ELECTRICAL AND
COMPUTER ENGINEERING
PURDUE UNIVERSITY

Heterostructure Tutorial

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1. Introduction

This tutorial is companion notes for Notes on Heterostructure Fundamentals written by Professor Mark S. Lundstrom [1]. The purpose of this tutorial is to help students learn to work with problems related to heterostructures by stepping through a series of excises.

This tutorial contains a set of exercises related to heterojunctions. The first part of tutorial will work on examples of drawing energy band diagram for abrupt heterojunctions. The first five examples are related to different doping profile $Al_{0.3}Ga_{0.7}As$/GaAs Heterojunction. The last example in part I is to draw energy band diagram for $In_{0.8}Ga_{0.2}As$/GaP n-P heterojunction. The second part of the tutorial will work on examples of drawing energy band diagram for graded heterojunctions and computing the grading distance. The first example of Part II will deal with $Al_{0.3}Ga_{0.7}As$/GaAs Heterojunction with different grading distance to see which grading distance to good enough get rid of the spike in energy band diagram for abrupt heterojunctions. The second example of Part II will calculate the grading distance needed to get rid of the spike in the energy band diagram for abrupt heterojunctions. The third part of the tutorial will work on I-V characteristics of heterojunctions.

In the tutorial, we will use a simulation program called Adept to plot energy band diagram for heterojunctions. In addition, Adept will plot the I-V characteristics for us in Part III of the tutorial. Adept is a simulation program on the Web. Go to Simulation Hub on Web. The WWW address for it is: http://www.ecn.purdue.edu/labs/punch Click on the list of Hubs. Then select Semiconductor Simulation Hub. Use guess acess to get in and select tools. Then, you will see a list of tools in Semiconductor Simulation Hub. Select Adept and go to first step of Run Adept -- Modify/Create Adept Input files. Go to example folder. You will find all input files for this tutorial under tutorial directory.

2. Part I: Energy Bands in Abrupt Heterojunctions

Example 1: Draw energy band diagram for $Al_{0.3}Ga_{0.7}As$/GaAs N-p Heterojunction under equilibrium condition.

Material parameters for $Al_{0.3}Ga_{0.7}As$:

E_G = 1.797eV	χ = 3.827	N_C = 0.857e18 cm^{-3}	N_V = 0.111e20 cm^{-3}
ni = 0.255e04 cm^{-3}	κ= 11.9	mng = 0.08034	mp = 0.57941
N_D = 1.0e16 cm^{-3}	N_A = 0.00		

Material parameters for GaAs:

E_G = 1.422eV	χ = 4.070	N_C = 0.462e18 cm^{-3}	N_V = 0.942e19 cm^{-3}
ni = 0.238e07 cm^{-3}	κ= 12.847	mng = 0.06700	mp = 0.5200
N_D = 0.00	N_A = 1.0e16 cm^{-3}		

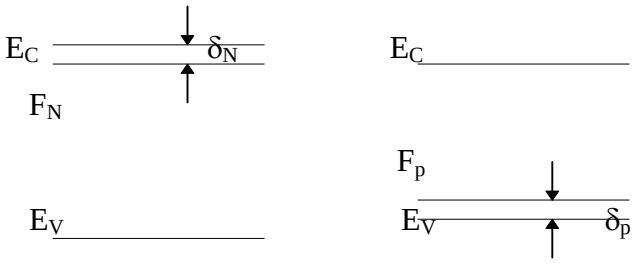
Note: The material parameters are also avaliable in the Semiconductor Simulation Hub Semiconductor Database on line.

Step1: Draw energy band diagram for isolated N type $Al_{0.3}Ga_{0.7}As$ and p type GaAs separatly.

Useful parameters:

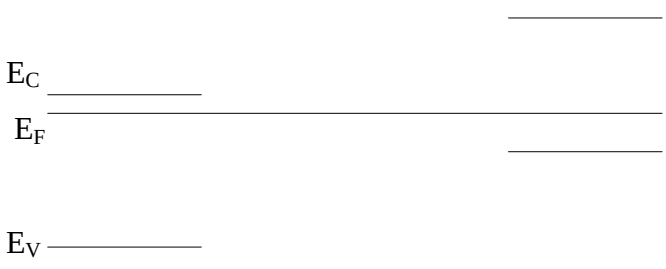
$$\delta_N = k*T*\log(N_C/n_0) = 0.0259*\log(0.875e18/1.0e16) = 0.115eV$$

$$\delta_p = k*T*\log(N_V/p_0) = 0.0259*\log(0.942e19/1.0e16) = 0.177eV$$



Step 2: Draw the trivial part of the energy band diagram after we put two material together.

We know that Fermi Level is a constant independent of position. So, we can draw a straight line for Fermi level. Then, it is reasonable to expect that regions for far away from the heterojunction to be identical in character to the isolated semiconductor.



Step 3: Draw the missing near-junction portion of the energy band diagram.

Go back to step 1 and take a look at the isolated energy band diagram. Since p tyep GaAs has a lower Fermi Level, electrons will flow to p side of junction when we put two material together. So, N side valence and conduction band will bend up and p side valence and conduction band will bend down. In addition, another important thing to keep in mind -- after putting two materials together, ΔE_C and ΔE_V will keep the same.

Step 4: Check energy band diagram by using Adept in Semiconductor Simulation Hub.

Go to Adept program on the Web. The simulation input file for this example will be found uner tutorial directory in the example folder with file name *example1*. Follow First Timer User's Guide in Adept to do the simulation. Also, check the energy band digram drawn by Adept by calculating the following parameters.

$$qV_{bi} = (\chi_p - \chi_N) + E_{Gp} - \delta_p - \delta_N = (4.07 - 3.827) + 1.422 - 0.115 - 0.177 = 1.373eV$$

$$V_{bi} = 1.373V$$

$$V_{Jp} = V_{bi} * [\frac{\kappa_N N_D}{\kappa_N N_D + \kappa_p N_A}] = 1.373 * [\frac{11.9 * 1.0e16}{11.9 * 1.0e16 + 12.847 * 1.0e16}] = 0.660V$$

