Solution problem 300-7 FYS9n4310 (maple work sheet)

Rerun of what the problem is
Si
CB=1e17 : bulk concentration in unit cm^-3
Pre-deposition
    T = 1000 C, Phosphorus , From Fig. 2.4, CS=1e21 cm^-3,
    NB electrical solubility is lower, while this is not explicitely mentioned in the textbook
    t =20*60 sec
Drive-in diffuion
  T =1100 C,
The problem is
 which t for drive in yields xj=4e-4 cm?
 what is the value of the surface concentration after drive in ?

We have to do simplifications here;
We approximate the real situation to one where the diffusivity is constant independent of the concentration,
This is obviously not correct since the diffusivity depends strongly on the electron concentration *n*.
We could have chosen two elctron concentrations in the range we have, to get an idea of how large effect this might have

Calculate diffusivities at 1000 C, predep and 1100 C drive-in

We have the following parameters from chapter 3.2 in the text book
See solution 300-2 for definition of symbols, We use units cm, eV, Kelvin.

```
> restart;
> pars32:={k=8.617065e-5, alpha=0.000473,Ego=1.17,beta=636,nio=
  7.3e15, Do=3.9,Ea=3.66,Dom=4.4,Eam=4,Dodm=44,Eadm=4.37};
```

$$pars32 := \{Do = 3.9, Dodm = 44, Dom = 4.4, Ea = 3.66, Eadm = 4.37, Eam = 4, Ego = 1.17, \alpha = 0.000473, \beta = 636, k = 0.00008617065, nio = 7.3\ 10^{15}\}$$

```
> pars:=pars32 union {ND=1e21};# We set ND equal to solid
  solubility
```

$$pars := \{Do = 3.9, Dodm = 44, Dom = 4.4, Ea = 3.66, Eadm = 4.37, Eam = 4, Ego = 1.17, ND = 1.\ 10^{21}, \alpha = 0.000473, \beta = 636, k = 0.00008617065, nio = 7.3\ 10^{15}\}$$

```
> #pars:=pars32 union {ND=1e20};# We set ND equal to some average
  concentration
```

We also have equations we can use for calculating ni and n

```
> eq1 := n = 1/2*ND+1/2*sqrt(ND^2+4*ni^2);# from neutrality
  condition
```

$$eq1 := n = \frac{1}{2} ND + \frac{1}{2} \sqrt{ND^2 + 4\, ni^2}$$

```
> eq2 := ni = nio*T^(3/2)*exp(-Eg/2/k/T);# from text book
```

$$eq2 := ni = nio\ T^{3/2}\ e^{-\frac{1}{2}\frac{Eg}{k\,T}}$$

```
> eq3 := Eg = Ego-alpha*(T)^2/(beta+T);#from text book
```

$$eq3 := Eg = Ego - \frac{\alpha T^2}{\beta + T}$$

```
> eq4:=delEg=-7.1e-10*sqrt(n/T);#from text book, high doping
  effects, we decide we will not use it
```

$$eq4 := delEg = -7.1\ 10^{-10} \sqrt{\frac{n}{T}}$$

Case a) T= 1000 C

```
> pars1000:=pars union {T=1273.0}:


> eq5a:=subs(pars1000,eq3);
```

$$eq5a := Eg = .768$$

```
> eq6a:=evalf(subs(pars1000 union {eq5a},eq2));
```

$$eq6a := ni = 9.985 \times 10^{18}$$

```
> eq7a:=subs(pars union {eq6a},eq1);
```

$$eq7a := n = 1.0000997 \times 10^{21}$$

```
> eq8 := Di = Do*exp(-Ea/(k*T));
```

$$eq8 := Di = Do\ e^{-\frac{Ea}{k T}}$$

```
> eq9a:=evalf(subs(pars1000,eq8));
```

$$eq9a := Di = 1.26 \times 10^{-14}$$

```
> eq10:=Dm=Dom*exp(-Eam/k/T)*(n/ni);
```

