Week5-Electronic Band Calculation(2)

ECE 695-O Semiconductor Transport Theory

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Contents

- k·p method
- Energy band structures – velocity and effective mass

k·p method

- k·p method is used to calculate band structures around a min. or max. (eg. valence band maximum and conduction band minimum)
- Consider Schrödinger Eq.

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = \mathcal{E}\psi$$

and Bloch form of ψ ,

$$\psi = u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} .$$

- By plugging the Block form into the Schrödinger Eq.

$$\mathcal{E}_{n\mathbf{k}} u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} = -\frac{\hbar^2}{2m}\nabla\cdot\left(e^{i\mathbf{k}\cdot\mathbf{r}}\nabla u_{n\mathbf{k}} + u_{n\mathbf{k}}\nabla e^{i\mathbf{k}\cdot\mathbf{r}}\right) + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= -\frac{\hbar^2}{2m}\nabla\cdot\left(e^{i\mathbf{k}\cdot\mathbf{r}}\nabla u_{n\mathbf{k}} + i\mathbf{k}\, u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\right) + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

※ ∇: gradient with respect to r (real space)

k·p method(2)

$$\mathcal{E}_{n\mathbf{k}} u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} = -\frac{\hbar^2}{2m} \nabla \cdot \left(e^{i\mathbf{k}\cdot\mathbf{r}} \nabla u_{n\mathbf{k}} + i\mathbf{k}\, u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \right) + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= -\frac{\hbar^2}{2m} \Big(\nabla e^{i\mathbf{k}\cdot\mathbf{r}} \cdot \nabla u_{n\mathbf{k}} + e^{i\mathbf{k}\cdot\mathbf{r}} \nabla^2 u_{n\mathbf{k}} + \\ + i\mathbf{k} \cdot \nabla u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + i\mathbf{k} \cdot u_{n\mathbf{k}} \nabla e^{i\mathbf{k}\cdot\mathbf{r}} \Big) + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= -\frac{\hbar^2}{2m} \Big(i\mathbf{k} \cdot \nabla u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i\mathbf{k}\cdot\mathbf{r}} \nabla^2 u_{n\mathbf{k}} + \\ + i\mathbf{k} \cdot \nabla u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} - k^2 u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \Big) + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= -\frac{\hbar^2}{2m} \left(e^{i\mathbf{k}\cdot\mathbf{r}} \nabla^2 u_{n\mathbf{k}} + 2 e^{i\mathbf{k}\cdot\mathbf{r}} i\mathbf{k} \cdot \nabla u_{n\mathbf{k}} - k^2 e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}} \right) + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= -\frac{\hbar^2}{2m} \left(e^{i\mathbf{k}\cdot\mathbf{r}} \nabla^2 + 2 e^{i\mathbf{k}\cdot\mathbf{r}} i\mathbf{k} \cdot \nabla - k^2 e^{i\mathbf{k}\cdot\mathbf{r}} \right) u_{n\mathbf{k}} + V u_{n\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

k·p method(3)

- By factoring out $e^{i\mathbf{k}\cdot\mathbf{r}}$

$$\left[-\frac{\hbar^2}{2m}\nabla^{\mathbf{2}}-\frac{i\hbar^2}{m}\mathbf{k}\cdot\ \nabla+\frac{\hbar^2k^2}{2m}+V(\mathbf{r})\right]u_{n\mathbf{k}}=\mathcal{E}_{n\mathbf{k}}u_{n\mathbf{k}}\quad .$$

- Let $\mathbf{p}=\frac{\hbar}{i}\nabla$ then,

$$\left[\ \frac{p^2}{2m}+\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}+\frac{\hbar^2k^2}{2m}+V(\mathbf{r})\ \right]u_{n\mathbf{k}}=\mathcal{E}_{n\mathbf{k}}u_{n\mathbf{k}}\quad .$$

- Near k=0

$$\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}+\frac{\hbar^2k^2}{2m}\approx\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}$$ can be treated

as perturbation.