$$\frac{V_{jp}}{V_{JN}} = \frac{\kappa_N N_D}{\kappa_p N_A}$$

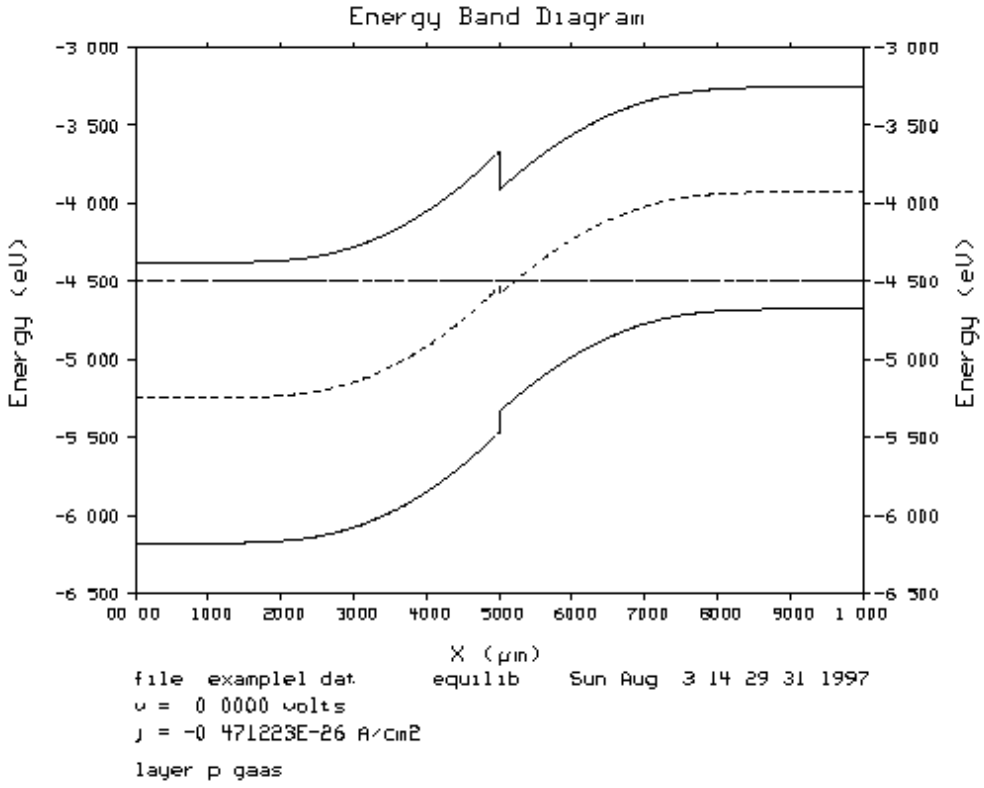
$$V_{JN} = V_{jp} * \frac{\kappa_p N_A}{\kappa_N N_D} = 0.660 * \frac{12.847 * 1.0e16}{11.9 * 1.0e16} = 0.713V$$

$$x_p = [\frac{2\kappa_p \varepsilon_0 V_{Jp}}{qN_A}]^{\frac{1}{2}} = [\frac{2*12.847*8.85e-14*0.660}{1.6e-19*1.0e16}]^{\frac{1}{2}} = 3.02e-05cm$$

$$N_A x_p = N_D x_N$$

$$x_N = \frac{N_A x_p}{N_D} = \frac{1.0e16*3.02e-05}{1.0e16} = 3.02e-05cm$$

Here is the complete energy band diagram generated by Adept:



Example 2: Draw energy band diagram for $Al_{0.3}Ga_{0.7}As$/GaAs N-p+ Heterojunction under equilibrium condition. What difference would you expect to see from example 1?

$Al_{0.3}Ga_{0.7}As$: $N_D = 1.0e16\ cm^{-3}$

GaAs: $N_A = 5.0e19\ cm^{-3}$

Step 1: Follow the first three steps in example 1 to draw the energy band diagram for this heterojunction.

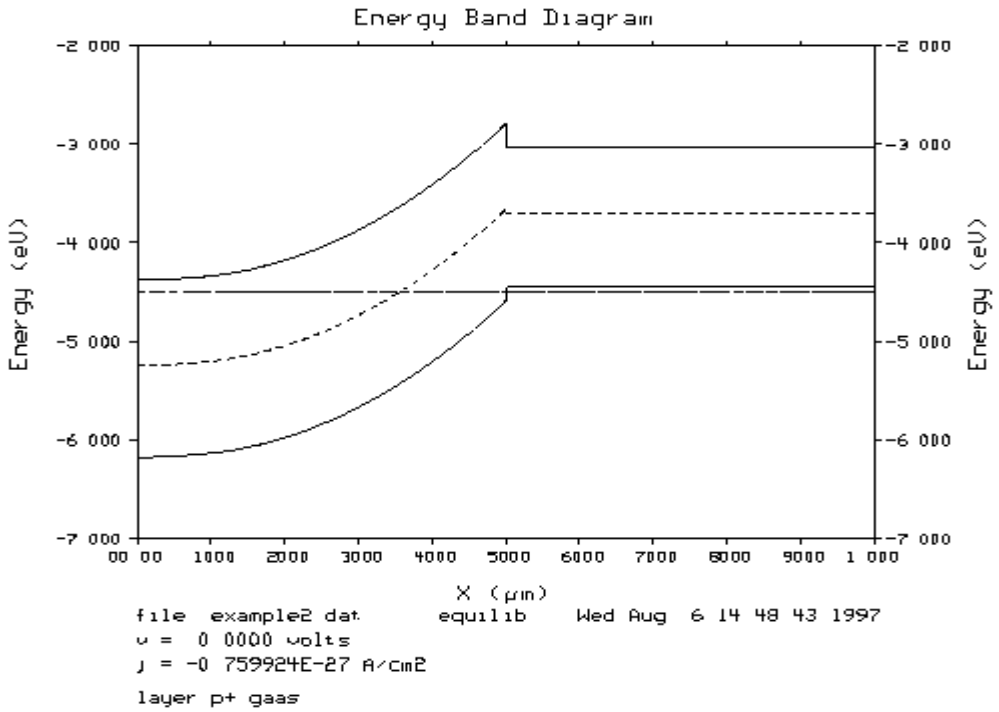
$$\delta_N = k * T * \log(N_C / n_0) = 0.0259 * \log(0.875e18 / 1.0e16) = 0.115eV$$

$$\delta_p = k * T * \log(N_V / p_0) = 0.0259 * \log(0.942e19 / 5.0e19) = -0.043eV$$

Step 2: Check the energy band diagram by using Adept in Semiconductor Simulation Hub.

Modify the input file for example 1 and see if you can get the right energy band diagram. You can check your input file by going to example folder and looking into *example2* under tutorial directory. Check the energy band diagram by calculating the same parameters as in example 1.

Here is the energy band diagram generated by Adept:



Example 3: Draw energy band diagram for $Al_{0.3}Ga_{0.7}As$/GaAs P-n Heterojunction under equilibrium condition. What difference would you expect to see from example 1?

$Al_{0.3}Ga_{0.7}As$: $N_A = 1.0e16\ cm^{-3}$

GaAs: $N_D = 1.0e16\ cm^{-3}$

Step 1: Follow the first three steps in example 1 to draw the energy band diagram for this heterojunction.

