Electronic Properties of the Materials: Computational Approach
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Module No # 08
Lecture No # 38
Semiconductors: Part 2 (Si, Ge and GaAs)

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Hello friends I already have discussed about some basics of semiconductor physics in this lecture I am going to discuss about 3 widely used semiconductors Silicon Germania and Gallium arsenide.

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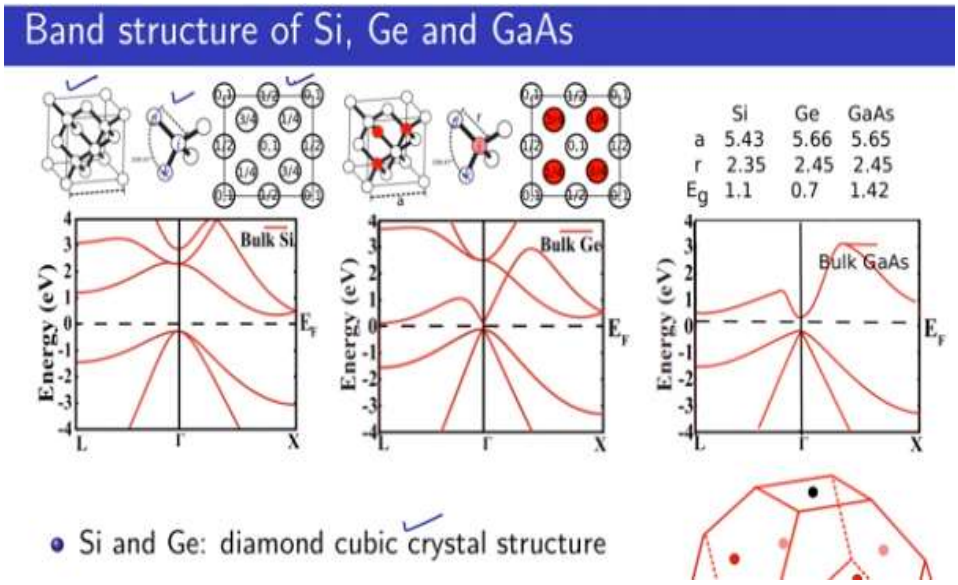

Silicon and germanium have a diamond cubic crystal structure. Diamond cubic crystal structure can be imagined as a cube with an atom at each corner and each face center like in a phase centered cubic crystal. In addition to that 4 out of the 8 tetrahedral voids are occupied by an atom. Each atom is tetrahedral coordinated this is the unit cell this is the atomic coordination and this is the top view of the unit cell.

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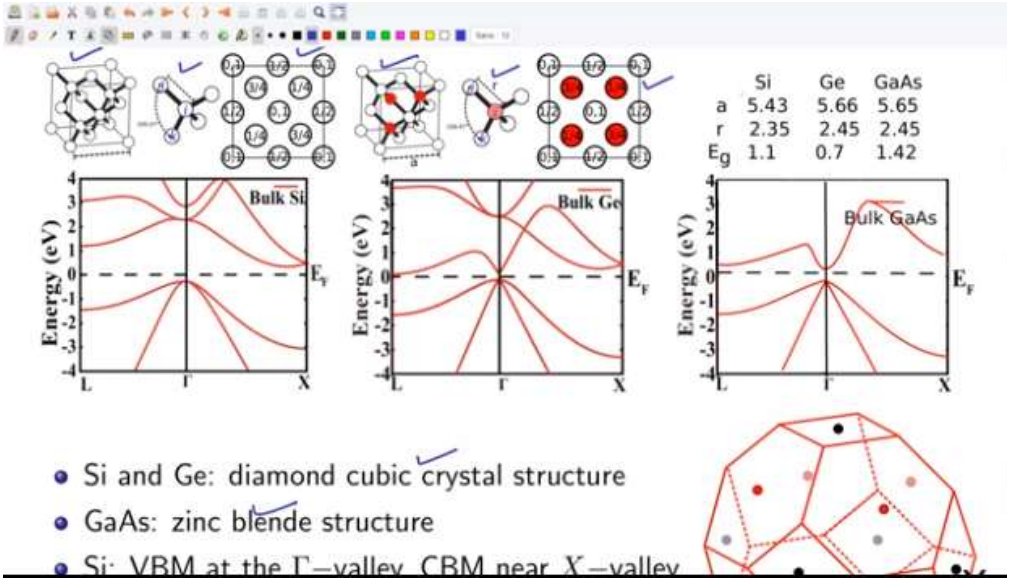

