Symmetry and the Brillouin Zones

Consider a two-dimensional square space lattice. The reciprocal lattice and Brillouin zones are shown in Fig. 10-7b. For simplicity assume that this lattice has point symmetry $C_{4v}(4mm)$ with the eight symmetry operations $\{E, C_4, C_{2v}, C_4^2, 2\sigma, 2\sigma_d\}$. The $2\sigma$ refers to mirror planes perpendicular to the $x$- and $y$-axes; $2\sigma_d$ are the two diagonal mirror planes; and the first four symbols refer to rotations about the axis out of the paper by 0, $\pi/2$, $\pi$, and $3\pi/2$.

Consider $k$ along $k_x$ as shown in Fig. 10-21a with the end point of the $k$-vector labeled $\Delta$. By applying all eight of the symmetry operations to this $k$-vector, we obtain the four $k$-values shown in this figure by the vectors with solid lines. Notice that under two of the symmetry operations, $E$ and $\sigma'$, the original $k$-vector, labeled $\Delta$, transforms into itself, that is, $Rk = k$ when $R = E, \sigma'$. These two symmetry operations form the group of $\Delta$. We will discuss its use but first let us look for other special points in the Brillouin zone.

Consider $k$ along the diagonal $k_x + k_y$, with the end point of the vector labeled $\Sigma$ in Fig. 10-21a. Again apply all eight symmetry operations to the $\Sigma$-vector and the four $k$-values shown in the figure with dashed vectors are obtained. Again we notice that this $k$-value, labeled $\Sigma$, transforms into itself under the symmetry operations $E$ and $\sigma'$, that is, $Rk = k$ when $R = E, \sigma'$. These two symmetry operations are called the group of $\Sigma$.

**Fig. 10-21** The first Brillouin zone of a two-dimensional square lattice showing special $k$-values: (a) the $\Delta$- and $\Sigma$-lines; (b) the $\Delta$ line; (c) a general point.

Brillouin Zones

of the BCC (a)
and FCC (b)
Lattice with Special Symmetry Points Indicated.

(a) Brillouin Zone
Def. \lq Wigner-Seitz\rq
Cell of the
Primitive Recip
Lattice.
(b) Symmetry
Group of Recip
Lattice is the
Same as for the lattice in
Configuration Space. (Should
Know Proof!)
(a) Special Points
are Sub-groups of
the full symmetry
Group.
Free Electron Approximations 3-Dimensional

(Empty Lattice)

\[ E = \frac{t^2}{2m} \left( (k_x - n \frac{2\pi}{a})^2 + (k_y - m \frac{2\pi}{a})^2 + (k_z - n \frac{2\pi}{a})^2 \right) \]

\[ E = \frac{t^2}{2m} \left( k_x^2 + k_y^2 + k_z^2 \right) \]

\[ E = \frac{t^2}{2m} \left( k_x^2 + k_y^2 + k_z^2 \right) \]

\[ a = \frac{b}{2} \]

\[ b = \text{cubic period} \]

\[ \frac{2\pi}{a} (x, y, z) \] 8-fold - obtained by going through the hexagons to the 8 centers of the second Brillouin zones.

\[ \frac{2\pi}{b} (x, y) \] 6-fold - obtained by going through the square end faces of the Brillouin zone to the centers.

\[ \frac{2\pi}{b} ( \pm 2y, 0) \] at the second Brillouin zones.

s-like

\[ 3\text{-fold} \]

p-like

\[ 2\text{-fold} \]

8-fold = \[ \Gamma_1 + \Gamma_{15} \] \( p \)-like set is the valence band

3-fold

6-fold = \[ \Gamma_2 + \Gamma_{16} + \Gamma_{17} \] rest are conduction band

all excited states of the conduction band
Character Analysis

Characters of Representations For the 43m Symmetry Group (GaAs)

Characters of The 18 point Symmetry Operations for Plane Waves is also Given

\[ \psi_{kn}(\bar{r}) = e^{i\bar{k} \cdot \bar{r}} U_{kn}(\bar{r}) \]

where \( \bar{k} \) is any reciprocal lattice vector

and where \( U_{kn} = e^{i\bar{k} \cdot \bar{r}} \)

Thus

\[ \varepsilon_n(\bar{k}) = \frac{h^2}{2m} (\bar{k} + \bar{R}) \cdot (\bar{k} + \bar{R}) \]

<table>
<thead>
<tr>
<th>Name</th>
<th>Basis Function</th>
<th>( E )</th>
<th>( 3C_2 )</th>
<th>( 8C_3 )</th>
<th>( 6\sigma_d )</th>
<th>( 6S_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Gamma_1 )</td>
<td>[ x^2, y^2, z^2 ]</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \Gamma_2 )</td>
<td>[ x^2, -y^2, z^2 ]</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>( \Gamma_3 )</td>
<td>[ x^2 - y^2, z^2 ]</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( \Gamma_{15} )</td>
<td>( x, y, z )</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>( \Gamma_{25} )</td>
<td>[ x(y^2 - z^2), y(x^2 - z^2), z(x^2 - y^2) ]</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>-1</td>
<td>+1</td>
</tr>
</tbody>
</table>

\[ \Pi = e^{i\frac{2\pi}{a} (x^2 + y^2 + z^2)} \]

Character Analysis:

\[ \Pi = \sum \alpha_i \Gamma_i \]

\[ \alpha_i = \frac{1}{h} \sum_{R \in \Gamma_i} \chi_i(R) \]

\( h = \text{order of the group} = \text{No of symmetry elements} = 24 \)

Thus

\[ \Pi = \chi (\Gamma_1 + \Gamma_{15}) \]