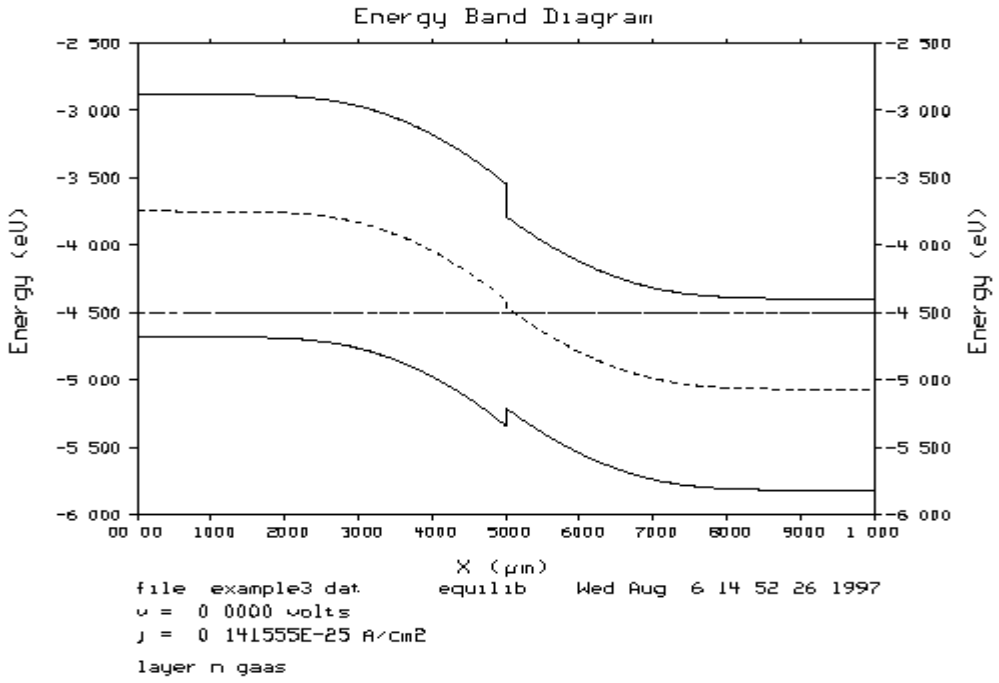
$$\delta_P = k * T * \log(N_V / p_0) = 0.0259 * \log(0.111e20 / 1.0e16) = 0.182eV$$

$$\delta_n = k * T * \log(N_C / n_0) = 0.0259 * \log(0.462e18 / 1.0e16) = 0.097eV$$

Step 2: Check the energy band diagram by using Adept in Semiconductor Simulation Hub.

Modify the input file for example 1 and see if you can get the right energy band diagram. You can check your input file by going to example folder and looking into *example3* under tutorial directory. Check the energy band diagram by calculating the same parameters as in example 1.

Here is the energy band diagram generated by Adept:



Example 4: Draw energy band diagram for $Al_{0.3}Ga_{0.7}As$/GaAs N-n Heterojunction under equilibrium condition.

$Al_{0.3}Ga_{0.7}As$: $N_D = 1.0e16\ cm^{-3}$

GaAs: $N_D = 1.0e16\ cm^{-3}$

Step 1: Follow the first three steps in example 1 to draw the energy band diagram for this heterojunction.

$$\delta_N = k * T * \log(N_C / n_0) = 0.0259 * \log(0.875e18 / 1.0e16) = 0.115eV$$

$$\delta_n = k * T * \log(N_C / n_0) = 0.0259 * \log(0.462e18 / 1.0e16) = 0.097eV$$

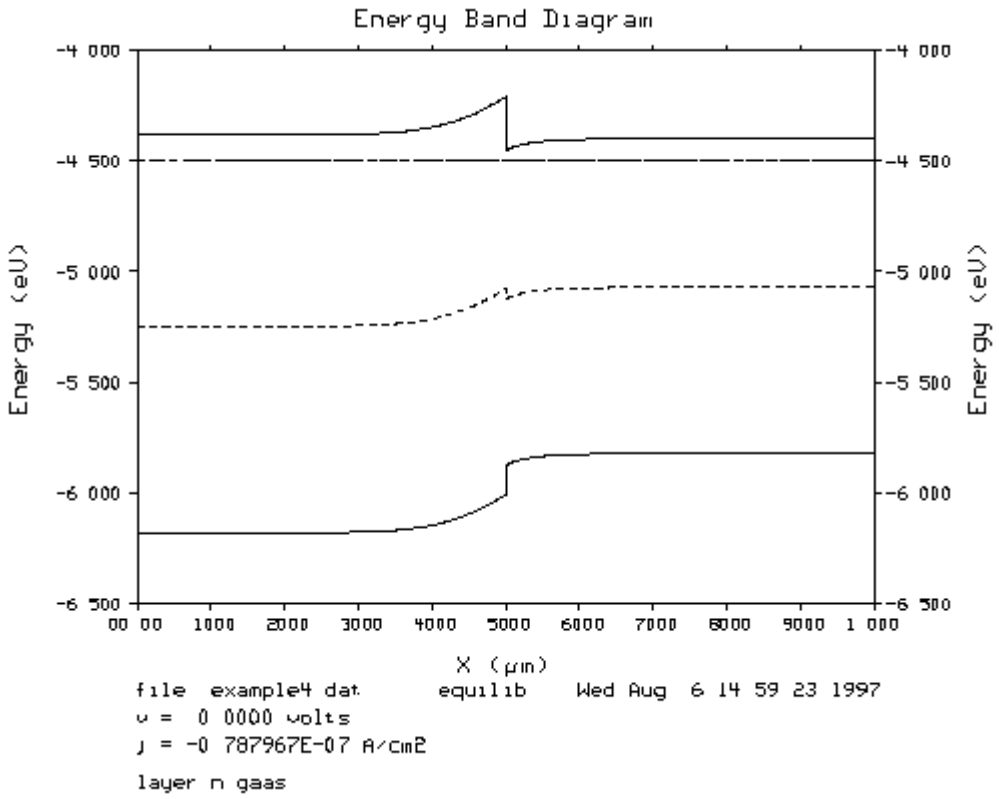
Step 2: Check the energy band diagram by using Adept in Semiconductor Simulation Hub.

Modify the input file for example 1 and see if you can get the right energy band diagram. You can check your input file by going to example folder and looking into

example4 under tutorial directory. Check the energy band diagram by calculating the same parameters as in example 1.

$$qV_{bi} = -[(\chi_N + \delta_N) - (\chi_n + \delta_n) = \chi_n - \chi_N + \delta_n - \delta_N$$
$$= 4.07 - 3.827 + 0.097 - 0.115 = 0.225eV$$
$$V_{bi} = 0.225V$$

Here is the energy band diagram energated by Adept:



Important Note: Other equations we used in example 1 to calculate other parameters will not work here because those equations are for pn junctions. Do simulation in Adept to see the energy band diagram. We can see that V_{JN} is approximately equal to V_{bi}. Not like what we expected that two side will have the same depletion width, most depletion region are on the N side.