Gallium arsenide has zinc blend structure the crystal structure can be imagined as a cube with an atom at each corner and each phase center like in a face centered cubic crystal. In addition to that 4 out of the 8 tetrahedral wires are occupied if you put gallium atom at the corners and face centers of the cube then you have to put Arsenic atom at the tetrahedral voids.

This is the unit cell this is the atomic coordination and this is the top view of the unit cell. Crystal structure related data and bend gap of silica germanium and gallium arsenide are reported in this table.

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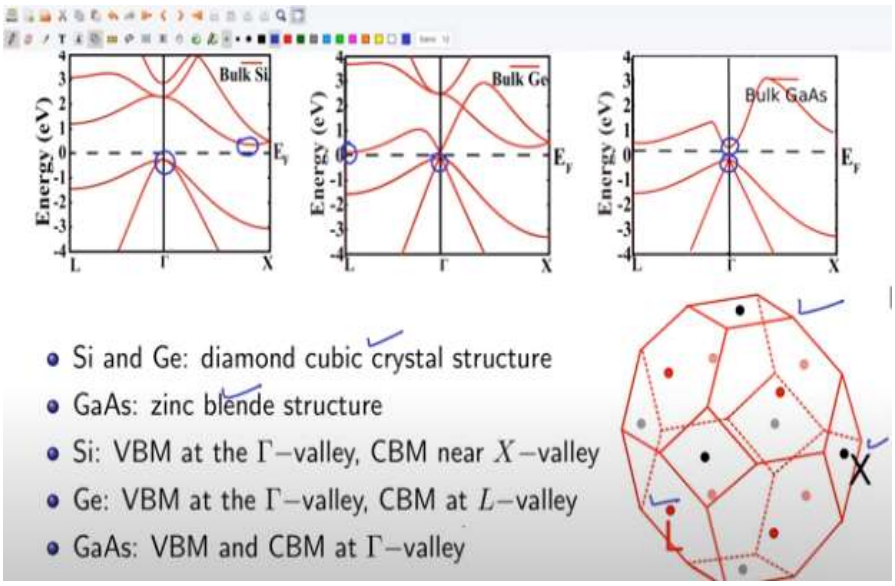

This is the first below in zone and I have shown 2 high symmetry points X point and L point shown by the black and red dots. There are 6 x points and 8 L points in case of silicon valence band maximum or VBM is located at the gamma point and conduction band minimum or CBM is located close to the x value. In case of germanium VBM is located at the gamma valley and CPM is located at the L valley. In case of gallium arsenide both VBM and CBM are located at the gamma valley where gamma is the center of the Brillouin zone.

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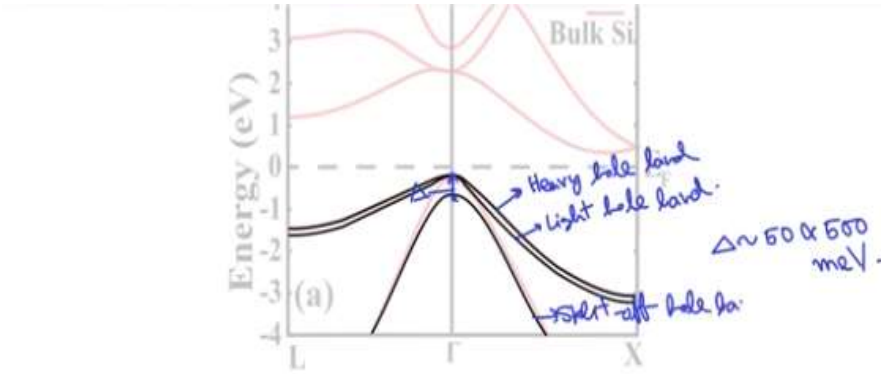

