

Problem 3 (a)

The bandgap of Si as found from the band structure lab is around 1.13 eV.

Problem 3 (b)

The band structure for a 3x3 nm rectangular nanowire is shown in Figure 3. The band gap in the nanowire is 1.51 eV.

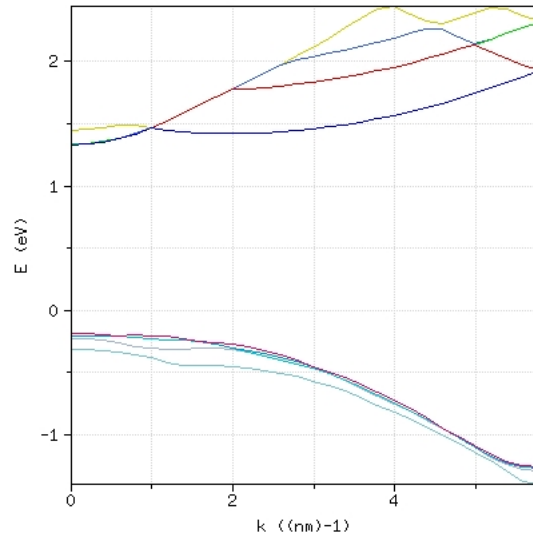


Figure 3: 3nm Si Nanowire Bandstructure

Problem 3 (c)

The band structure for a 4x4 nm rectangular nanowire is shown in Figure 4. The band gap in the nanowire is 1.37 eV.

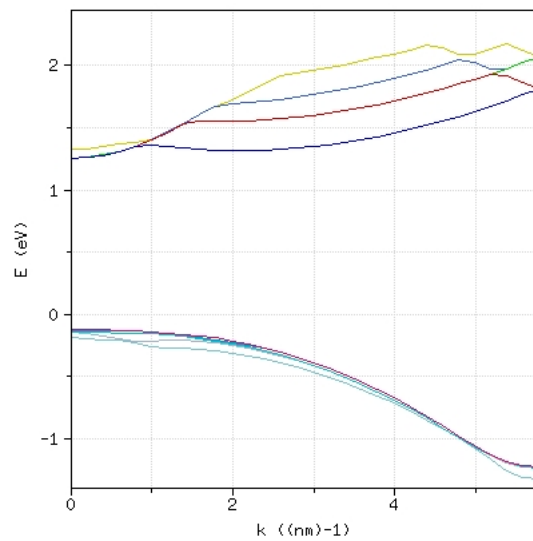


Figure 4: 4nm Si Nanowire Bandstructure

Problem 3 (d)

The rectangular nanowire boundaries confine the electrons in two directions, say x and y . Only the z direction is free. As the wire boundaries spread out, the quantum wells in each direction expand. As the quantum wells expand the spacing of the k values decreases ($2\pi/L_{(x,y)}$). This results in an increased number of energy levels and a decrease in their separation. As a result, the nanowire band structure begins to approach the bulk band structure which has a lower band gap.

Problem 3 (e)

There are many physical parameters that will change as a result of the dimensions of the nanowire. The effective mass will be different as the bands in the nanowire are sharper (lower effective mass). Additionally, the confinement will make the density of states in the nanowire quite different than bulk silicon. This in turn will make the carrier concentrations different in the nanowire than in bulk.

Problem 3 (f)

In essence, the z direction has no confinement and will follow the traditional band structure in this dimension (e.g. parabolic). However, the confinement in the other two directions causes the allowed energy levels to take discrete values as they did in the classical quantum well problem. The way to think of this is that there are two energy sub-bands (each confined direction) and a single dispersion relation that should be considered (the free direction). These energy sub-bands are classified by the traditional particle in a box problem, $E = n^2\hbar^2\pi^2/2mL_{(x,y)}^2$.

Problem 3 (g)

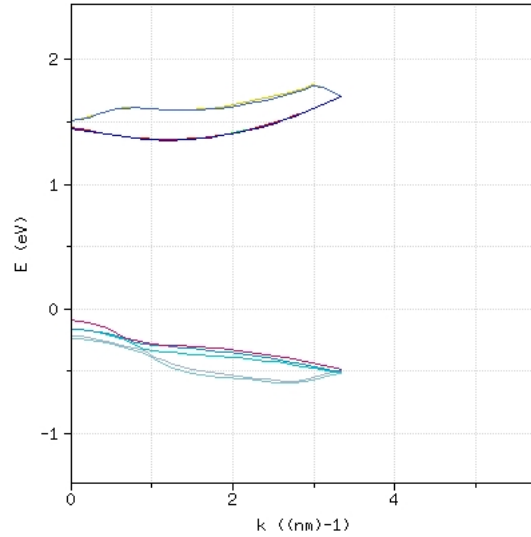


Figure 5: 3nm Si Nanowire Bandstructure along [111] transport direction

Unlike the [100]-oriented Si nanowire, the [111]-oriented one has indirect bandgap 1.44 eV. The most significant difference between these two wires is the effective mass. According to the data given by the Bandstructure Lab, the effective masses of [100] and [111] wires are $1.33 m_0$ and $1.44 m_0$ respectively. As a result, we can conclude that electron must have lower injection velocity in the [111] wire due to the higher effective mass. For more detailed discussion, please see [2].

