Homework #3 Solutions, EE/MSE 486. Spring 2017

Problem 1

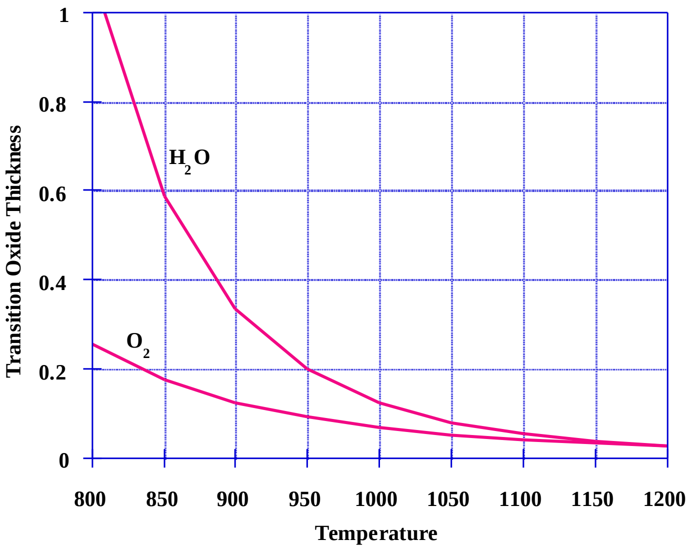
The transition from linear to parabolic growth is a gradual one and therefore there is no specific thickness at which an abrupt transition takes place. We can "define" the transition, as occurring when

$$\frac{k_S x_o}{D} \approx 1 \quad \text{or when} \quad x_o = \frac{D}{k_S} = \frac{B}{2(B/A)}$$

Taking the values for dry O_2 as an example, from notes, we have

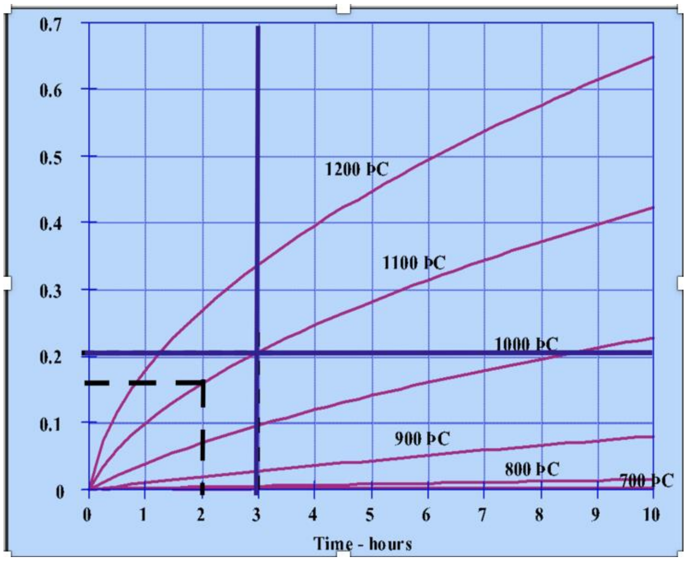
$$x_o = \frac{B}{2(B/A)} = \frac{7.72\text{x}10^2 \exp\left(-\frac{1.23\text{eV}}{kT}\right)}{(2)6.23\text{x}10^6 \exp\left(-\frac{2\,\text{eV}}{kT}\right)} = 0.619\text{x}10^{-4} \exp\left(\frac{0.77\text{eV}}{kT}\right)$$

This equation is plotted below along with the H_2O result also using values from notes. The values in notes apply to (111) silicon as does the graph below. (100) curves are easily generated by dividing the respective B/A values by 1.68.

