In This Lecture:

- Luttinger-Kohn Hamiltonian
- Refreshment on Defects & Elasticity
- Pikus-Bir Hamiltonian
- Atomic Units

k·p and Similar Band Edge Techniques

Brief Overview

- Kane's Hamiltonian
  - 8 bands (CB+3 VB with spin) treated exactly
  - Coupling with the other bands neglected
  - HH band comes out with wrong sign and value (due above approximation)
  - No warping predicted (i.e., isotropic) for finite **k**
- Luttinger-Kohn Hamiltonian (for degenerate bands with spin-orbit)
  - 6 VBs treated exactly; can be extended to include CBs as well
  - Other bands are included via Löwdin's technique
  - Warping of the VBs is predicted
- Pikus-Bir Hamiltonian
  - Just like LK Hamiltonian, but includes the effects of strain in the xtal

Luttinger-Kohn Hamiltonian

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Motion of Electrons and Holes in Perturbed Periodic Fields

2113 citations!

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Bell Telephone Laboratories, Murray Hill, New Jersey
(Received October 13, 1954)

A new method of developing an "effective-mass" equation for electrons moving in a perturbed periodic structure is discussed. This method is particularly adapted to such problems as arise in connection with impurity states and cyclotron resonance in semiconductors such as Si and Ge. The resulting theory generalizes the usual effective-mass treatment to the case where a band minimum is not at the center of the Brillouin zone, and also to the case where the band is degenerate. The latter is particularly striking, the usual Wannier equation being replaced by a set of coupled differential equations.

Begin with the total Hamiltonian for the cell-periodic fn's dropping their band indices for convenience:

$$H u_{\mathbf{k}}(\mathbf{r}) = E(\mathbf{k}) u_{\mathbf{k}}(\mathbf{r})$$

$$H = H_0 + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{4m_0^2 c^2} \nabla V \times \mathbf{p} \cdot \boldsymbol{\sigma} + H'$$

Neglect compared to

$$H_0 = \frac{p^2}{2m} + V(\mathbf{r})$$

$$H' = \frac{\hbar}{m_0} \mathbf{k} \cdot \Pi$$

p

$$\Pi = \mathbf{p} + \frac{\hbar}{4m_0 c^2} \boldsymbol{\sigma} \times \nabla V$$

Ref: Chuang

Expand any cell-periodic wf in terms of the **k**=0 basis:

$$u_{\mathbf{k}}(\mathbf{r}) = \sum_{j'}^{A} a_{j'}(\mathbf{k}) u_{j'0}(\mathbf{r}) + \sum_{\gamma}^{B} a_{\gamma}(\mathbf{k}) u_{\gamma 0}(\mathbf{r})$$

where, according to Kane's model **k**=0 solutions (exc. Class B) are of the form:

$$u_{10}(\mathbf{r}) = \left|\frac{3}{2}, \frac{3}{2}\right\rangle = \frac{-1}{\sqrt{2}}|(X + iY)\uparrow\rangle$$

$$u_{20}(\mathbf{r}) = \left|\frac{3}{2}, \frac{1}{2}\right\rangle = \frac{-1}{\sqrt{6}}|(X + iY)\downarrow\rangle + \sqrt{\frac{2}{3}}|Z\uparrow\rangle$$

$$u_{30}(\mathbf{r}) = \left|\frac{3}{2}, \frac{-1}{2}\right\rangle = \frac{1}{\sqrt{6}}|(X - iY)\uparrow\rangle + \sqrt{\frac{2}{3}}|Z\downarrow\rangle$$

$$u_{40}(\mathbf{r}) = \left|\frac{3}{2}, \frac{-3}{2}\right\rangle = \frac{1}{\sqrt{2}}|(X - iY)\downarrow\rangle$$

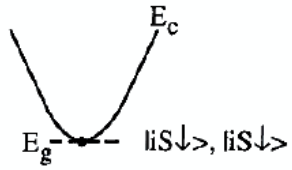
$$u_{50}(\mathbf{r}) = \left|\frac{1}{2}, \frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}|(X + iY)\downarrow\rangle + \frac{1}{\sqrt{3}}|Z\uparrow\rangle$$

$$u_{60}(\mathbf{r}) = \left|\frac{1}{2}, \frac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}|(X - iY)\uparrow\rangle - \frac{1}{\sqrt{3}}|Z\downarrow\rangle$$

Ref: Chuang

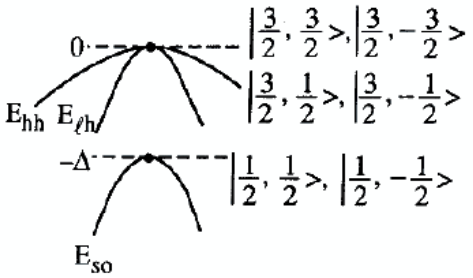
Also recall that at **k**=0, band edge fn's satisy:

$$H(\mathbf{k}=0)u_{j0}(\mathbf{r}) = E_j(0)u_{j0}(\mathbf{r})$$



$$E_j(0) = E_p + \frac{\Delta}{3} = 0 \qquad \text{for } j = 1,2,3,4$$

$$E_j(0) = E_p - \frac{2\Delta}{3} = -\Delta \qquad \text{for } j = 5,6$$



where $E_p = -\Delta/3$

Now, apply Löwdin's method:

$$\sum_{j'}^{A}\left(U_{jj'}^{A} - E\delta_{jj'}\right)a_{j'}(\mathbf{k}) = 0$$

Effect of remote bands are here

Ref: Chuang

where

$$U^A_{jj'} = H_{jj'} + \sum_{\gamma \neq j,\, j'}^{B} \frac{H_{j\gamma} H_{\gamma j'}}{E_0 - E_\gamma} = H_{jj'} + \sum_{\gamma \neq j,\, j'}^{B} \frac{H'_{j\gamma} H'_{\gamma j'}}{E_0 - E_\gamma}$$

$$H_{jj'} = \langle u_{j0} | H | u_{j'0} \rangle = \left[E_j(0) + \frac{\hbar^2 k^2}{2m_0} \right] \delta_{jj'} \qquad (j, j' \in A)$$

$$H'_{j\gamma} = \langle u_{j0} | \frac{\hbar}{m_0} \mathbf{k} \cdot \boldsymbol{\Pi} | u_{\gamma 0} \rangle \cong \sum_\alpha \frac{\hbar k_\alpha}{m_0} p^\alpha_{j\gamma} \qquad (j \in A, \gamma \notin A)$$

p

where we note that $\Pi_{jj'} = 0$, for $j, j' \in A$, and $\Pi^\alpha_{j\gamma} \simeq p^\alpha_{j\gamma}$ for $j \in A$ and $\gamma \notin A$. Since $\gamma \neq j$, adding the unperturbed part to the perturbed part in $H'_{j\gamma}$ does not affect the results, i.e., $H_{j\gamma} = H'_{j\gamma}$. We thus obtain