- Valence bands splits due to spin-orbit coupling
- Top band splits into heavy and light hole band
- Third band separated from the heavy and light hole band by Δ - known as split-off hole band

The valence band of silicon germanium and Gallia arsenide splits because of spin orbit coupling spinner orbit coupling is a relativistic effect that splits the electronic bands in many materials. Since I did not discuss about spin-orbit coupling I shall only mention about it without going into detail. Without spin orbit coupling there are degenerate valence bands due to spin orbit coupling degeneracy is partly lifted as the bands split.

The top band splits into 2 bands known as the heavy hole band and light hole bend. The third band is now separated from the heavy and light one band at the gamma point by an energy delta. Delta is approximately between 50 and 500 milli electron volt in different semiconductors this band is known as the split off whole band.

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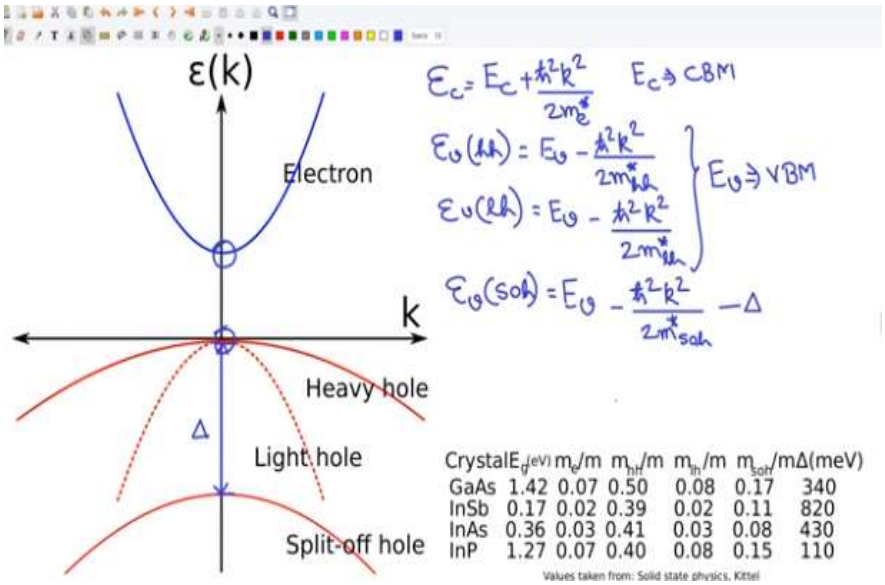

Let me discuss about some general features of band structure of direct gap materials like gallium arsenide. For Semiconductor like gallium arsenide the conduction bandage is at the gamma value that is the center of the Brillouin zone. The conduction bandage is spherical with effective mass m e star such that we can write the energy dispersion relation as E C where C stands for conduction band is equals to EC + h cross square K square divided by 2 m e star.

$$\varepsilon_c = E_c + \frac{\hbar^2 k^2}{2m_e^*}$$

there are 3 valence bands at the gamma valley heavy hole band, light hold band, and split of hold band. The heavy hole and light hole bands are degenerate at the gamma point and we can write the energy dispersion as

$$\text{Heavy hole, } \varepsilon_v(hh) = E_v - \frac{\hbar k^2}{2m_{hh}^*}$$

$$\text{Light hole, } \varepsilon_v(lh) = E_v - \frac{\hbar k^2}{2m_{lh}^*}$$

In these equations E v is valence band maximum this is the spin orbits splitting delta and energy dispersion for the split of hole band is given by

$$\text{Split of hole, } \varepsilon_v(soh) = E_v - \frac{\hbar k^2}{2m_{soh}^*} -$$

Since the whole bands are not spherical equations for whole bands are only some approximation this is going to be discussed again when we discuss all bands of silicon and germanium.