(generally speaking, this should be $\frac{\hbar}{m}(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{p}+\frac{\hbar^2(\mathbf{k}-\mathbf{k}_0)^2}{2m}\approx\frac{\hbar}{m}(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{p}$)

k·p method(4)

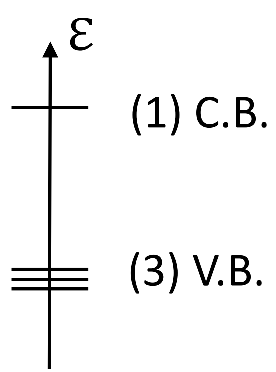
Example) Application to conduction and valence bands:

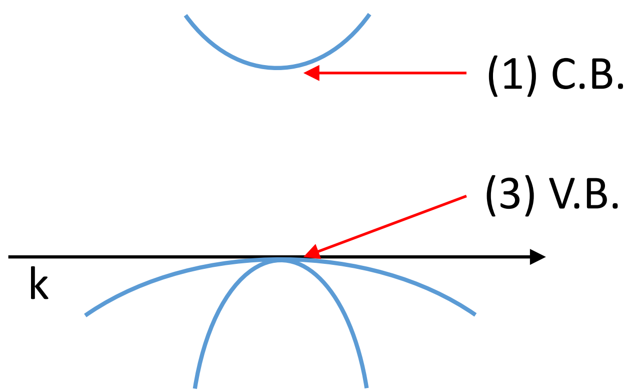
- First we need to solve

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]U_0 = \mathcal{E}U_0 \quad .$$

- From the previous study, we know there are 3 valence bands and 1 major conduction band → sp3 bonding like Ge or GaAs.

We know that:





k·p method(4)

- It's also know that the 3 V.B. states are "p-like" and 1 C.B. is s-like.
- We can write down 4 possible solutions as

$u_1 \longrightarrow u_c$: function of r only (s like)

$u_2 \longrightarrow u_x$: function of r and x/r

$u_3 \longrightarrow u_y$: function of r and y/r

$u_4 \longrightarrow u_z$: function of r and z/r

- Wave functions have certain symmetry characteristics.
- u_x is antisymmetric about the x=0 plane.

i.e.

$$u_x(-x, y, z) = -u_x(x, y, z)$$
$$u_x(x, -y, z) = u_x(x, y, z)$$
$$u_x(x, y, -z) = u_x(x, y, z)$$

- Likewise, for u_y and u_z.

k·p method(5)

- The u_i (i= c, x, y, z) functions are normalized and orthogonal
- Let's call $\mathcal{E}_{10} = \mathcal{E}_c$ and $\mathcal{E}_{20} = \mathcal{E}_{30} = \mathcal{E}_{40} = \mathcal{E}_v$.
- In the Schrödinger Eq.

$$\left[\frac{p^2}{2m} + \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar^2 k^2}{2m} + V(\mathbf{r})\right]u_{n\mathbf{k}} = \mathcal{E}_{n\mathbf{k}}u_{n\mathbf{k}}$$

we neglect $\frac{\hbar^2 k^2}{2m}$ term near k = 0 (to 1st order) and consider $\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}$ as a perturbation term.

$$\left[\frac{p^2}{2m} + \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p} + V(\mathbf{r})\right]u_{n\mathbf{k}} = \mathcal{E}_{n\mathbf{k}}u_{n\mathbf{k}}$$

- From perturbation theory we need to solve:

$$\begin{vmatrix} H'_{11} - (\mathcal{E} - \mathcal{E}_c) & H'_{12} & H'_{13} & \cdots \\ H'_{21} & H'_{22} - (\mathcal{E} - \mathcal{E}_v) & H'_{23} & \cdots \\ H'_{31} & H'_{32} & H'_{33} - (\mathcal{E} - \mathcal{E}_v) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix} = 0$$

k·p method(6)

- We will evaluate each matrix element.

$$\Longrightarrow H'_{11} = \int u_c^* H' u_c \; d^3r \qquad \text{Perturbation: } H' = \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}$$

$$= -i\frac{\hbar^2}{m}\int u_c^* \left(k_x\frac{\partial}{\partial x} + k_y\frac{\partial}{\partial y} + k_z\frac{\partial}{\partial z}\right) u_c \;\; d^3r$$

- Consider $\dfrac{\partial}{\partial x}u_c(r) = \dfrac{\partial}{\partial r}u_c(r)\dfrac{\partial r}{\partial x} = \dfrac{x}{r}\;\dfrac{\partial u_c}{\partial r}$.