$$U^A_{jj'} = \left[E_j(0) + \frac{\hbar^2 k^2}{2m_0} \right] \delta_{jj'} + \frac{\hbar^2}{m_0^2} \sum_{\gamma \neq j,\, j'}^{B} \sum_{\alpha,\, \beta} \frac{k_\alpha k_\beta p^\alpha_{j\gamma} p^\beta_{\gamma j'}}{E_0 - E_\gamma}$$

couples bands *j* and *j'* via band γ in class B

Change of notation; let $U^A_{jj'} \equiv D_{jj'}$

Ref: Chuang

$$D_{jj'} = E_j(0)\,\delta_{jj'} + \sum_{\alpha,\beta} D_{jj'}^{\alpha\beta} k_\alpha k_\beta$$

where $$D_{jj'}^{\alpha\beta} = \frac{\hbar^2}{2m_0}\left[\delta_{jj'}\delta_{\alpha\beta} + \sum_{\gamma}^{B} \frac{p_{j\gamma}^{\alpha} p_{\gamma j'}^{\beta} + p_{j\gamma}^{\beta} p_{\gamma j'}^{\alpha}}{m_0(E_0 - E_\gamma)}\right]$$

For *j=j'*, similar to single-band effective mass tensor

The couplings within class A can be expressed using three so-called Luttinger parameters: $\gamma_1, \gamma_2, \gamma_3$

They are actually fitted to experimental data to generate faithful band dispersions

Ref: Chuang

In terms of Luttinger parameters, the LK Hamiltonian becomes:

$$\overline{\overline{\mathbf{H}}}^{\mathrm{LK}} = -\begin{bmatrix} P+Q & -S & R & 0 & -S/\sqrt{2} & \sqrt{2}R \\ -S^{+} & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{3/2}S \\ R^{+} & 0 & P-Q & S & \sqrt{3/2}S^{+} & \sqrt{2}Q \\ 0 & R^{+} & S^{+} & P+Q & -\sqrt{2}R^{+} & -S^{+}/\sqrt{2} \\ -S^{+}/\sqrt{2} & -\sqrt{2}Q^{+} & \sqrt{3/2}S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^{+} & \sqrt{3/2}S^{+} & \sqrt{2}Q^{+} & -S/\sqrt{2} & 0 & P+\Delta \end{bmatrix} \begin{matrix} \text{HH} \\ \text{LH} \\ \text{LH} \\ \text{HH} \\ \text{SO} \\ \text{SO} \end{matrix}$$

complex conjugate

where

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

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

$$R = \frac{\hbar^2}{2m_0}\left[-\sqrt{3}\gamma_2\left(k_x^2 - k_y^2\right) + i2\sqrt{3}\gamma_3 k_x k_y\right]$$

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

Ref: Chuang

So, essentially we have solved the Hamiltonian

$$\left[\frac{p^2}{2m_0} + V(\mathbf{r}) + \frac{\hbar}{4m_0^2c^2}\nabla V \times \mathbf{p}\cdot\boldsymbol{\sigma}\right]\psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\,\psi_{n\mathbf{k}}(\mathbf{r})$$

where

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r}) \qquad u_{n\mathbf{k}}(\mathbf{r}) = \sum_{j=1}^{6} a_j(\mathbf{k})\,u_{j0}(\mathbf{r})$$

For the expansion eigenvectors and eigenvalues:

$$\sum_{j'=1}^{6} H_{jj'}^{\mathrm{LK}} a_{j'}(\mathbf{k}) = E a_j(\mathbf{k}) \qquad E_n(\mathbf{k}) = E$$

But now, the effect of remote bands are also taken into account through the Löwdin renormalization. It reveals indirect band couplings among those within class A via direct couplings with those in class B.

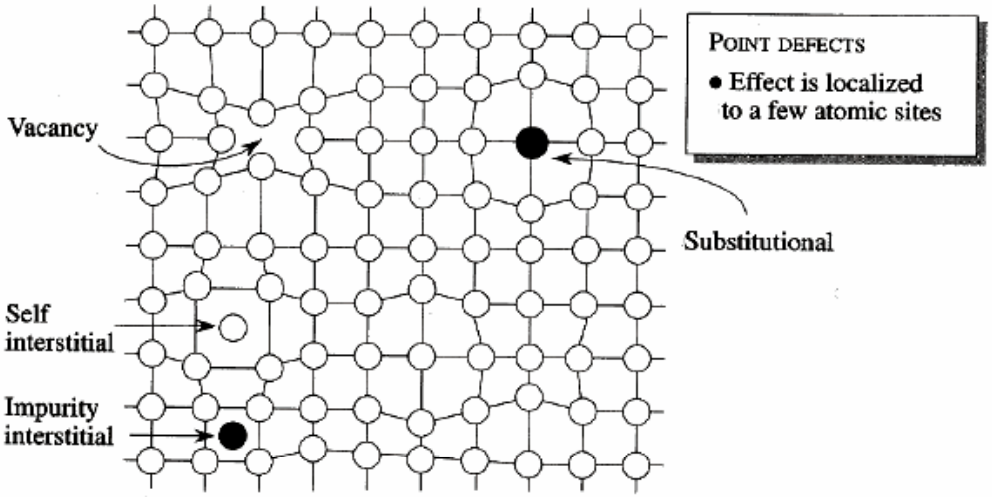
Ref: Chuang

Common defects in semiconductors

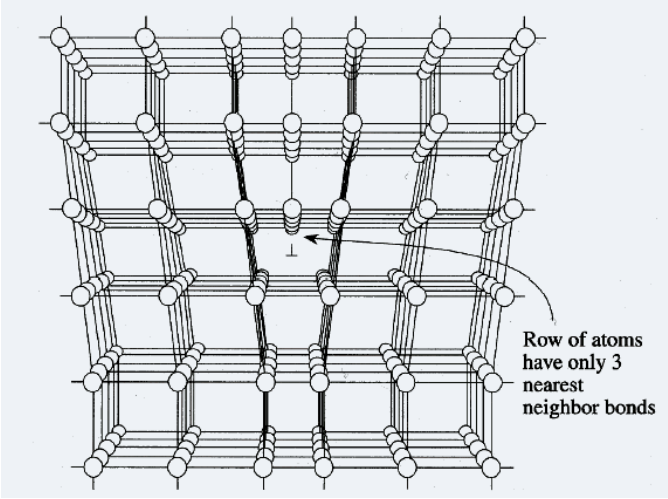
- **Point defects**

A function of the xtal growth temperature

$$\frac{N_d}{N_{tot}} = k_d \exp\left(-\frac{E_d}{k_B T_{growth}}\right)$$



- **Line defects (dislocations)**



- **Planar & volume defects**

Important in poly-xtalline mat'ls

Ref: Singh

Strain in heterostructures

Strain: $\varepsilon = \dfrac{a_S - a_I}{a_I}$

A simplistic estimate of the critical thickness:

