Physics of strained band structure of semiconductors

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Outline

1. Pikus-Bir Hamiltonian for bulk semiconductors
2. Band structure of strained QWs
3. Strained QW lasers:

   1) Compressive strain and tensile strain

   2) Advantage of strained QW lasers

   3) Critical thickness

1. Pikus-Bir Hamiltonian (1)

- Luttinger-Kohn Hamiltonian w/o strain

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

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

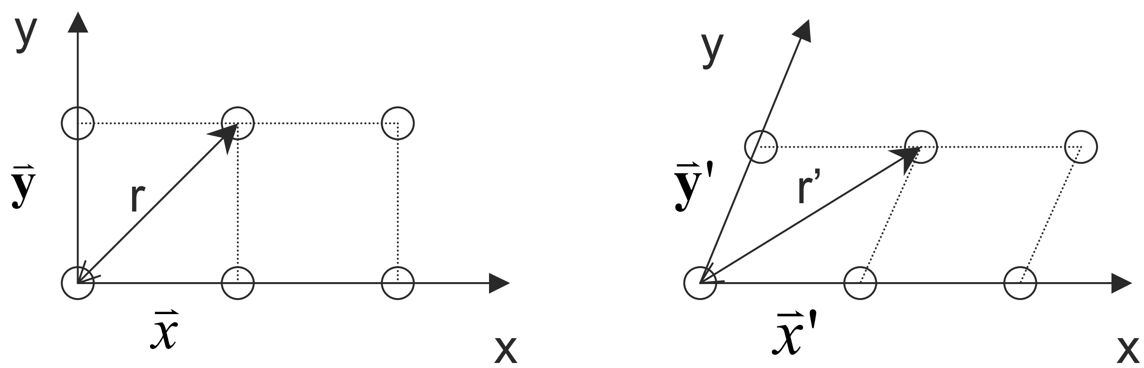
$$Q = \left(\frac{\hbar^2}{2m_0}\right)\gamma_2(k_x^2 + k_y^2 - 2k_z^2)$$

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

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

1. Pikus-Bir Hamiltonian (2)

- Derivation of Pikus-Bir Hamiltonian using the transform of coordinates methods:



(a) Unstrained lattice (b) Strained lattice

$$\vec{x}' = (1+\varepsilon_{xx})\vec{x} + \varepsilon_{xy}\vec{y} + \varepsilon_{xz}\vec{z}$$

$$\vec{y}' = \varepsilon_{yx}\vec{x} + (1+\varepsilon_{yy})\vec{y} + \varepsilon_{yz}\vec{z}$$

$$\vec{z}' = \varepsilon_{zx}\vec{x} + \varepsilon_{zy}\vec{y} + (1+\varepsilon_{zz})\vec{z}$$

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

$$\frac{V+\delta V}{V} = x' \bullet y' \times z' = 1 + \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

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

1. Pikus-Bir Hamiltonian (3)

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

$$P = P_k + P_\varepsilon \qquad Q = Q_k + Q_\varepsilon$$

$$R = R_k + R_\varepsilon \qquad S = S_k + S_\varepsilon$$

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

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

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

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

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

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

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

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

1. Pikus-Bir Hamiltonian (4)

- For simplifying purpose, we treat the special case for biaxial strain:

$$\varepsilon_{xx} = \varepsilon_{yy} \neq \varepsilon_{zz},$$
$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0$$

$$\Rightarrow \quad R_{\varepsilon} = S_{\varepsilon} = 0$$

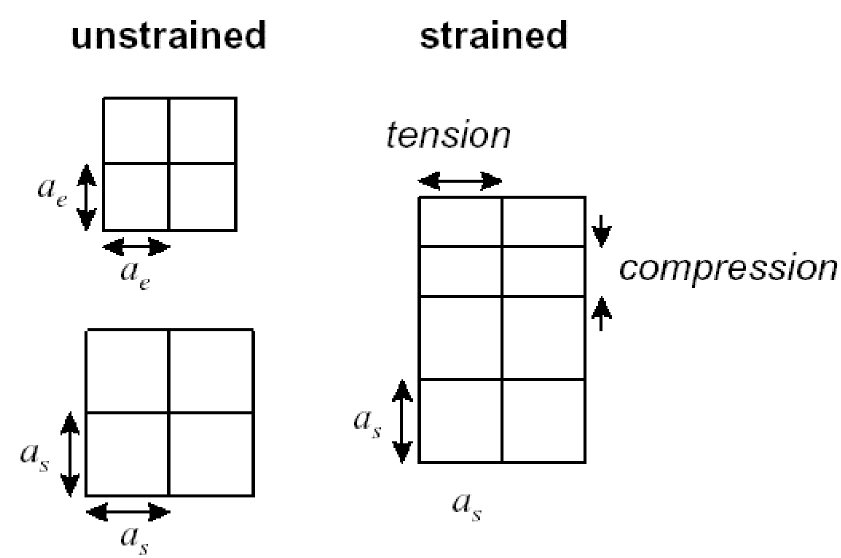
where $$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_0 - a}{a}, \varepsilon_{zz} = -\frac{2C_{12}}{C_{11}}\varepsilon_{xx}$$

