1. CHARGE CARRIERS IN SEMICONDUCTORS

(A).   The doping type of a semiconductor can be determined from the steady-state equilibrium position of the Fermi level, E_F, with respect to the intrinsic energy level, E_i. The Fermi level is the energy of a state that has a probability of 1/2 of being occupied by an electron (assuming there is actually an available state). If the Fermi level is closer to the conduction band (above E_i) then there is a higher concentration of electrons in the conduction band than holes in the valence band and the material is *n*-type. Conversely, if the Fermi level is closer to the valence band (below E_i) then there is a higher concentration of holes in the valence band compared to electrons in the conduction band and the material is *p*-type. Along with the fact that E_i is located at approximately the middle of the band gap, we can see that region (1) is *n*-type, region (2) is *p*-type, region (3) is *n*-type, and region (4) is *p*-type .

(B).   The real-space energy diagram drawn in this problem represents the energy bands and hole energies as a function of some zero-energy reference level (typically this E = 0 eV level is chosen to be the upper-most valence band, which in this case is located in region (2)). In the case of holes, the energy of a hole increases the further down you go from the valence band, so hole (3) has the highest total energy, holes (1) and (2) have the second highest, and hole (4) has the lowest total energy. The energy band diagram also gives the potential energy at each position in the semiconductor. Similar to a ball on a hill, a hole located exactly at the valence band will have potential energy equal to the energy difference between that valence band and the upper-most valence band (if a hole is located at the upper-most valence band it is said to have no potential energy). Thus, hole (3) has the highest potential energy and hole (2) has the lowest potential energy .

(C).   From example 3-2, it is shown that the band diagram in **k**-space is parabolic and representative of the electron or hole's kinetic energy (meaning that if a hole has a non-zero wavevector **k**, it has non-zero kinetic energy). When **k** = 0 (the vertex of the parabola), the **k**-space energy diagram is touching the valence band of the real-space band diagram, like so:
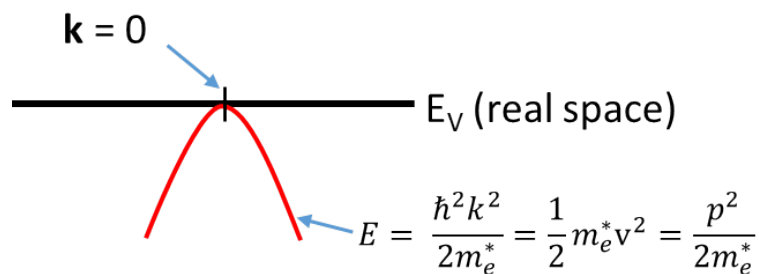

Figure 1.1: Real-space energy diagram showing the valence band edge E_V and the **k**-space relationship for a free hole in the valence band.

As seen in the previous figure, the further the hole is from the valence band (the higher up it is on the **k**-space diagram) the more kinetic energy it has, seen in the following figure:
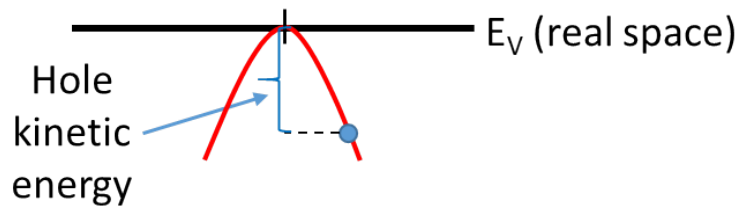
Figure 1.2: The further the hole is from the valence band (the higher up it is on the **k**-space diagram) the more kinetic energy it has.

Either of the two diagrams above are acceptable . Using these facts, hole (2) has the highest kinetic energy while hole (1) has the lowest kinetic energy .

(D).   The occupation probability is given by the Fermi function, Equation 3-10 in the book:

$$f(E) \;=\; \frac{1}{1 + e^{(E - E_F)/kT}} \tag{1.1}$$

However, this equation is the occupation probability for **electrons**. If a state is not occupied by an electron then it is by default occupied by a hole. Since the probability of a state being occupied by either an electron or a hole is 1, we can subtract the Fermi function from 1 to get the occupation probability of a hole:

$$f_{\text{hole}}(E) \;=\; 1 - \frac{1}{1 + e^{(E - E_F)/kT}} \tag{1.2}$$

As the quantity $E - E_F$ becomes more negative, representative of moving down from the Fermi level which applies for holes in the valence band, f_{hole} becomes smaller. Thus, the further a hole state in the valence band is from the Fermi level, the smaller the chance is that it will be occupied by a hole. Knowing this, the energy state of hole (4) has the highest occupation probability while the energy state of hole (3) has the lowest occupation probability .