$$d_c \cong \frac{a_S}{2|\varepsilon|}$$

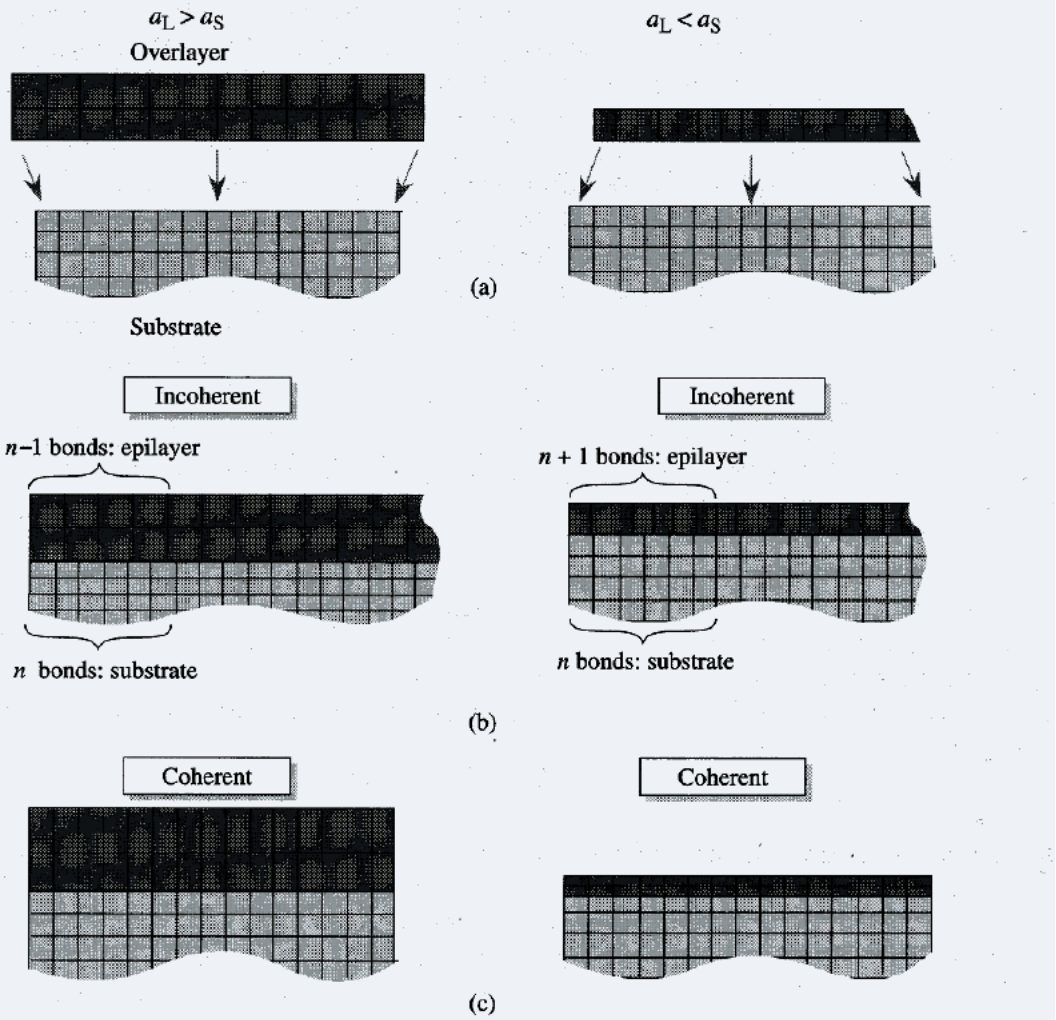
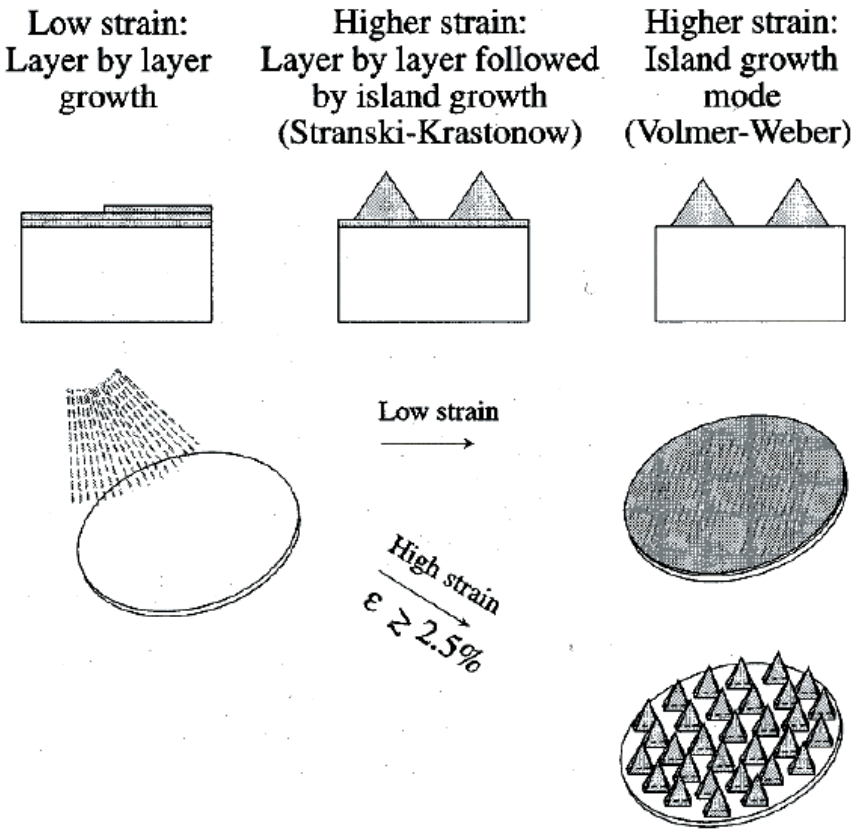


Figure 1.20: (a) The conceptual exercise in which an overlayer with one lattice constant is placed without distortion on a substrate with a different lattice constant. (b) Dislocations are generated at positions where the interface bonding is lost. (c) The case is shown where the overlayer is distorted so that no dislocation is generated.

Ref: Singh

Self-assembled structures



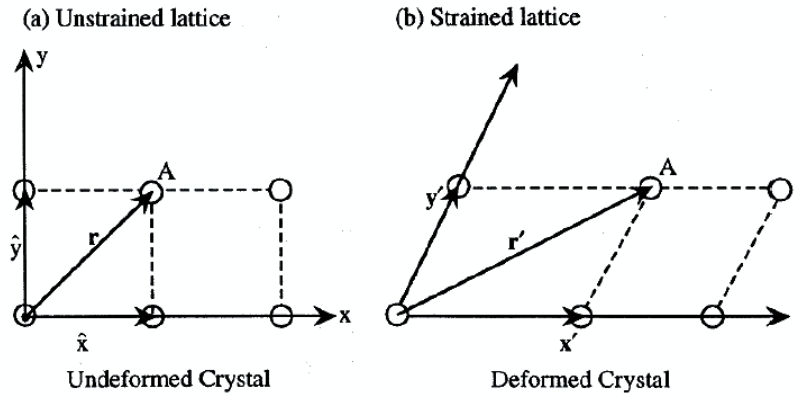
Lateral feature sizes can be controlled from 100Å -1000Å
$\Longrightarrow 10^{12}$ features per wafer can be produced without lithography

Figure 1.22: Growth modes in strained epitaxy. The island mode growth can be exploited to make "self-assembled" quantum dot structures.