C_{11} and C_{12} are elastic stiffness constants

1. Pikus-Bir Hamiltonian (5)

- Derivation of ε_{zz} by the linear relationship of stress vs strain :

$$\begin{bmatrix} \tau_{xx} \\ \tau_{yy} \\ \tau_{zz} \\ \tau_{xy} \\ \tau_{yz} \\ \tau_{zx} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

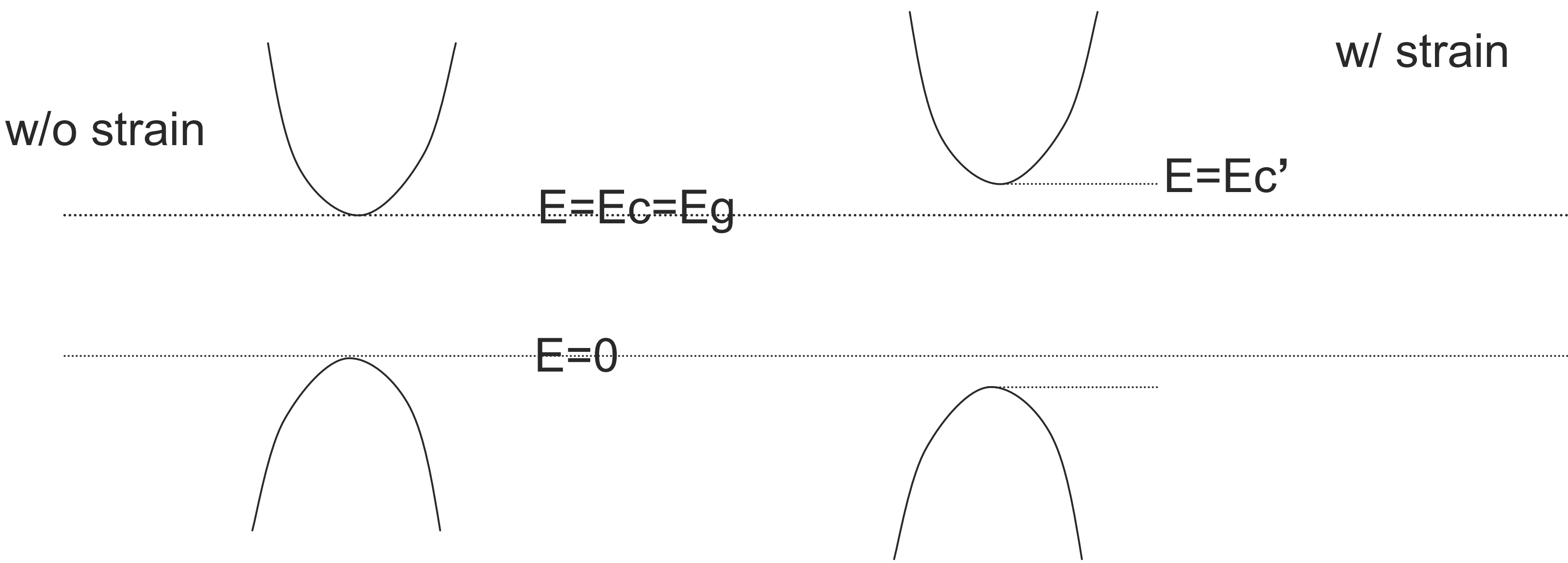


$$\tau_{zz} = C_{12}(\varepsilon_{xx} + \varepsilon_{yy}) + C_{11}\varepsilon_{zz} = 0$$

$$\varepsilon_{zz} = -\frac{2C_{12}}{C_{11}}\varepsilon_{xx}$$

1. Pikus-Bir Hamiltonian (6)

- Band structures w/o the spin-orbit split-off band coupling:
  - Set the reference level E=0 at the bulk valence band edge:



1. Pikus-Bir Hamiltonian (7)

- From the PB Hamiltonian, we know when k=0, P=Pε, Q=Qε, R=Rε

$$E_{HH}(k=0) = -(P_\varepsilon + Q_\varepsilon) = a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

$$E_{LH}(k=0) = -(P_\varepsilon - Q_\varepsilon) = a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) - \frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

$$E_C(k=0) = Eg + a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$where:$$

$$a_c = \frac{\hbar}{2m_e^*}, a_v = -\frac{\hbar\gamma_1}{2m_0}, b = -\frac{\hbar\gamma_2}{m_0}$$

1. Pikus-Bir Hamiltonian (8)

Set $a = a_c - a_v$, which is the hydrostatic deformation potential,

$$E_{C-HH}(k=0) = Eg + a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) - \frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

$$E_{C-LH}(k=0) = Eg + a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

Let's define:

$$\delta E_{hy} = -a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}),\ and$$

$$\frac{1}{2}\delta E_{sh} = Q_{\varepsilon} - \frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

So we have:

$$E_{C-HH}(k=0) = Eg - \delta E_{hy} + \frac{1}{2}\delta E_{sh}$$

$$E_{C-LH}(k=0) = Eg - \delta E_{hy} - \frac{1}{2}\delta E_{sh}$$

1. Pikus-Bir Hamiltonian (9)

- For k≠0, we have general equations:

$$\det[H_{ij}(k)-\delta_{ij}E]=0$$

$$E_{HH}(k)=-P_\varepsilon-P_k-\mathrm{sgn}(Q_\varepsilon)\sqrt{(Q_\varepsilon+Q_k)^2+|R_k|^2+|S_k|^2}$$

$$E_{LH}(k)=-P_\varepsilon-P_k+\mathrm{sgn}(Q_\varepsilon)\sqrt{(Q_\varepsilon+Q_k)^2+|R_k|^2+|S_k|^2}$$

For biaxial compression: $\Rightarrow Q_\varepsilon<0\Rightarrow \mathrm{sgn}(Q_\varepsilon)=-1$

For biaxial tension: $\Rightarrow Q_\varepsilon>0\Rightarrow \mathrm{sgn}(Q_\varepsilon)=+1$

1. Pikus-Bir Hamiltonian (10)

- By approximation for small-expansion:

$$E_{HH}(k) = -P_\varepsilon - Q_\varepsilon - \left(\frac{\hbar^2}{2m_0}\right)[(\gamma_1+\gamma_2)(k_x^2+k_y^2)+(\gamma_1-2\gamma_2)k_z^2]$$

$$E_{LH}(k) = -P_\varepsilon + Q_\varepsilon - \left(\frac{\hbar^2}{2m_0}\right)[(\gamma_1-\gamma_2)(k_x^2+k_y^2)+(\gamma_1-2\gamma_2)k_z^2]$$

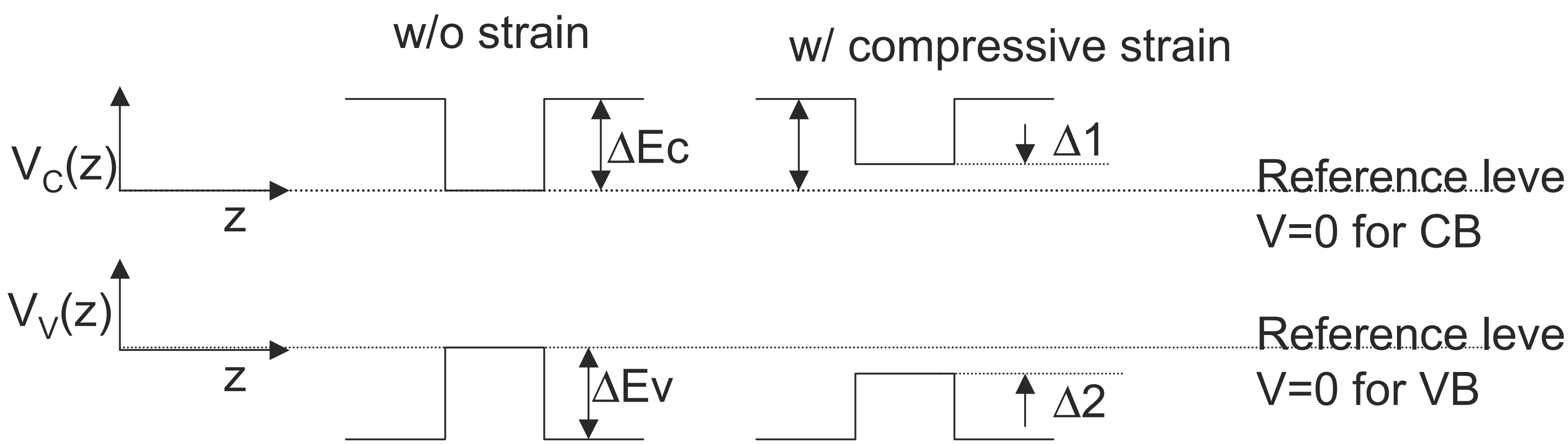
$$\frac{m_{hh}^z}{m_0} = \frac{1}{\gamma_1 - 2\gamma_2}, \frac{m_{hh}^t}{m_0} = \frac{1}{\gamma_1 + \gamma_2}$$