Example 5: Draw energy band diagram for $Al_{0.3}Ga_{0.7}As$/GaAs P-p Heterojunction under equilibrium condition.

$Al_{0.3}Ga_{0.7}As$: $N_A = 1.0e16\ cm^{-3}$

GaAs: $N_A = 1.0e16 cm^{-3}$

Step 1: Follow the first three steps in example 1 to draw the energy band diagram for this heterojunction.

$$\delta_P = k * T * \log(N_V / p_0) = 0.0259 * \log(0.111e20 / 1.0e16) = 0.182eV$$

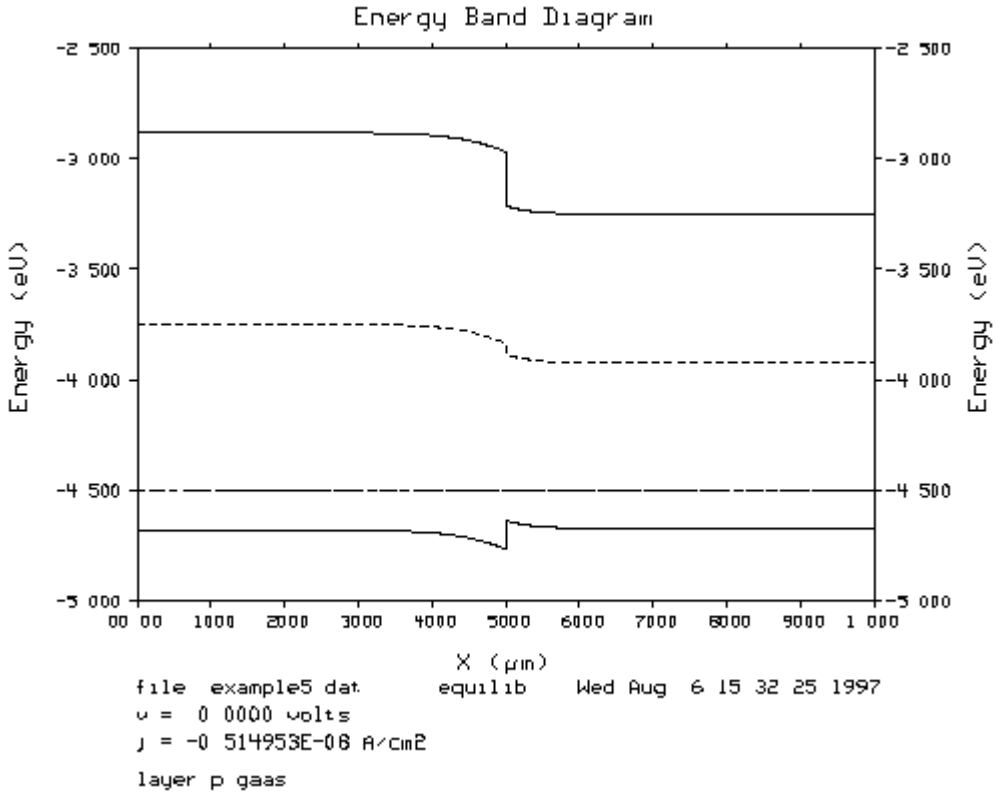
$$\delta_p = k * T * \log(N_V / p_0) = 0.0259 * \log(0.924e19 / 1.0e16) = 0.177eV$$

Step 2: Check the energy band diagram by using Adept in Semiconductor Simulation Hub.

Modify the input file for example 1 and see if you can get the right energy band diagram. You can check your input file by going to example folder and looking into *example4* under tutorial directory. Check the energy band diagram by calculating the same parameters as in example 1. Do you notice any differece from our expectation? Yes, as pointed in example 4, the equations are used to calculate parameters can't be used in these example either.

$$qV_{bi} = -[(\chi_P + E_{GP} + \delta_P) - (\chi_p + E_{Gp} + \delta_p) = (\chi_p - \chi_P) + (E_{Gp} - E_{GP}) - \delta_p + \delta_P$$
$$= 4.07 - 3.827 + 1.422 - 1.797 - 0.177 + 0.182 = -0.127eV$$
$$V_{bi} = -0.127V$$

Here is the energy band diagram generated by Adept:



Example 6: Draw energy band diagram for $In_{0.8}Ga_{0.2}As$/GaP n-P Heterojunction under equilibrium condition.

Material parameters for $In_{0.8}Ga_{0.2}As$:

E_G =0.550eV	χ = 4.00	N_C = 0.137e18 cm^{-3}	N_V = 0.659e19 cm^{-3}
ni = 0.229e14 cm^{-3}	κ= 15.15	mng = 0.031	mp = 0. 41
N_D = 0.3e19 cm^{-3}	N_A = 0.00		

Material parameters for GaP:

E_G = 2.26eV	χ = 2.04	N_C = 0.186e20 cm^{-3}	N_V = 0.123e20cm^{-3}
ni = 0.16e01cm^{-3}	κ= 11.1	mng = 0.8200	mp = 0.6200
N_D = 0.00	N_A = 0.1e20 cm^{-3}		

Note: The material parameters are also avaliable in the Semiconductor Simulation Hub Semiconductor Database on line.

Step 1: Follow the first three steps in example 1 to draw the energy band diagram for this heterojunction.

$$\delta_n = k * T * \log(N_C / n_0) = 0.0259 * \log(0.137e18 / 0.3e19) = -0.034eV$$

$$\delta_P = k * T * \log(N_V / p_0) = 0.0259 * \log(0.123e20 / 0.1e20) = 0.0023eV$$

Step 2: Check the energy band diagram by using Adept in Semiconductor Simulation Hub.

Go to Semiconductor Simulation Hub and select Adept. You can find input file for this example named *example6* in example folder under tutorial directory. Check the envergy band diagram by Adept by calculating the following parameters.