Ref: Singh

Some background on elasticity

Strain & volume dilation



$$\mathbf{x}' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$
$$\mathbf{y}' = \varepsilon_{yx}\hat{x} + (1+\varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$
$$\mathbf{z}' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1+\varepsilon_{zz})\hat{z}$$

No longer unit vectors

We define six independent components of strain

$$e_1 = \varepsilon_{xx} \qquad e_2 = \varepsilon_{yy} \qquad e_3 = \varepsilon_{zz}$$
$$e_4 = \mathbf{x}' \cdot \mathbf{y}' = \varepsilon_{xy} + \varepsilon_{yx}$$
$$e_5 = \mathbf{y}' \cdot \mathbf{z}' = \varepsilon_{yz} + \varepsilon_{zy}$$
$$e_6 = \mathbf{z}' \cdot \mathbf{x}' = \varepsilon_{zx} + \varepsilon_{xz}$$

Another common notation

$$e_{xx},\ e_{yy},\ e_{zz},\ e_{xy},\ e_{yz},\ e_{zx}$$

Ref: Chuang

Strain & volume dilation (cont'd)

$$\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z} \equiv (x, y, z)$$

$$\mathbf{r}' = x\mathbf{x}' + y\mathbf{y}' + z\mathbf{z}'$$

$$\mathbf{r}' = x'\hat{x} + y'\hat{y} + z'\hat{z} \equiv (x', y', z')$$

$$\frac{V + \delta V}{V} = \mathbf{x}' \cdot \mathbf{y}' \times \mathbf{z}' = 1 + (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$\frac{\delta V}{V} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

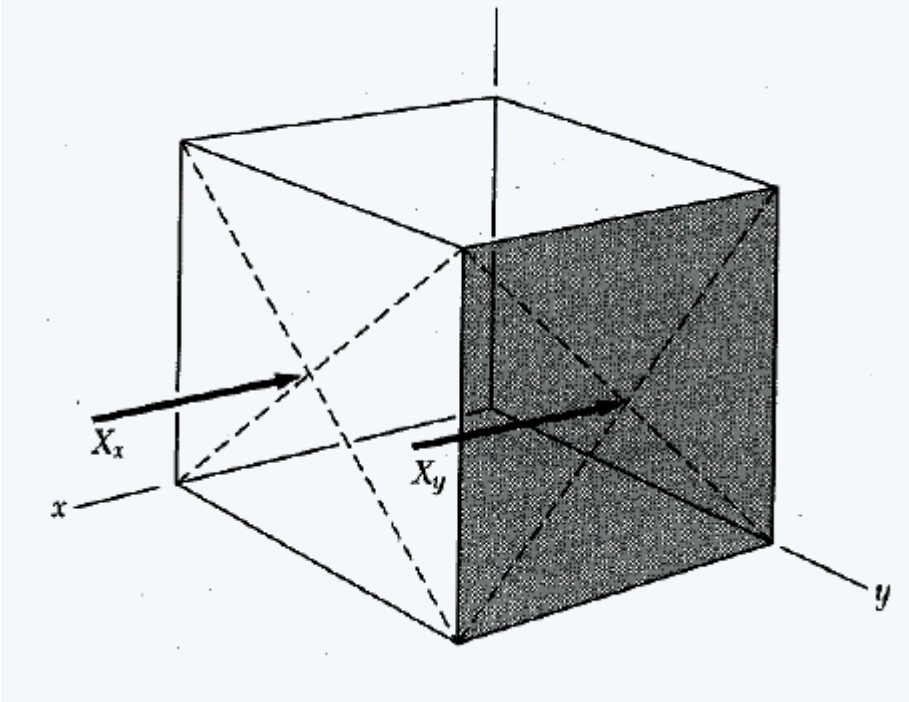
Fractional change of xtal volume under uniform deformation

Ref: Chuang

Some background on elasticity (cont'd)

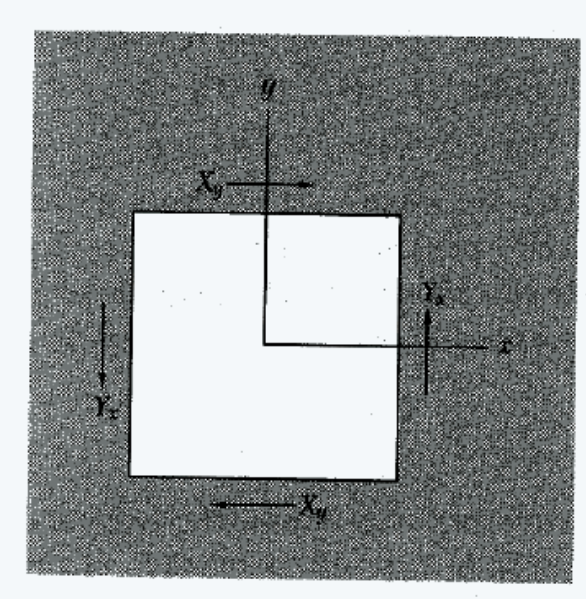
Stress

$X_x,\ X_y,\ X_z,\ Y_x,\ Y_y,\ Y_z,\ Z_x,\ Z_y,\ Z_z$ Stress components in general



Under static equilibrium (total torque around origin should vanish)

$$Y_z = Z_y \ ; \qquad Z_x = X_z \ ; \qquad X_y = Y_x$$



Ref: Kittel

Some background on elasticity (cont'd)

Six independent components can be chosen as: $X_x, Y_y, Z_z, Y_z, Z_x, X_y$

Stress-Strain relation: extension of Hooke's law (linear regime)

$$
\begin{aligned}
X_x &= C_{11}e_{xx} + C_{12}e_{yy} + C_{13}e_{zz} + C_{14}e_{yz} + C_{15}e_{zx} + C_{16}e_{xy} \\
Y_y &= C_{21}e_{xx} + C_{22}e_{yy} + C_{23}e_{zz} + C_{24}e_{yz} + C_{25}e_{zx} + C_{26}e_{xy} \\
Z_z &= C_{31}e_{xx} + C_{32}e_{yy} + C_{33}e_{zz} + C_{34}e_{yz} + C_{35}e_{zx} + C_{36}e_{xy} \\
Y_z &= C_{41}e_{xx} + C_{42}e_{yy} + C_{43}e_{zz} + C_{44}e_{yz} + C_{45}e_{zx} + C_{46}e_{xy} \\
Z_x &= C_{51}e_{xx} + C_{52}e_{yy} + C_{53}e_{zz} + C_{54}e_{yz} + C_{55}e_{zx} + C_{56}e_{xy} \\
X_y &= C_{61}e_{xx} + C_{62}e_{yy} + C_{63}e_{zz} + C_{64}e_{yz} + C_{65}e_{zx} + C_{66}e_{xy}
\end{aligned}
$$