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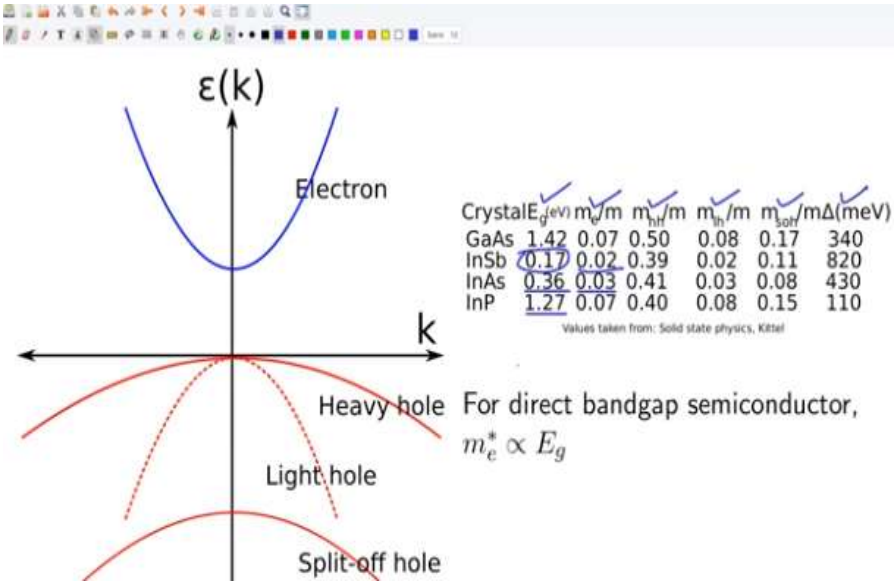

Crystal	E_g(eV)	m_e/m	m_{hh}/m	m_{lh}/m	m_{soh}/m	Δ(meV)
GaAs	1.42	0.07	0.50	0.08	0.17	340
InSb	0.17	0.02	0.39	0.02	0.11	820
InAs	0.36	0.03	0.41	0.03	0.08	430
InP	1.27	0.07	0.40	0.08	0.15	110

Values taken from: Solid state physics, Kittel

Values of band gap electron effective mass, heavy hole effective mass, light hole effective mass, spin orbital effective mass, and spin orbit splitting delta have been given in this table for different direct gap materials. From the table we observe an interesting factor a crystal having lower band gap has lower electron effective mass. For example in Sb has the smallest band gap of 0.17 electron volt and it also has the smallest effective mass of electron = 0.02.

Band gap increases in As to 0.36 electron volt and electron effective mass also increases to 0.03. Finally pan gap increases to 1.27 electron volt in case of in P which also has the highest electron effective mass of 0.07 in the in gap series.

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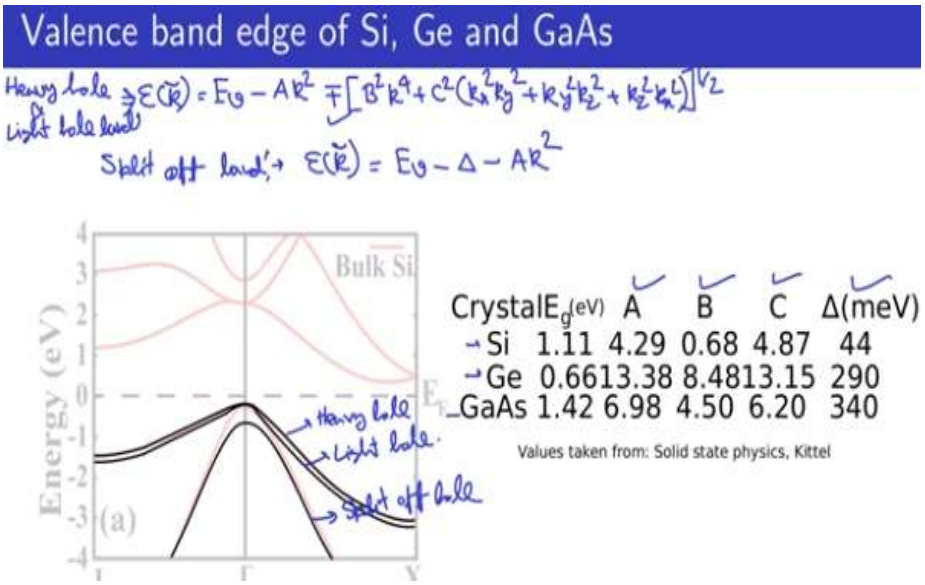

