# Band structures

1. k·p theory
2. Kohn-Luttinger theory
3. Effective bond-orbital model (EBOM)
4. Band structures of superlattices
5. Transfer matrix method
6. Quantum dot electronic states

HW assignment: Ch. 7, Problem 12.

# k·p theory

$$[-\frac{\hbar^2\nabla^2}{2m}+U(\mathbf{r})]\psi_{n\mathbf{k}}(\mathbf{r})=\mathcal{E}_n(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{r}),\ \psi_{nk}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$$

$$H_k u_{n\mathbf{k}}(\mathbf{r})=\mathcal{E}_n(\mathbf{k})u_{n\mathbf{k}}(\mathbf{r}),$$

$$\text{where } H_{\mathbf{k}}=\frac{\hbar^2}{2m}(-i\nabla+\mathbf{k})^2+U(\mathbf{r})=\frac{1}{2m}(p^2+2\hbar\mathbf{k}\cdot\mathbf{p}+k^2)+U(\mathbf{r})$$

$$\Rightarrow[-\frac{\hbar^2\nabla^2}{2m}+U(\mathbf{r})+\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p})]u_{n\mathbf{k}}(\mathbf{r})=[\mathcal{E}_n(k)-\frac{\hbar^2k^2}{2m}]u_{n\mathbf{k}}(\mathbf{r})$$

$$\Rightarrow[H_0+\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p})]u_{n\mathbf{k}}(\mathbf{r})=\mathcal{E'}_n(\mathbf{k})u_{n\mathbf{k}}(\mathbf{r})$$

$\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p})$ is treated as a perturbation.

⋆ Zeroth-order solutions are: $u_{no}(r)$ with energies $\mathcal{E}_n(0)$.

$$\text{Expansion: } u_{n\mathbf{k}}(\mathbf{r})=\sum_{n'}C^n_{n'}(\mathbf{k})u_{n'o}(\mathbf{r})$$

$$\Rightarrow\sum_{n'}\{[\mathcal{E}_n(0)-\mathcal{E}'_n(\mathbf{k})]\delta_{nn'}+<u_{no}|\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p})|u_{n'o}>\}C^n_{n'}(\mathbf{k})=0.$$

# Full zone k·p theory

[Cardona & Pollak, Phys. Rev. **142** ,530 (1966)]

Keep sufficiently large number of $u_{no}$ [ e.g. lowest 15 states corresponding to $k = (000)$, 8(111)'s, and 6(200)'s].

• Comments:

Solutions obtained are good for **k** throughtout the entire Brillouin zone.

Matrix elements $< u_{n0}|\mathbf{p}|u_{n0} >$ can be computed from pseudopotential method or taken from experimental data (cyclotron resonance).

When the group theory (symmetry) is used, only the independent matrix elements need to be determined for covalent material (Si,Ge,$\alpha$-Sn,etc.).

For III-V materials, one needs additional six parameters. The band structures do not have correct periodicity (not valid in repeated zone scheme)

Most accurate near the zone center, predicting best effective masses among all the models. Near the zone-center, band structures can be calculated by second-order perturbation theory.

[ E. O. Kane, J. Phys. Chem. Sol. 1, (1960)]:

A. Non-degenerate case: [e.g. conduction band of most semiconductors (s-like band)]

$$E_n(\mathbf{k}) = E_n(0) + \frac{\hbar^2 k^2}{2m} + < u_{n0}|\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p})|u_{n0} > + \sum_{n'\neq n} \frac{|< u_{n0}|\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}|u_{n'0}>|^2}{E_n(0) - E_{n'}(0)}$$

[ NOTE: $< u_{n0}|\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}|u_{n0} >= 0$ by symmetry]

$$= E_n(0) + \frac{\hbar^2 k^2}{2}\sum_{ij}(1/m^*)_{ij}k_i k_j$$

$$\text{where } (\frac{1}{m^*})_{ij} = \frac{1}{m}\delta_{ij} + \frac{1}{m^2}\sum_{n'\neq n}\frac{p_i^{n,n'}p_j^{n,n'} + p_j^{n,n'}p_i^{n,n'}}{E_n(0) - E_{n'}(0)}$$

is called the effective-mass tensor.

$$p_i^{n,n'} \equiv < u_{n0}|p_i|u_{n'0} > .$$

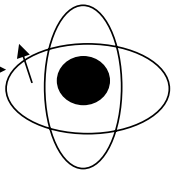
For cublic crystals (including sc, bcc, fcc, diamond, and zincblende), we have

$$E_n(\mathbf{k}) = E_n(0) + \frac{\hbar^2 k^2}{2m^*}.$$

Here the effective mass tensor is reduced to a scalar.

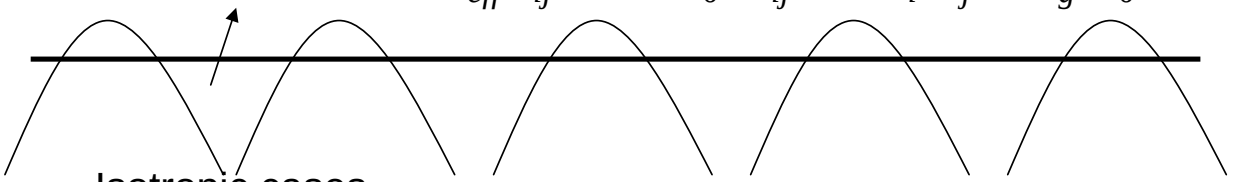
# Meaning of the effective mass

- Bare electron mass $m_0$



- Effective mass

$$(1/m_{eff})_{ij} = 1/m_0(\delta_{ij} \pm 2p_i p_j/(E_g m_0))$$



Isotropic cases

- For electrons in conduction band +
- For electrons in valence band –
- Effective mass can be measured by cycltron resonance experiment

$$(m_{c,v})_{eff} = \frac{m_0}{1 \pm \frac{2 < c \mid p \mid v >^2}{m_0 E_g}}$$

# Band with degenerated states

- Isolated atom Si $3s^2 3p^2$
- Semiconductor $3sp^3$
- In the presence of spin – orbital interaction only the total angular
- Momentum,i.e. the sum of the orbital and spin angular momentum,
- is a conserved quantity.

$$[H=\frac{p^2}{2m_0}+V_0(r)+\frac{\hbar}{4m_0^2c^2}\sigma\cdot\nabla V(r)\times\vec{p}]\psi_b(k,r)=E_b(k)\psi_b(k,r)$$

$$\{\frac{p^2}{2m_0}+V(r)+\frac{\hbar}{m_0}\vec{k}\cdot\vec{p}+\frac{\hbar}{4m_0^2c^2}[\nabla V(r)\times(\vec{p}+\vec{k})]\cdot\sigma\}u_b(k,r)=$$

$$(E_b(k)-\hbar^2k^2/2m_0)u_b(k,r)$$ ← Time reversal symmetry

B. Degenerate case: [e.g. valence bands of semiconudctors]

Let $|u_\nu(0)>$ denote the J-fold degenerate states at the zone center ($\Gamma$ point). Ignore the interactions among $|u_\nu(0)>$'s first. The first-order correction to the perturbed state due coupling to other states is given by

$$|u_\nu(\mathbf{k})>=|u_\nu(0)>+\sum_{n'\neq J}\frac{<u_\nu(0)|\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}|u_{n'}(0)>}{E_\nu(0)-E_{n'}(0)}|u_{n'}(0)>.$$

Thus, the first-order correction to the energy for states $|u_\nu>$'s are given by diagonalizing the perturbed matrix within the J-fold basis (degenerate perturbation theory)

$$H^{(1)}_{\nu,\nu'}\equiv E_\nu(0)\delta_{\nu,\nu'}+\sum_{n'\neq J}\frac{<u_\nu(0)|\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}|u_{n'}(0)><u_{n'}(0)|\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}|u_{\nu'}(0)>}{E_\nu(0)-E_{n'}(0)}.$$

For cubic crystals with $p$-like valence bands (e.g. Si, Ge, GaAs, InAs,...), we have

$$H^{(1)}=\begin{pmatrix} Ak_x^2+B(k_y^2+k_z^2) & Ck_xk_y & Ck_xk_z \\ - & Ak_y^2+B(k_x^2+k_z^2) & Ck_xk_z \\ - & - & Ak_z^2+B(k_y^2+k_x^2) \end{pmatrix},$$

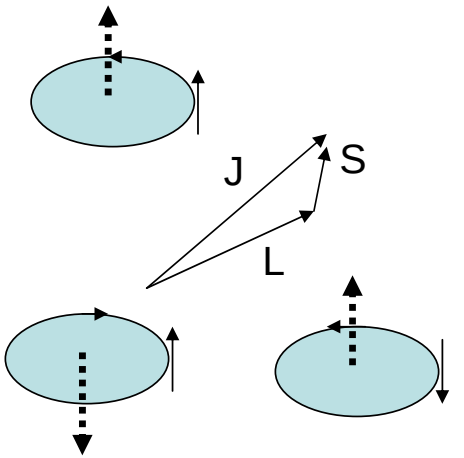
where $A, B, C$ are three band parameters, which are determined experimentally (typically via cyclotron resonance measurements).

# Valence bands with spin-orbit interaction

- J=3/2

$$|3/2,\pm 3/2>=|m_L=\pm 1,\left[\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right]>$$

$$|3/2,\pm 1/2>=\frac{1}{\sqrt{3}}[\sqrt{2}\,|m_L=0,\left[\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right]>+|m_L=\pm 1,\left[\begin{matrix}\downarrow\\ \uparrow\end{matrix}\right]>]$$

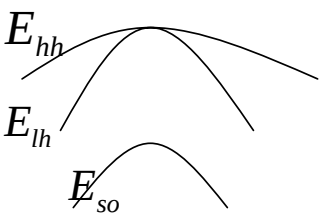



- J=1/2

$$|1/2,\pm 1/2>=\frac{1}{\sqrt{3}}[-|m_L=0,\left[\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right]>+\sqrt{2}\,|m_L=\pm 1,\left[\begin{matrix}\downarrow\\ \uparrow\end{matrix}\right]>]$$


Kane's model ×

Luttinger-Kohn's model ✓



The valence bands become 6-fold, since $J = 1 \oplus 1/2 = 1/2, 3/2$. The top four valence bands are given by $|3/2, 3/2 >= -\frac{1}{\sqrt{2}}(|x > +i|y >) \uparrow, |3/2, 1/2 >= -\frac{1}{\sqrt{6}}(|x > +i|y >) \downarrow -2|z >\uparrow$, $|3/2, -1/2 >= \frac{1}{\sqrt{6}}(|x > -i|y >) \uparrow +2|z >\downarrow$ ,$|3/2, -3/2 >= \frac{1}{\sqrt{2}}(|x > -i|y >) \downarrow$.

$$H^{(off)} = \frac{\hbar^2}{2m} \begin{pmatrix} A_+ & L & M & 0 \\ L^* & A_- & 0 & M \\ M^* & 0 & A_- & -L \\ 0 & M^* & -L^* & A_+ \end{pmatrix},$$

where

$$A_\pm \equiv (\gamma_1 \pm \gamma_2)(k_x^2 + k_y^2) + (\gamma_1 \mp 2\gamma_2)k_z^2,$$

$$L = -2i\sqrt{3}\gamma_3 K^- k_z,$$

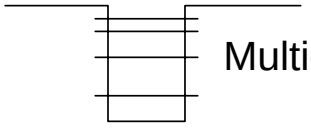
$$M = -\sqrt{3}\bar{\gamma} K^{-2} + (\gamma_2 - \gamma_3)k_x k_y$$

$$K^\pm \equiv (k_x \pm i k_y),$$

$\gamma_1, \gamma_2, \gamma_3$ are called "Luttinger parameters" and they are related to $A, B, C$ by $\gamma_1 = \frac{1}{3}(A + B), \gamma_2 = \frac{1}{6}(A - B)$, and $\gamma_3 = \frac{1}{6}C$.

