Solution problem 300-6 FYS9n4310

Short rerun of what the problem is:
Si , As predeposition:
T=1100 C, t=10*60 sec

Drive-in diffusion:
t=24*60*60 sec, T=1000 C

What will be the max carrier concentratiom? (See eq 3.23)
Explain equation 3.23

```
> restart;
```
We have the following parameters from chapter 3.2 and table 3.2, See solution 300-2 for symbol definitions
The units are eV, cm, sec, K,
```
> pars:={k=8.617065e-5, alpha=0.000473,Ego=1.17,beta=636,nio=7.3e15,
  Do=0.0066,Ea=3.44, Dom=12.0,Eam=4.05};
```
$pars := \{Do = 0.0066, Dom = 12.0, Ea = 3.44, Eam = 4.05, Ego = 1.17, \alpha = 0.000473, \beta = 636, k$

$= 0.00008617065, nio = 7.3\ 10^{15}\}$

The idiffusivity will be given by

$$> eq1 := D = Do\ e^{-\frac{Ea}{kT}} + \frac{Dom\ e^{-\frac{Eam}{kT}}\ n}{ni}\ :$$

The intrinsic carrier concentration is given by (book eq 3.8)

$$> eq2 := ni = nio\ T^{\frac{3}{2}}\ e^{-\frac{Eg}{2kT}}\ :$$

The bandgap is given by (exept for highdoping effects) is given by (book eq 3.9)

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

We calculate the intrinsic carrier concentration ni at 1100C
```
> eq4a:=evalf(subs(pars union {T=1100+273},subs(eq3,eq2)));
```
$$eq4a := ni = 1.726021439\ 10^{19}$$

```
> eq5:=nmax=1.9e22*exp(-0.453/k/T);# = equation (3.23) in textbook
```
$$eq5 := nmax = 1.9\ 10^{22}\ e^{-\frac{0.453}{kT}}$$

We calculate the maximum electron concentration for As doping at 1100 °C
```
> evalf(subs(pars union {T=1100+273},eq5));
```
$$nmax = 4.129575315\ 10^{20}$$

While we see from Fig 2.4 that the As solid solibility is 1.4e21 at 1100 C (also at 1000 C)
So *n*max is lower than Cmax, thus we will use nmax as the electron concentration when calculating the diffusivity

```
> eq6a:=n=evalf(subs(pars union {T=1100+273},rhs(eq5)));
```
$$eq6a := n = 4.129575315 \ 10^{20}$$

We can then calculate the diffusivity from eq1 by plugging the given and calculated parameters
```
> eq7a:=evalf(subs(pars union {T=1100+273} union {eq6a} union {eq4a},
  eq1));
```
$$eq7a := D = 3.919628108 \ 10^{-13}$$

Notice that we have calculated the diffusivity for a particular value of n, but in the diffusion experiment the eleectron concetration goes frm nmax and down to ni;
we could check what the diffusivity is if D had followed the equilibrium value of n; We do it in particular for the lowest value of n, namely $n=ni$. Not asked for in the text, but the diffusivity is then
```
> eq7a2:=evalf(subs(pars union {T=1100+273} union {n=rhs(eq4a)} union
  {eq4a},eq1));
```
$$eq7a2 := D = 1.787424144 \ 10^{-14}$$

So D is an order of magnitude lower if the equuilibrium concentration of vacancies is present at the lowest concentrations of As.
The different contributions to D are then
```
> Dneautral=evalf(subs(pars union {T=1100+273},Do*exp(-Ea/(k*T))));
```
$$Dneautral = 1.556595018 \ 10^{-15}$$

```
> Dm_max=evalf(subs(pars union {T=1100+273}union{eq4a}union{eq6a},
  Dom*exp(-Eam/(k*T))*n*(1/ni)));
```
$$Dm\_max = 3.904062158 \ 10^{-13}$$

```
> Dm_min=evalf(subs(pars union {T=1100+273}union{eq4a}union{n=rhs
  (eq4a)},Dom*exp(-Eam/(k*T))*n*(1/ni)));
```
$$Dm\_min = 1.631764642 \ 10^{-14}$$

Since we were not asked to solve the problem numerically, we will use the formulas fro 'predeposition' assuming a constant diffusivity given by eq7a
For the total amount of predopsited dopands for the case of constant diffusivity, we have
```
> eq8:=QT=2/sqrt(Pi)*Cs*sqrt(D*t);
```
$$eq8 := QT = \frac{2 \ Cs \ \sqrt{D \ t}}{\sqrt{\pi}}$$

We put in the value of the surface concentration, Cs, from the solid solubility from fig.2.4 in the book, and the maximum diffusivity
```
> eq9a:=evalf(subs(pars union {T=273+1100,Cs=1.4e21,t=10*60} union
  {eq7a},eq8));
```
$$eq9a := QT = 2.422596871 \ 10^{16}$$

Then we calculate on the drive-in case:
```
> eq4b:=evalf(subs(pars union {T=1000+273},subs(eq3,eq2)));
```
$$eq4b := ni = 9.984573047 \ 10^{18}$$

```
> evalf(subs(pars union {T=1000+273},eq5));
```
$$nmax = 3.056898526 \ 10^{20}$$

```
> eq6b:=n=evalf(subs(pars union {T=1000+273},rhs(eq5)));
```

$$eq6b := n = 3.056898526 \ 10^{20}$$

The carrier concentration could be this high(it will be so at the surface at the beginning of the drive-in),
the carrier concentration would be lower at larger depth and for longer times.
If we calculate the diffusivity with a too high carrier conc the diffusivity is too high (but not much) and
we will calculate a too low carrier concentration,
So we should calculate this problem numerically, but that's too time consuming for now so we calcute the
diffuion profile as if all the diffusion was occurring at a concentration given by the max electrical
solubility, just as we did in a)

```
> eq7b:=evalf(subs(pars union {T=1000+273} union {eq6b} union {eq4b},
  eq1));
```
$$eq7b := D = 3.410353488 \ 10^{-14}$$

We have equations we can use for calculating concentration profiles , here we only need the surface
concentration
```
> #eq10:=C=QT/sqrt(Pi*D*t)*exp(-(z^2)/4/D/t);
> eq11:=Cs=QT/sqrt(Pi*D*t);
```
$$eq11 := Cs = \frac{QT}{\sqrt{\pi \ D \ t}}$$

```
> evalf(subs(pars union {eq9a} union {eq7b} union {t=24*60*60},eq11))
  ;
```
$$Cs = 2.517964751 \ 10^{20}$$

OK we see that this is lower than the electrical solubility

Answer: The maximum electron concentration will be 2.5x10^{20} cm^{-3}

Regarding equation (3.23)
I have called these terms *elctrical solubility* and *solid solubility*.
The maximum solid solubility is given as the concentration one needs to be below in order to not get
precipitation of other phases. In this case SiliconArsenides (- or ArsenoSilicides). However not all
Arsenic that is not in precipitates will be electrically active. That seems to be confirmed experimentally.
There can be many reasons for this. One is cluster formation of As. For example two or more As atoms
together or two or more together with Vacancies to form electrically inactive and relatively stable clusters.
Dislocation, or defect compensation is another effect. Dislocation trapping another.