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Computational Electronics

# Simplified Band-Structure Models and Carrier Dynamics

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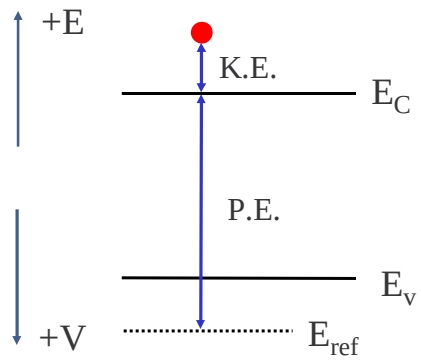
## Notation

**Basic convention:**




Kinetic energy:

$$K.E. = E - E_C$$

Potential Energy:

$$P.E. = -qV = E_C - E_{ref}$$

$$V = -\frac{1}{q}\left(E_C - E_{ref}\right)$$

Electric field: $\boldsymbol{\varepsilon} = -\nabla V$, or in 1D $\boldsymbol{\varepsilon} = -\frac{dV}{dx} = \frac{1}{q}\frac{dE_C}{dx}$

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## E-k Relation for Free Electrons

➔ Definition:

$$E = \frac{p^2}{2m_0}, \quad m_0 = \text{free electron mass}$$

➔ de Broglie hypothesis:

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}k = \hbar k \quad \Longrightarrow \quad E = \frac{\hbar^2 k^2}{2m_0}$$

**Energy-wavevector relation for electrons in a crystal:**

The dispersion relation in a crystal (*E-k* relation) is obtained by solving the Schrödinger wave equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\phi_{\mathbf{k}}(\mathbf{r}) = E_k\phi_{\mathbf{k}}(\mathbf{r})$$



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## Bloch Theorem

If the potential energy $V(\mathbf{r})$ is periodic, then the solutions of the SWE are of the form:

$$\phi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})u_n(\mathbf{k},\mathbf{r})$$

where $u_n(\mathbf{k},\mathbf{r})$ is periodic in $\mathbf{r}$ with the periodicity of the direct lattice and $n$ is the band index.

**Methods used to calculate the energy band structure:**

- ➔ Tight-binding method
- ➔ Orthogonal plane-wave method
- ➔ Pseudopotential method
- ➔ **k•p** method
- ➔ Density functional technique (DFT)

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## Prototypical Band Structure

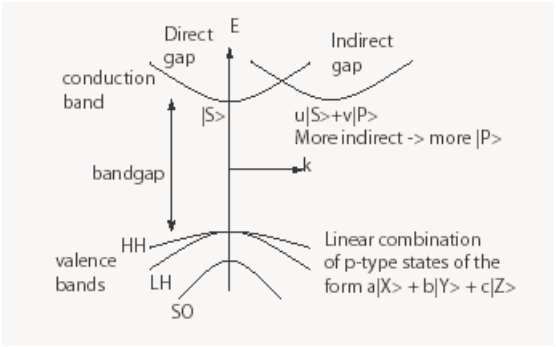
- Typically semiconductors have an average of 4 valence electrons per atom composed of partially-filled *s*- and *p*-type orbitals that contribute to tetrahedral bonds that form through $sp^3$ hybridization.
- The symmetry properties of these atomic orbitals are apparent from consideration of their angular components:

$$s = 1$$

$$p_x = \frac{x}{r} = \sqrt{3}\sin\theta\cos\varphi$$

$$p_y = \frac{y}{r} = \sqrt{3}\sin\theta\sin\varphi$$

$$p_z = \frac{z}{r} = \sqrt{3}\cos\theta$$



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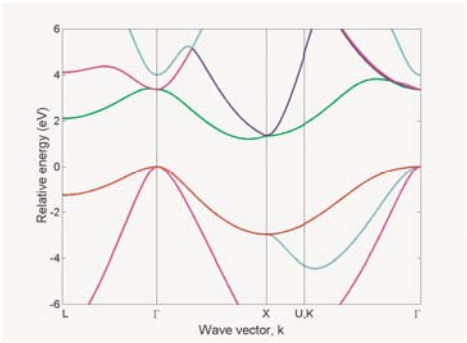
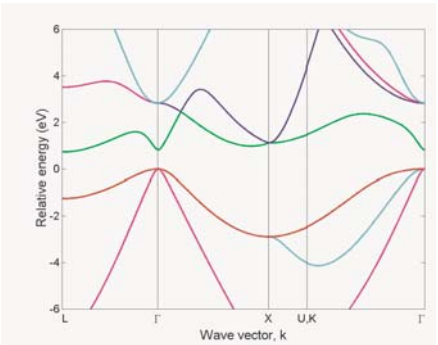
## Empirical Pseudopotential Calculations for Si and Ge




Silicon

Germanium

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## Simplified Band-Structure Models

•Parabolic Band Model

$$E(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k}|^2}{2m_0^*} \qquad \mathbf{v} = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k}) = \frac{\hbar \mathbf{k}}{m_0^*}$$

•Non-Parabolic Band Model

$$E(\mathbf{k})\left(1+\alpha E(\mathbf{k})\right) = \frac{\hbar^2 |\mathbf{k}|^2}{2m_0^*} \qquad E(k) = \frac{\sqrt{1+\frac{4\alpha\hbar^2 |\mathbf{k}|^2}{2m_0^*}}-1}{2\alpha}$$

$$\mathbf{v} = \frac{1}{\hbar}\nabla_k E(\mathbf{k}) = \frac{\hbar \mathbf{k}}{m_0^*}\left(1+4\alpha\frac{\hbar^2 |\mathbf{k}|^2}{2m_0^*}\right)^{-1/2}$$



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## Effective Masses

Curvature of the band determines the effective mass of the carriers in a crystal, which is different from the free electron mass.

Smaller curvature ➔ heavier mass
Larger curvature ➔ lighter mass

$$\frac{1}{m_{ij}^*} = \frac{1}{\hbar^2}\cdot\frac{\partial^2 E}{\partial k_i \partial k_j} \quad \Rightarrow \quad \frac{1}{m^*} = \begin{bmatrix} \frac{1}{m_{xx}^*} & 0 & 0 \\ 0 & \frac{1}{m_{yy}^*} & 0 \\ 0 & 0 & \frac{1}{m_{zz}^*} \end{bmatrix}$$

- For parabolic bands, the components of the effective mass tensor are calculated according to:

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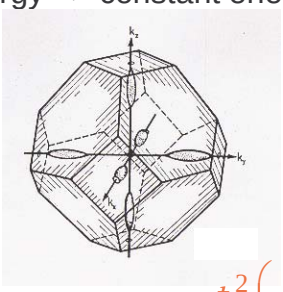
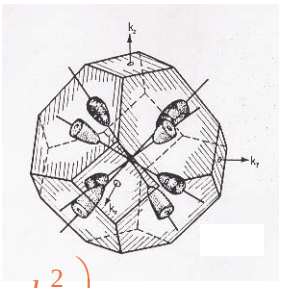
## Constant Energy Surfaces

From the knowledge of the energy band structure, one can construct the plot for the allowed k-values associated with a given energy => constant energy surfaces

Si 

Ge 

$$(E - E_C)_i = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_{xi}^*} + \frac{k_y^2}{m_{yi}^*} + \frac{k_z^2}{m_{zi}^*}\right)$$

Note: The electron effective mass in GaAs is isotropic, which leads to spherically symmetric constant energy surfaces.



