# Lecture8:
# Band structure

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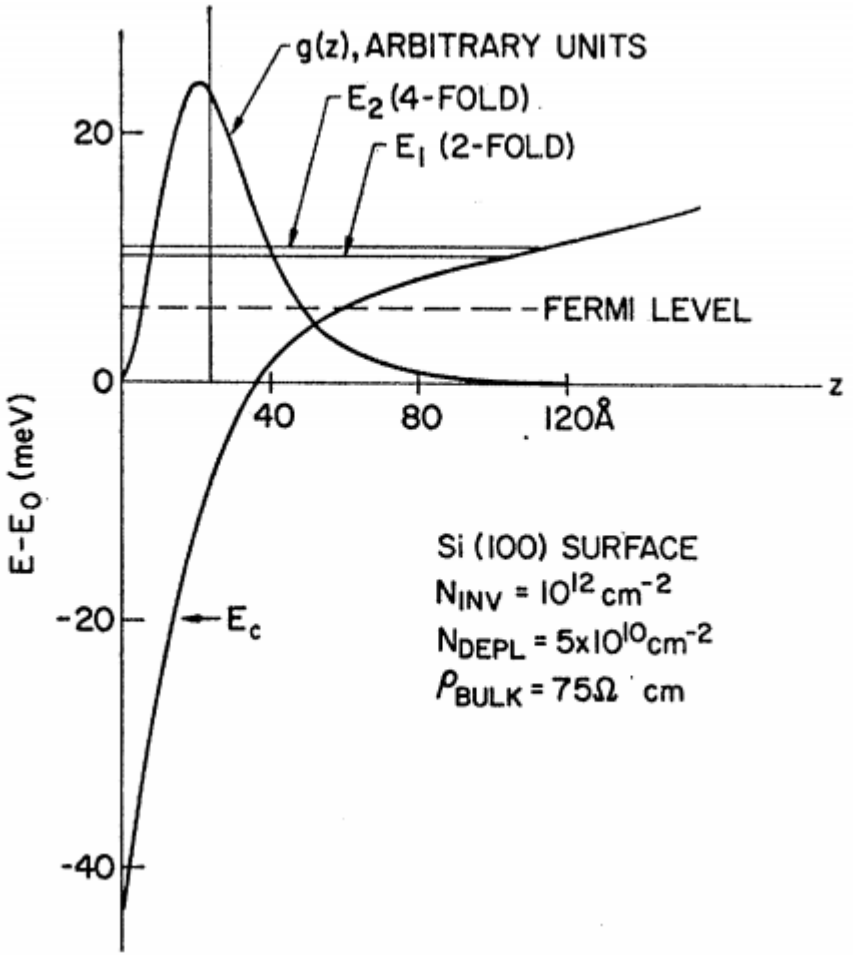
# Homework#3

- Additional Q&A session for Homework#3
  - Stern & Howard, Physical Review, 1967



# Band structure of Si (1)

- Conduction band
  - Ellipsoidal model

$$E(\mathbf{k}) = \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2}{2m_t}\left(k_x^2 + k_y^2\right)$$

  - Non-parabolicity

$$E^{NP}(\mathbf{k})\left(1 + E^{NP}(\mathbf{k})\right) = E(\mathbf{k})$$

# Band structure of Si (2)

- Valence band
  - Six-band k.p model (Taken from S-Band manual)

$$
H_{LK} = -\begin{array}{|cccccc|c}
\multicolumn{6}{c}{\left|\frac{3}{2},\frac{3}{2}\right\rangle \quad \left|\frac{3}{2},\frac{1}{2}\right\rangle \quad \left|\frac{3}{2},-\frac{1}{2}\right\rangle \quad \left|\frac{3}{2},-\frac{3}{2}\right\rangle \quad \left|\frac{1}{2},\frac{1}{2}\right\rangle \quad \left|\frac{1}{2},-\frac{1}{2}\right\rangle} & \\
\hline
P+Q & -S & R & 0 & -\frac{S}{\sqrt{2}} & \sqrt{2}R & \left|\frac{3}{2},\frac{3}{2}\right\rangle \\
 & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{\frac{3}{2}}S & \left|\frac{3}{2},\frac{1}{2}\right\rangle \\
 & & P-Q & S & \sqrt{\frac{3}{2}}S^{*} & \sqrt{2}Q & \left|\frac{3}{2},-\frac{1}{2}\right\rangle \\
 & & & P+Q & -\sqrt{2}R^{*} & -\frac{S^{*}}{\sqrt{2}} & \left|\frac{3}{2},-\frac{3}{2}\right\rangle \\
 & & & & P+\Delta & 0 & \left|\frac{1}{2},\frac{1}{2}\right\rangle \\
 & & & & & P+\Delta & \left|\frac{1}{2},-\frac{1}{2}\right\rangle \\
\hline
\end{array}
$$

*Complex conjugate*

# Band structure of Si (3)

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

Luttinger–Kohn:

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

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

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

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

Bir–Pikus:

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

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

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

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

- $\gamma_1, \gamma_2, \gamma_3$ are the Luttinger parameters.
- $a, b, d$ are the Bir–Pikus deformation potentials.
- $\Delta$ is the spin-orbit split-off energy.

# Band structure of Si (4)

- Valence band
  - Parameters

| Symbol | Parameter name | Si default value | Ge default value | Unit |
|---|---|---|---|---|
| $\gamma_1$ | gamma1 | 4.306 | 10.536 | 1 |
| $\gamma_2$ | gamma2 | 0.345 | 3.107 | 1 |
| $\gamma_3$ | gamma3 | 1.44 | 4.397 | 1 |
| $\Delta_{so}$ | Delta | 0.0434 | 0.297 | eV |

| Symbol | Parameter name | Si default value | Ge default value | Unit |
|---|---|---|---|---|
| $a$ | a_v | 2.46 | 1.25 | eV |
| $b$ | b | –2.316 | –2.067 | eV |
| $d$ | d | –5.514 | –3.836 | eV |

# Homework#4

- Repeat Homework#3 with realistic band structures.
  - a) Ellipsoidal model without non-parabolicity
    - $m_l = 0.914$
    - $m_t = 0.196$
  - b) Consider the non-parabolicity ($\alpha = 0.5$ eV$^{-1}$)
    - How can we consider the non-parabolicity?

- Calculate the bulk hole band structure.
  - For a while, neglect the strain terms.