Homework #2 Solutions, EE/MSE 486, Spring 2017

Problem 1:

$$D_P = D^o + D^- \frac{n}{n_i} + D^= \left(\frac{n}{n_i}\right)^2 + D^+ \left(\frac{p}{n_i}\right)$$

Here $\frac{n}{n} = \left(\frac{N_D - N_A}{2} + \sqrt{\frac{(N_D - N_A)^2}{4} + {n_i}^2} \right) / n_i = \frac{n_i}{p}$ for n type doping;

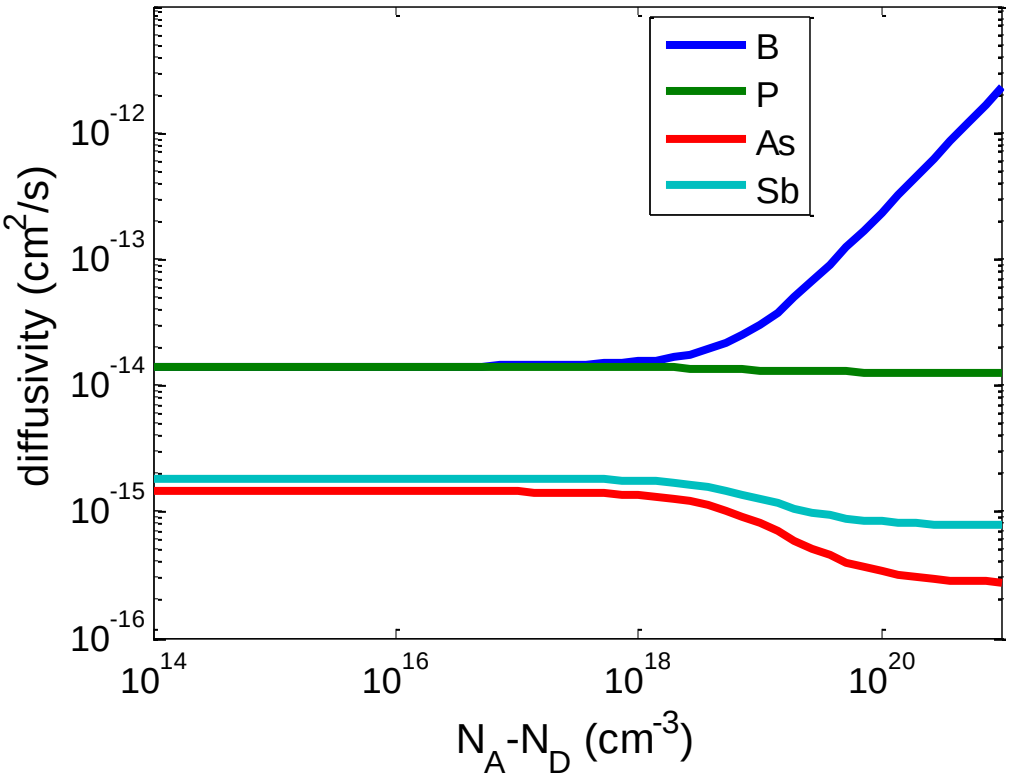
$\frac{p}{n_i} = \left(\frac{N_A - N_D}{2} + \sqrt{\frac{(N_A - N_D)^2}{4} + {n_i}^2} \right) / n_i = \frac{n_i}{n}$ for p type doing.

At 1000C, $n_i = 3.1*10^{16} T^{3/2} \exp(-\frac{0.603eV}{kT}) cm^{-3} = 5.8*10^{18} cm^{-3}$