# Degenerate Valence Bands

- Quantum well

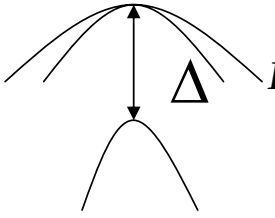


Multi-subbands

- For valence band

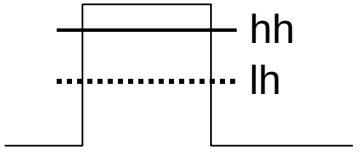
| $Semi$ | $\Delta(eV)$ |
|---|---|
| $Si$ | 0.044 |
| $Ge$ | 0.29 |
| $GaAs$ | 0.35 |
| $InAs$ | 0.41 |
| $InSb$ | 0.82 |
| $InP$ | 0.14 |
| $GaP$ | 0.094 |

Bulk




$$E_{hh}(k_z) = \frac{-\hbar^2}{2m_0}(\gamma_1 - 2\gamma_2)k_z^2 = \frac{\hbar^2}{2m_{hh}^z}k_z^2$$

$$E_{lh}(k_z) = \frac{-\hbar^2}{2m_0}(\gamma_1 + 2\gamma_2)k_z^2 = \frac{\hbar^2}{2m_{lh}^z}k_z^2$$

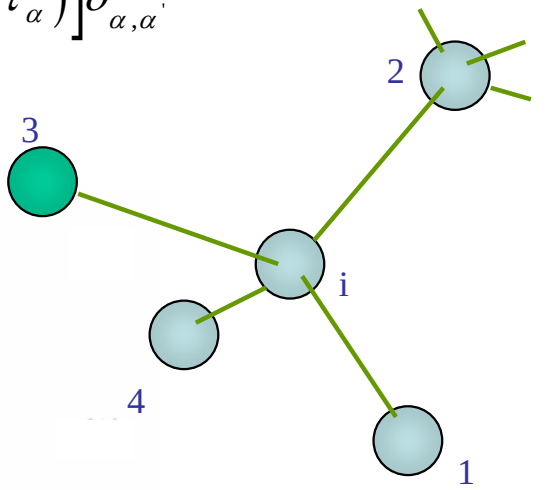



$$[\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_m^z}\frac{\partial}{\partial z} + V(z)]\varsigma_m(z) = E\varsigma_m(z); \quad m = hh, lh$$

# Effective bond-orbital Model
## [Y.C.Chang, PRB 37, 8215 (1988)]

$$H_{\alpha,\alpha'}(\vec{k}) = E_p \delta_{\alpha,\alpha'} +$$

$$\sum_{\tau} e^{i\vec{k}\cdot\vec{\tau}} \left\{ E_{xy}\tau_\alpha \tau_{\alpha'} + \left[ \left( E_{xx} - E_{xy} \right) \tau_\alpha^2 + E_{zz}\left(1 - \tau_\alpha^2\right) \right] \delta_{\alpha,\alpha'} \right.$$




$$\langle \mathbf{R},s \mid H \mid \mathbf{R}',s \rangle = E_s \delta_{\mathbf{R}',\mathbf{R}} + E_{ss} \delta_{\mathbf{R}'-\mathbf{R},\tau}$$

and

$$\langle \mathbf{R},s \mid H \mid \mathbf{R},\alpha \rangle = E_{sx} \delta_{\mathbf{R}'-\mathbf{R},\tau} \tau_\alpha \ ,$$

where $|\mathbf{R},s\rangle$ denote an $s$-like orbital located at $\mathbf{R}$. Taking the Taylor expansion over $\mathbf{k}$ and omitting terms higher than the second order in $\mathbf{k}$, we obtain the Hamiltonian in the $sp^3$ basis

Taking the Taylor expansion over **k** and omitting terms higher than the second order, we obtain

$$H(\mathbf{k})=\begin{vmatrix} E_v-\lambda_1 k_x^2-\lambda_2 k^2 & -\lambda_3 k_x k_y & -\lambda_3 k_x k_z \\ -\lambda_3 k_x k_y & E_v-\lambda_1 k_y^2-\lambda_2 k^2 & -\lambda_3 k_y k_z \\ -\lambda_3 k_x k_z & -\lambda_3 k_y k_z & E_v-\lambda_1 k_z^2-\lambda_2 k^2 \end{vmatrix} ,$$

where

$$\begin{aligned} E_v &= E_p + 8E_{xx} \ , \\ \lambda_1 &= (E_{zz}-E_{xx})a^2/2 \ , \\ \lambda_2 &= (3E_{xx}-E_{zz})a^2/2 \ , \\ \lambda_3 &= E_{xy}a^2 \ . \end{aligned} \tag{3'}$$

Comparing $H(\mathbf{k})$ with the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for the valence bands, we have

$$(L-M)=\lambda_1, \ M=\lambda_2, \ N=\lambda_3 \ , \tag{4}$$

where $L$, $M$, and $N$ are $\mathbf{k}\cdot\mathbf{p}$ band parameters defined as A, B, C.

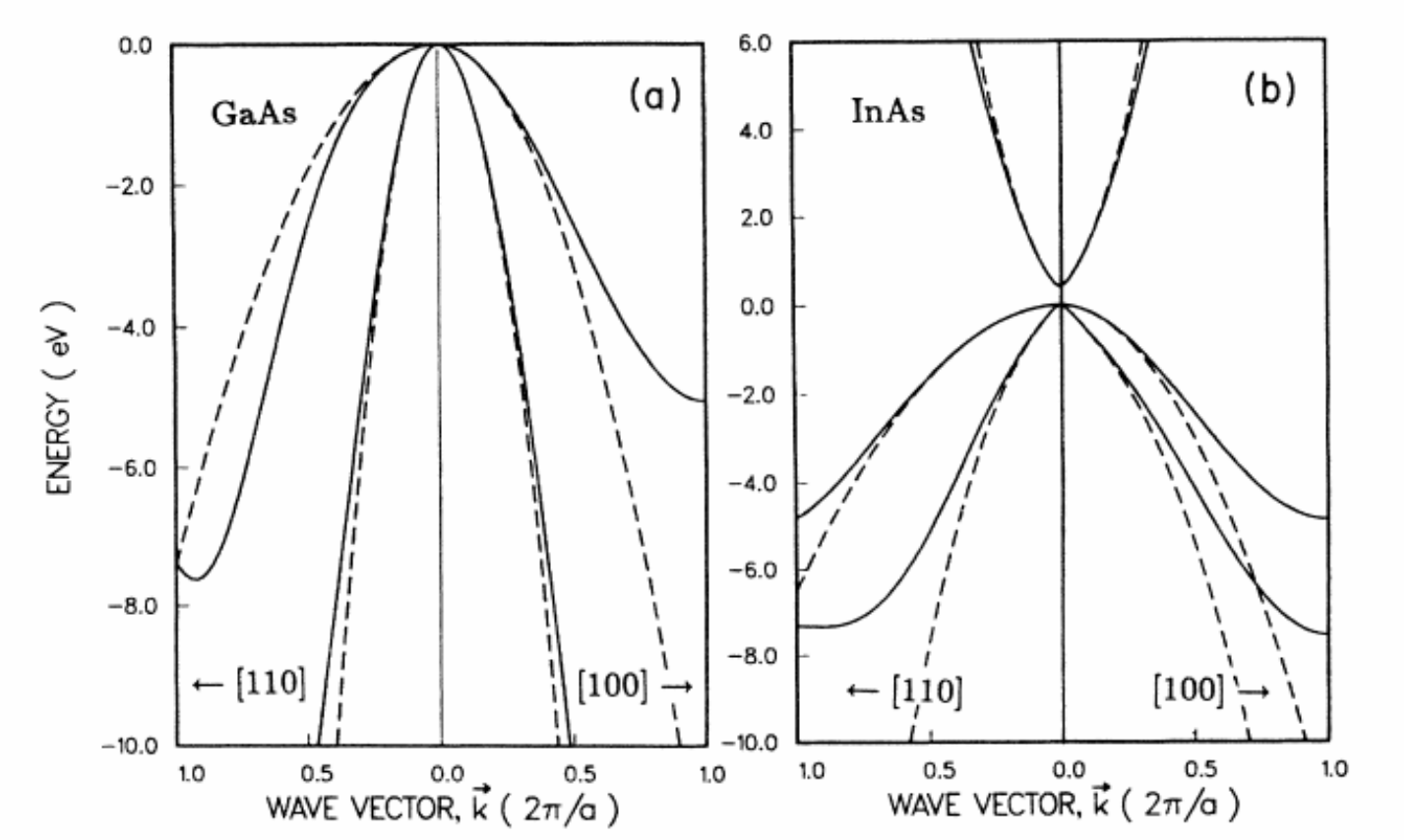
# Tayler expansion up to $k^2$

$$H(\mathbf{k}) = \begin{pmatrix} E_c - E_{ss}a^2k^2 & i4E_{sx}ak_z & i4E_{sx}ak_y & i4E_{sx}ak_z \\ -i4E_{sx}ak_x & E_v - \lambda_1 k_x^2 - \lambda_2 k^2 & -\lambda_3 k_x k_y & -\lambda_3 k_x k_z \\ -i4E_{sx}ak_y & -\lambda_3 k_x k_y & E_v - \lambda_1 k_y^2 - \lambda_2 k^2 & -\lambda_3 k_y k_z \\ -i4E_{sx}ak_z & -\lambda_3 k_x k_z & -\lambda_3 k_y k_z & E_v - \lambda_1 k_z^2 - \lambda_2 k^2 \end{pmatrix}$$

TABLE II. Relations between bond-orbital parameters and $\mathbf{k}\cdot\mathbf{p}$ parameters. $R_0=\hbar^2/2m_0a^2$, $X_{hl}=4$ eV.

| VBM | CVBM |
|---|---|
| | $E_{sx}^2=E_g(12\gamma_2R_0-X_{hl}/8)/32$ |
| $E_{xy}=6\gamma_3R_0$ | $E_{xy}=6\gamma_3R_0-16E_{sx}^2/E_g$ |
| $E_{xx}=(\gamma_1+4\gamma_2)R_0$ | $E_{xx}=\gamma_1R_0-16E_{sx}^2/(3E_g)+X_{hl}/24$ |
| $E_{zz}=(\gamma_1-8\gamma_2)R_0$ | $E_{zz}=E_{xx}+X_{hl}/8$ |
| $E_p=E_v-12\gamma_1R_0$ | $E_p=E_v-12E_{xx}+X_{hl}/2$ |
| | $E_{ss}=-\frac{m_0}{m_c}R_0+64E_{sx}^2\left[\frac{2}{E_g}+\frac{1}{E_g+\Delta}\right]/3$ |

# Band structures obtained with EBOM versus k.p method



# Band structures of superlattices

• General Considerations:

a. A superlattice consists of two (or more) kinds of bulk materials [e.g. GaAs-AlAs superlattice], stacked in layers along a given directions (called growth direction)

b. A superlattice has well-defined unit cell and periodicity e.g. a unit cell of $(M, N)$ GaAs AlAs superlattice.

periodicity $= (M + N)a' = d$ in the growth direction $(z)$ and $a'$ in the $x, y$ directions.

c. Electronic States can be labelled by crystal wave vectors $\mathbf{k} = (\mathbf{k}_{\|}, q)$ [cf: $\mathbf{k} = (\mathbf{k}_{\|}, k_z)$ for bulk]

d. Bloch states of the superlattice are denoted by $\psi_{n\mathbf{k}}(\mathbf{r})$, where $n =$ band index, $\mathbf{k} = (\mathbf{k}_{\|}, q)$.