$$eq10 := Dm = \frac{Dom\ e^{-\frac{Eam}{k T}}\ n}{ni}$$

```
> eq11a:=evalf(subs(pars1000 union{eq7a} union{eq6a},eq10));
```

$$eq11a := Dm = 6.42 \times 10^{-14}$$

```
> eq12:=Ddm=Dodm*exp(-Eadm/k/T)*(n/ni)^2;
```

$$eq12 := Ddm = \frac{Dodm\ e^{-\frac{Eadm}{k T}}\ n^2}{ni^2}$$

```
> eq13a:=evalf(subs(pars1000 union{eq7a} union{eq6a},eq12));
```

$$eq13a := Ddm = 2.21 \times 10^{-12}$$

```
> eq14:=D=Di+Dm+Ddm;
```

$$eq14 := \mathrm{D} = Di + Dm + Ddm$$

```
> eq15a:=subs({eq13a} union {eq11a}union{eq9a},eq14);
```

$$eq15a := \mathrm{D} = 2.28 \times 10^{-12}$$

case b) T= 1100 C

```
> pars1100:=pars union {T=1373.0}:
> eq5b:=subs(pars1100,eq3);
```

$$eq5b := Eg = .7262$$

```
> eq6b:=evalf(subs(pars1000 union {eq5b},eq2));
```

$$eq6b := ni = 1.21 \times 10^{19}$$

```
> eq7b:=subs(pars union {eq6b},eq1);
```

$$eq7b := n = 1.00 \times 10^{21}$$

```
> eq9b:=evalf(subs(pars1100,eq8));
```

$$eq9b := Di = 1.43 \times 10^{-13}$$

```
> eq11b:=evalf(subs(pars1100 union{eq7b} union{eq6b},eq10));
```

$$eq11b := Dm = 7.54 \times 10^{-13}$$

```
> eq13b:=evalf(subs(pars1100 union{eq7b} union{eq6b},eq12));
```

$$eq13b := Ddm = 2.73 \times 10^{-11}$$

```
> eq15b:=subs({eq13b} union {eq11b}union{eq9b},eq14);
```

$$eq15b := \mathrm{D} = 2.82 \times 10^{-11}$$

We calculate the total amount of dopants by the predeposition
Measured as atoms pr surface area

```
> eq16:=QT=2/sqrt(Pi)*Cs*sqrt(D*t);
```

$$eq16 := QT = \frac{2\, Cs \sqrt{\mathrm{D}\, t}}{\sqrt{\pi}}$$

We got this from the predeposition, so we put in the values from the a) case 1000 C

```
> eq17a:=evalf(subs({eq15a} union {Cs=1.0e21,t=20*60} ,eq16));
```

$$eq17a := QT = 5.91 \times 10^{16}$$

From equation 3.19 of textbook we have

```
> eq18:=xj=sqrt(4*D*t*ln(QT/(CB*sqrt(Pi*D*t))));
```

$$eq18 := xj = 2 \sqrt{\mathrm{D}\, t \ln\left(\frac{QT}{CB \sqrt{\pi\, \mathrm{D}\, t}}\right)}$$

We require xj to be 4e-4 and solve the equation with respect to t

```
> eq19:=evalf(subs({eq17a} union {eq15b} union {CB=1e17,xj=4e-4},
  eq18));
```

$$eq19 := 4.00 \times 10^{-4} = 1.06 \times 10^{-5} \sqrt{t \ln\left(\frac{6.27 \times 10^{4}}{\sqrt{t}}\right)}$$

```
> sol_t:=solve(eq19,t);
```

$$sol\_t := 3.94 \times 10^{9},\ 1.67 \times 10^{2}$$

For n= 1e21 we get 4e9 sec and 167 sec . It is almast eternity, so we pick 167 seconds, the other solution 4e9 is perfectly valid, just impractical
For n= 1e20 we get 4e9 sec and 12603 sec . The last is 4 hours

```
> 167/60.0;
```

$$2.78 \times 10^{0}$$

This is a little short to be practical reasonable practical time
2 min is the required drive in time for n=1e21 and 4 h for n=1e20