Now let me discuss about balance bandage of silicon germanium and gallium arsenide valence band edges in silicon germanium and gallium arsenide are not very simple. Holes at the valence bandage are characterized by 2 effective masses heavy hole and light hole there is another band split off due to the inaudible interaction and this is known as the split off hole band.

Constant energy surfaces are not spherical but given by

For light and heavy hole band $\varepsilon(\vec{k}) = E_v - Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}$

The choice of sine distinguishes between 2 masses.

The energy dispersion relation for the split off band can be written as

$$\varepsilon(\vec{k}) = E_v - \Delta - Ak^2$$

values of A B C and delta are reported in this table for silicon germanium and gallium arsenide.

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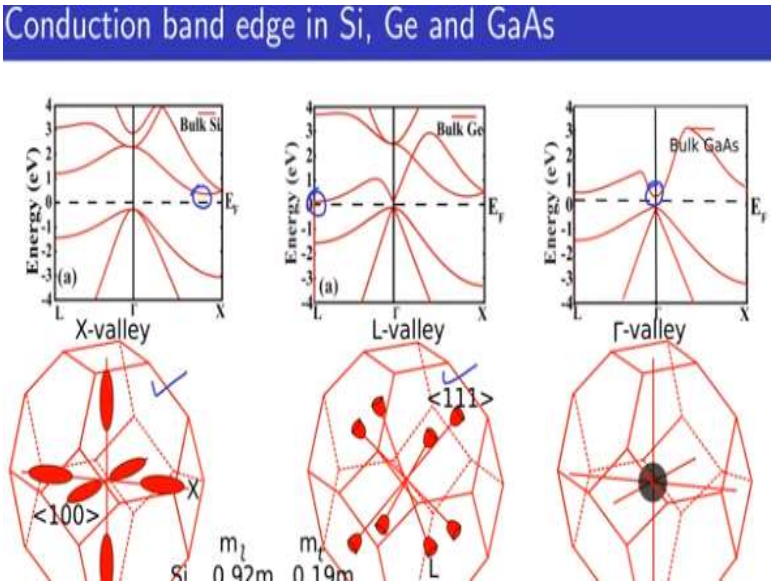

Now let us discuss about the conduction bandage of silicon germanium and gallium arsenide. In case of silica CBM is located near the x value now there are 6 x points in the first Brillouin zone and thus there are 6 constant energy ellipsoids in case of silicon. In case of germanium CVM is located at the L value there are 8 L points in the first Brillouin zone. And thus there are 8 constant energy ellipsoids in case of germanium in case of gallium arsenide CBM is located at the gamma value and the constant energy surface is spherical.

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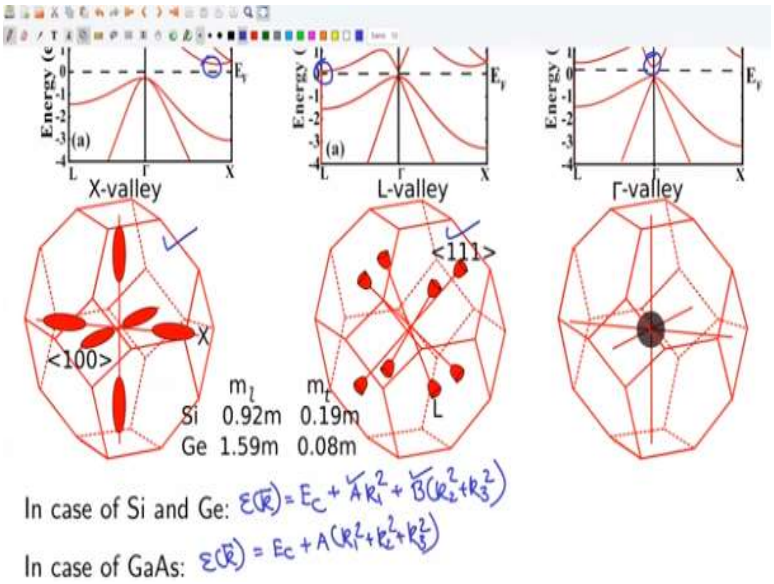