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}) \quad \text{... Bloch theorem,}$$

where $\mathbf{R}$ is any lattice vector of the superlattice. Let $\mathbf{R} = d\hat{z}$ (along the growth direction then $\psi_{n\mathbf{k}}(\mathbf{r} + d\hat{z}) = e^{iqd}\psi_{n\mathbf{k}}(\mathbf{r})$.

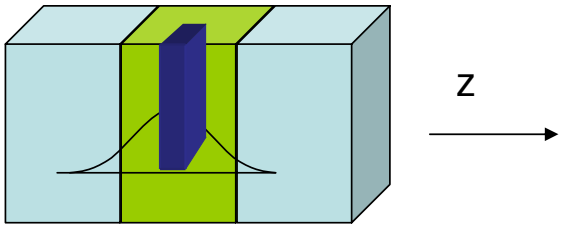
e. Concept of zone-folding (e.g. $d = 4a'$).

# Envelope Function Approximation

(Single electron picture)

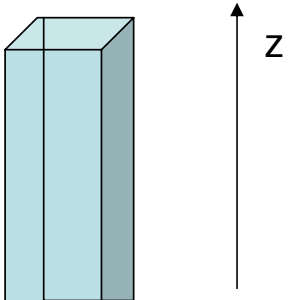
- Quantum wells

$$\psi(r) = \varsigma_n(z) e^{i(k_x x + k_y y)} u_b(k \approx 0, r)$$




- Quantum wires

$$\psi(r) = \varsigma_n(x)\varsigma(y) e^{ik_z z} u_b(k \approx 0, r)$$

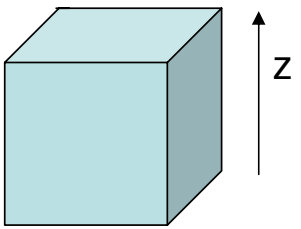



- Quantum dots

$$\psi(r) = \varsigma_n(x)\varsigma_m(y)\varsigma_p(z) u_b(k \approx 0, r)$$

$$\downarrow$$

$$\varsigma_{n,m,l}(x, y, z)$$



• Envelope-function Approach: (Ideal for flat-band superlattices)

Procedures:

a. Find general solutions to the Shrodinger equation in each flat-band region

$$H^{(\sigma)}\psi = E\psi; \sigma = A \text{ or } B.$$

Note: $H^{(\sigma)}$ in each region is the same as in bulk material $\sigma$, apart from a constant shift in energy (V). The solution is known for each quantum number, $\mathbf{k}$

$$H^{(\sigma)}\phi^{(\sigma)}_{\mathbf{k}} = E^{(\sigma)}(\mathbf{k})\phi^{(\sigma)}_{\mathbf{k}}, \mathbf{k} = (\mathbf{k}_{\parallel}, q).$$

For each fixed energy, $E$ and in-plane wave vector, $\mathbf{k}_{\parallel}$, there are finite number of solutions (in general copmlex) for $k_z$, which satisfy

$$E = E^{(\sigma)}(\mathbf{k}_{\parallel}, k_z) + V_{\sigma}, k_z = \text{ complex},$$

$V_{\sigma}$ is called the band offset for material $\sigma$ . The solution can be depicted as the "complex band structure" One can use different theoretical methods to describe the complex band structure, e.g., tight-binding or $\mathbf{k}\cdot\mathbf{p}$ methods.[Y. C. Chang and J. N. Schulman, Phys. Rev. B25, 3975-86 (1982)]

The description must be accurate near the energy of interest. For most applications, the energy of interest is near the conduction-band minimum or valence-band maximum of the smaller-gap material. So, the $\mathbf{k}\cdot\mathbf{p}$ approach is adequate. If the tight-binding method is used, the interaction parameters must be selected so that the band structure is accurate near band extrema ( or $\mathbf{k}=0$ for direct semiconductors). The number of complex $k_z$ solutions depends on which method is used.

Example: $\mathbf{k}\cdot\mathbf{p}$(effective-mass) method for conduction band

$$E^{(\sigma)}(\mathbf{k}) = \frac{\hbar^2}{2m_\sigma^*}k^2 = \frac{\hbar^2}{2m_\sigma^*}(k_\parallel^2 + k_z^2).$$

To find complex roots, let

$$E - V_\sigma = \frac{\hbar^2}{2m\sigma*}(k_\parallel^2 + k_z^2).$$

So, $k_z = \pm\sqrt{2m_\sigma^*(E-V_\sigma)/\hbar^2 - k_\parallel^2}$.

Denote the complex $k_z$ roots by $k_i^{(\sigma)}$, $i = 1, ..., p$ and the corresponding Bloch states by $\phi_{\mathbf{k}_\parallel,i}^{(\sigma)}$, then

$$\psi = \sum_{i=1}^{p} A_i^{(\sigma)}\phi_{\mathbf{k}_\parallel,i}^{(\sigma)} \quad \text{in each region } \sigma,$$

where $A_i^{(\sigma)}$ are coefficients to be determined by matching boundary conditions.

$\star$ Example: In the effective-mass approximation

$$k_z^{(\sigma)} = \pm\sqrt{2m_\sigma^*(E - V_\sigma)}/\hbar \text{ (assume } k_\parallel = 0) \equiv \pm k_\sigma;\ \sigma = A, B.$$

$$\text{So, } \psi = \begin{cases} A_1^{(A)}\psi_{k_A} + A_2^{(A)}\psi_{-k_A} & \text{in region A} \\ A_1^{(B)}\psi_{k_B} + A_2^{(B)}\psi_{-k_B} & \text{in region B} \end{cases}$$

Note: $\phi_{k_z}^{(\sigma)} = e^{ik_z^{(\sigma)}z}u_0^{(\sigma)}$ ... periodic part.

$$\text{Then, } \psi = \begin{cases} (A_1^{(A)}e^{ik_Az} + A_2^{(A)}e^{-ik_Az})u_0^{(A)} = F_A(z)u_0^{(A)} & \text{in region A} \\ (A_1^{(B)}e^{ik_Bz} + A_2^{(B)}e^{-ik_Bz})u_0^{(A)} = F_B(z)u_0^{(B)} & \text{in region B} \end{cases}$$

$F_A(z)$ and $F_B(z)$ are called envelope functions. For convenience, rewrite

$$F_A(z) = A_1\cos k_Az + A_2\sin k_Az,\ F_B(z) = B_1\cos k_B(z - l_A) + B_2\sin k_B(z - l_A).$$

b. Find relations between coefficients $\{A_i^{(\sigma)}\}$ through boundary conditions (B.C.):

(i) Effective-mass theory:

B.C. for $\psi$: both $\psi$ and $\partial_z\psi$ continuous

B.C. for $F$: Both $F(z)$ and $\frac{1}{m*(z)}\partial_z F(z)$ continuous.

Two boundary conditions give rise to a $2\times 2$ matrix equation

$$\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = t_{BA} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$$

for interface 1.

⋆ Exercise: Show that

$$t_{BA} = \begin{pmatrix} \cos k_A l_A & \sin k_A l_a \\ -\xi \sin k_A l_A & -\xi \cos k_A l_A \end{pmatrix}, \ \xi = (\frac{k_A}{k_B})(\frac{m_B^*}{m_A^*}).$$

Similarly, $e^{iqd}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = t_{AB}\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = t_{AB}t_{BA}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$

$T = (t_{AB})(t_{BA})$ is called the "transfer matrix". It has two eigenvalues $e^{\pm iqd}$. Thus, we have

$$Tr(T) = 2\cos qd = 2\cos k_A l_A \cos k_B l_B - (\xi + \xi^{-1})\sin k_A l_A \sin k_B l_B.$$

# Local orbital basis

- Transfer matrix approach (applicable for any superlattice)

Example: sawtooth superlattice.

Using tight-binding method, we write superlattice Bloch states as

$$\psi_{\mathbf{k}} = \sum_{L} e^{iqLd} \sum_{l\alpha} F_{\alpha}(l) |\mathbf{k}_{\parallel}; la' + Ld; \alpha > \quad [l = 1, ..., N]$$

$$0 = (H - E)\psi_{\mathbf{k}} = \sum_{L} e^{iqLd} \sum_{l\alpha} F_{\alpha}(l)(H - E)|\mathbf{k}_{\parallel}; la' + Ld; \alpha > .$$

Multiplying $< l; a'|$ from the left gives

$$\sum_{\alpha} \{F_{\alpha}(l+1) < l; \alpha'|H|l+1; \alpha > + < l; \alpha'|H - E|l; \alpha > F_{\alpha}(l) + < l; \alpha'|H|l-1; \alpha > F_{\alpha}(l-1) >= 0$$

$$\Rightarrow F(l+1) = -[H^{(+)}(l)]^{-1}[H^{(0)}(l)F(l) + H^{(-)}(l)F(l-1)],$$

where $H^{(\pm)}_{\alpha'\alpha}(l) =< l; \alpha'|H|l\pm; \alpha >$, and $H^{(0)}_{\alpha'\alpha}(l) =< l; \alpha'|H|l\alpha > -E\delta_{\alpha\alpha'}$

$$\Rightarrow \begin{pmatrix} F(l+1) \\ F(l) \end{pmatrix} = t(l) \begin{pmatrix} F(l) \\ F(l-1), \end{pmatrix}$$

where $t(l) = \begin{pmatrix} -[H^{(+)}(l)]^{-1} H^{(0)}(l) & -[H^{(+)}(l)]^{-1} H^{(-)}(l) \\ 1 & 0 \end{pmatrix}$.

Repeat $N$ times...

$$\Rightarrow \begin{pmatrix} F(N+1) \\ F(N) \end{pmatrix} = T_N \begin{pmatrix} F(1) \\ F(0) \end{pmatrix} = e^{iqd} \begin{pmatrix} F(1) \\ F(0) \end{pmatrix},$$

where $T_N = t(N)t(N-1)\cdots t(2)t(1)$.