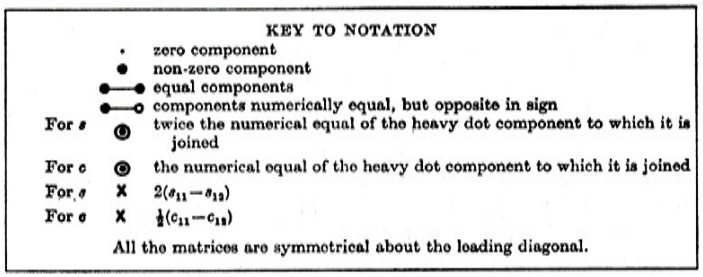
C's : elastic stiffness constants, moduli of elasticity

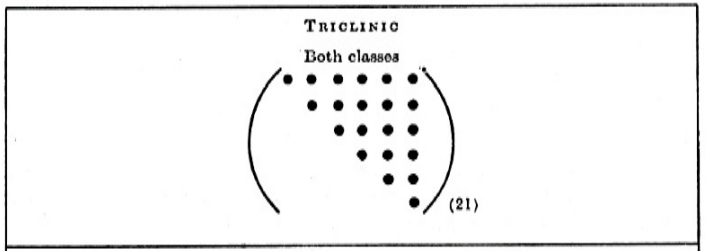
For a cubic xtal:

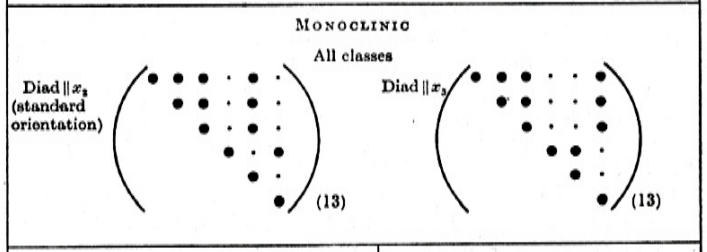
	e_{xx}	e_{yy}	e_{zz}	e_{yz}	e_{zx}	e_{xy}
X_x	C_{11}	C_{12}	C_{12}	0	0	0
Y_y	C_{12}	C_{11}	C_{12}	0	0	0
Z_z	C_{12}	C_{12}	C_{11}	0	0	0
Y_z	0	0	0	C_{44}	0	0
Z_x	0	0	0	0	C_{44}	0
X_y	0	0	0	0	0	C_{44}

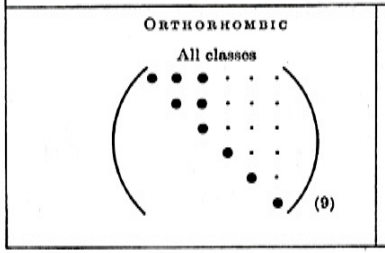
Ref: Kittel

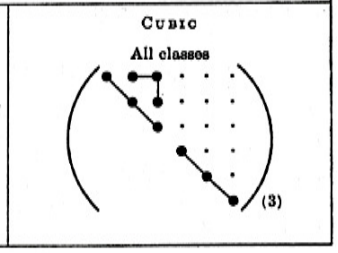
Effects of xtal symmetry on elastic constants

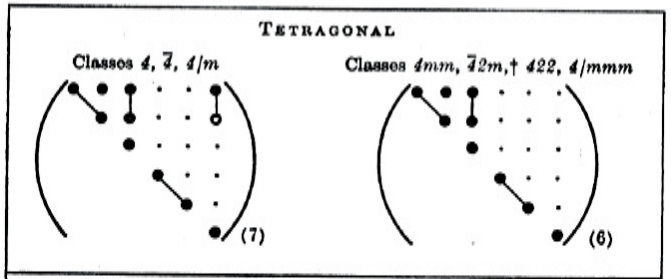


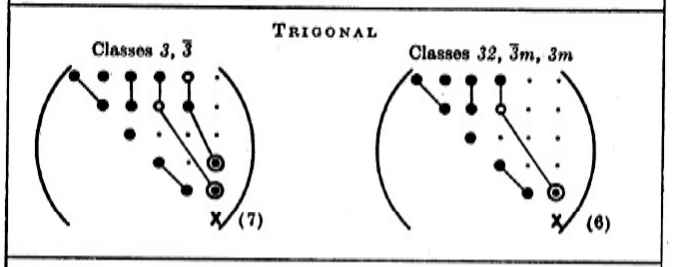


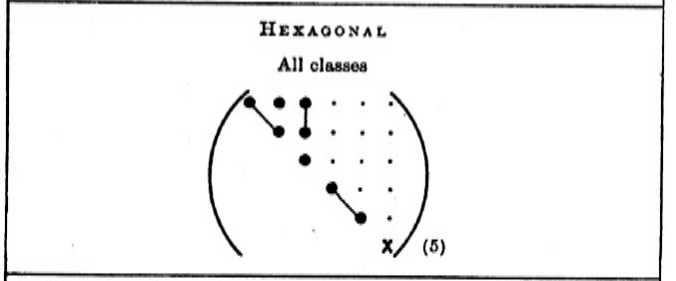


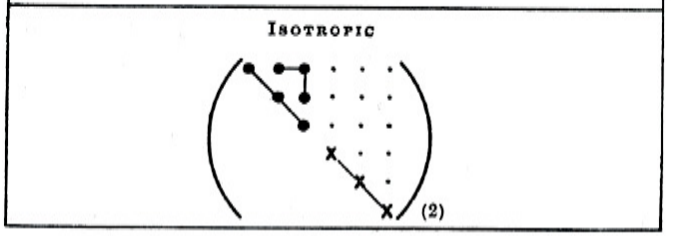












Ref: Nye

Back to pseudomorphic epitaxial growth

$$\begin{aligned} e_{\parallel} &= \frac{a_S}{a_L} - 1 \\ &= \epsilon \end{aligned}$$

No stress along the growth direction!

$$\begin{aligned} \epsilon_{xx} &= \epsilon_{\parallel} \\ \epsilon_{yy} &= \epsilon_{xx} \\ \epsilon_{zz} &= \frac{-2c_{12}}{c_{11}}\epsilon_{\parallel} \\ \epsilon_{xy} &= 0 \\ \epsilon_{yz} &= 0 \\ \epsilon_{zx} &= 0 \end{aligned}$$