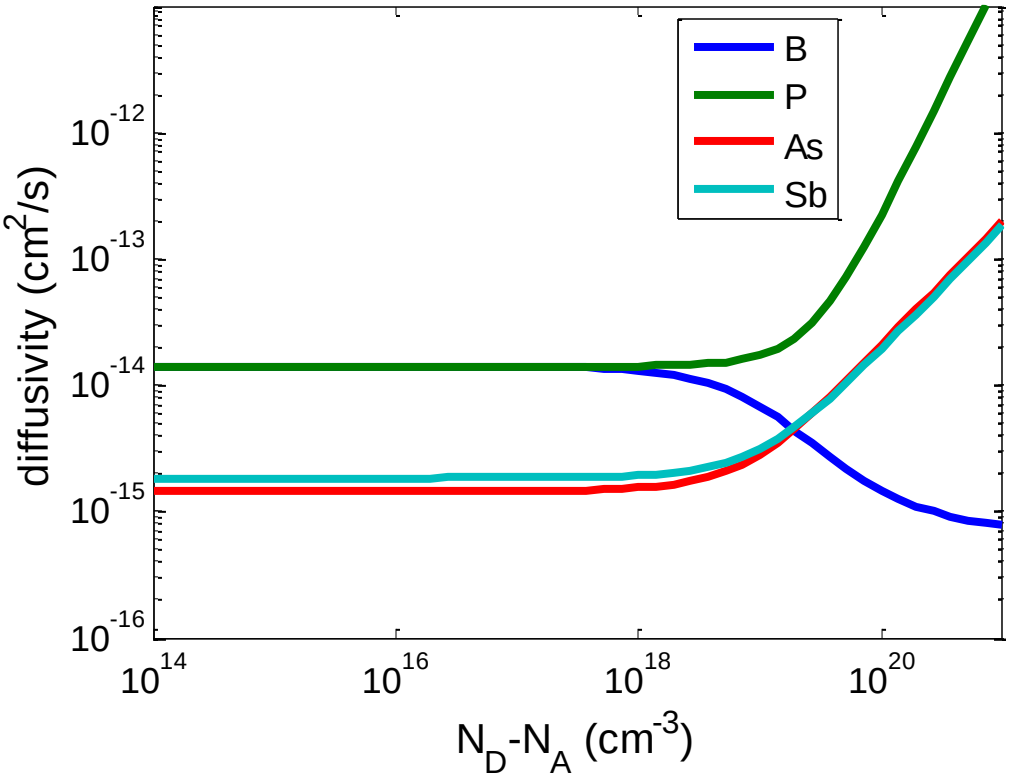
From the table in the notes, we have

	D^o (cm^2/s)	D^+ (cm^2/s)	D^- (cm^2/s)	$D^=$ (cm^2/s)
B	7.04e-16	1.34e-14		
P	1.27e-14		6.58e-16	2.25e-16
As	2.68e-16		1.17e-15	
Sb	7.70e-16		1.07e-15	

The plot for p type is:



The plot for n type is:



Problem 2

The intrinsic carrier concentration in Silicon is given by

$$n_i = 3.1*10^{16} T^{3/2} \exp(-\frac{0.603eV}{kT}) cm^{-3}$$

The electric field enhancement factor for diffusion is

$$h = 1 + \frac{N_D}{\sqrt{N_D{}^2 + 4n_i^2}}$$

where N_D is $1*10^{19}cm^{-3}$ in the problem.

Considering the concentration dependent diffusion for As, we have

$$D_{As} = D^o + D^- \frac{n}{n_i}$$

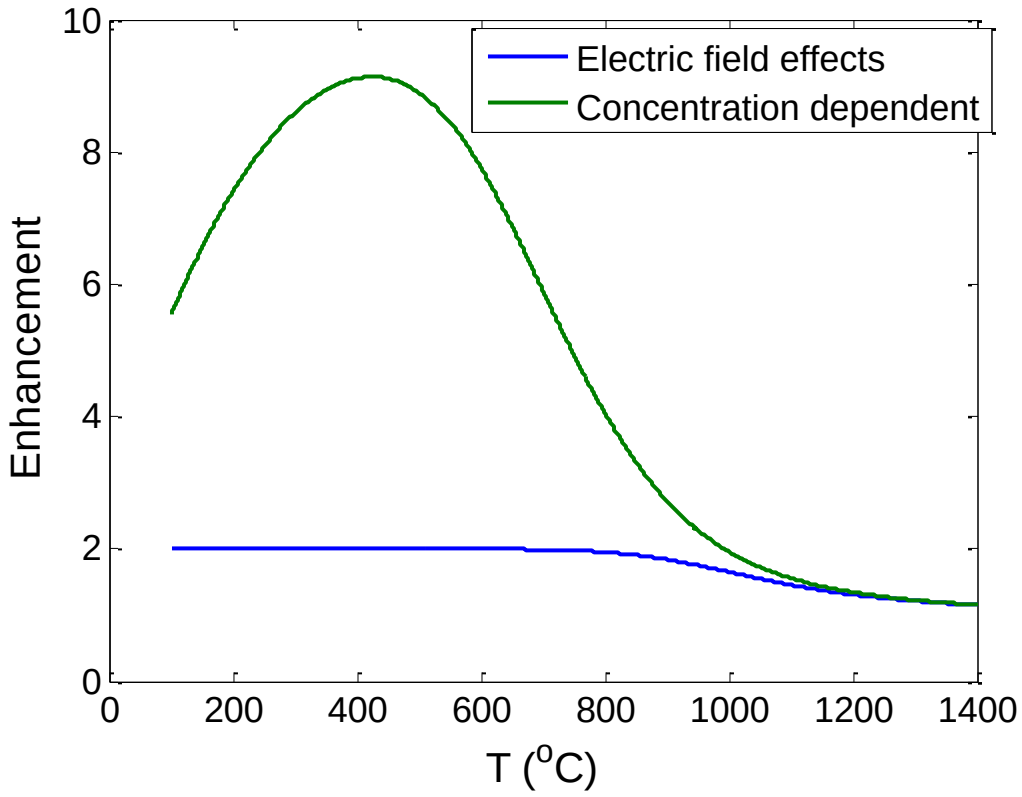
Here, $n = \frac{N_D}{2} + \sqrt{\frac{N_D^2}{4} + n_i^2}$