Solve $|TN(E) - e^{iqd}1| = 0$ for $E(q)$.

# Superlattice bands obtained with EBOM

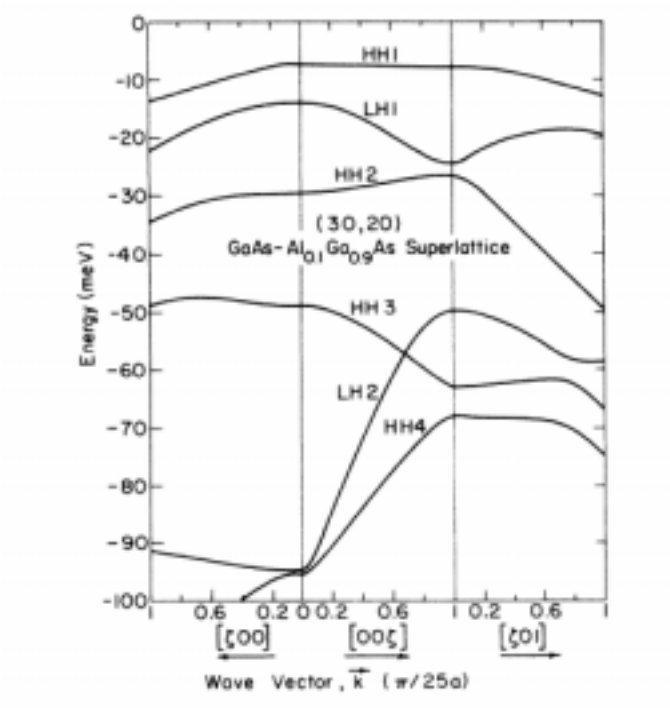



FIG. 2. Valence-subband structures of a (30,20) GaAs-$Al_{0.1}Ga_{0.9}As$ superlattice obtained in the VBM.

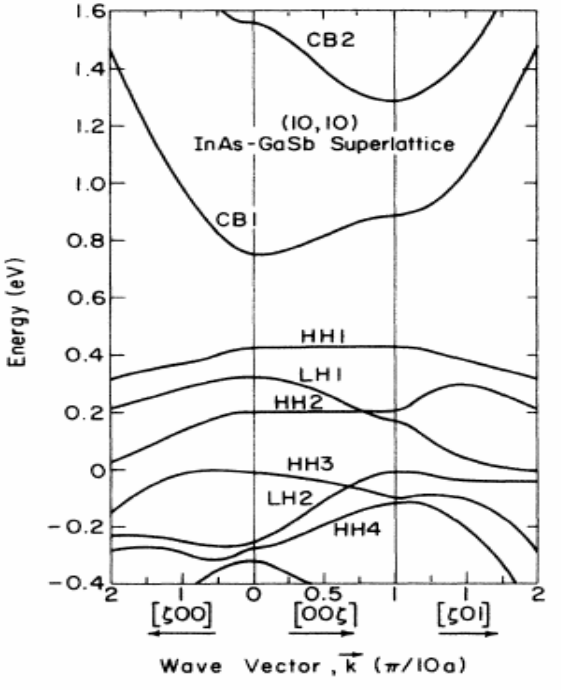
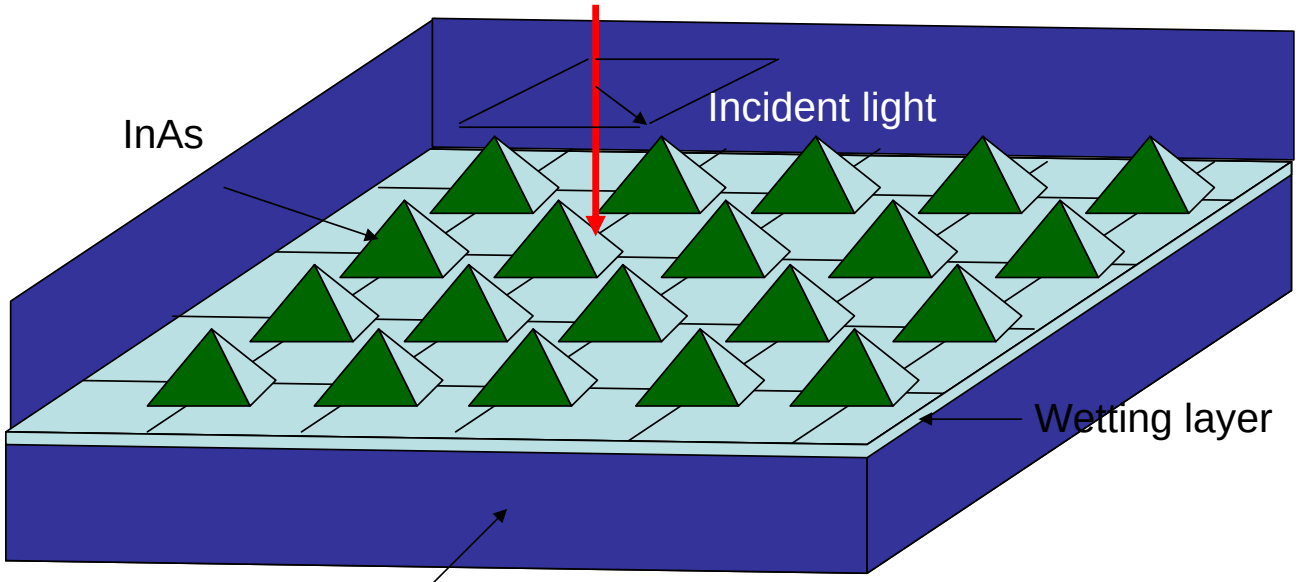



FIG. 3. Subband structures of a (10,10) InAs-GaSb superlattice obtained in the CVBM.

# Self assembled quantum dots




Lattice mismatch 7%

Infrared detector
Laser

Area density

$10^{11} / cm^2$

# Physical effects in QD

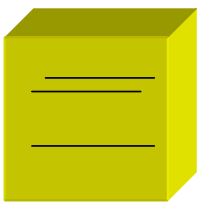
Quantum confinement (size effect)

Selection rule (light polarization)

Discrete energy levels (0-d density of states)

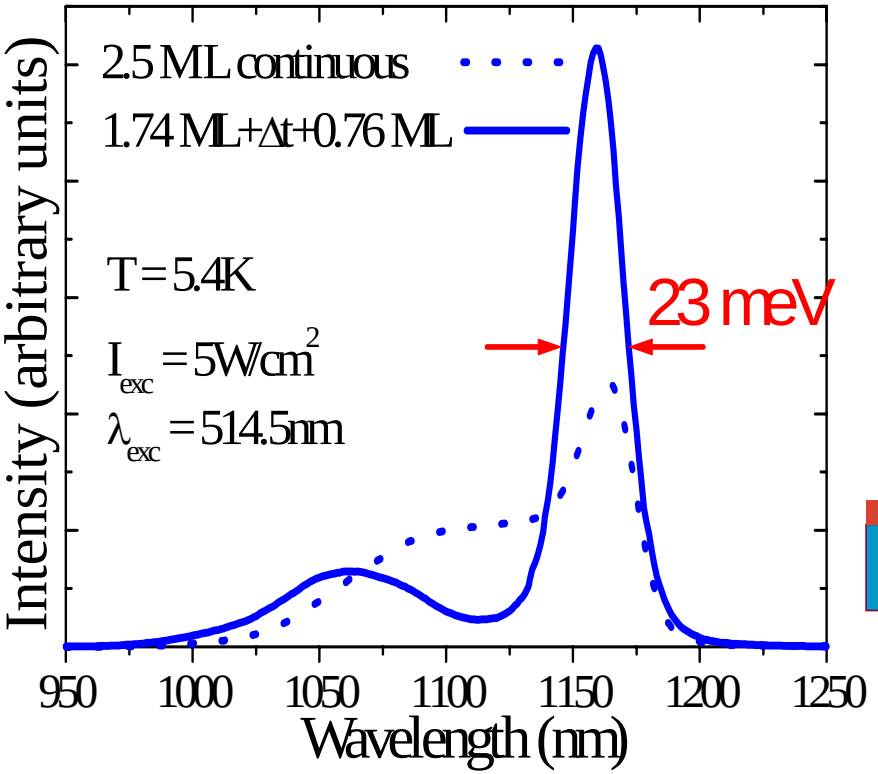
Strong Coulomb interaction (Coulomb blockade)

Strong electron correlation (many-body effect)