2. DOPING IN A SEMICONDUCTOR

GaAs is a III-V semiconductor (**Ga** - group III, **As** - group V), while **Si** is a group IV atom. If a group IV atom replaces a group V atom, there will be an extra hole that can easily be thermalized into the valence band by the excitation of an electron from the valence band into the acceptor impurity level. So if **Si** (IV) replaces only **As** (V), the semiconductor is doped *p*-type .

If $\frac{3}{5}$ of the **Si** atoms replace **As** while $\frac{2}{5}$ of the **Si** atoms replace **Ga**, the material is still doped *p*-type (there are more free holes in the valence band than free electrons in the conduction band since more **As** atoms are replaced than **Ga** atoms). However, the doping compared to the previous situation is $\frac{3}{5}$ - $\frac{2}{5}$ = $\frac{1}{5}$ the amount (due to the extra electrons created by **Si** replacing **Ga** and the reduction in free holes since those **Si** atoms don't replace **As**). This is a very common doping method and is known as counter-doping or compensation.

Si is known as an amphoteric dopant. At low temperature (T $\sim$ 700 °C), **Si** prefers to replace **As** atoms and act as an acceptor, while at high temperatures (T $\sim$ 900 °C), **Si** prefers to replace **Ga** atoms and act as a donor. Also, if using **Si** in a **GaAs** melt, a large concentration of **Si** will produce an *n*-type material while a small concentration will actually produce a *p*-type **GaAs** semiconductor.

3.   THE FERMI DISTRIBUTION AND DOPING

(A).   The electron concentration n_0 can be easily calculated using Equation 3-24 in the book:

$$n_0 p_0 = n_i^2 \tag{3.1}$$

Solving for n_0 gives:

$$n_0 = \frac{n_i^2}{p_0} = 5 \times 10^{13} \text{ cm}^{-3} \tag{3.2}$$

Since the equilibrium electron concentration is higher than the equilibrium hole concentration, the material is *n*-type doped . This can be seen without even solving for n_0 since the hole concentration given in the problem is less than the intrinsic carrier concentration n_i. If the material is intrinsic then $p_0 = n_0 = n_i$. Doping the semiconductor will increase or decrease p_0 or n_0 depending on the doping type.

(B).   This part can be solved using either n_0 (Equation 3-25a) or p_0 (Equation 3-25b) and solving for (E_F - E_i) or (E_i - E_F), respectively. Since we know the material is *n*-type, E_F will be above E_i and we will use Equation 3-25a:

$$n_0 = n_i e^{(E_F - E_i)/kT} \tag{3.3}$$

Solving for (E_F - E_i) and using kT = 25.9 meV:

$$(E_F - E_i) = kT * \ln\left(\frac{n_o}{n_i}\right) = 0.441 \text{ eV} \tag{3.4}$$

(C).   The answer to this part is simply the definition of the Fermi level. The occupation probability of an energy state at the Fermi level is 1/2 .

(D).   The occupation probability can be calculated using the Fermi function and the energy of the conduction band, E_C:

$$f(E_C) = \frac{1}{1 + e^{(E_C - E_F)/kT}} \tag{3.5}$$

In order to arrive at an answer we need the difference between the conduction band energy level and the Fermi level. In part (b) you calculated the quantity (E_F - E_i). Since you were told to assume E_i is at the center of the band gap, we know that (E_C - E_i) = E_g/2. The band gap of GaAs at room temperature can be found in Appendix III of the book and is 1.43 eV. (E_C - E_F) = (E_C - E_i) - (E_F - E_i) = E_g/2 - (E_F - E_i):

$$(E_C - E_F) = \frac{E_G}{2} - (E_F - E_i) = 0.715 - 0.441 = 0.274 \text{ eV} \tag{3.6}$$

Plugging this value into the Fermi function and using kT = 25.9 meV, we find the occupation probability to be:

$$f(E_C) = \frac{1}{1 + e^{(E_C - E_F)/kT}} = \frac{1}{1 + e^{(0.274)/0.0259}} = 2.54 \times 10^{-5} \tag{3.7}$$

(E). The real-space energy band diagram should look like the following (labeling the difference between E_i and E_V is not necessary):
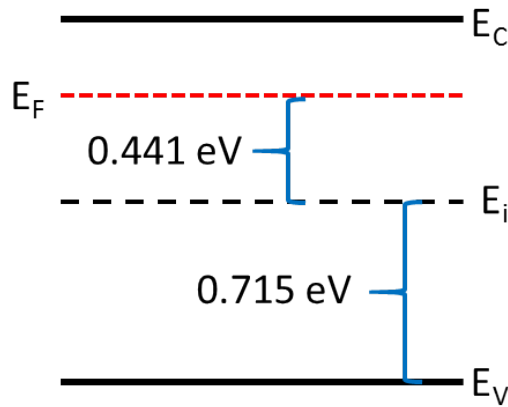

Figure 3.1: Real-space energy diagram showing the conduction band, valence band, the Fermi level, the intrinsic energy level, and the quantity E_F - E_i.