The method to get D^o and D^- is the same as the problem 1. We can define the enhancement from the concentration dependent diffusion as:

$$Enhancement = \frac{D^o + D^- \frac{n}{n_i}}{D^o + D^-}$$

We can plot the enhancement from electric field effect and from the concentration-dependent diffusion together as a function of temperature, as shown below.

When the temperature is lower the 1300C, both of the enhancement factor is larger than 1.2. At 1300C, n/n_i is about 1.25. When reducing temperature, n/ni would increase remarkably. Thus the enhancement factor will also increase.



Problem 3:

Sentaurus input file is:

```
line x  location=0    spacing=0.01  tag=SiDevTop
line x  location=1    spacing=0.01
line x  location=5 spacing=0.1  tag=SiDevBot
region silicon xlo=SiDevTop xhi=SiDevBot

init concentration=2e18<cm-3> field=Phosphorus wafer.orient=100
```

deposit material=oxide type=isotropic thickness=1 Boron conc=1e22
diffuse temperature=900<C> time=22<min>
struct tdr=predep

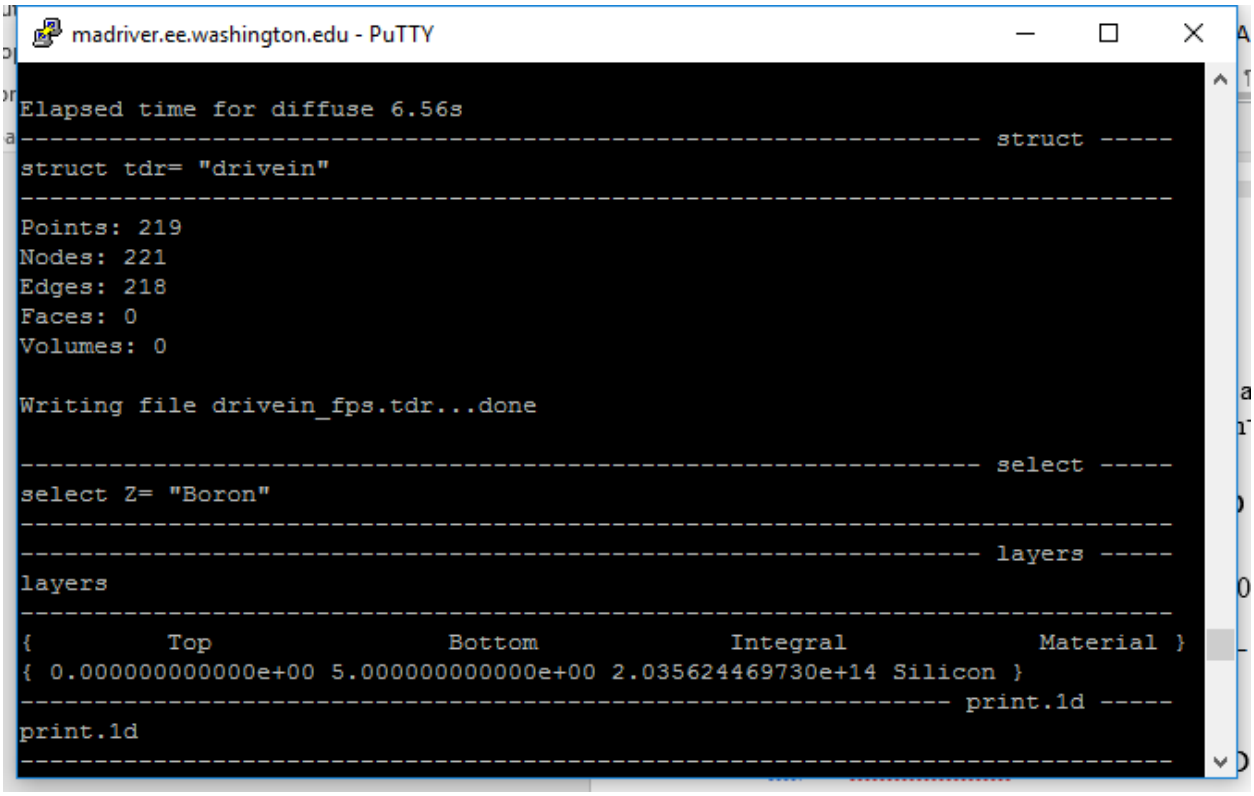
strip oxide

diffuse temperature=1000<C> time=60<min>

struct tdr=drivein

select z=Boron
layers
print.1d

In this input file, we can tune the predeposition time to match the dose requirement. The "layers" command would output the dose (cm^{-2}) at certain layer in the terminal window as shown below:



The intrinsic diffusivity for boron at 900 C is: $D_B^{900C} = 1.0\exp\left(-\frac{3.5}{kT}\right) = 9.3\times10^{-16}\, cm^2 s^{-1}$

The relation between dose and predeposition time with fixed surface concentration is:

$$Q = \frac{2C_S}{\sqrt{\pi}}\sqrt{Dt}$$

C_s is the surface concentration which is about $6*10^{19}/cm^{-3}$ from the Sentaurus simulation. To get $Q=2*10^{14}cm^{-2}$, we need $Dt=9.2*10^{-12}cm^{-2}$

So the predeposition time for intrinsic D should be: $t = \frac{9.2*10^{-12}}{9.3*10^{-16}} = 9.9*10^3 s$

The extrinsic diffusivity for boron at 900 C is:

$$D_B^{900C} = h\left[0.05\exp\left(-\frac{3.5}{kT}\right) + 0.95\exp\left(-\frac{3.5}{kT}\right)\frac{p}{n_i}\right] = 3.4\times10^{-14}\ cm^2 s^{-1} \text{ with h~2}$$

So the predeposition time for extrinsic D should be: $t = \frac{9.2*10^{-12}}{3.4*10^{-14}} = 2.7*10^2 s$

Based on TCAD simulation, the predeposition time is about 22 min which is smaller than the value based on the constant intrinsic diffusivity while larger the value using extrinsic diffusivity. This is because Sentaurus use pair diffusion model as default, which consider electrical field effect, concentration dependence and coupled diffusion between dopant and point defects.

Problem 4:

Based on the mass relation for the chemical reaction, in equilibrium the concentration of active As and inactive As4V has the relation below:

$$C_{As4V} = kC_V C_{As}^4 \quad (1)$$

Here C_X stands for the concentration of x and k is the equilibrium constant. C_{As} is the concentration of active As and we will use $C_{As,tot}$ to stand the total concentration of As.

$$C_{As,tot} = C_{As} + 4 * C_{As4V} \quad (2)$$

When $C_{As,tot} = 2 * 10^{20} cm^{-3}$, the inactive As4V is 10% of the total As. So we have