$$\frac{m_{lh}^z}{m_0} = \frac{1}{\gamma_1 + 2\gamma_2}, \frac{m_{lh}^t}{m_0} = \frac{1}{\gamma_1 - \gamma_2}$$

1. Pikus-Bir Hamiltonian (11)

- This Hamiltonian also introduces the *Luttinger parameters*, $\gamma 1$, $\gamma 2$, and $\gamma 3$. *They can be derived from matrix elements between various bands,*
- *But in practice are experimentally measured parameters*
- Experimental parameters improves the accuracy - corrections to these parameters through experimentally automatically accounts for any effects from other bands that are not in the theory.

2. Strained band structure for QW (1)



$$H_C = -\frac{\hbar^2}{2m_e^*}\left[k_x^2 + k_y^2 + \frac{\partial^2}{\partial z^2}\right] + V_C(z)$$

$$H_{hh} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1+\gamma_2)(k_x^2+k_y^2) - (\gamma_1 - 2\gamma_2)\frac{\partial^2}{\partial z^2}\right] + V_V(z)$$

$$H_{lh} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1-\gamma_2)(k_x^2+k_y^2) - (\gamma_1 + 2\gamma_2)\frac{\partial^2}{\partial z^2}\right] + V_V(z)$$

2. Strained band structure for QW (2)

- The Hamiltonian:

$$V_C(z) = \begin{cases} 0 & |z| \le \dfrac{L_w}{2} \\ \Delta E_c & |z| > \dfrac{L_w}{2} \end{cases}$$

$$V_V(z) = \begin{cases} 0 & |z| \le \dfrac{L_w}{2} \\ \Delta E_v & |z| > \dfrac{L_w}{2} \end{cases}$$

w/o strain

$$V_C(z) = \begin{cases} a_c(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) & |z| \le \dfrac{L_w}{2} \\ \Delta E_c & |z| > \dfrac{L_w}{2} \end{cases}$$

$$V_V(z) = \begin{cases} a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) & |z| \le \dfrac{L_w}{2} \\ \Delta E_v & |z| > \dfrac{L_w}{2} \end{cases}$$

w/ strain

3. Strained QW lasers (1)

(1) Compressive strain and tensile strain

- Compressive strain: hh is above ll
- Tensile strain: ll is above hh

↓

- Compressive strained laser: TE polarization
- above Tensile strain: TM polarization

3. Strained QW lasers (2)

(2) Advantage of strained QW lasers

- Lower Ith
- Better temperature performance
- Improved lifetime
- Higher speed

3. Strained QW lasers (3)

(3) Critical thickness:

- Lattice mismatch < 10%, otherwise, dislocation problem becomes serious and strain relaxes.
- Different materials have different critical thickness

Conclusion

- Since 1980s, as strained epitaxy has become reliable, strained semiconductor structures have been more intensively studied theoretically and have more and more applications in:
  - Semiconductor lasers
  - Microwave devices
  - Detectors

  and this trend will continue.

Reference

- Jasprit Singh, “Physics of semiconductors and their heterostructures”, MaGraw-Hill, Inc., 1993, chapter 4, 5.
- Shun Lien Chuang, “Physics of optoelectronics devices”, John Wiley & Sons, Inc., 1995, chapter 7.