So, $$k_x \int u_c^* \frac{\partial}{\partial x} u_c \;\; d^3r = k_x \int dxdydz \;\; u_c^* \frac{x}{r}\frac{\partial u_c}{\partial r} = 0$$

since $u_c^* \frac{x}{r}\frac{\partial u_c}{\partial r}$: odd function of x

k·p method(7)

- Similarly $$k_y \int u_c^* \frac{\partial}{\partial y} u_c \;\; d^3r = k_y \int dxdydz \;\; u_c^* \frac{y}{r}\frac{\partial u_c}{\partial r} = 0$$

$$k_z \int u_c^* \frac{\partial}{\partial z} u_c \;\; d^3r = k_z \int dxdydz \;\; u_c^* \frac{z}{r}\frac{\partial u_c}{\partial r} = 0$$

$$\Longrightarrow H'_{11} = 0$$

- Let's check H'_{12} .

$$H'_{12} = \int u_c^* H' u_x \, d^3r$$

$$= -i\frac{\hbar^2}{m}\int u_c^* \left(k_x \frac{\partial}{\partial x} + k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z}\right) u_x \;\; d^3r$$

$$= -i\frac{\hbar^2}{m}\left[\int u_c^* k_x \frac{\partial}{\partial x} u_x \;\; d^3r + \int u_c^* k_y \frac{\partial}{\partial y} u_x \;\; d^3r + \int u_c^* k_z \frac{\partial}{\partial z} u_x \;\; d^3r\right]$$

k·p method(8)

$$= -i\frac{\hbar^2}{m}\left[\int u_c^* k_x \frac{\partial}{\partial x} u_x \ \ d^3r + \int u_c^* k_y \frac{\partial}{\partial y} u_x \ \ d^3r + \int u_c^* k_z \frac{\partial}{\partial z} u_x \ \ d^3r\right]$$

- Here, we have $u_c^* \frac{\partial}{\partial y} u_x$ and $u_c^* \frac{\partial}{\partial z} u_x$ that are odd functions of x and $u_c^* \frac{\partial}{\partial x} u_x$ that is an even function of x, y, z.

- So

$$H'_{12} = -i\frac{\hbar^2}{m}\int u_c^* k_x \frac{\partial}{\partial x} u_x \ \ d^3r = k_x \frac{\hbar}{m}\int u_c^* p_x u_x \ \ d^3r$$

$$= k_x P$$

where $P \equiv \frac{\hbar}{m}\int u_c^* p_x u_x \ \ d^3r = \frac{\hbar}{m}\int u_c^* p_y u_y \ \ d^3r = \frac{\hbar}{m}\int u_c^* p_z u_z \ \ d^3r$

(=>momentum matrix element).

k·p method(9)

- Similarly,

$$H'_{13} = \int u_c^* H' u_y \, d^3r = k_y \frac{\hbar}{m} \int u_c^* p_y u_y \, d^3r$$

$$= k_y P$$

$$H'_{14} = k_z P$$

$$H'_{21} = k_x P$$

$$H'_{22} = 0 \qquad H'_{23} = 0 \qquad H'_{24} = 0$$

- Then the matrix becomes

$$\begin{vmatrix} \mathcal{E}_c - \mathcal{E} & k_x P & k_y P & k_z P \\ k_x P & \mathcal{E}_v - \mathcal{E} & 0 & 0 \\ k_y P & 0 & \mathcal{E}_v - \mathcal{E} & 0 \\ k_z P & 0 & 0 & \mathcal{E}_v - \mathcal{E} \end{vmatrix} = 0$$

which gives the characteristic eq. $(\mathcal{E}_v - \mathcal{E})^2\{(\mathcal{E}_v - \mathcal{E})(\mathcal{E}_c - \mathcal{E}) - k^2P^2\} = 0.$

k·p method(10)