In case of silicon and germanium equation of the constant energy ellipsoid is E K = E C; which is the conduction band minimum + A K 1 square + B K 2 square + K 3 square. Note that we need 2 constants A and B because we have to fit and ellipsoid in case of gallium arsenide the constant

energy surface is E K = E C + a A K 1 square +B K 2 square + K 3. In this case we need only 1 constant a because the constant energy surface is a sphere.

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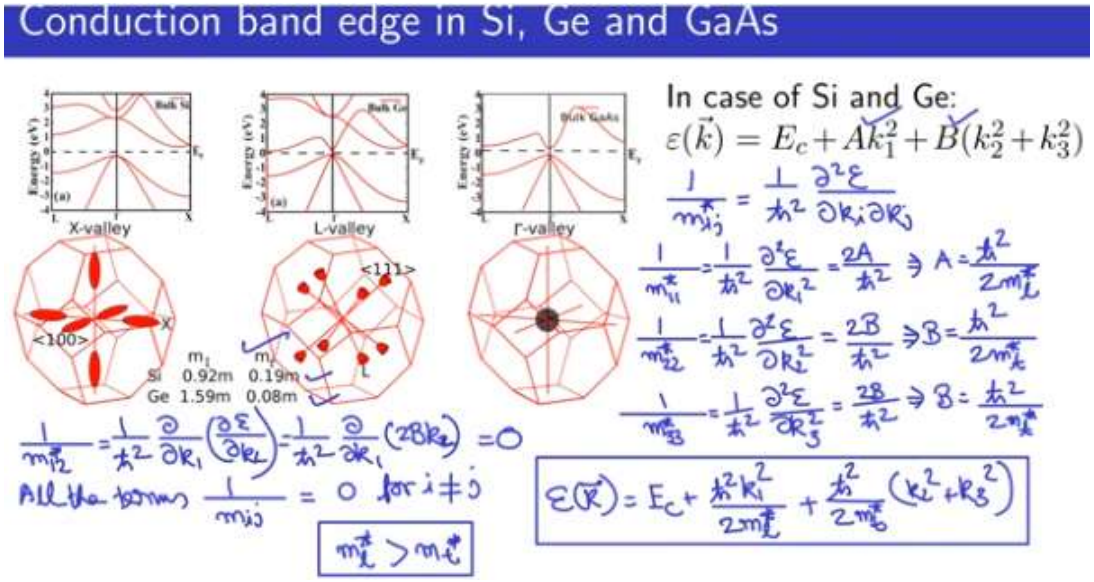

We know the equation of constant energy ellipsoid in k-space. Now let us calculate the effective mass, effective mass is defined as

$$\frac{1}{m_{ij}^*} = \frac{1}{\hbar}\frac{\partial^2 \varepsilon}{\partial k_i \partial k_j}$$

$$\frac{1}{m_{11}^*} = \frac{1}{\hbar}\frac{\partial^2 \varepsilon}{\partial k_1^2} = \frac{2A}{\hbar^2} \Rightarrow A = \frac{\hbar^2}{2m_l^*}$$
$$\frac{1}{m_{22}^*} = \frac{1}{\hbar}\frac{\partial^2 \varepsilon}{\partial k_2^2} = \frac{2B}{\hbar^2} \Rightarrow B = \frac{\hbar^2}{2m_t^*}$$

Similarly,

$$\frac{1}{m_{33}^*} = \frac{1}{\hbar}\frac{\partial^2 \varepsilon}{\partial k_3^2} = \frac{2B}{\hbar^2} \Rightarrow B = \frac{\hbar^2}{2m_t^*}$$

Note that $m_{22} = m_{33}$ and I write both of them as m_t.

