k_2^2 - k_3^2 - 2\sqrt{2}k_1k_3) - i(2k_1k_2 - \sqrt{2}k_2k_3)]$
 $R = -\frac{\sqrt{3}}{6}\gamma_2[(k_2^2 - k_3^2 + 2\sqrt{2}k_1k_3) + i(8k_1k_2 + 4\sqrt{2}k_2k_3)]$
 $+ \frac{\sqrt{3}}{6}\gamma_3[(6k_1^2 - 5k_2^2 - k_3^2 + 2\sqrt{2}k_1k_3) - i(4k_1k_2 - 4\sqrt{2}k_2k_3)]$

N=∞

$P = -\gamma_1 k^2$
 $Q = -\gamma_2(k_1^2 + k_2^2 - 2k_3^2)$
 $S = 2\sqrt{3}\gamma_3(k_1 - ik_2)k_3$
 $R = \sqrt{3}[\gamma_3(k_1^2 - k_2^2) - i2\gamma_2k_1k_2]$