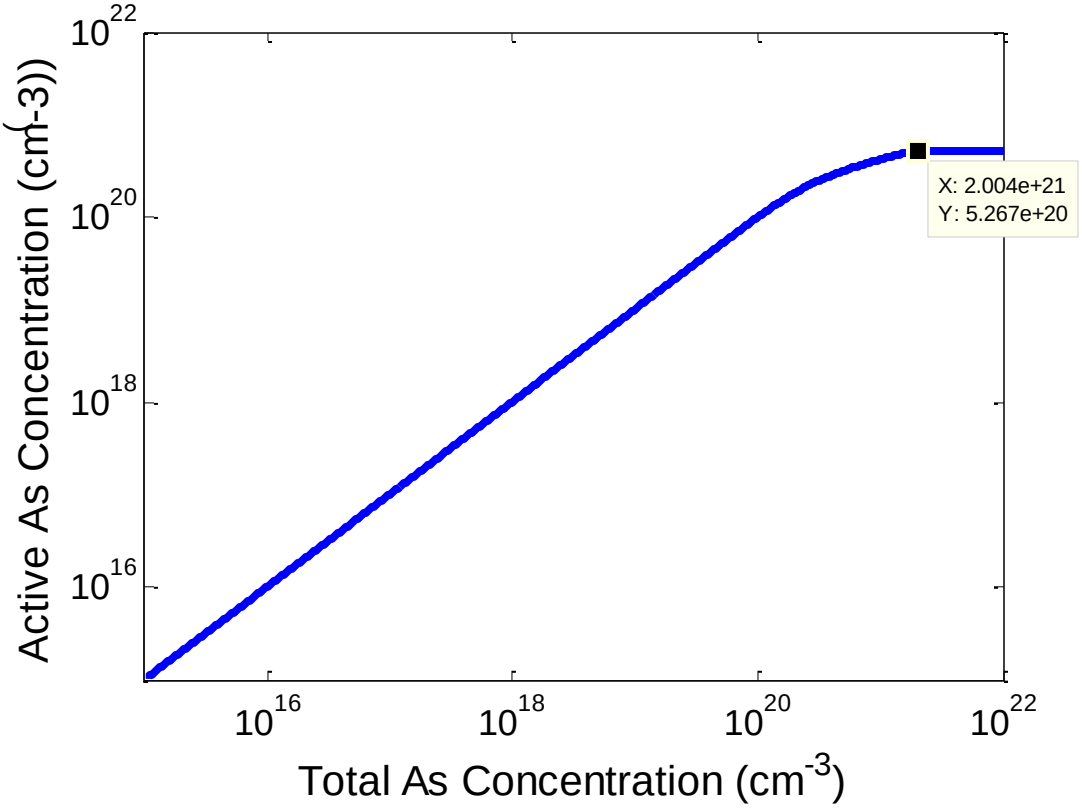
$$4 * C_{As4V} = 0.1 * 2 * 10^{20} cm^{-3} \text{ and } C_{As} = 0.9 * 2 * 10^{20} cm^{-3} \quad (3)$$

Put (3) back to (1), we can get $kC_V = 4.8 * 10^{-63} cm^9$

(2) then becomes

$$C_{As,tot} = C_{As} + 4 * 4.8 * 10^{-63} * C_{As}^4 \quad (4)$$

(4) describes the relation between C_{As} and $C_{As,tot}$ which can be plotted as follows:



The peak stable electron density before precipitation is 5.267*10^{20}cm^{-3} when $C_{As,tot} = 2 * 10^{21} cm^{-3}$.

Problem 5.

Sentaurus input file:

line x location=0 spacing=0.01 tag=SiDevTop

line x location=1 spacing=0.01

line x location=5 spacing=0.1 tag=SiDevBot

region silicon xlo=SiDevTop xhi=SiDevBot

init concentration=2e16<cm-3> field=Phosphorus wafer.orient=100

pdbSet Silicon Dopant DiffModel Fermi

#pdbSet Silicon Dopant DiffModel Pair

pdbSet Gas_Silicon Phosphorus BoundaryCondition Dirichlet

pdbSetDouble Silicon Phosphorus Cstar 3e20

diffuse temperature=900<C> time=1<hr>

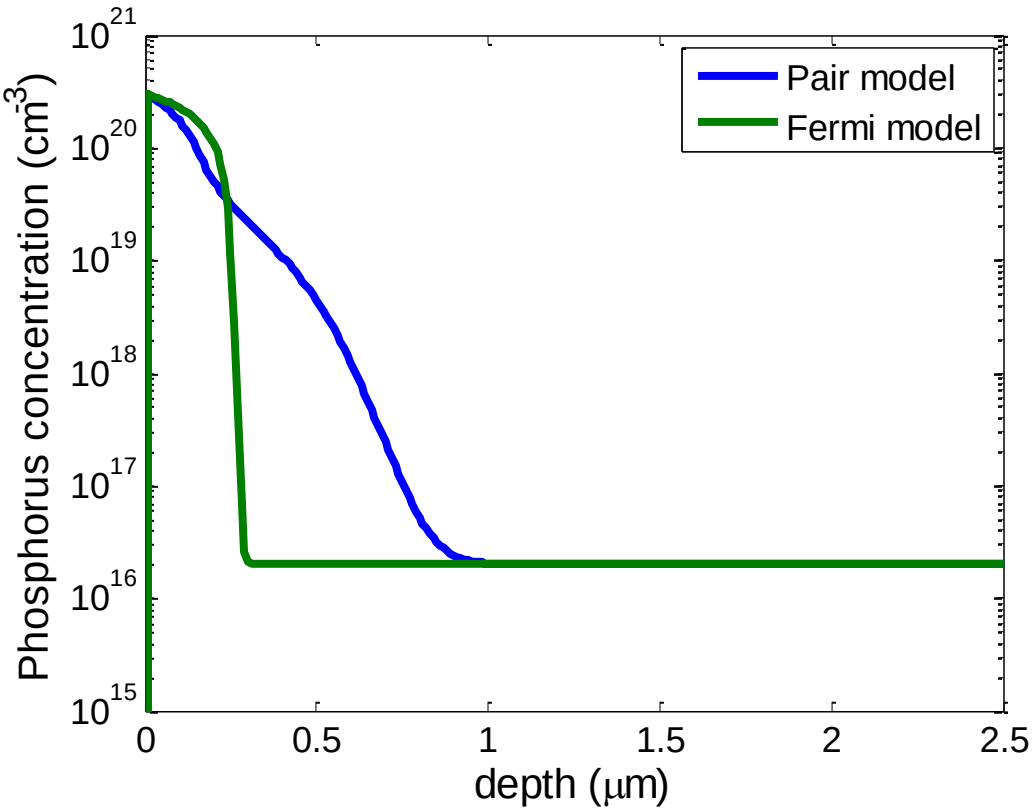
struct tdr=Fermi

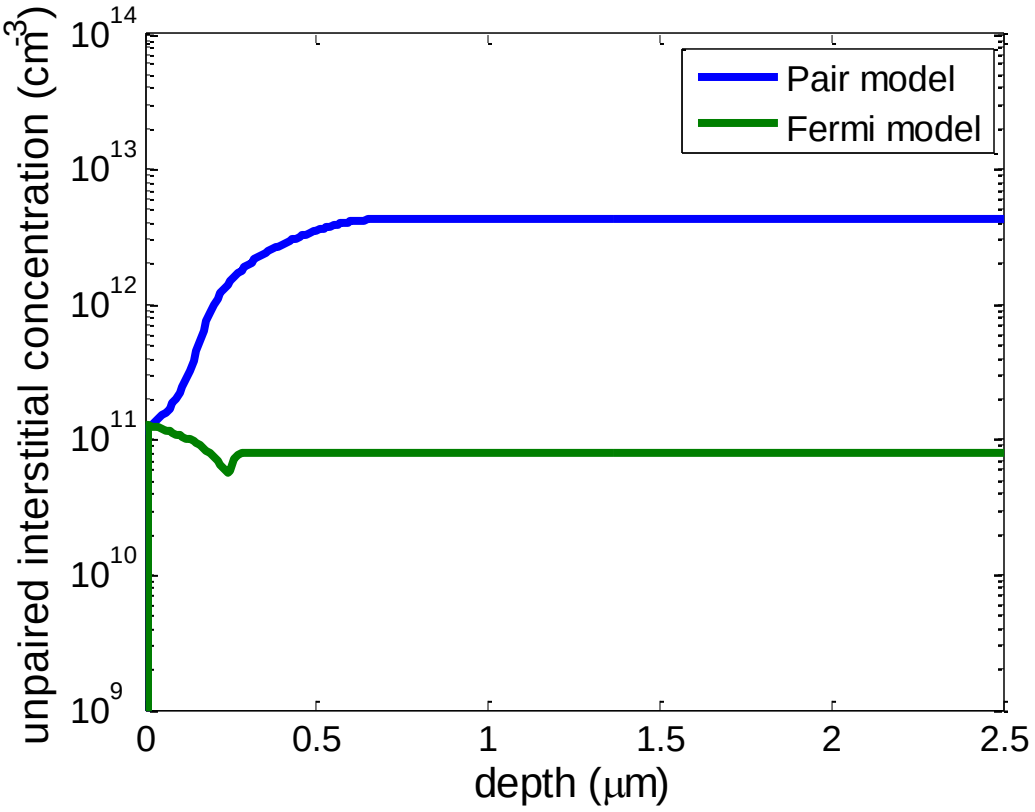
 # struct tdr=Pair

select z=Phosphorus

print.1d

The comparison between pair model and Fermi model is shown in following plots:





There is strong interstitial supersaturation in the bulk region in the Pair model while the unpaired interstitial is in equilibrium for Fermi model. The supersaturation of interstitial of Pair model is due to the diffusion of PI pairs into the bulk and dissociated into phosphorus and unpaired interstitial (chemical pumping effect). While the small dip of Int profile for Femi model is due to the doping dependence of interstitial equilibrium concentration.

Kink of phosphorus profile is due to the negative gradient of Int near surface, while the “tail” is the result of enhanced diffusion caused by interstitial supersaturation.