(F). In part (b) you calculated (E_F - E_i) tp be 0.441 eV. Now, (E_F - E_i) is equal to a third of that value, which is 0.147 eV. Solving for n_0 using Equation 3-25a and using kT = 25.9 meV:

$$n_0 = n_i e^{(E_F - E_i)/kT} = 2 \times 10^6 * e^{(0.147)/0.0259} = 5.8 \times 10^8 \text{ cm}^{-3} \tag{3.8}$$

We can then use Equation 3-24 to solve for p_0:

$$p_0 = \frac{n_i^2}{n_0} = 6.9 \times 10^3 \text{ cm}^{-3} \tag{3.9}$$

4. THE INTRINSIC ENERGY LEVEL

(A). The first thing to note is that this is not room temperature, so kT is not equal to 25.9 meV. Instead, we must recalculate the value of kT using T = 500K. Since k = 8.62×10^{-5} eV/K, kT = 0.0431 eV or 43.1 meV. We know the band gap of the semiconductor along with the effective density of states at the conduction and valence band edges and using these we can solve for the intrinsic carrier concentration with Equation 3-23:

$$n_i = \sqrt{(N_C N_V)}e^{-E_g/2kT} = 3.24 \times 10^{14} \text{ cm}^{-3} \tag{4.1}$$

Since we were given the value of the equilibrium electron concentration, we can solve for p_0 using Equation 3-24:

$$p_0 = \frac{n_i^2}{n_0} = 2.1 \times 10^{17} \text{ cm}^{-3} \tag{4.2}$$

(B). Solving for the difference between E_F and E_i is the same as in the previous problem. However, we can tell from the fact that p_0 is greater than n_i and greater than n_0 that the material is *p*-type doped . This means E_F will be below E_i so we should use Equation 3-25b and solve for (E_i - E_F), once again remembering that since we are at T = 500K, kT = 0.0431 eV:

$$(E_i - E_F) = kT * \ln\left(\frac{p_o}{n_i}\right) = 0.279 \text{ eV} \tag{4.3}$$

(C). For this part, we need to calculate how far E_i is from the center of the band gap. This difference will be labeled simply as ΔE_i from this point. The first thing to note is that we can write ΔE_i as (E_i - E_V) - E_g/2. If this quantity is negative then we know that E_i is closer to the valence band than the conduction band and if it is positive then we know E_i is closer to the conduction band than the valence band. The quantity (E_i - E_V) = (E_i - E_F) + (E_F - E_V). (E_F - E_V) can be calculated from Equation 3-19:

$$(E_F - E_V) = -kT * \ln\left(\frac{p_o}{N_v}\right) = 0.16 \text{ eV} \tag{4.4}$$

Using the value of (E_i - E_F) calculated in part (b) we can solve for (E_i - E_V):

$$(E_i - E_V) = (E_i - E_F) + (E_F - E_V) = 0.16 + 0.279 = 0.439 \text{ eV} \tag{4.5}$$

We can now calculate ΔE_i:

$$\Delta E_i = (E_i - E_V) - \frac{E_g}{2} = 0.439 - 0.375 = 0.064 \text{ eV} = 64 \text{ meV} \tag{4.6}$$

Thus, <mark>E_i is actually 6.4 meV above the center of the band gap</mark>. This is due to the difference in the electron and hole effective masses, which changes the shape of the parabola of the (E,**k**) relationship and the effective density of states at the band edges. It is easiest to think of what happens to E_i by assuming an intrinsic semiconductor, so $n_0 = p_0 = n_i$. If the effective density of states at the conduction band edge, N_c, is less than the effective density of states at the valence band edge, N_v, there are fewer states per unit volume at the conduction band edge for electrons to occupy compared to the number of states per unit volume that holes can occupy at the valence band edge. Since E_F is located at E_i in an intrinsic semiconductor, the concentration of electrons in the conduction band, n_0, will be less than the concentration of holes in the valence band, p_0, if E_i is located at the center of the band gap. Since we know this cannot be true for an intrinsic semiconductor, E_i (and by association E_F) must shift upwards towards the conduction band. Just like in an n-type doped semiconductor, n_0 will increase and p_0 will decrease. Since the semiconductor is intrinsic, when they are both equal to each other and to n_i, E_i is in the correct position.

As it turns out, when the electron effective mass is smaller than the hole effective mass, N_c is less than N_v and the intrinsic energy level E_i is closer to the conduction band than the valence band. If the hole effective mass is less than the electron effective mass, E_i is closer to the valence band than the conduction band.