$$qV_{bi} = (\chi_P - \chi_n) + E_{GP} - \delta_P - \delta_n = 2.4 - 4.0 + 2.26 - 0.0023 + 0.034 = 0.6917eV$$
$$V_{bi} = 0.6917V$$

$$V_{JP} = V_{bi} * [\frac{\kappa_n N_D}{\kappa_n N_D + \kappa_P N_A}] = 0.6917 * [\frac{15.05 * 0.3e19}{15.15 * 0.3e19 + 11.1 * 0.1e20}] = 0.2009V$$

$$\frac{V_{jP}}{V_{Jn}} = \frac{\kappa_n N_D}{\kappa_P N_A}$$

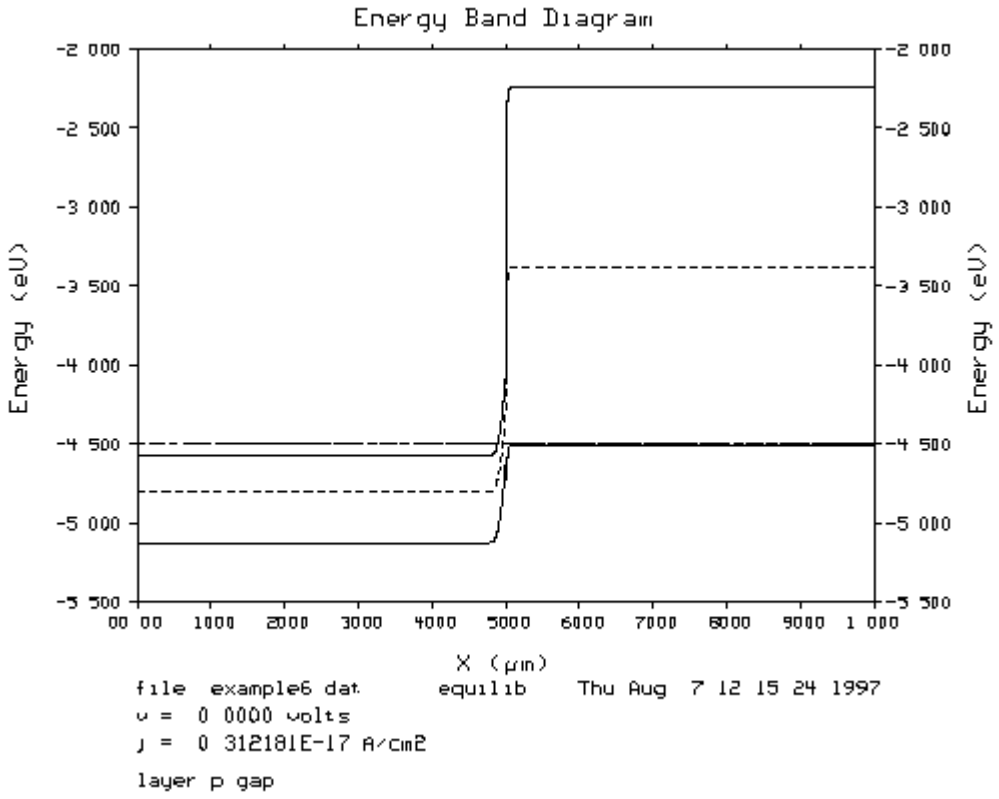
$$V_{Jn} = V_{jP} * \frac{\kappa_P N_A}{\kappa_n N_D} = 0.2009 * \frac{11.1 * 0.1e20}{15.15 * 0.3e19} = 0.4906V$$

$$x_P = [\frac{2\kappa_P \varepsilon_0 V_{JP}}{qN_A}]^{\frac{1}{2}} = [\frac{2 * 11.1 * 8.85e-14 * 0.2009}{1.6e-19 * 0.1e20}]^{\frac{1}{2}} = 4.9668e-07cm$$

$$N_A x_P = N_D x_n$$

$$x_n = \frac{N_A x_P}{N_D} = \frac{0.1e20 * 4.9668e-07}{0.3e19} = 1.6556e-06cm$$

Here is the energy band diagram generated by Adept:



3. Part II: Energy Bands in Graded Heterojunctions

Example 7: Draw energy band diagram for $Al_{0.3}Ga_{0.7}As$/GaAs N-p Heterojunction under equilibrium condition with linearly graded over the following distances:

a) 500 Angstroms b) 0.2 μm c) 0.5 μm

Material parameters for $Al_{0.3}Ga_{0.7}As$:

E_G = 1.797eV	χ = 3.827	N_C = 0.857e18 cm^{-3}	N_V = 0.111e20 cm^{-3}
ni = 0.255e04 cm^{-3}	κ= 11.9	mng = 0.08034	mp = 0.57941
N_D = 1.0e16 cm^{-3}	N_A = 0.00		

Material parameters for GaAs:

E_G = 1.422eV	χ = 4.070	N_C = 0.462e18 cm^{-3}	N_V = 0.942e19 cm^{-3}
ni = 0.238e07 cm^{-3}	κ= 12.847	mng = 0.06700	mp = 0.5200
N_D = 0.00	N_A = 1.0e16 cm^{-3}		

Note: The material parameters are also avaliable in the Semiconductor Simulation Hub Semiconductor Database on line.

Step 1: Sketch the electrostatic potential profile for the junction.

Usefuly parameters for drawing the profiles:

$$\delta_N = k*T*\log(N_C/n_0) = 0.0259*\log(0.875e18/1.0e16) = 0.115eV$$

$$\delta_p = k*T*\log(N_V/p_0) = 0.0259*\log(0.942e19/1.0e16) = 0.177eV$$

$$qV_{bi} = (\chi_p - \chi_N) + E_{Gp} - \delta_p - \delta_N = (4.07 - 3.827) + 1.422 - 0.115 - 0.177 = 1.373eV$$

$$V_{bi} = 1.373V$$

$$V_{Jp} = V_{bi} * [\frac{\kappa_N N_D}{\kappa_N N_D + \kappa_p N_A}] = 1.373 * [\frac{11.9*1.0e16}{11.9*1.0e16 + 12.847*1.0e16}] = 0.660V$$

$$\frac{V_{jp}}{V_{JN}} = \frac{\kappa_N N_D}{\kappa_p N_A}$$

$$V_{JN} = V_{jp} * \frac{\kappa_p N_A}{\kappa_N N_D} = 0.660 * \frac{12.847*1.0e16}{11.9*1.0e16} = 0.713V$$

$$x_p = [\frac{2\kappa_p \varepsilon_0 V_{Jp}}{qN_A}]^{\frac{1}{2}} = [\frac{2*12.847*8.85e-14*0.660}{1.6e-19*1.0e16}]^{\frac{1}{2}} = 3.02e-05cm$$

$$N_A x_p = N_D x_N$$

$$x_N = \frac{N_A x_p}{N_D} = \frac{1.0e16*3.02e-05}{1.0e16} = 3.02e-05cm$$

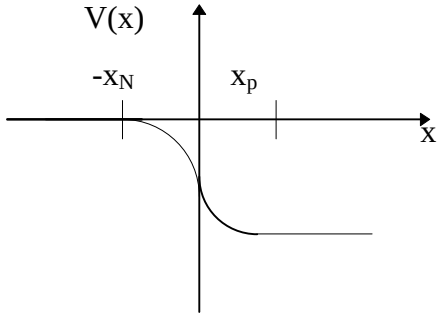
Then, use the following equation to draw the electrostatic potential profile.

$$V(x) = \frac{qV_A}{2\kappa_p \varepsilon_0}(x + x_p)^2 = \frac{1.6e-19*1.0e16}{2*12.847*8.85e-14}(x + 3.02e-05)^2$$

$$= 7.0363e08*(x + 3.02e-05) \; for - x_p < x < 0$$

$$V(x) = V_{bi} - \frac{qV_D}{2\kappa_N \varepsilon_0}(x_N - x)^2 = 1.373 - \frac{1.6e-19*1.0e16}{2*11.9*8.85e-14}(3.02e-05 - x)^2$$