References

- [1] S. Das Sarma, S. Adam, E. H. Hwang, and E. Rossi. Electronic transport in two-dimensional graphene. *Rev. Mod. Phys.*, 83:407–470, May 2011.
- [2] N. Neophytou, A. Paul, M. S. Lundstrom, and G. Klimeck. Bandstructure effects in silicon nanowire electron transport. *IEEE TRANSACTIONS ON ELECTRON DEVICES*, 55:1286 – 1297, June 2008.

$$n = \frac{N_D - N_A}{2} + \left[\left(\frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2} \quad (7)$$

$$p = \frac{N_A - N_D}{2} + \left[\left(\frac{N_A - N_D}{2} \right)^2 + n_i^2 \right]^{1/2} \quad (8)$$

At 300 K, the intrinsic carrier concentration in Si is $1 \times 10^{10} \text{ (cm}^{-3}\text{)}$. With the provided doping concentration, $N_D \gg n_i$. This means that the material is in the extrinsic region so that the carrier concentration is equivalent to the doner concentration in the conduction band. Therefore

$$n \approx N_D = 10^{14} / \text{cm}^3 \quad (9)$$

$$p \approx n_i^2 / N_D = 10^6 / \text{cm}^3 \quad (10)$$

Problem 2 (b)

At 300 K, the intrinsic carrier concentration in Si is $1 \times 10^{10} \text{ (cm}^{-3}\text{)}$. With the provided doping concentration, $N_A \gg n_i$. This means that the materials in in the extrinsic region so that the carrier concentration is equivalent to the acceptor concentration in the valence band. Therefore

$$p \approx N_A = 10^{15} / \text{cm}^3 \quad (11)$$

$$n \approx n_i^2 / N_A = 10^5 / \text{cm}^3 \quad (12)$$

Problem 2 (c)

At 300 K, the intrinsic carrier concentration in Si is $1 \times 10^{10} \text{ (cm}^{-3}\text{)}$. With the provided doping concentrations, $N_D - N_A = 10^{15} / \text{cm}^3$. This difference is much larger than the intrinsic carrier concentration so it is still in the extrinsic region. In this scenario, N_D is not significantly larger than N_A and equations 4.79a and 4.79b from ASF should be used:

$$n = N_D = 10^{15} / \text{cm}^3 \quad (13)$$

$$p = n_i^2 / N_D = 10^5 / \text{cm}^3 \quad (14)$$

Problem 2 (d)

At 470 K, the intrinsic carrier concentration in Si is approximately $1 \times 10^{14} \text{ (cm}^{-3}\text{)}$. Again using the equations in ASF:

$$n = N_D = 1.618 \times 10^{14} / \text{cm}^3 \quad (15)$$

$$p = n_i^2 / N_D = 6.180 \times 10^{13} / \text{cm}^3 \quad (16)$$

At this temperature, Silicon is beginning enter the intrinsic region where $n \approx n_i$ and no longer N_D .

Problem 2 (e)

At 645 K, the intrinsic carrier concentration in Si is about $1 \times 10^{16} \text{ (cm}^{-3}\text{)}$. In this situation, the device is in the intrinsic region, $n_i \gg |N_D - N_A|$, where the carrier concentration is dominated by the number of intrinsic carriers:

$$n_i \approx n = 1 \times 10^{16} \text{ cm}^{-3} \quad (17)$$

$$n_i \approx p = n_i^2/n = 1 \times 10^{16} \text{ cm}^{-3} \quad (18)$$

Problem 3 (a)

At 545 K, Si has an intrinsic carrier concentration of approximately $10^{15}/\text{cm}^3$. Using the following equations from ASF, the electron and hole concentrations can be found:

$$n = \frac{N_D - N_A}{2} + \left[\left(\frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2} \quad (19)$$

$$p = \frac{N_A - N_D}{2} + \left[\left(\frac{N_A - N_D}{2} \right)^2 + n_i^2 \right]^{1/2} \quad (20)$$

Table 1: Carrier Concentrations in Si at 545 K v N_D

Donor Doping (N_D)(cm^{-3})	Electron (n) (cm^{-3})	Hole (p)(cm^{-3})
10^{13}	1.005×10^{15}	9.9501×10^{14}
10^{14}	1.051×10^{15}	9.5123×10^{14}
10^{15}	1.618×10^{15}	6.1803×10^{14}
10^{16}	1.010×10^{16}	9.9020×10^{13}
10^{17}	1.000×10^{17}	9.9990×10^{12}

This table shows that at large doping concentrations, the material is in the extrinsic operating region, but at $10^{15}/\text{cm}^3$ the material begins to obey an intrinsic relation.