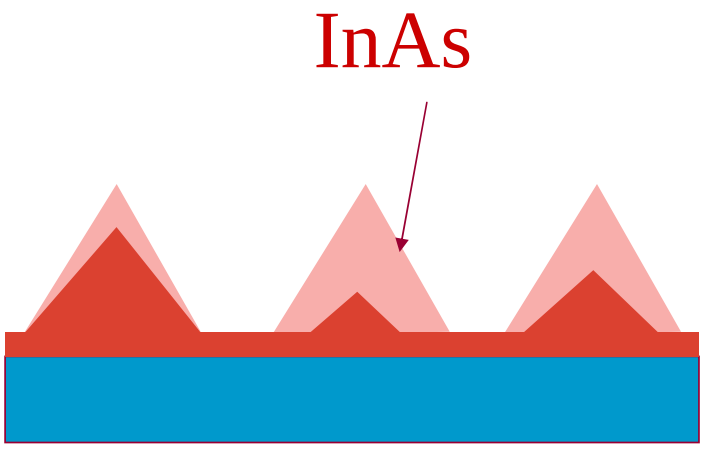


Artificial atom

# PL of InAs/GaAs self-assembled QDs




Stranski-Krastanov growth

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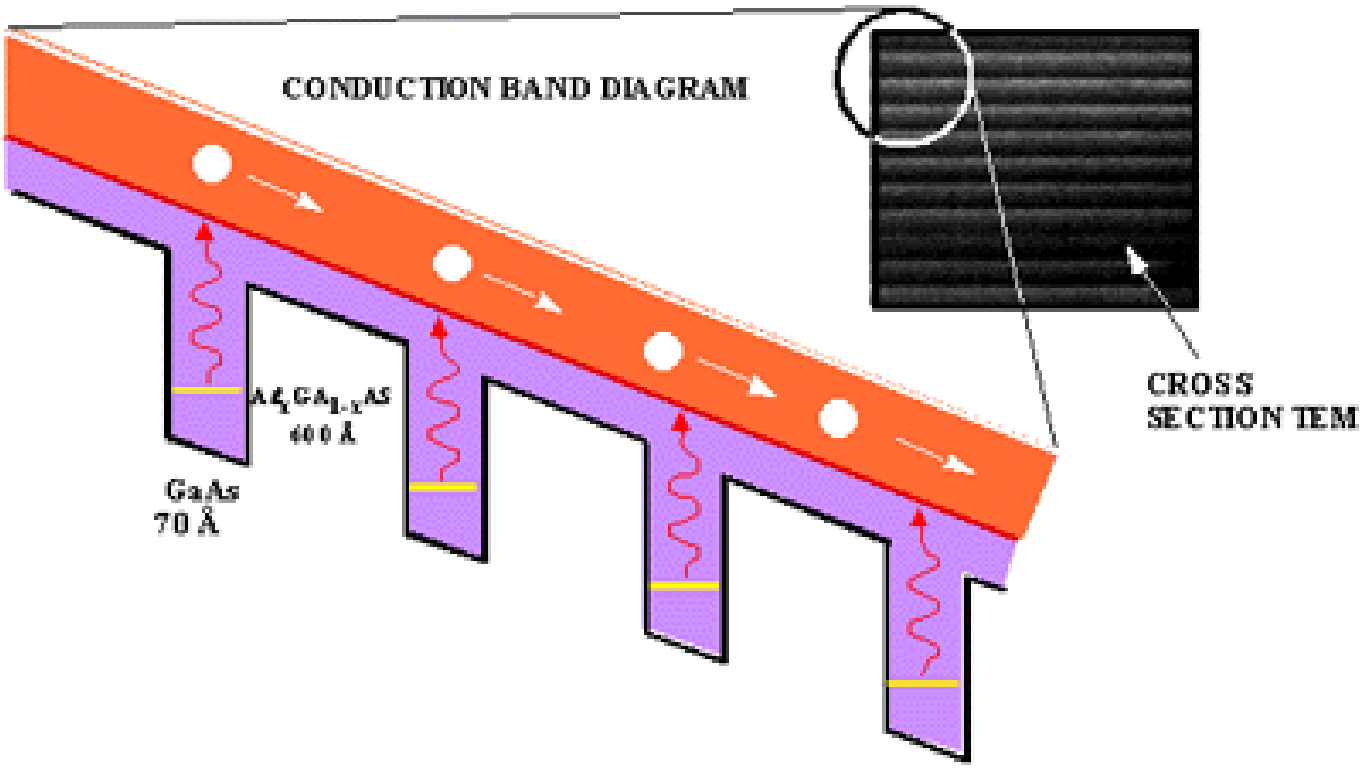
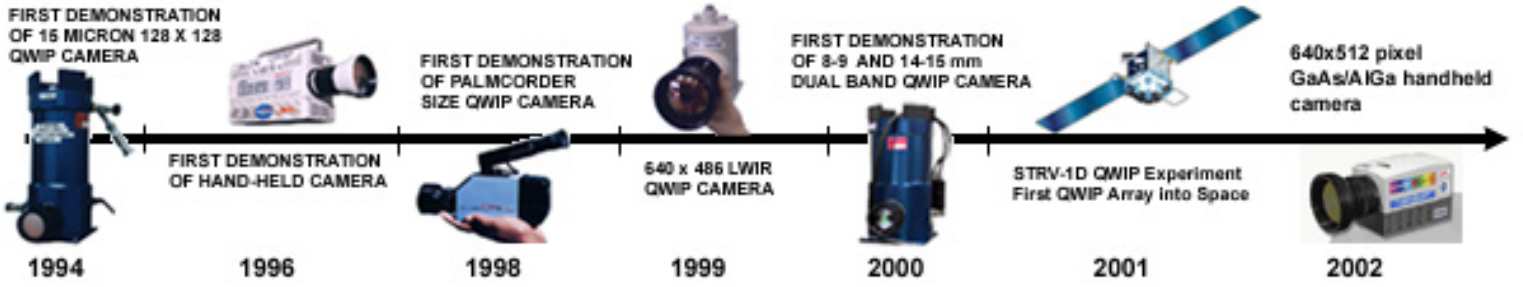
# 量子井紅外線偵測器(QWIP)

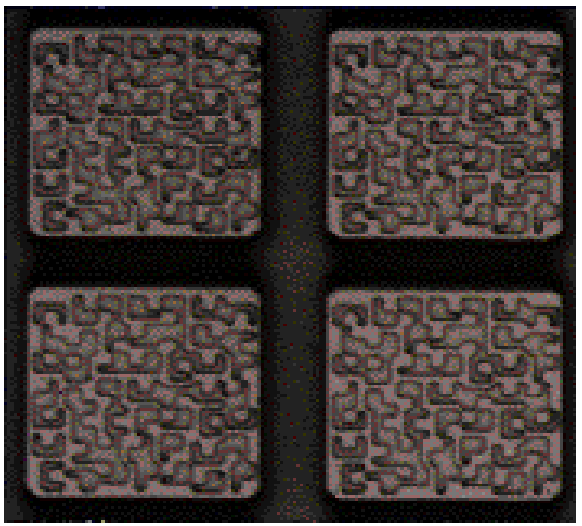



http://qwip.jpl.nasa.gov/tutorial.html

# 紅外線偵測器 (Infrared detector)

# 量子井紅外線偵測器 (QWIP)

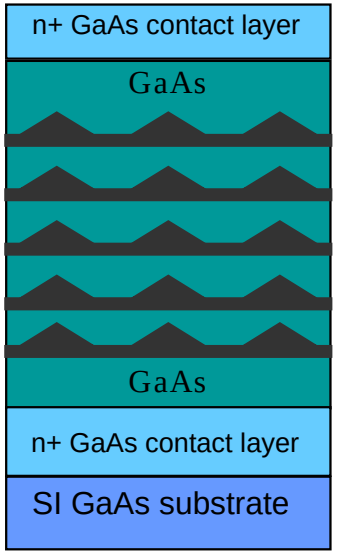


http://qwip.jpl.nasa.gov/tutorial.html

# Schematics of QDIP test structures

[Z. Chen and A. Madhukar (USC)]

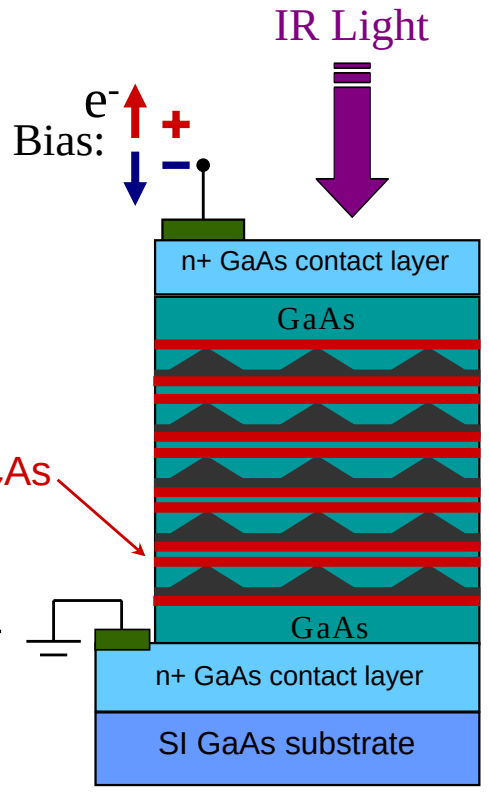


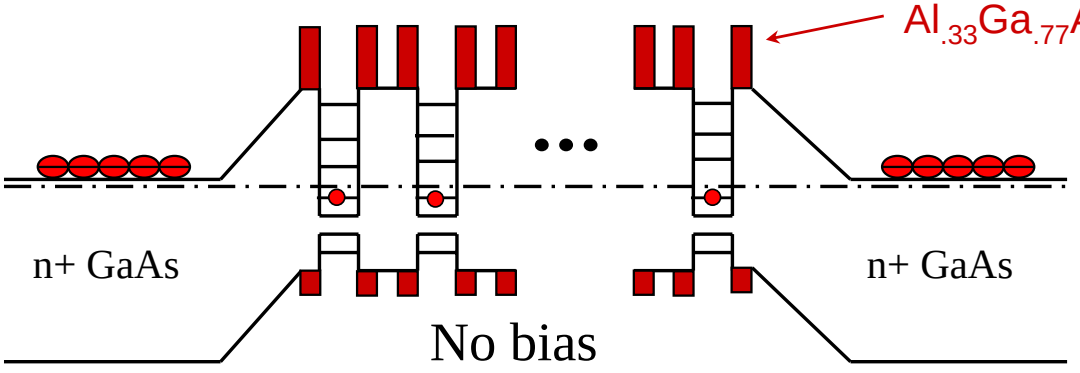

*Doping: Balance between PC & Dark Current*

*n-i(MQD)-n*

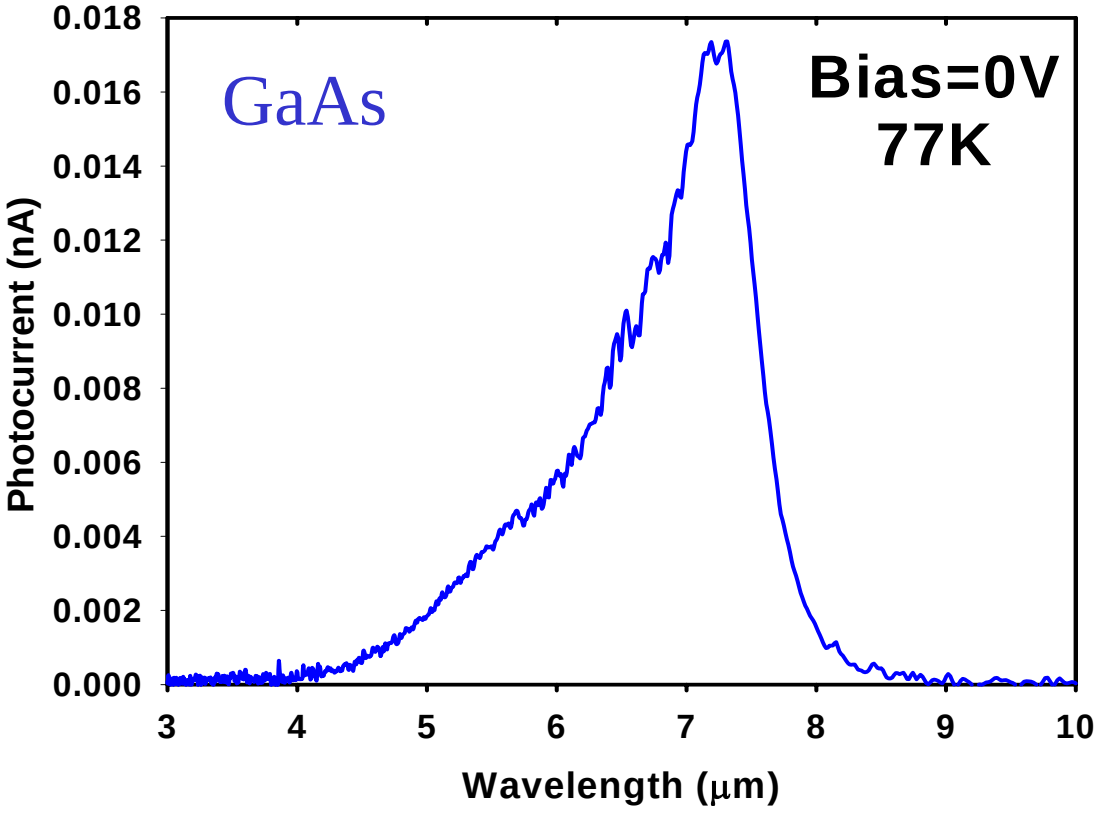
*n-n(MQD)-n*

5 layers of
PIG 3ML InAs QDs:
(2ML + Δt + 1ML)
with 150ML GaAs/AlGaAs spacers



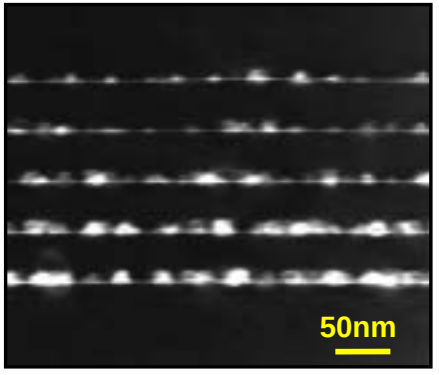
# Photovoltaic Effect




- Photovoltaic Effect is due to asymmetric potential of QDs
- Potential for normal-incidence photovoltaic MIR Photodetector