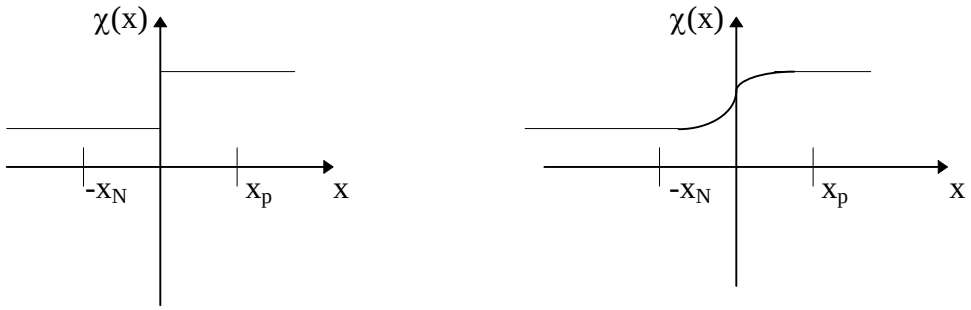
$$= 1.373 - 7.563e08*(3.02e-05 - x)^2 \; for 0 < x < x_N$$



Note: The compositional grading does not change the electrostatics, which are determined by the depletion approximation.

Step 2: Sketch the electron affinity profile for the junction.

First, let's sketch an assumed electron affinity profile without grading. Then, smooth the jump through the grading distance. So, we have the electron affinity profile with grading.



Step 3: Sketch the energy band diagram for the junction.

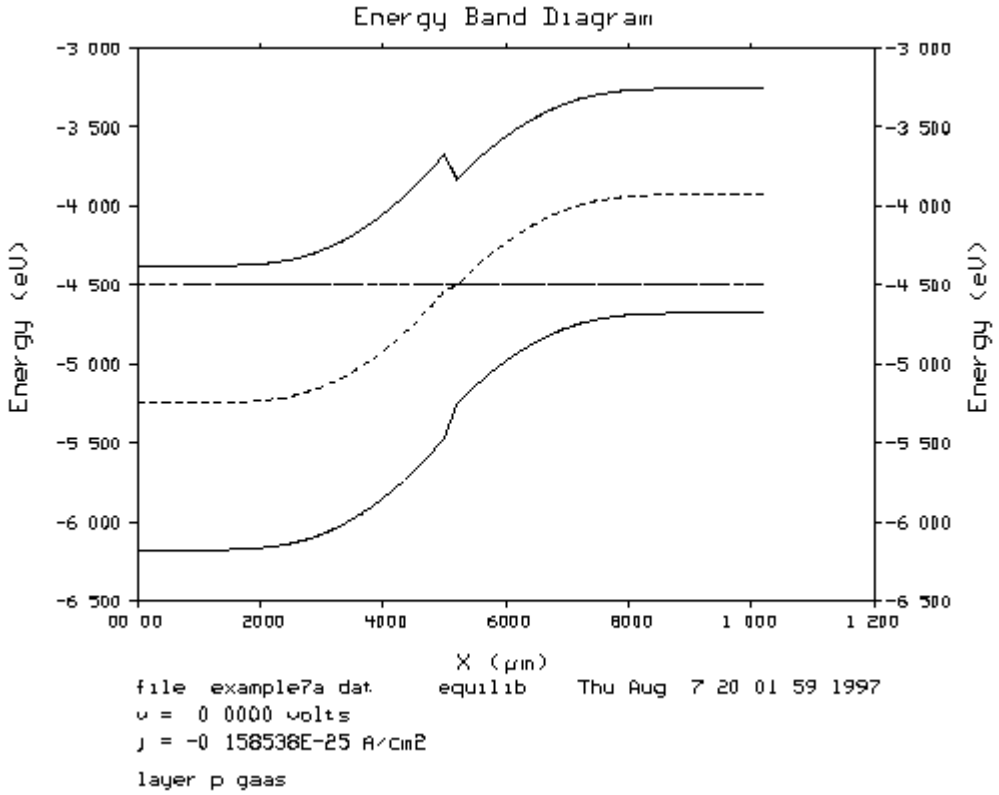
By turning the electrostatic potential and electron affinity profiles upside down and adding these two, we get the conduction band profile. We then find the valence band profile by substracting the position dependent bandgap for Ec(x).

Step 4: Check the energy band diagram by using Adept in Semiconductor Simulation Hub.

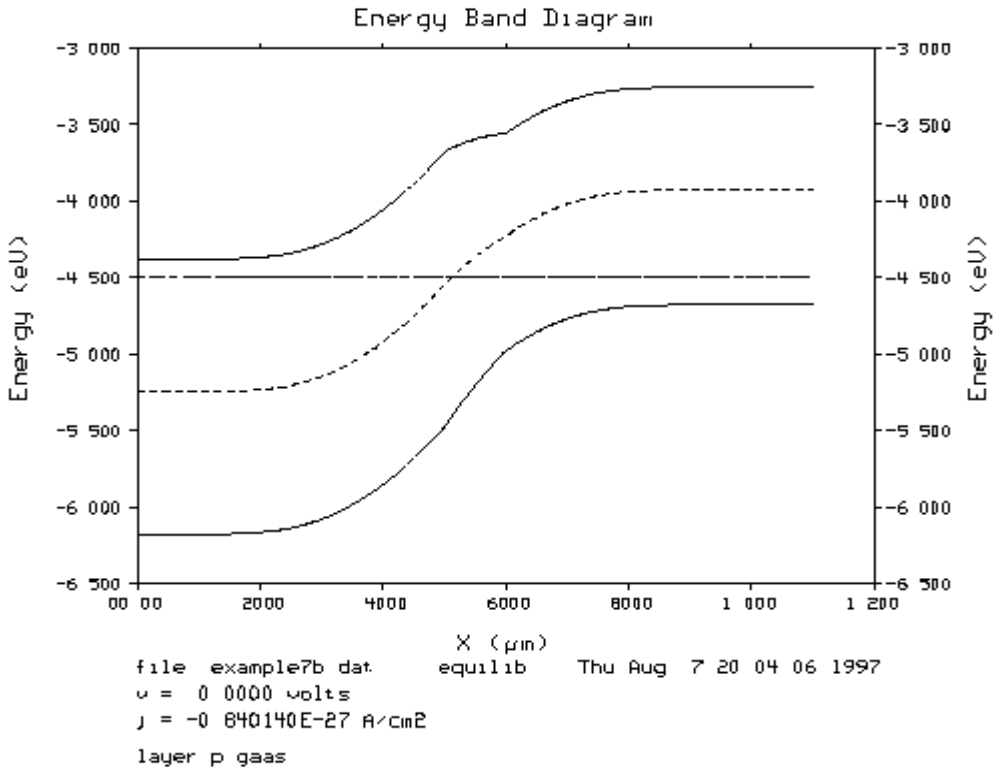
Go to Semiconductor Simulation Hub and select Adept. You can find input file for this example named *example7a, example7b and example7c* in example folder under tutorial directory. Check the energy band diagram by Adept to see if the spike is goine.