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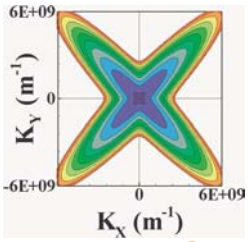
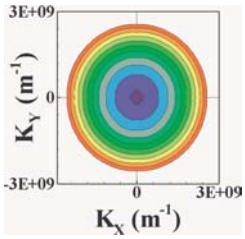
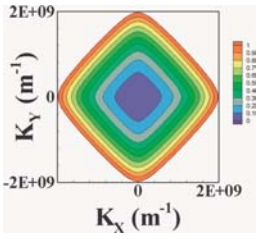
## Valence Bands

Due to the *p*-like symmetry and mixing of the V.B. states, the constant energy surfaces are warped spheres:

- ➔ The *hh*-band is most warped
- ➔ The *lh*- and *so*-band are more spherical




$$E(k) = -\frac{\hbar^2}{2m}\left\{Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}\right\}$$

$$m_{hh}^* = \frac{m_o}{A - \sqrt{B^2 + C^2/6}},\quad m_{lh}^* = \frac{m_o}{A + \sqrt{B^2 + C^2/6}},\quad m_{so}^* = \frac{m_o}{A}$$

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## Important Parameters

| Name | Symbol | Germanium | Silicon | Gallium Arsenide |
|---|---|---|---|---|
| **Band minimum at $k = 0$** | | | | |
| Minimum energy | $E_{g,direct}$ [eV] | 0.8 | 3.2 | 1.424 |
| Effective mass | $m_e^*/m_0$ | 0.041 | 0.2 | 0.067 |
| **Band minimum *not* at $k = 0$** | | | | |
| Minimum energy | $E_{g,indirect}$[eV] | 0.66 | 1.12 | 1.734 |
| Longitudinal effective mass | $m_{e,l}^*/m_0$ | 1.64 | 0.98 | 1.98 |
| Transverse effective mass | $m_{e,t}^*/m_0$ | 0.082 | 0.19 | 0.37 |
| Wavenumber at minimum | $k$ [1/nm] | xxx | xxx | xxx |
| Longitudinal direction | | (111) | (100) | (111) |
| **Heavy hole valence band maximum at $E = k = 0$** | | | | |
| Effective mass | $m_{hh}^*/m_0$ | 0.28 | 0.49 | 0.45 |
| **Light hole valence band maximum at $k = 0$** | | | | |
| Effective mass | $m_{lh}^*/m_0$ | 0.044 | 0.16 | 0.082 |
| **Split-off hole valence band maximum at $k = 0$** | | | | |
| Split-off band valence band energy | $E_{v,so}$ [eV] | -0.028 | -0.044 | -0.34 |
| Effective mass | $m_{h,so}^*/m_0$ | 0.084 | 0.29 | 0.154 |



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## Effective Masses

In transport calculations there are two different masses in use:

**Density of States effective mass** – used in DOS calculations

$$m_{e,dos}^* = M_C^{2/3}\left(m_l m_t m_t\right)^{1/3}$$

**Conductivity effective mass** – used in conductivity calculations, which for ellipsoidal constant energy surfaces is calculated using:

$$m_{e,cond}^* = \frac{3}{\frac{1}{m_l}+\frac{1}{m_t}+\frac{1}{m_t}}$$

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# Values of Effective Masses

| Name | Symbol | Germanium | Silicon | Gallium Arsenide |
|---|---|---|---|---|
| Smallest energy bandgap at 300 K | $E_g$ (eV) | 0.66 | 1.12 | 1.424 |
| **Effective mass for density of states calculations** | | | | |
| Electrons | $m_{e,dos}^*/m_0$ | 0.56 | 1.08 | 0.067 |
| Holes | $m_{h,dos}^*/m_0$ | 0.29 | 0.57/0.8 | 0.47 |
| **Effective mass for conductivity calculations** | | | | |
| Electrons | $m_{e,cond}^*/m_0$ | 0.12 | 0.26 | 0.067 |
| Holes | $m_{h,cond}^*/m_0$ | 0.21 | 0.36/0.38 | 0.34 |