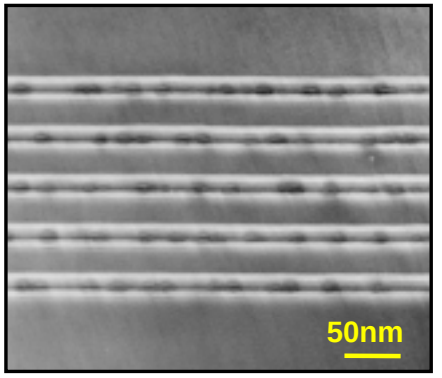
# Optical and Structural Characterization of QDIPs

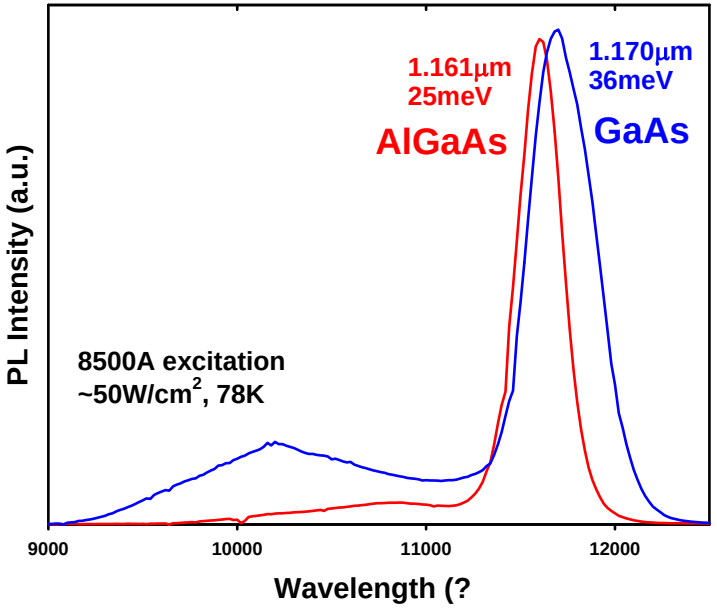
TEM GaAs

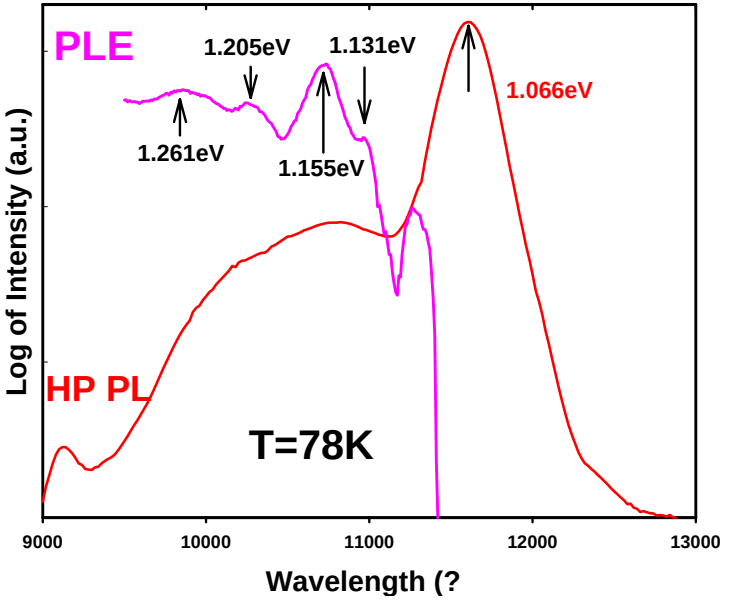



*Energies of transitions (from PL/PLE data):*
*65meV, 89meV*
*139meV, 195meV*

TEM AlGaAs

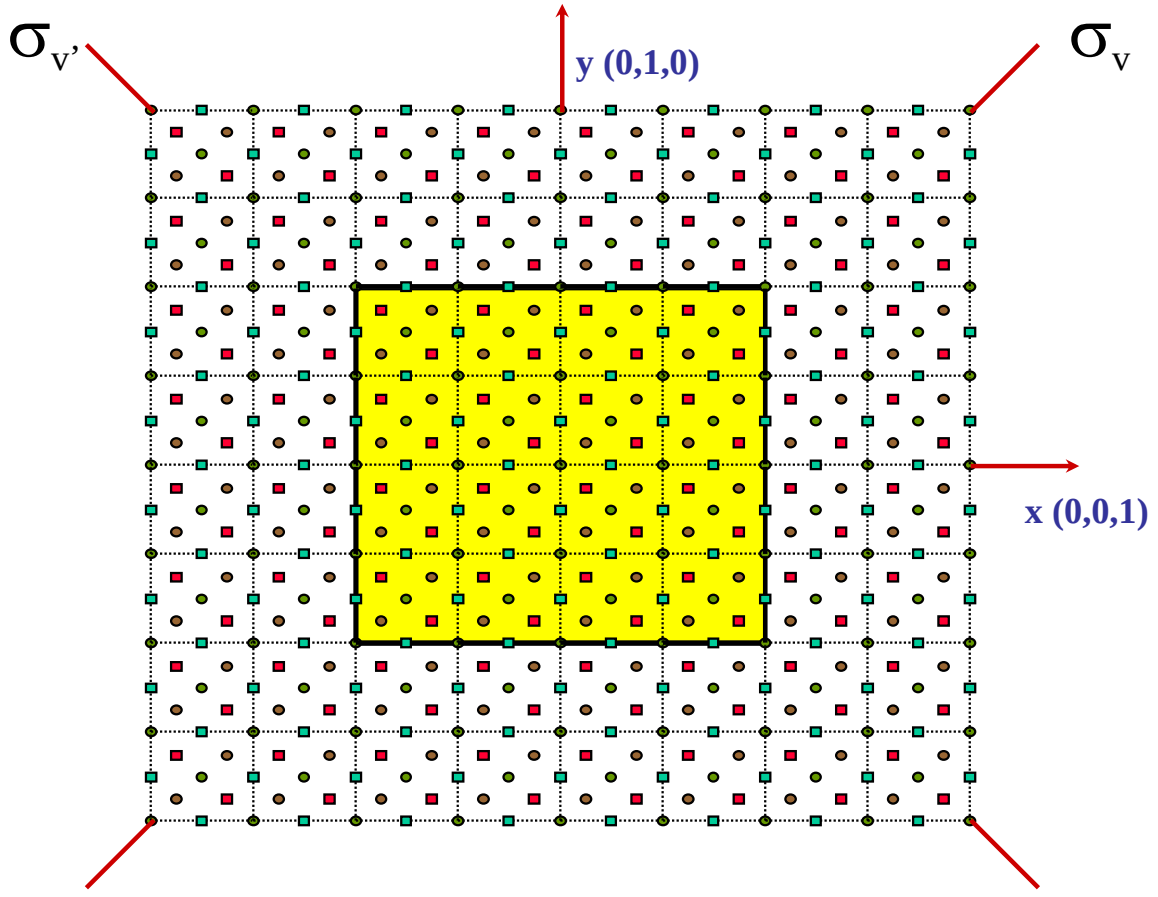


# Microscopic modeling

[S. Sun,Y. C. Chang, PRB 62, 13631 (2000)]

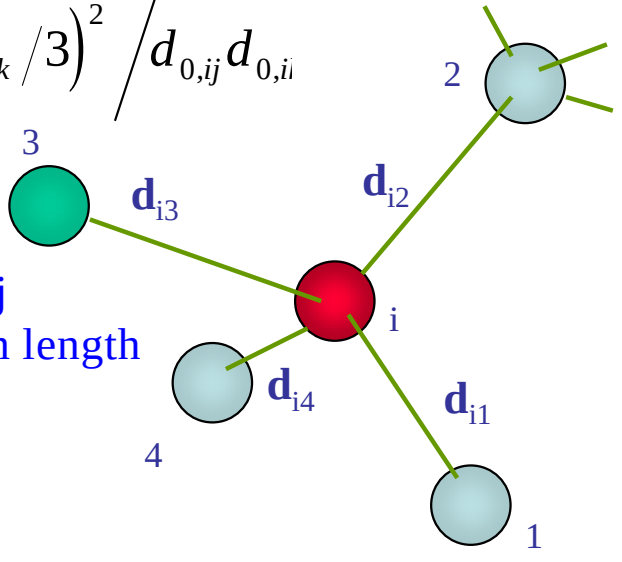


# Valence force field (VFF) Model

$$V = \frac{1}{4}\sum_{ij}\frac{3}{4}\alpha_{ij}\left(d_{ij}^2 - d_{0,ij}^2\right)^2 \Big/ d_{0,ij}^2$$

$$+\frac{1}{4}\sum_{i}\sum_{j\neq k}\frac{3}{4}\beta_{ijk}\left(\vec{d}_{ij}\cdot\vec{d}_{ik} + d_{0,ij}d_{0,ik}/3\right)^2 \Big/ d_{0,ij}d_{0,ik}$$

i labels atom positions
j , k label nearest-neighbors of i
$d_{ij}$ = bond length joining sites i and j
$d_{0,ij}$ is the corresponding equilibrium length
$\alpha_{ij}$= bond stretching constants
$d_{ijk}$= bond bending constants
We take $d_{ijk}^2 = d_{ij}d_{ik}$



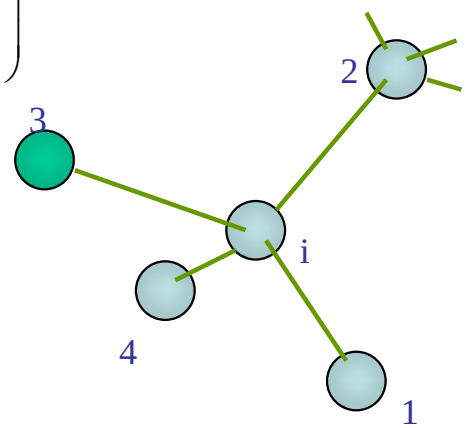
# Effective bond-orbital Model
## [Y.C.Chang, PRB 37, 8215 (1988)]

$$H_{\alpha,\alpha'}(\vec{k}) = E_p \delta_{\alpha,\alpha'} +$$
$$\sum_{\tau} e^{i\vec{k}\cdot\vec{\tau}} \left\{ E_{xy} \tau_\alpha \tau_{\alpha'} + \left[ \left( E_{xx} - E_{xy} \right) \tau_\alpha^2 + E_{zz} \left( 1 - \tau_\alpha^2 \right) \right] \delta_{\alpha,\alpha} \right.$$

### Strain Hamiltonian

$$H_{st} = \begin{pmatrix} -\Delta V_H + D_1 & \sqrt{3} d e_{xy} & \sqrt{3} d e_{xz} \\ \sqrt{3} d e_{xy} & -\Delta V_H + D_2 & \sqrt{3} d e_{yz} \\ \sqrt{3} d e_{xz} & \sqrt{3} d e_{yz} & -\Delta V_H + D_3 \end{pmatrix}$$

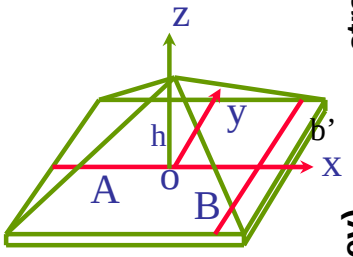
$e_{ij} = (\varepsilon_{ij} + \varepsilon_{ji})/2$
$\Delta V_H = (a_1 + a_2)(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$
$D_1 = b(2\varepsilon_{xx} - \varepsilon_{yy} - \varepsilon_{zz})$
$D_2 = b(2\varepsilon_{yy} - \varepsilon_{xx} - \varepsilon_{zz})$
$D_3 = b(2\varepsilon_{zz} - \varepsilon_{xx} - \varepsilon_{yy})$
$a_1$, $a_2$, b, d = deformation potentials.

