EE-606: Solid State Devices
Lecture 7: Energy Bands in Real Crystals

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Outline

1) E-k diagram/constant energy surfaces in 3D solids

2) Characterization of E-k diagram: Bandgap

3) Characterization of E-k diagram: Effective Mass

4) Conclusions

Reference: Vol. 6, Ch. 3 (pages 71-77)
Electronic States

Original Problem

Periodic Structure
Brillouin Zone in Cubic Lattice ...

Follow W-S algorithm, but now for reciprocal lattice
Brillouin Zone in *Real* FCC Lattices ...

Real Space FCC (for Si, Ge, GaAs)

Reciprocal Lattice

Note unlike cubic lattice, zone edge is not at \( \pi/a \)
Analogy for E-k Diagram: 4D info throught 2D Plots

Density (x,y,z)

4D information

A series of line-sections can represent the 4D info in 2D plots

Cut along (θ₁, φ₁) ...

ρ

r
E-k along Γ-X Direction
E-k along Γ-L direction
3 valence bands (light hole, heavy hole, split-off) valence bands near \( k=0 \) is essentially \( E \sim k^2 \)

- Minima may not be at zone center
- (Ge: 8 L valleys, Si: 6 X valleys, and GaAs: \( \Gamma \) valleys)
E-k diagram for GaAs

Direct bandgap material

Zone-edge gaps ($L_6$-$\Gamma_8$, $X_6$-$\Gamma_8$) close to direct gap

Has important implications
For transport
Analogy for E-k Diagram

Contours of density ....

Density (x,y,z)
Constant-E surface for Conduction Band

\[ E = E_c + A k_1^2 + B (k_2^2 + k_3^2) \]

\[ E = E_c + A (k_1^2 + k_2^2 + k_3^2) \]
Constant E-surface ...

\[ E = E_c + A k_1^2 + B (k_2^2 + k_3^2) \]

\[ \frac{1}{m_{ij}} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \]

\[ \frac{1}{m_{11}} = \frac{2A}{\hbar^2}; \quad \frac{1}{m_{22}} = \frac{1}{m_{33}} = \frac{2B}{\hbar^2}; \quad \frac{1}{m_{ij}}(i \neq j) = 0 \]

\[ \frac{1}{m_{11}} = \frac{1}{m_{22}} = \frac{1}{m_{33}} = 2A; \quad \frac{1}{m_{ij}}(i \neq j) = 0 \]
Four valleys inside BZ for Germanium
Constant E-surface for Valence Band

\[ E = E_v - Ak^2 \pm \sqrt{B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)} \]

Si: \( A=4.29, B=0.68, C=4.87 \); Ge: \( A=13.38, B=8.48, C=13.15 \)
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Measurement of Band Gap

Photons are only absorbed between bands that have filled and empty states.
Measurement of Energy Gap

\[ \Delta h \nu \]

\[ I_{\text{out}}(E_{\text{out}} - E_{\text{in}}) \sim \left(E - E_{23} - E_{ph}\right)^2 \]

\[ \sim \sqrt{E - E_{23}} \]
Temperature-dependent Band Gap

\[ E_G(T) = E_G(0) - \frac{\alpha T^2}{T + \beta} \]

<table>
<thead>
<tr>
<th>Material</th>
<th>( E_G(300 \text{ K}) )</th>
<th>( E_G(0) )</th>
<th>( \alpha )</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ge</td>
<td>0.663</td>
<td>0.7437</td>
<td>4.774 \times 10^{-4}</td>
<td>235</td>
</tr>
<tr>
<td>Si</td>
<td>1.125</td>
<td>1.170</td>
<td>4.730 \times 10^{-4}</td>
<td>636</td>
</tr>
<tr>
<td>GaAs</td>
<td>1.422</td>
<td>1.519</td>
<td>5.405 \times 10^{-4}</td>
<td>204</td>
</tr>
</tbody>
</table>
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Measurement of Effective Mass
Measurement of Effective Mass

\[ \nu_0 = 24 \text{ GHz (fixed)} \]

B field variable ...

\[
\nu_0 = \frac{qB_0}{2\pi m^*} \quad m^* = \frac{qB_0}{2\pi \nu_0}
\]
Derive the Cyclotron Formula \[ m^* = \frac{qB_0}{2\pi\nu_0} \]

For an particle in (x-y) plane with B-field in z-direction, the Lorentz force is ...

\[ \frac{m^*\nu^2}{r_0} = q\nu \times B_z = q\nu B_z \]

\[ \nu = \frac{qB_0r_0}{m^*} \]

\[ \tau = \frac{2\pi r_0}{\nu} = \frac{2\pi m^*}{qB_0} \]

\[ \nu_0 \equiv \frac{1}{\tau} = \frac{qB_0}{2\pi m^*} \]

\[ \omega_0 = 2\pi\nu_0 = \frac{qB_0}{m^*} \]
Conclusions

1) E-k diagram/constant energy surfaces are simple ways to represent the locations where electrons can sit. They arise from the solution of Schrodinger equation in periodic lattice.

2) E-k diagram and energy bands contain equivalent information. In principle, any one can be used to construct the other.

3) Experimental measurements are key to making sure that the theoretical calculations are correct. We will discuss them in the next class.