Now let us calculate this term

$$\frac{1}{m_{12}^*} = \frac{1}{\hbar^2}\frac{\partial}{\partial k_1}\left(\frac{\partial \varepsilon}{\partial k_L}\right) = \frac{1}{\hbar^2}\frac{\partial}{\partial k_1}(2Bk_2) = 0$$

Thus we can conclude that all the terms

$$\frac{1}{m_{ij}} = 0 \text{ for } i \neq j$$

Equation of the constant energy ellipsoid now can be written in terms of effective mass and

$$\varepsilon(\vec{k}) = E_c + \frac{\hbar^2 k_1^2}{2m_l^*} + \frac{\hbar^2}{2m_t^*}(k_2^2 + k_3^2)$$

Note that m l star is the major axis and m t star is the minor axis of the ellipsoid $m_l^* > m_t^*$. Value for effective mass in l for longitudinal and p for transverse direction for silicon and germanium are reported in this table. Note that the anisotropy of effective mass in case of germanium is much higher than the anisotropy of effective mass in case of silicon.

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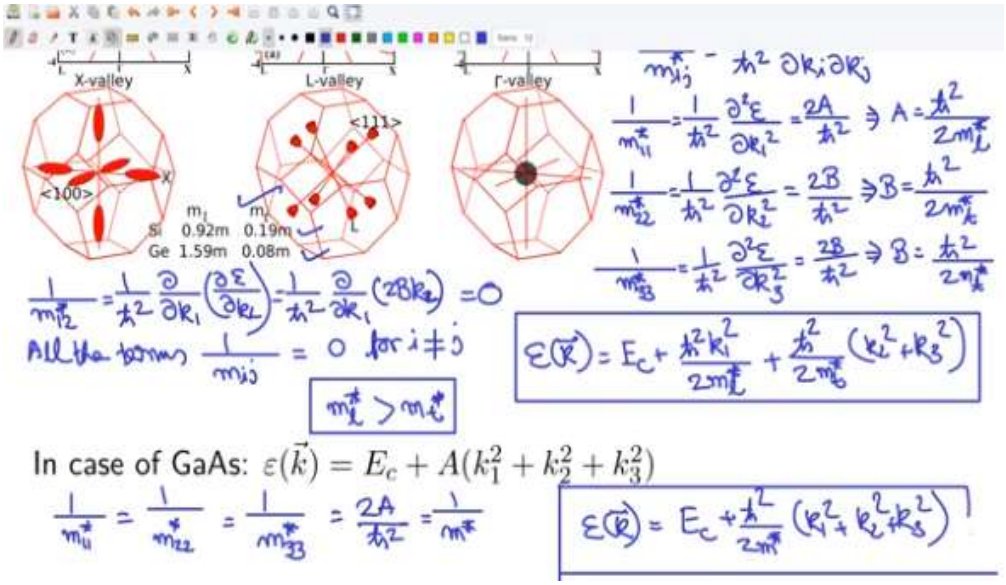

In case of gallium arsenide effective mass in all the directions are equal as the constant energy surface is spherical. Thus 1 by m 1 1 star = 1 by m 2 2 star = 1 by m 3 3 star = 2 A by h cross square; and I just write it as 1 by m star. And the equation of constant energy surface is