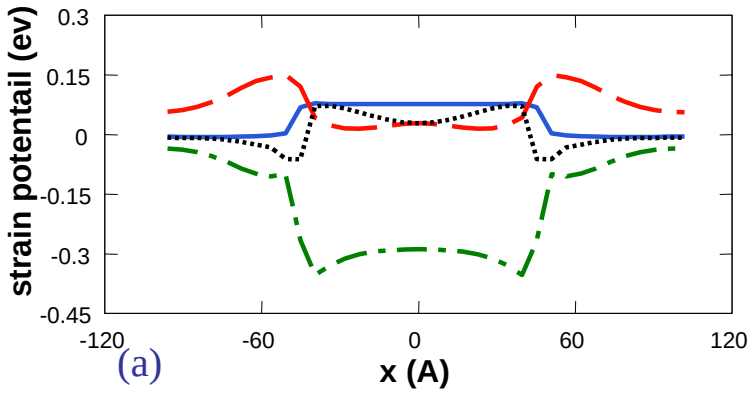


# Strain Potential
# Along Line A and B of Dot 1

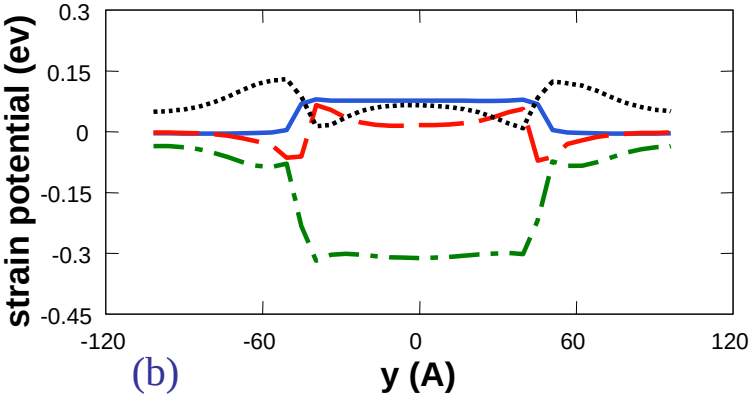
- **Fig.(a):**
  **strain potential along line A**
- **Fig.(b):**
  **strain potential along line B**

$V_{ss}$
$V_{xx}$
$V_{yy}$
$V_{zz}$




(a)

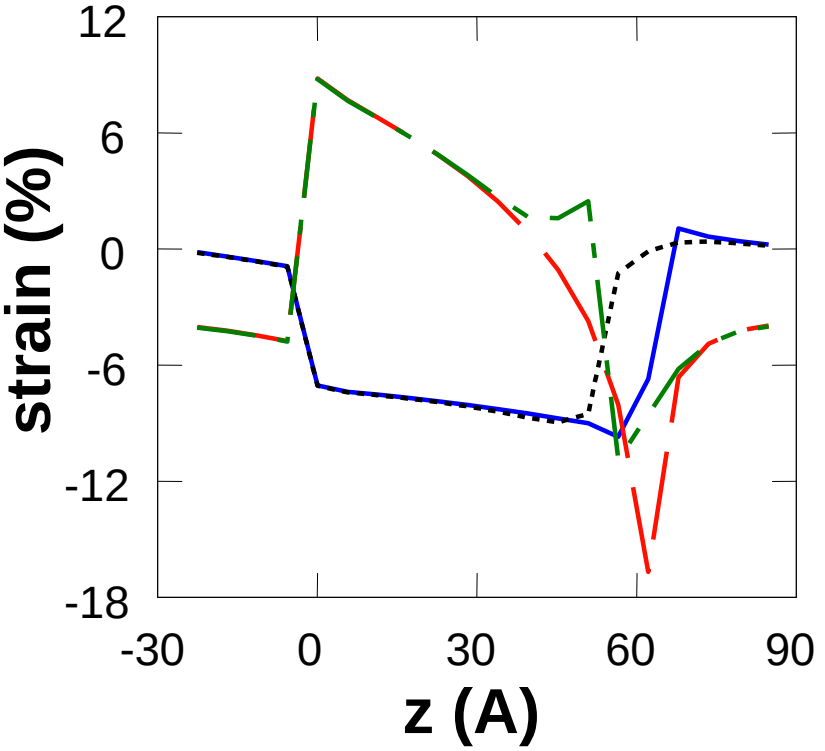



(b)

- **Band offset:**
  **CB: 0.833eV**
  **VB: 0.260eV**

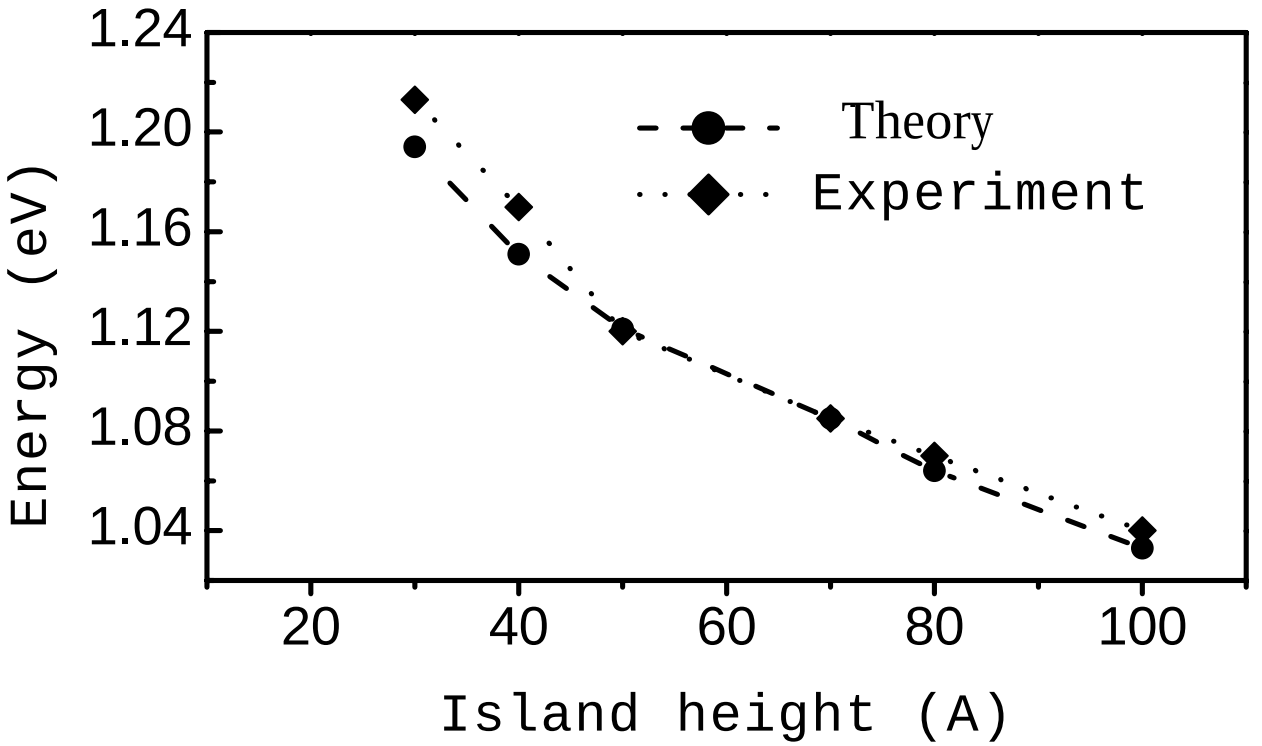
# Strain Distribution Along [001] of Dot 1 and Dot 2

- **Hydrostatic Strain :**
  **Dot 1:** ——
  **Dot 2:** .....
- **Biaxial Strain:**
  **Dot 1:** - - - - - -
  **Dot 2:** — · — · —
- **[001] is growth direction**
- **Dot 1: 0-62.5 A**
  **Dot 2: 0-50A**