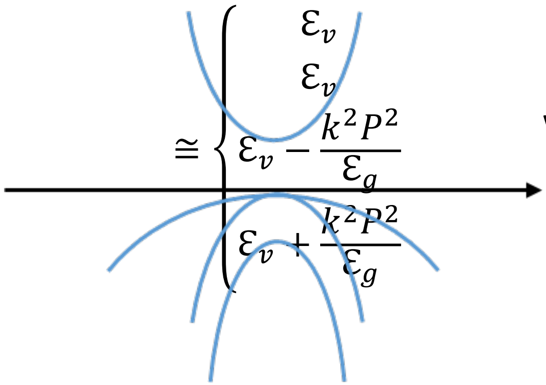
- The equation have 4 roots:

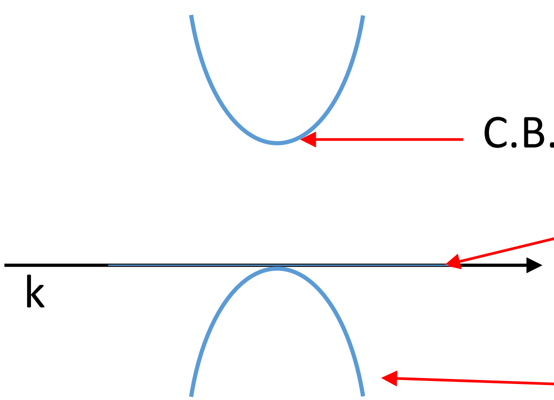
$$\mathcal{E} = \begin{cases} \mathcal{E}_v \\ \mathcal{E}_v \\ \dfrac{\mathcal{E}_c + \mathcal{E}_v}{2} \pm \sqrt{\dfrac{(\mathcal{E}_c - \mathcal{E}_v)^2}{4} + k^2P^2} \end{cases}$$

for small k

$$\cong \begin{cases} \mathcal{E}_v \\ \mathcal{E}_v \\ \mathcal{E}_v - \dfrac{k^2P^2}{\mathcal{E}_g} \\ \mathcal{E}_v + \dfrac{k^2P^2}{\mathcal{E}_g} \end{cases}$$

where $\mathcal{E}_g = \mathcal{E}_c - \mathcal{E}_v$

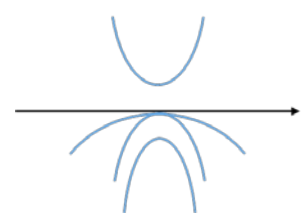




Heavy hole band and Split off band — usually do not show up in 1st order perturbation theory

Light hole-“like” band (this is not light hole)

The real band shape is like :



C.B.
H.H.
L.H.
S.O

k·p method(11)

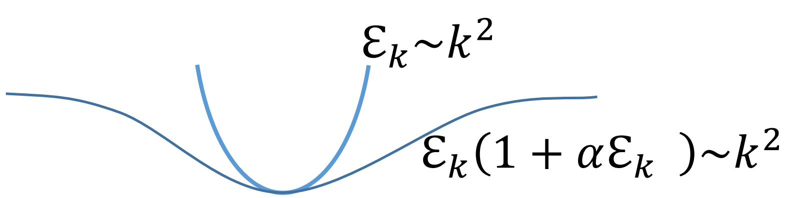
- Let $\mathcal{E} = \mathcal{E}_c + \mathcal{E}_k$ where $\mathcal{E}_k$: kinetic energy above $\mathcal{E}_c$.
- This gives

$$(\mathcal{E}_v - \mathcal{E})^2\{(\mathcal{E}_v - \mathcal{E})(\mathcal{E}_c - \mathcal{E}) - k^2P^2\} = 0$$

$$(\mathcal{E}_v - \mathcal{E}_c - \mathcal{E}_k)^2\{-\mathcal{E}_k(\mathcal{E}_v - \mathcal{E}_c - \mathcal{E}_k) - k^2P^2\} = 0$$