We have done all the calculations again with two electron concentration since, 1) the elctron concentration will be lower than the P one, 2) An average concentration is lower than the max

Some of uncertainties as to wether this will be observed relates to our assumptions and approximations
We have assumed a constant space independent diffusivity, that will not be the case, we overesstimate the diffusivity corresponding to underestimation of time.
We do not make an explicit high concentration effect of bandgap narrowing, that by neglection we are underestimating ni , coresponding to overestimation of diffusivity from neg and double neg diffusion, it also corresponds to underestimation of n, the result is though an overestimation of diffusivity.

```
> if sol_t[1]>1e6 then eq20:=t=sol_t[2] else eq20:=t=sol_t[1];fi;
```

$$eq20 := t = 167.11$$

So calculation of surface concentration

```
> eq21:=Cs=solve(eq16,Cs);
```

$$eq21 := Cs = \frac{1}{2}\,\frac{QT\sqrt{\pi}}{\sqrt{D\,t}}$$

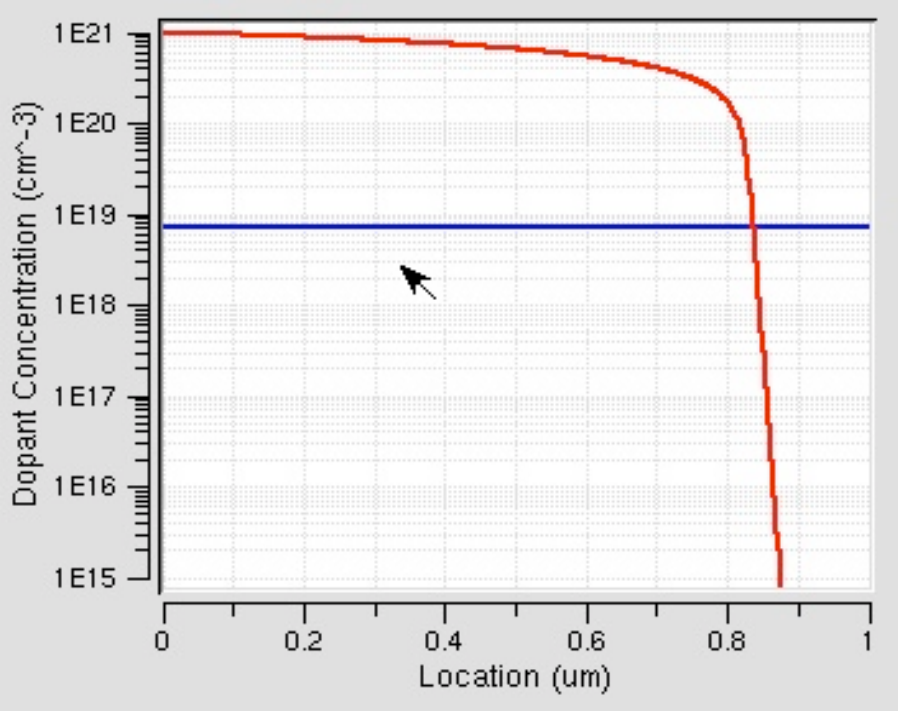
```
> eq22:=evalf(subs({eq17a}union{eq20}union{eq15b},eq21));
```

$$eq22 := Cs = 7.62 \times 10^{20}$$

The surface concentration after drive in is 8.9E19 cm^-3 for n=1e20;

NanoHUB http://www.nanohub.org/tools/atcadlab
or
http://www.nanohub.org/tools/prolabcdd/