Here is the energy band diagram generated by Adept:

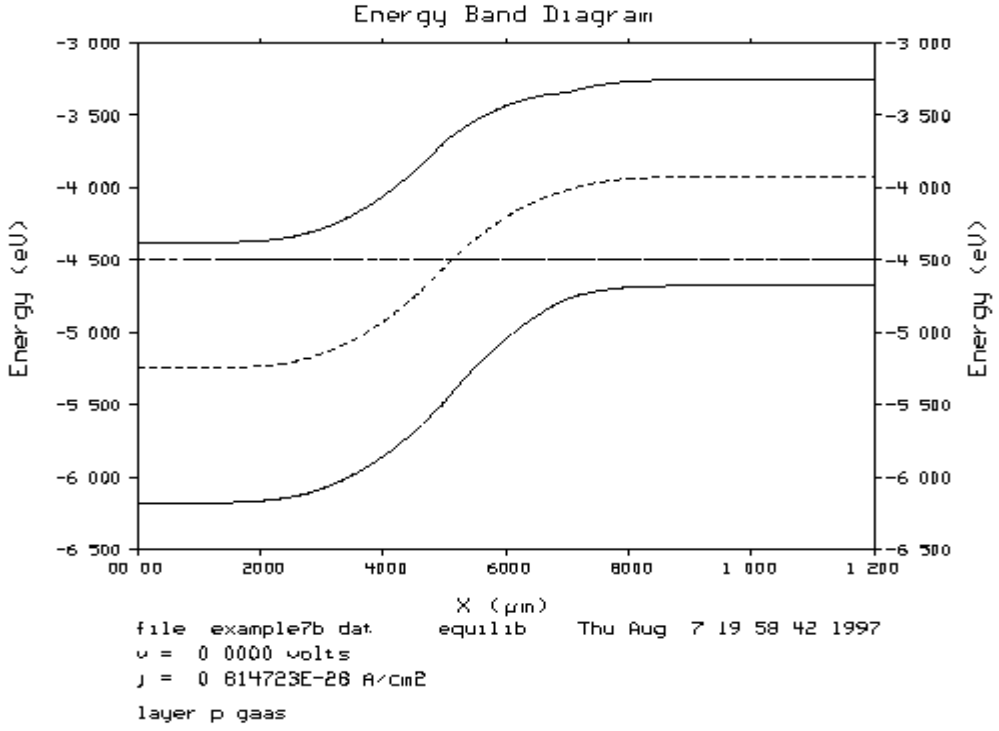
a)



b)


Energy Band Diagram
-3 000
-3 500
-4 000
-4 500
-5 000
-5 500
-6 000
-6 500
Energy (eV)
00 00
2000
4000
6000
8000
1 000
1 200
X (μm)
file example7b dat equilib Thu Aug 7 20 04 06 1997
v = 0 0000 volts
j = -0 840140E-27 A/cm2
layer p gaas

c)

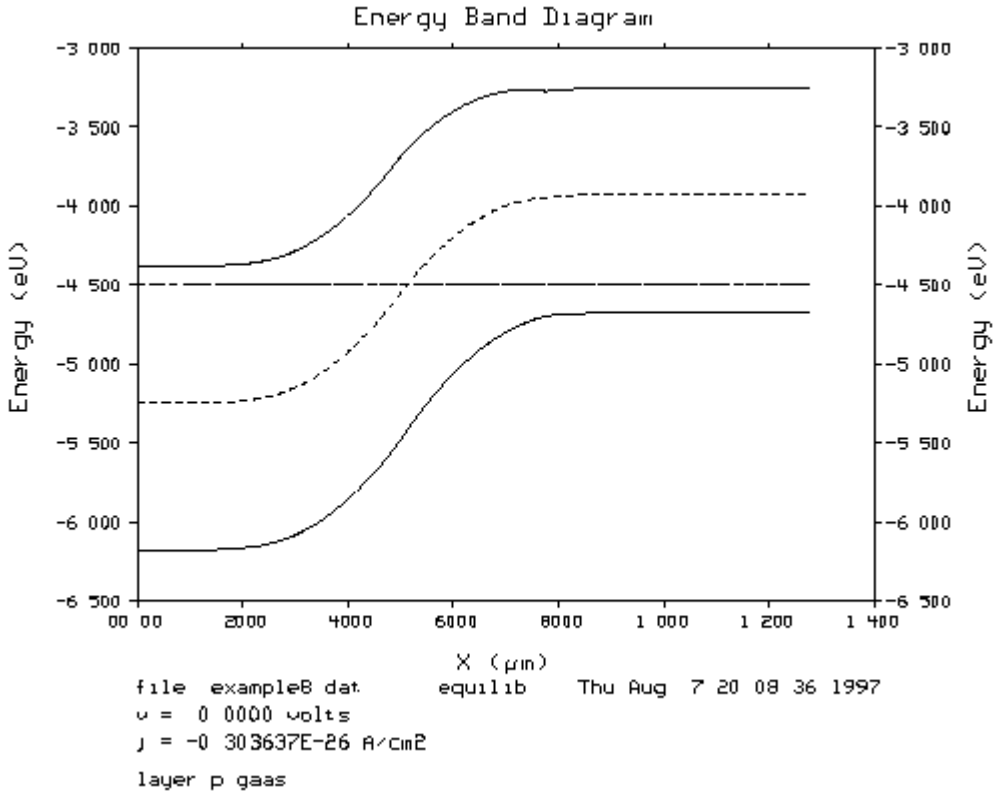

Energy Band Diagram
-3 000
-3 500
-4 000
-4 500
-5 000
-5 500
-6 000
-6 500
Energy (eV)
00 00
2000
4000
6000
8000
1 000
1 200
X (μm)
file example7b dat equilib Thu Aug 7 19 58 42 1997
v = 0 0000 volts
j = 0 814723E-28 A/cm2
layer p gaas

Example 8: Compute the grading distance x_g for example 7. Use Adept to draw energy band diagram and see if the spike is gone.

$$x_g = x_n(1-\sqrt{1-\Delta E_C / qV_{bi}}) = 3.02e-05*(1-\sqrt{1-\frac{0.23}{1.373}}) = 2.76e-05cm$$

Go to Semiconductor Simulation Hub and select Adept. You can find the input file for this example under tutorial directory with name example8 in example folder. Do the simulation and check the energy band diagram. Compare the energy band diagram in example 1, is the spike gone?