$$-\mathcal{E}_k(\mathcal{E}_v - \mathcal{E}_c - \mathcal{E}_k) - k^2P^2 = 0$$

$$\mathcal{E}_k\left(1 + \frac{\mathcal{E}_k}{\mathcal{E}_c - \mathcal{E}_v}\right) = \frac{P^2}{\mathcal{E}_c - \mathcal{E}_v}k^2$$



$$k^2 \sim \mathcal{E}_k(1 + \alpha\mathcal{E}_k)$$

Non-parabolicity

Other band structure calculation methods

- Cellular Method
- Muffin-Tin Potential
- Augmented Plane Wave(APW) method
- Green's Function (KKR) method
- Orthogonal Plane Wave(OPW) method
- etc

Energy Band Structures

- Velocity and Effective Mass
  - Using the analogy to classical mechanics

$$\underbrace{\mathbf{v} = \nabla_{\mathbf{k}}\omega}_{\text{Group velocity}} = \underbrace{\frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}}_{\mathcal{E} = \hbar\omega}$$

  - In a similar way, we can define electron velocity inside a crystal:

$$\mathbf{v} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E} \qquad \text{(here k is the crystal wave vector)}$$

Energy Band Structures

- In classical mechanics, a Hamiltonian (H) is the summation of kinetic energy (T) and potential energy (V).

$$H = T + V$$

- T is described by momentum, p_i and
- V is described by coordinate, q_i.

- The force acting on an object can be found by

time derivative

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

- In a similar way, we can define the external force acting on an electron:

$$\begin{aligned}\mathbf{F}_{ext} &= (\text{time derivative of crystal momentum } \hbar\mathbf{k}) \\ &= \hbar\frac{\boldsymbol{dk}}{\boldsymbol{dt}}\end{aligned}$$

Effective Mass

- The underlying idea of these definitions are like this.
- In quantum mechanics, $p = \frac{\hbar}{i}\nabla$.
- And Hamiltonian is $H = \frac{\hbar^2}{2m}\nabla^2 + V$.
- If $V = 0$, $[H, p] = 0$ (commute) -> we can measure momentum and energy simultaneously.
- To make $V = 0$, we need the concept of effective mass.
- This is, in a way, that we will wrap all the influence from the crystal potential into the effective mass term and treat the particle like a free particle (without potential).

- In classical mechanics, acceleration $\mathbf{a}$ is

$$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \frac{1}{\hbar}\frac{d}{dt}(\nabla_{\mathbf{k}}\mathcal{E})$$

- By using the chain rule,

$$\mathbf{a} = \frac{1}{\hbar}\left(\frac{d\mathbf{k}}{dt}\cdot\nabla_{\mathbf{k}}\right)\nabla_{\mathbf{k}}\mathcal{E} = \frac{1}{\hbar^2}(\mathbf{F}_{ext}\cdot\nabla_{\mathbf{k}})\nabla_{\mathbf{k}}\mathcal{E}$$

Effective Mass(2)

$$\mathbf{a} = \frac{1}{\hbar^2}(\mathbf{F}_{ext} \cdot \nabla_{\mathbf{k}})\nabla_{\mathbf{k}}\mathcal{E} \longrightarrow a_i = \frac{1}{\hbar^2}\left(\sum_j F_{ext\ j}\frac{\partial}{\partial k_j}\right)\frac{\partial}{\partial k_i}\mathcal{E}$$

- From the form of F = m a,   a = F/m.
- By the analogy,

$$a_i = \frac{1}{\hbar^2}\left(\sum_j \frac{\partial^2}{\partial k_j \partial k_i}\mathcal{E}\right)F_{ext\ j}$$

$$= [m^*]^{-1}\ F_{ext\ j}$$

- And we define the inverse mass tensor

$$\boxed{[m^*]^{-1}_{ij} \equiv \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}}{\partial k_j \partial k_i}}$$:definition of effective mass.

$$[\mathbf{a}] = [m^*]^{-1}[\mathbf{F}]$$