NanoHUB Concentration Dependant Simulation, T=1000 C, Cs=1e21, dvs predep 1

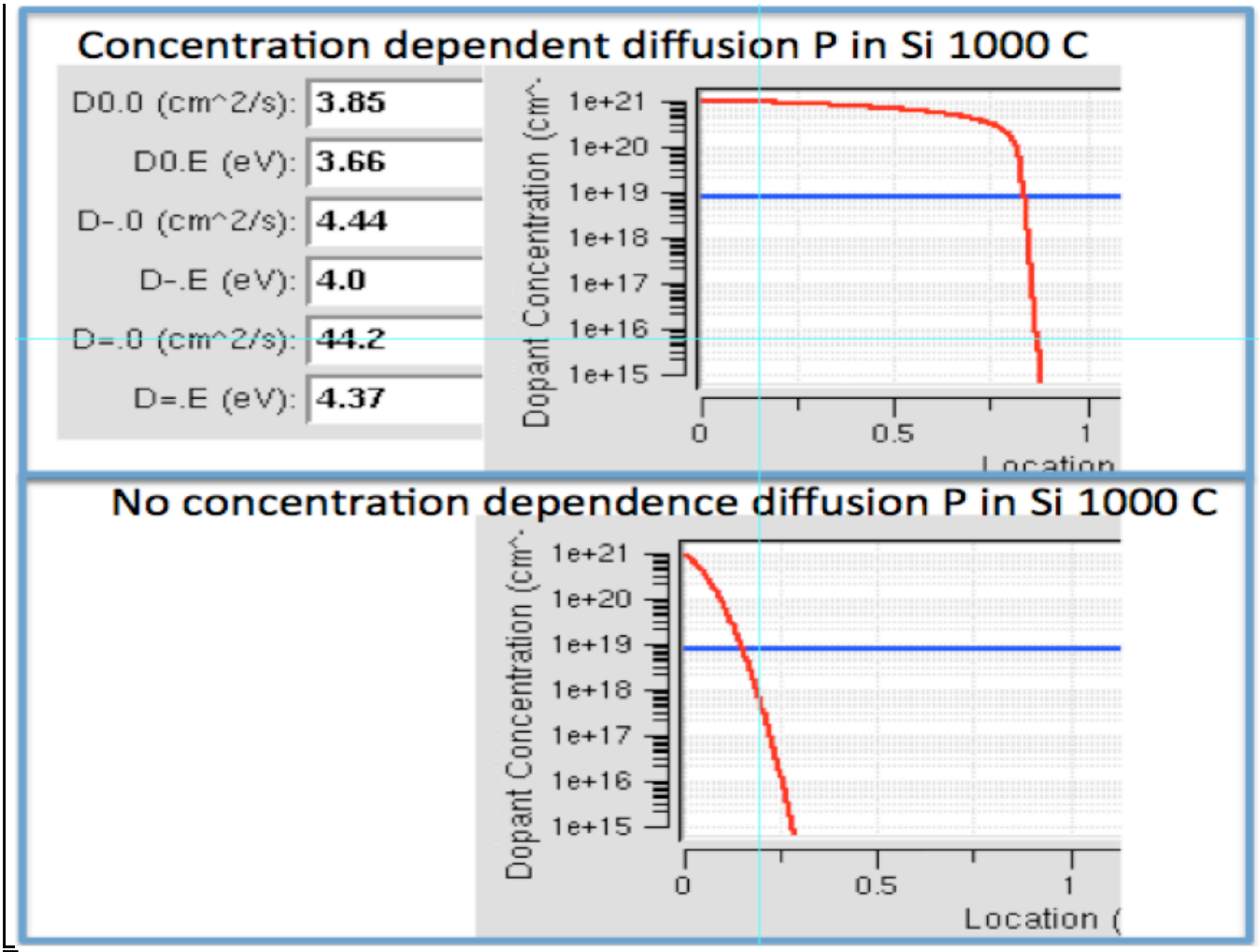


Estimate QT from above (1e21x0.6e21)/2*0.6e-4+0.6+0.2/2*0.2e-4, just by geometry, we can also download the data and integrate

```
> QT=(1e21+0.6e21)/2*0.6e-4+(0.6e21+0.2e21)/2*0.2e-4;
```

$$QT = 5.60 \times 10^{16}$$

Just a comment on concentration dependence, no concentration depemdence, both can be simulated in nanohub
Below you see the difference



So Drive-in simulation nanoHub:

nanoHUB simulation w QT=5.6 e16, Drivein diffusion, 5 min