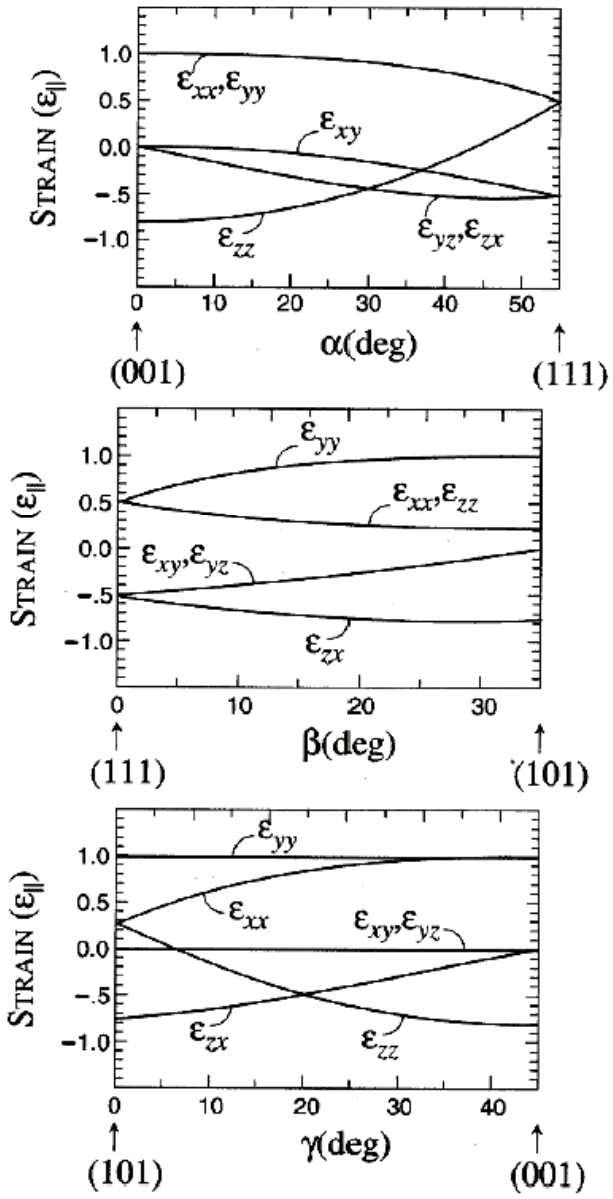
For strained growth on (001) substrate & fcc lattice

For strained growth on (111) substrate & fcc lattice

$$\begin{aligned} \epsilon_{xx} &= \left[\frac{2}{3} - \frac{1}{3}\left(\frac{2c_{11}+4c_{12}-4c_{44}}{c_{11}+2c_{12}+4c_{44}}\right)\right]\epsilon_{\parallel} \\ \epsilon_{yy} &= \epsilon_{xx} \\ \epsilon_{zz} &= \epsilon_{xx} \\ \epsilon_{xy} &= \left[\frac{-1}{3} - \frac{1}{3}\left(\frac{2c_{11}+4c_{12}-4c_{44}}{c_{11}+2c_{12}+4c_{44}}\right)\right]\epsilon_{\parallel} \\ \epsilon_{yz} &= \epsilon_{xy} \\ \epsilon_{zx} &= \epsilon_{yz} \end{aligned}$$

Ref: Singh

On arbitrary growth planes



Ref: Singh

Strained tensor for self-organized quantum dots

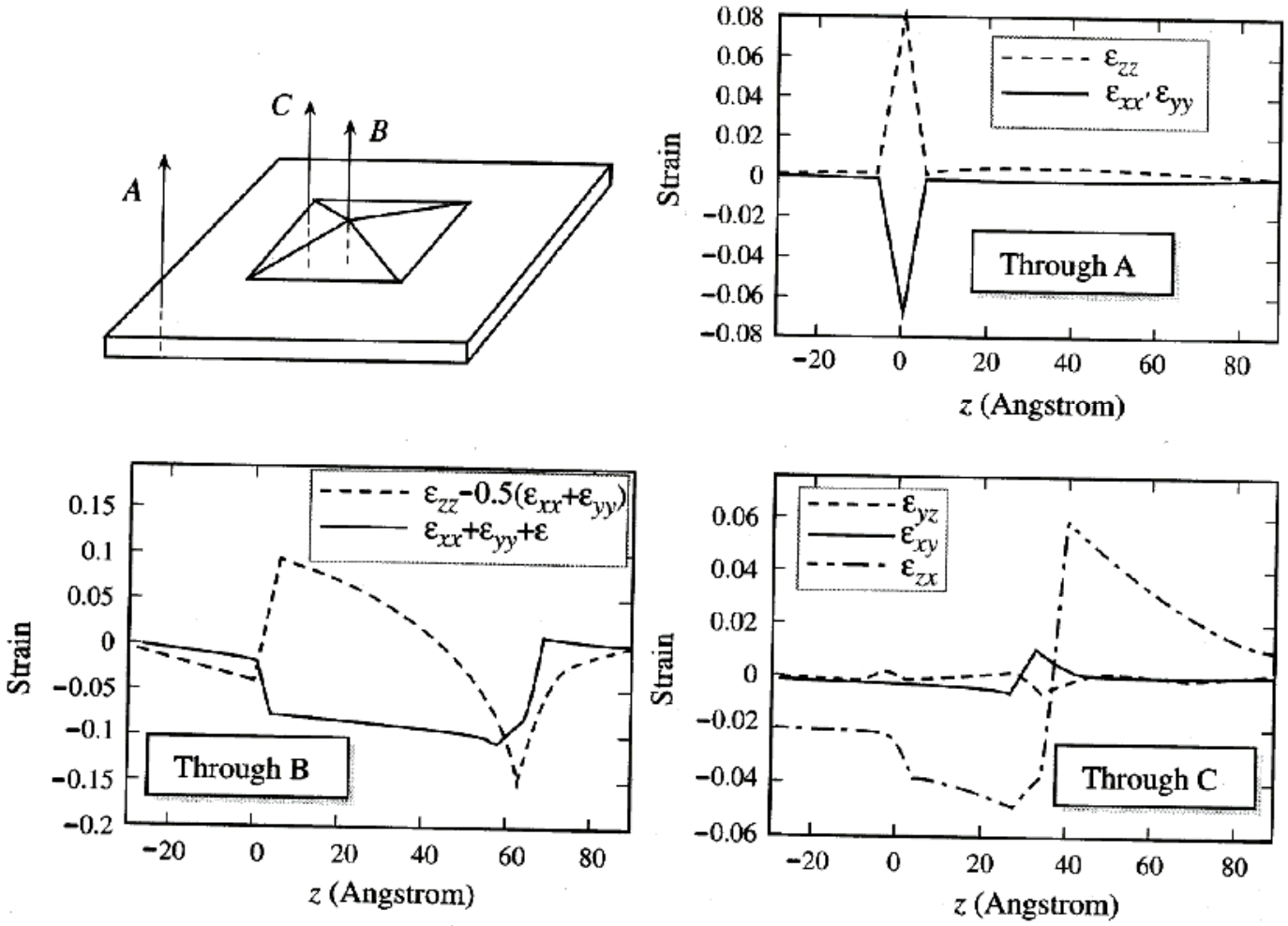
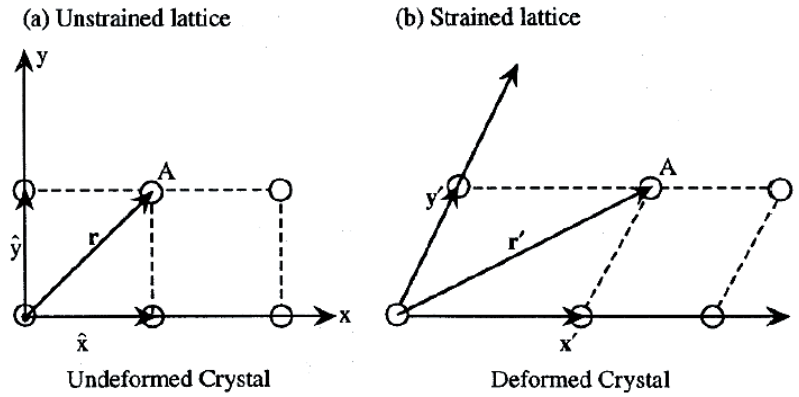