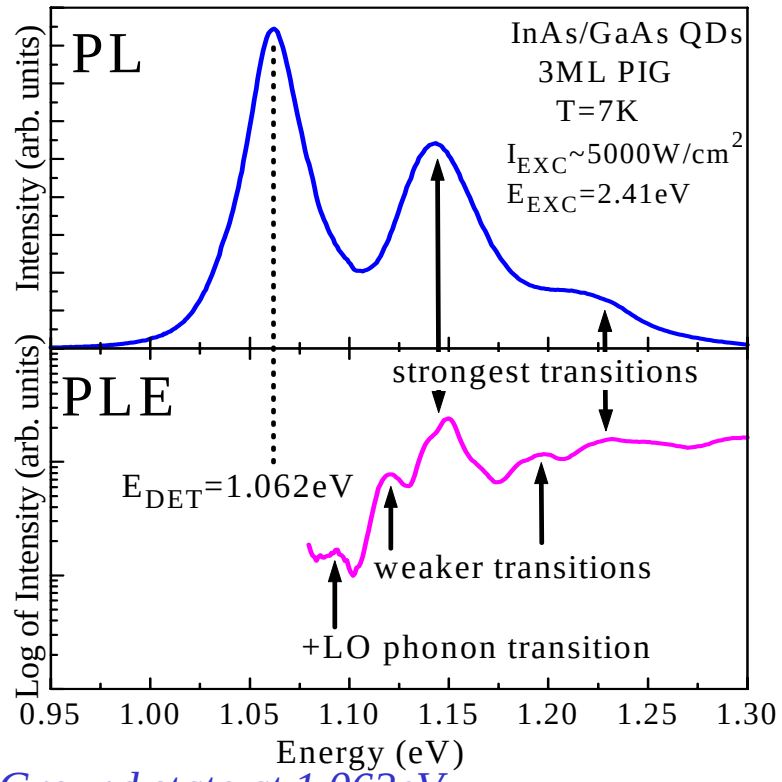


# Ground Transition Energy Varying With Dot Height (comparing to Experiment)

Dot base length 200Å



# PL/PLE Characterization: Electronic Structure

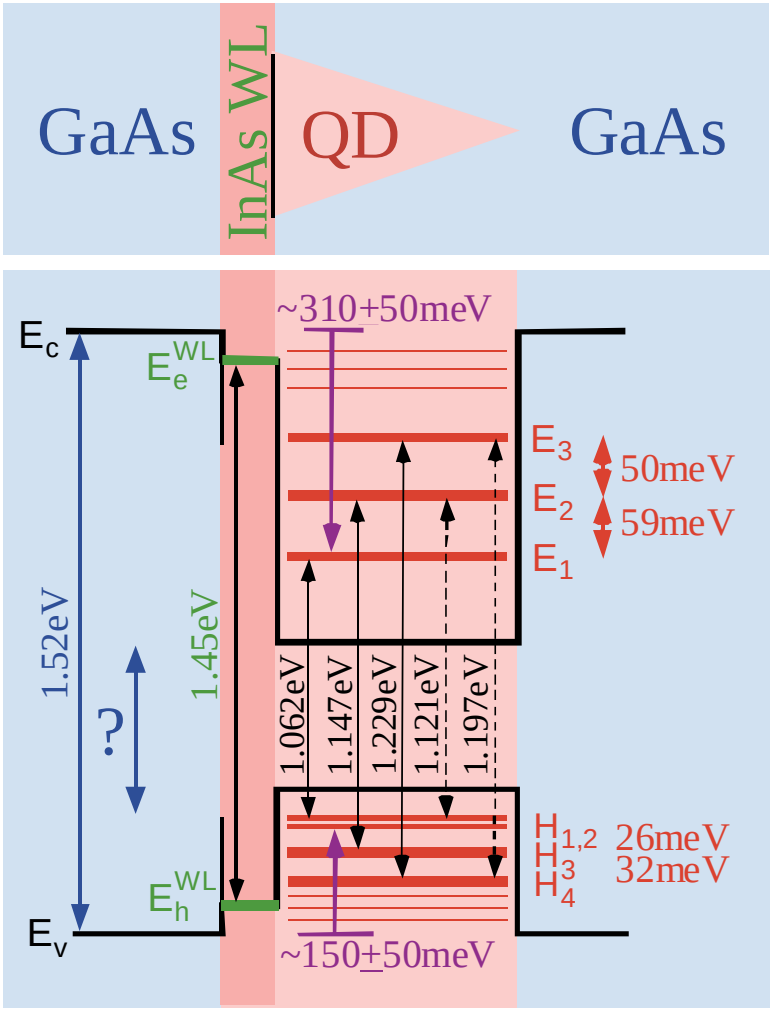



*Ground state at 1.062eV*

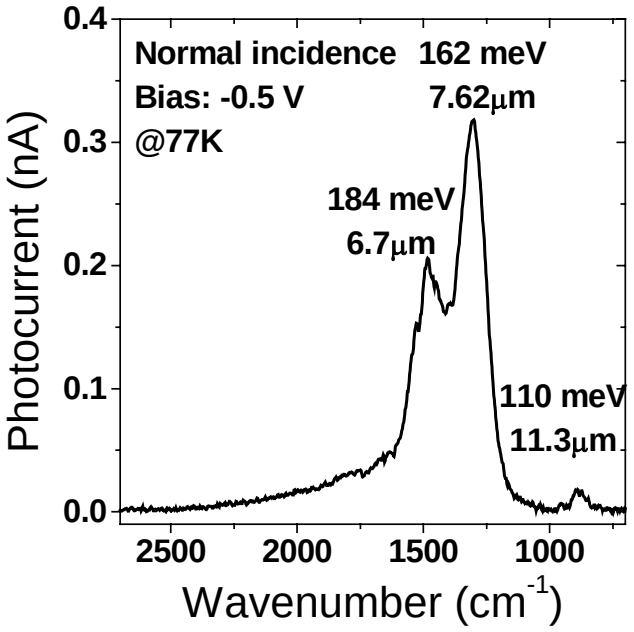
*Excited states:*

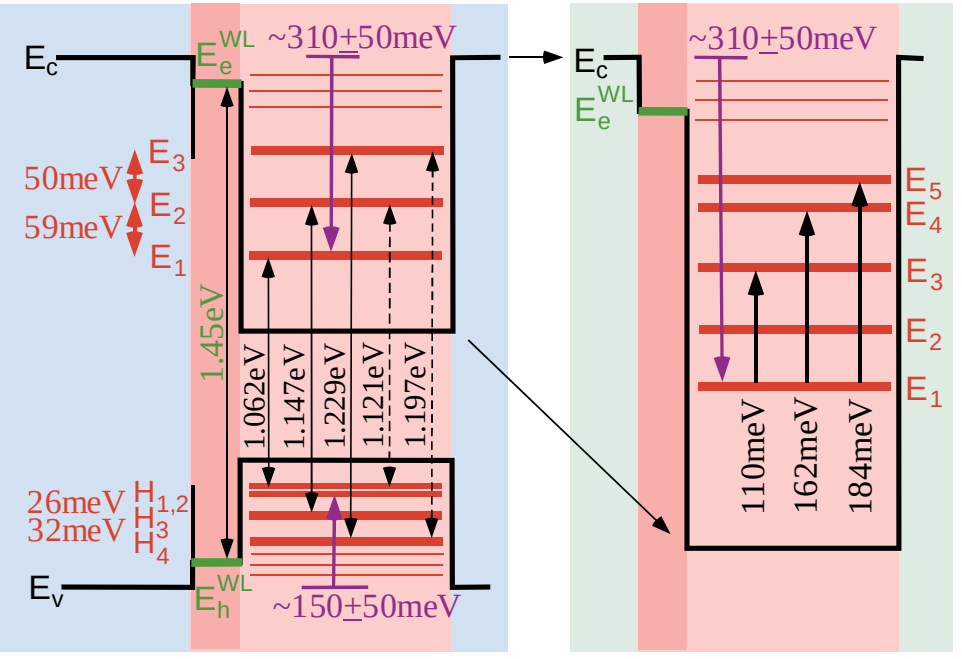
*Strongest at 1.147eV and 1.229eV*

*Weaker at 1.121eV and 1.197eV*



# Intra-band Transitions




A. Madhkar (USC)

# Intra-band Transitions

Table 4 Inter-sub band transition matrix elements of ground electron state to upper three electron states, $\left|\langle \phi_{1,c}|\bar{r}|\phi_{i,c}\rangle\right|^2$. B=200A, h=80A.

| Symmetry | state i | x | y | z |
|---|---|---|---|---|
| A1 | #2 (0.111) | 0 | 0 | 0.2 |
| | #3 (0.123) | 0 | 0 | 57 |
| | #4 (0.197) | 0 | 0 | 201 |
| A2 | #2 (0.106) | 0 | 0 | 28.5 |
| | #3 (0.114) | 0 | 0 | 0 |
| B1,B2 | #2 (0.109) | 0 | 0 | 15 |
| | #3 (0.138) | 0 | 0 | 42 |
| | #4 (0.201) | 0 | 0 | 14 |
| A1-B1n | #1 (0.062) | 446 | 446 | 0 |
| | #2 (0.162) | 0.2 | 0.2 | 0 |
| | #3 (0.218) | 0.4 | 0.4 | 0 |
| B1-A1n | #2(0.049) | 536 | 536 | 0 |
| | #3(0.061) | 659 | 659 | 0 |
| | #4(0.135) | 376 | 376 | 0 |
| | #5(0.161) | 10.2 | 10.2 | 0 |

# Transfer-matrix approach

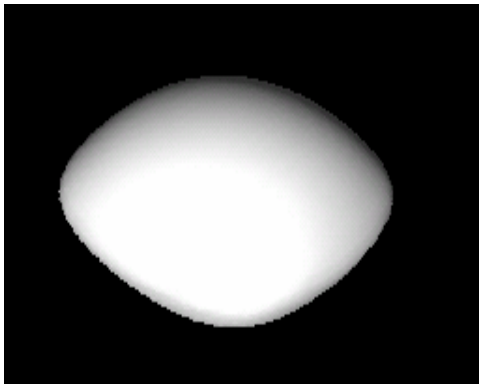
- Energy and wave functions computed using a stabilized transfer matrix technique by dividing the system into many slices along growth direction.
- Envelope function approximation with energy-dependent effective mass is used.
- Effective-mass Hamiltonian in k-sapce:

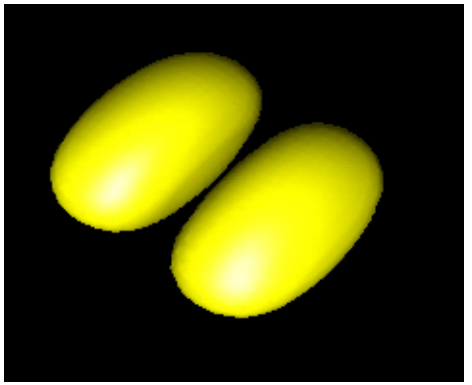
  $[(k_x^2+k_y^2)/m_t(E)+\partial_z^2/m_l(E)-E]F(\mathbf{k}) + \sum_{\mathbf{k}'}[V(\mathbf{k},\mathbf{k}')+V_{imp}(\mathbf{k},\mathbf{k}')]F(\mathbf{k}')=0$

  is solved via plane-wave expansion in each slice.
- 14-band k·p effects included perturbatively in optical matrix elements calculation
- Dopant effects incorporated as screened Coulomb potential
- The technique applies to quantum wells and quantum dots (or any 2D periodic nanostructures)

# Charge densities of low-lying states in lens-shaped QD

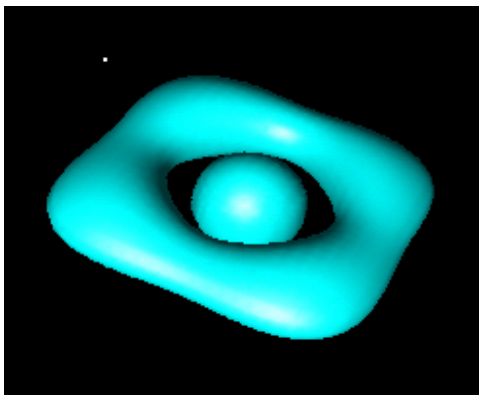
s-like

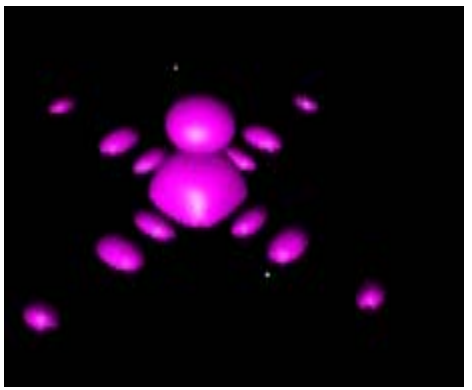




$p_x/p_y$ like

d-like





$p_z$ like