Here is the energy band diagram generated by Adept:



4. Par III: I-V Characteristics of Heterojunctions

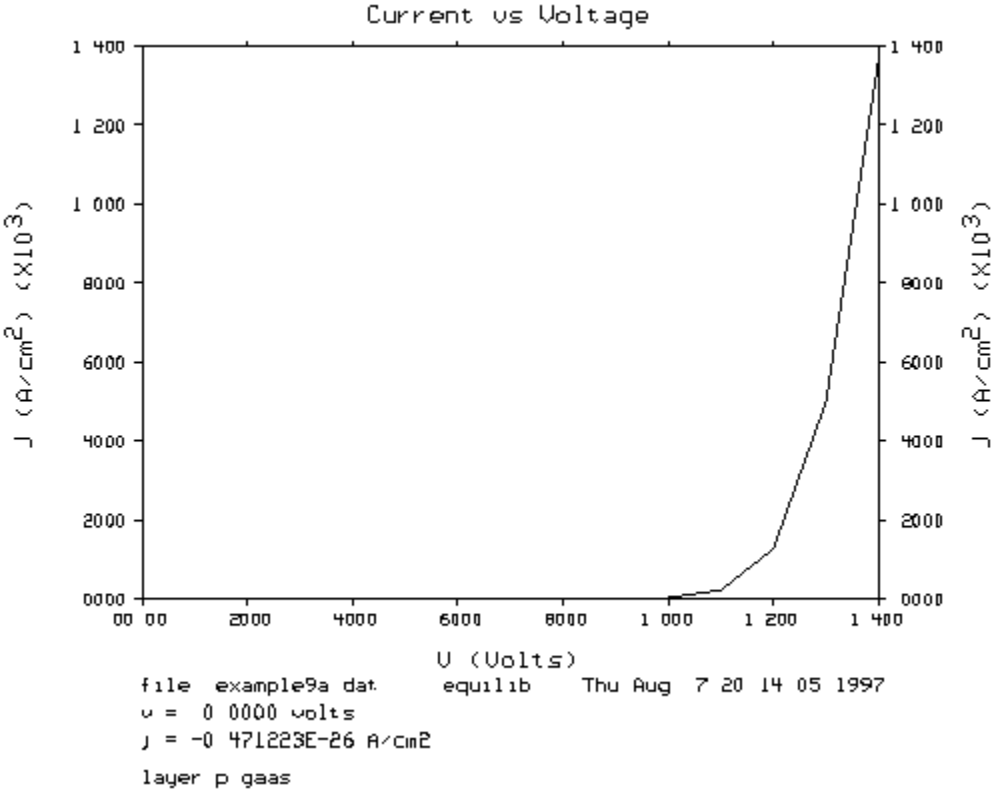
Example 9: Draw I-V characteristics of $Al_{0.3}Ga_{0.7}As$/GaAs N-p Heterojunction.

a) Draw I-V characteristic of N-p abrupt heterojunction with applying forward bias voltage from 0 to 1.4 volts.

b) Draw I-V characteristic of N-p graded heterojunction with applying forward bias voltage from 0 to 1.4 volts. Use the grading distance calculated in example 8. Then, compare these two plots.

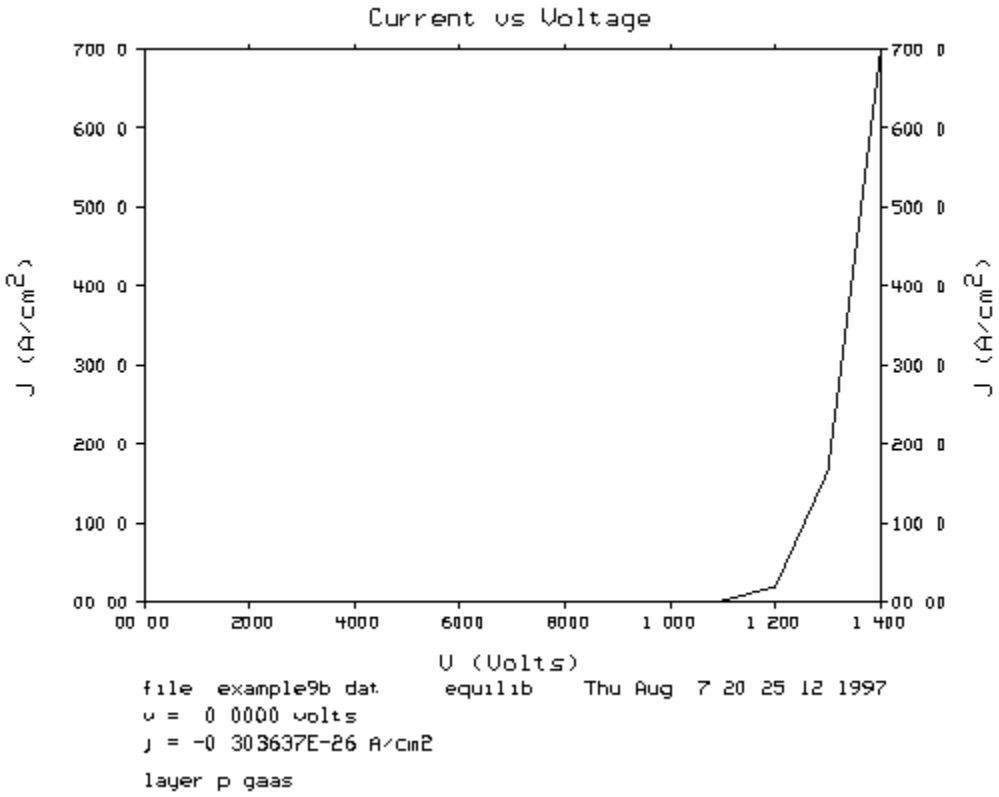
Step 1: Go to Adept and open the example folder. You can find the input file named example9a under tutorial directory in example folder. Run the simulation and examine the I-V plot.

Here is the I-V plot generated by Adept:



Step 2: Go to Adept and open the example folder. You can find the input file named example9a under tutorial directory in example folder. Run the simulation and examine the I-V plot.

Here is the I-V plot generated by Adept:



Step 3: Compare the above two plots. What difference do you see from these two plots?

Yes, graded heterojunction has a much higher current than the abrupt heterojunctions. Because graded heterojunctions have a alomst constant Fermi Lever under bias. However, abrupt heterojunctions do not have this characteristic as that of graded ones. For abrupt heterojunctions, how the Fermi Level line up is best shown in Fig 6.4 (p. 244) in Semiconductor Device Fundamentals[2]. So, in practice, we often use graded heterojunction to increase the current.

References:

[1] Lundstrom, Mark S., "Notes on Heterostructure Fundamentals", fall 1995.

[2] Pierret, Robert F., Semicondctor Device Fundamentals, 1996.