$$\varepsilon(\vec{k}) = E_c + \frac{\hbar^2}{m^*}(k_1^2 + k_2^2 + k_3^2)$$

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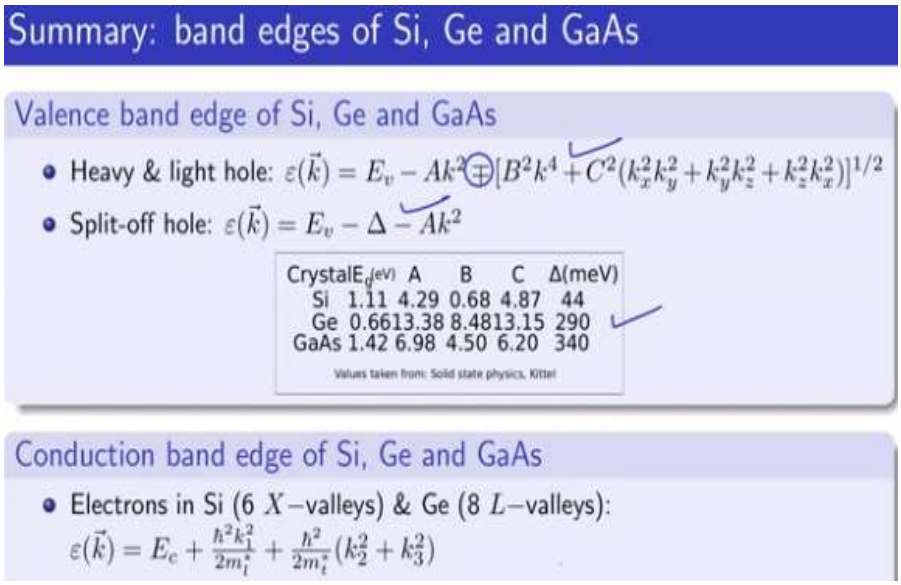

This is the summary of what we discussed about band edges of silicon germanium and gallium arsenide. The valence band edges are not simple we have 1 heavy hole band and 1 light hole band degenerate at the gamma point. The constant energy surfaces corresponding to heavy and light fold band are not spherical and given by this expression. The choice of sign distinguishes the heavy and light hole effective mass.

There is another band split off from the heavy and light hole band at the gamma point due to the spin orbit coupling. This is known as the split of whole band the constant energy surface is given by these expression relevant parameters are given in this table.

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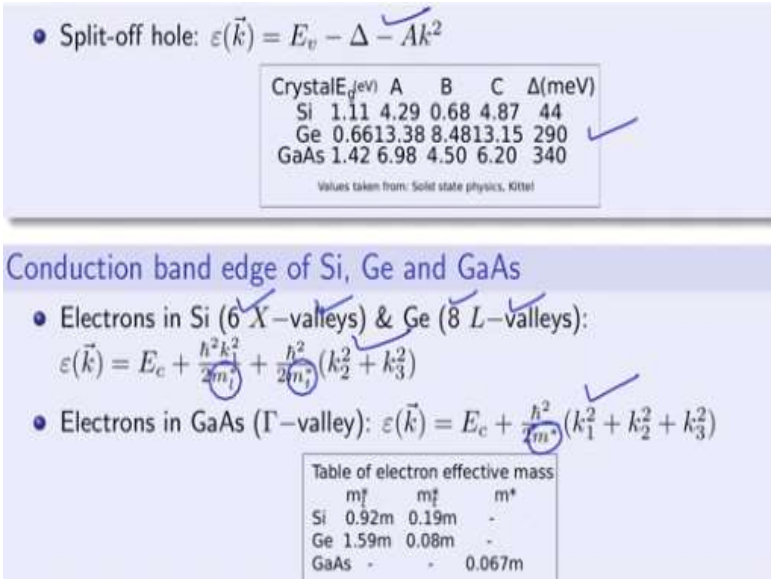

Constant energy surfaces or electrons in silicon and germanium are ellipsoids given by this expression. There are 6 ellipsoids for silicon near 6 X values and there are 8 ellipsoids for germanium near the 8 L valleys. M l star is the longitudinal effective mass which is greater than the transverse effective mass m t star. In case of gallium arsenide constant energy surface is spherical given by this expression and effective mass m star is isotropic electron effective masses are reported in this table