Figure 1.24: Strain tensor in a pyramidal InAs on GaAs self-assembled quantum dot.

Ref: Singh

Pikus-Bir Hamiltonian: Including Strain

Uniformly deformed crystal



$$\mathbf{x}' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$
$$\mathbf{y}' = \varepsilon_{yx}\hat{x} + (1+\varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$
$$\mathbf{z}' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1+\varepsilon_{zz})\hat{z}$$

No longer unit vectors

$$\mathbf{r}' = \mathbf{r} + \bar{\bar{\varepsilon}} \cdot \mathbf{r} = (1 + \bar{\bar{\varepsilon}}) \cdot \mathbf{r}$$

invert

$$r_i = r_i' - \sum_j \varepsilon_{ij} r_j'$$

$$\mathbf{r} = (1 - \bar{\bar{\varepsilon}}) \cdot \mathbf{r}'$$

Back in the deformed xtal coordinate system:

$$\left[\frac{\mathbf{p}'^2}{2m_0} + V(\mathbf{r}')\right]\psi_{n\mathbf{k}'}(\mathbf{r}') = E_n(\mathbf{k}')\psi_{n\mathbf{k}'}(\mathbf{r}')$$

Ref: Chuang

Now comes some manipulations

using the chain rule $\frac{\partial}{\partial r_i'} = \sum_j \frac{\partial r_j}{\partial r_i'}\frac{\partial}{\partial r_j} = \frac{\partial}{\partial r_i} - \sum_j \varepsilon_{ji}\frac{\partial}{\partial r_j}$

therefore $\mathbf{p}' = \mathbf{p}\cdot(1-\bar{\bar{\varepsilon}})$ $\qquad p'^2 = p^2 - 2\sum_{i,j} p_i \varepsilon_{ij} p_j$

expanding the potential $V\left[(1+\bar{\bar{\varepsilon}})\cdot\mathbf{r}\right] = V_0(\mathbf{r}) + \sum_{i,j} V_{ij}\varepsilon_{ij}$ $\qquad V_{ij} = \left.\frac{\partial V}{\partial \varepsilon_{ij}}\right|_{\varepsilon_{ij}\to 0}$

$$[H_0 + H_\varepsilon]\psi_{n\mathbf{k}'}\left[(1+\bar{\bar{\varepsilon}})\cdot\mathbf{r}\right] = E_n(\mathbf{k}')\psi_{n\mathbf{k}'}\left[(1+\bar{\bar{\varepsilon}})\cdot\mathbf{r}\right]$$

$$H_0 = \frac{p^2}{2m_0} + V_0(\mathbf{r})$$

$$H_\varepsilon \equiv \sum_{\alpha,\beta}\hat{D}^{\alpha\beta}\varepsilon_{\alpha\beta} = \sum_{\alpha,\beta}\left(-\frac{1}{m_0}p_\alpha p_\beta + V_{\alpha\beta}\right)\varepsilon_{\alpha\beta}$$

$$\begin{aligned}\psi_{n\mathbf{k}'}\left[(1+\bar{\bar{\varepsilon}})\cdot\mathbf{r}\right] &= e^{i\mathbf{k}'\cdot\mathbf{r}'}u_{n\mathbf{k}'}(\mathbf{r}') \\ &= e^{i\mathbf{k}'\cdot(1+\bar{\bar{\varepsilon}})\cdot\mathbf{r}}u_{n\mathbf{k}'}\left[(1+\bar{\bar{\varepsilon}})\cdot\mathbf{r}\right] \\ &= e^{i\mathbf{k}\cdot\mathbf{r}}u^s_{n\mathbf{k}}(\mathbf{r})\end{aligned}$$

Ref: Chuang

Arriving at the Pikus-Bir Hamiltonian

$$H_0\left[e^{i\mathbf{k}\cdot\mathbf{r}}u^s_{n\mathbf{k}}(\mathbf{r})\right] = e^{i\mathbf{k}\cdot\mathbf{r}}\left(H_0 + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar^2k^2}{2m_0}\right)u^s_{n\mathbf{k}}(\mathbf{r})$$

$$H_\varepsilon\left[e^{i\mathbf{k}\cdot\mathbf{r}}u^s_{n\mathbf{k}}(\mathbf{r})\right] = e^{i\mathbf{k}\cdot\mathbf{r}}\left(H_\varepsilon - \frac{2\hbar}{m_0}\sum_{\alpha,\beta}k_\alpha\varepsilon_{\alpha\beta}p_\beta\right)u^s_{n\mathbf{k}}(\mathbf{r})$$

$$[H_0 + H']u^s_{n\mathbf{k}}(\mathbf{r}) = \left(E - \frac{\hbar^2k^2}{2m_0}\right)u^s_{n\mathbf{k}}(\mathbf{r})$$

$$H' = H_k + H_\varepsilon + H_{\varepsilon k}$$

$$H_k = \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}$$

$$H_\varepsilon = \sum_{\alpha,\beta}\hat{D}^{\alpha\beta}\varepsilon_{\alpha\beta}$$

$$H_{\varepsilon k} \equiv -2\frac{\hbar}{m_0}\sum_{\alpha,\beta}k_\alpha\varepsilon_{\alpha\beta}p_\beta$$

correspondence with LK Hamiltonian: $k_\alpha k_\beta \leftrightarrow \varepsilon_{\alpha\beta}$

Ref: Chuang

keeping terms to second order in **k** and first order in strain reduces to

$$H = H^{\mathrm{LK}} + H_\varepsilon \qquad (H_\varepsilon)_{jj'} = \sum_{\alpha,\beta} \hat{D}^{\alpha\beta}_{jj'} \varepsilon_{\alpha\beta}$$