Problem 3 (b)

The intrinsic energy level E_i can be found using ASF 4.86:

$$E_i = \frac{E_c + E_v}{2} + \frac{3}{4}kT \ln(m_p^*/m_n^*) \quad (21)$$

For this calculation, I am assuming that the effective mass ratio's dependence on temperature will be minimal and can be safely approximated by the 300 K ratio of .685. Using Figure 4.19 from ASF, the band gap is approximately 1.06 eV.

$$E_i = \frac{1.2\text{eV}}{2} + \frac{3}{4}(8.617 \times 10^{-5}\text{eV K}^{-1})(545\text{K}) \ln(0.685) = 0.5117 \text{ eV} \quad (22)$$

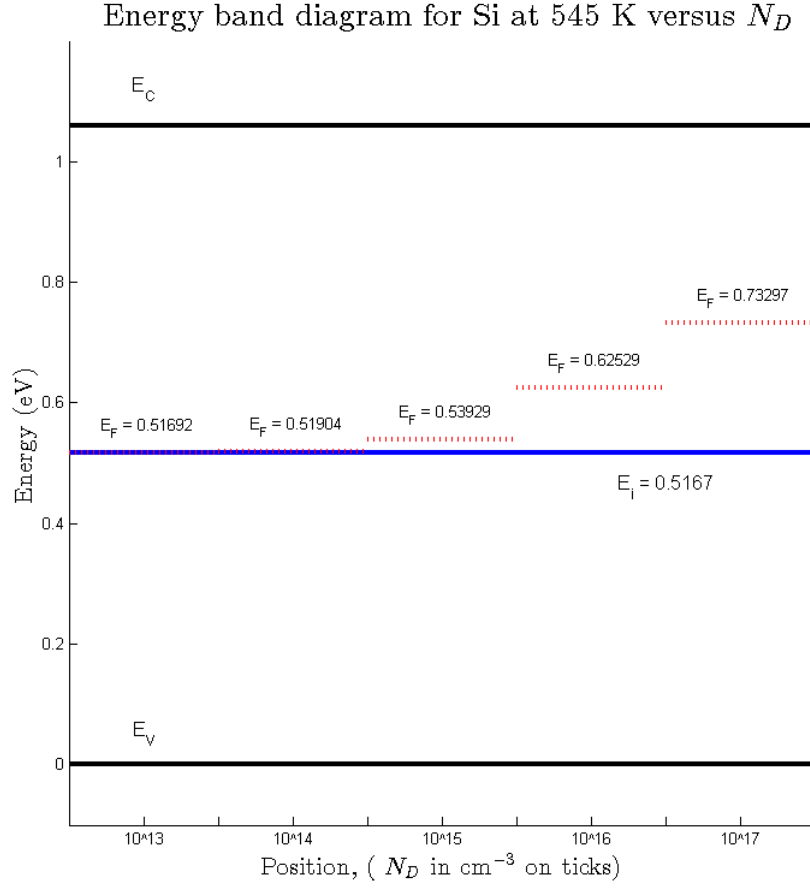


Figure 1: Band Diagram for Si versus Doping Concentration

Table 2: $E_F - E_i$ v Donor Doping Concentration (cm^{-3})

Donor Doping (N_D)(cm^{-3})	$E_F - E_i$	E_F
10^{13}	0.0002	0.5169
10^{14}	0.0023	0.5190
10^{15}	0.0226	0.5393
10^{16}	0.1086	0.6253
10^{17}	0.2163	0.7330

using the valence band as the reference. With this value and ASF 4.89 (shown below), the $E_F - E_i$ relation can be computed for each sample

$$E_F - E_i = kT \ln(n/n_i) \quad (23)$$

The band diagrams derived from these results are shown in Figure 1.

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Fall 2025 ECE 60600 Homework 4 Problem 4 Solution

Monday, September 29, 2025 12:08 PM

The process of drawing band diagram is outlined in the following recorded lectures

<https://nanohub.org/courses/ECE606Alam/01a/outline/week8pnandmsdiodeelectrostatics-i-vcharacteristics/lecture20electrostaticsofp-njunctiondiodes> (35:00-40:00)

[ECE 606 Solid State Devices L19.2: PN Junctions - Drawing Band-Diagrams in Equilibrium](#) (1:53-4:40)