For the CB: (isotropic case)

$$\frac{\hbar^2}{2m_e^*} \leftrightarrow a_c$$

Pikus-Bir CB deformation potential

$$E(\mathbf{k}) = E_c(0) + \frac{\hbar^2}{2} \sum_{\alpha,\beta} \left(\frac{1}{m^*}\right)_{\alpha\beta} k_\alpha k_\beta + a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

For the VB:

$$\frac{\hbar^2\gamma_1}{2m_0} \leftrightarrow D_v^d = -a_v$$

$$\frac{\hbar^2\gamma_2}{2m_0} \leftrightarrow \frac{D_u}{3} = -\frac{b}{2}$$

$$\frac{\hbar^2\gamma_3}{2m_0} \leftrightarrow \frac{D_u'}{3} = \frac{-d}{2\sqrt{3}}$$

Ref: Chuang

The final form including strain

$$H = -\begin{bmatrix} P+Q & -S & R & 0 & -\frac{1}{\sqrt{2}}S & \sqrt{2}R \\ -S^{+} & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{\frac{3}{2}}S \\ R^{+} & 0 & P-Q & S & \sqrt{\frac{3}{2}}S^{+} & \sqrt{2}Q \\ 0 & R^{+} & S^{+} & P+Q & -\sqrt{2}R^{+} & -\frac{1}{\sqrt{2}}S^{+} \\ -\frac{1}{\sqrt{2}}S^{+} & -\sqrt{2}Q & \sqrt{\frac{3}{2}}S & -\sqrt{2}R & P+\Delta & 0 \\ \sqrt{2}R^{+} & \sqrt{\frac{3}{2}}S^{+} & \sqrt{2}Q & -\frac{1}{\sqrt{2}}S & 0 & P+\Delta \end{bmatrix} \begin{matrix} |\tfrac{3}{2},\tfrac{3}{2}\rangle \\ |\tfrac{3}{2},\tfrac{1}{2}\rangle \\ |\tfrac{3}{2},-\tfrac{1}{2}\rangle \\ |\tfrac{3}{2},-\tfrac{3}{2}\rangle \\ |\tfrac{1}{2},\tfrac{1}{2}\rangle \\ |\tfrac{1}{2},-\tfrac{1}{2}\rangle \end{matrix}$$

same basis

Luttinger-Kohn part

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

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

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

$$S_k = \left(\frac{\hbar^2}{2m_0}\right)2\sqrt{3}\,\gamma_3(k_x-ik_y)k_z$$

$$P = P_k + P_\varepsilon \qquad Q = Q_k + Q_\varepsilon$$
$$R = R_k + R_\varepsilon \qquad S = S_k + S_\varepsilon$$

strain (Pikus-Bir) part

$$P_\varepsilon = -a_v(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})$$

$$R_\varepsilon = \frac{\sqrt{3}}{2}b(\varepsilon_{xx}-\varepsilon_{yy}) - id\varepsilon_{xy}$$

$$Q_\varepsilon = -\frac{b}{2}(\varepsilon_{xx}+\varepsilon_{yy}-2\varepsilon_{zz})$$

$$S_\varepsilon = -d(\varepsilon_{xz}-i\varepsilon_{yz})$$

Ref: Chuang

Table K.2 Important Band Structure Parameters[a–f] for GaAs, AlAs, InAs, InP, and GaP

	Materials				
	GaAs	AlAs	InAs	InP	GaP
Parameters					
a_0 (Å)	5.6533	5.6600	6.0584	5.8688	5.4505
E_g (eV)					
0 K	1.519	3.13 2.229*	0.42	1.424	2.90 2.35*
300 K	1.424	3.03 2.168*	0.354	1.344	2.78 2.27*
Δ (eV)	0.34	0.28	0.38	0.11	0.08
$E_{v,\mathrm{av}}$ (eV)	−6.92	−7.49	−6.67	−7.04	−7.40
Optical matrix parameter E_p (eV)	25.7 (25.0)[f]	21.1	22.2	20.7 (16.7)[f]	22.2
Deformation potentials (eV)					
a_c (eV)	−7.17	−5.64	−5.08	−5.04	−7.14
a_v (eV)	1.16	2.47	1.00	1.27	1.70
$a = a_c - a_v$ (eV)	−8.33	−8.11	−6.08	−6.31	−8.83
b (eV)	−1.7	−1.5	−1.8	−1.7	−1.8
d (eV)	−4.55	−3.4	−3.6	−5.6	−4.5
C_{11} (10^{11} dyne/cm^2)	11.879	12.5	8.329	10.11	14.05
C_{12} (10^{11} dyne/cm^2)	5.376	5.34	4.526	5.61	6.203
C_{44} (10^{11} dyne/cm^2)	5.94	5.42	3.96	4.56	7.033
Effective masses					
m_e^*/m_0	0.067	0.15	0.023	0.077	0.25
m_{hh}^*/m_0	0.50	0.79	0.40	0.60	0.67
m_{lh}^*/m_0	0.087	0.15	0.026	0.12	0.17
$m_{hh,z}/m_0 = \dfrac{1}{\gamma_1 - 2\gamma_2}$	0.333	0.478	0.263	0.606	0.326
$m_{lh,z}/m_0 = \dfrac{1}{\gamma_1 + 2\gamma_2}$	0.094	0.208	0.027	0.121	0.199
γ_1	6.8 (6.85)	3.45	20.4	4.95	4.05
γ_2	1.9 (2.1)	0.68	8.3	1.65	0.49
γ_3	2.73 (2.9)	1.29	9.1	2.35	1.25

Ref: Chuang

(Hartree) Atomic Units

In any computational project on semiconductors, use atomic units (a.u.), not cgs/SI

cgs (Gaussian) → Atomic Units:

Set in expressions: $e = m_0 = \hbar = 1$

SI→ Atomic Units:

Set in expressions: $\frac{e}{\sqrt{4\pi\varepsilon_0}} = m_0 = \hbar = 1$

Derived Units in a.u. :

Energy: 1 Ha = 2 Ry = 27.12 eV

Length: 1 a_B = Bohr Radius

Demonstration on Schrödinger Eq.

Start with the following expression in SI for the exciton bound states

$$\left[-\frac{\hbar^2}{2\mu_X}\nabla^2-\frac{e^2}{4\pi\kappa\varepsilon_0 r}\right]\psi_X(\vec{r})=E\psi_X(\vec{r})$$

Setting above: $$\frac{e}{\sqrt{4\pi\varepsilon_0}}=m_0=\hbar=1$$

Results in the expression in terms of variables in a.u. (denoted with tilde)

$$\left[-\frac{1}{2\tilde{\mu}_X}\tilde{\nabla}^2-\frac{1}{\kappa\tilde{r}}\right]\tilde{\psi}_X(\vec{\tilde{r}})=\tilde{E}\tilde{\psi}_X(\vec{\tilde{r}})$$