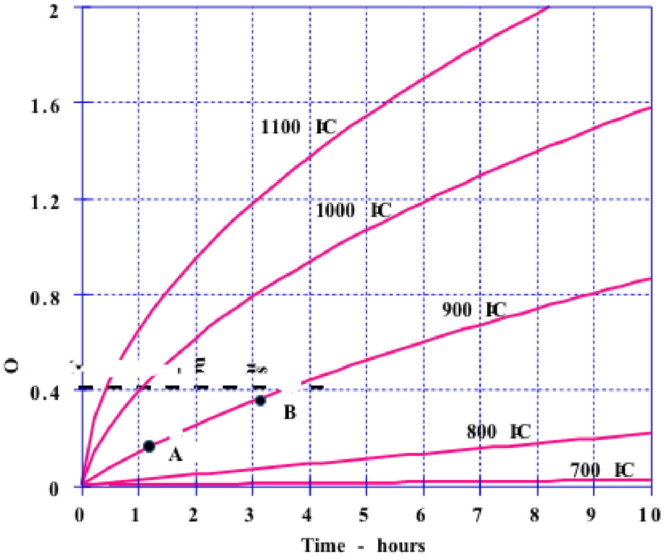


Problem 2

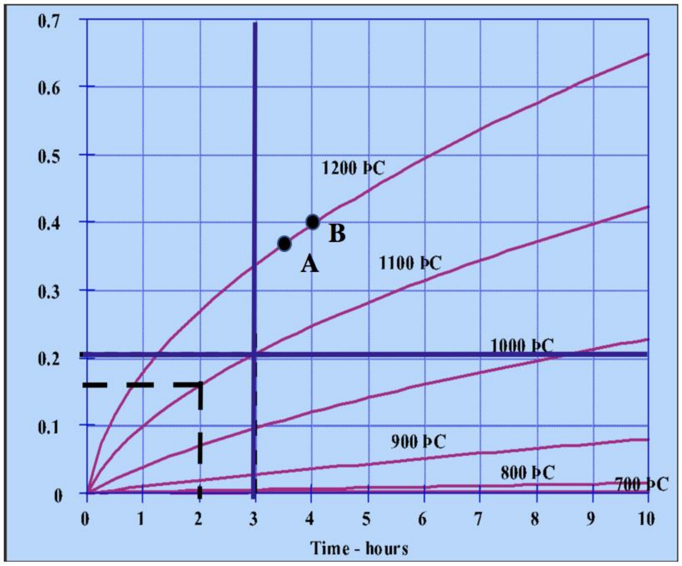
We can use these figures to estimate the oxide thickness as follows. First, we use figure in page 10 of the notes for the first dry oxidation cycle



A two hour oxidation at 1100˚C produces an oxide thickness of about 0.16 µm. We next use figure in page 11 for the wet oxidation as shown below. Then oxidation is 2 hrs in H_2O at 900 ˚C. We start by finding the point on the 900˚C curve that corresponds to 0.16 µm since this is the starting oxide thickness. This is point A. We then move along the 900˚C curve by two hours to point B. This corresponds to a thickness of about 0.36 µm which is the thickness at the end of the wet oxidation.



We now go back to the figure of page 10 of the note for the final dry O_2 cycle. This process is 0.5 hrs at 1200˚C. We start by finding the point on the 1200˚C curve that corresponds to a starting oxide thickness of 0.36 µm. This is point A below. We then increment the time by 0.5 hrs along the 1200˚C curve, to arrive at a final oxide thickness of about 0.4 µm.



Problem 3.

(a) At 1000C, and 1 atm $B = 7.72 * 10^2 \frac{\mu m^2}{h} \exp\left(-\frac{1.23eV}{kT}\right) = 1.05 * 10^{-2} \frac{\mu m^2}{h}$

$$\frac{B}{A} = \frac{6.23}{1.68} * 10^6 \frac{\mu m}{h} \exp\left(-\frac{2.0eV}{kT}\right) = 4.5 * 10^{-2} \frac{\mu m}{h}$$

Note that the factor 1.68 is used in the <100> case.

Since $B \propto P_{O2}$ $and \frac{B}{A} \propto P_{O2}^{0.75}$, at 0.2 atm we can get

$$B = 2.1 * 10^{-3} \frac{\mu m^2}{h} \; and \frac{B}{A} = 1.3 * 10^{-2} \frac{\mu m}{h}$$

To get the oxide thickness, we use the following equation:

$$x_o^2 + Ax_o + B(t + \tau) = 0$$

Assume $\tau \sim 0$ $i.e.$ $x_i \sim 0$, we can get

$$x_o = \frac{-A + \sqrt{A^2 + 4Bt}}{2} = \begin{cases} 0.0064\,\mu m\, for\; t = 0.5hr \\ 0.0233\mu m\, for\; t = 2hr \end{cases}$$

(b) The Sentaurus input file is listed below:

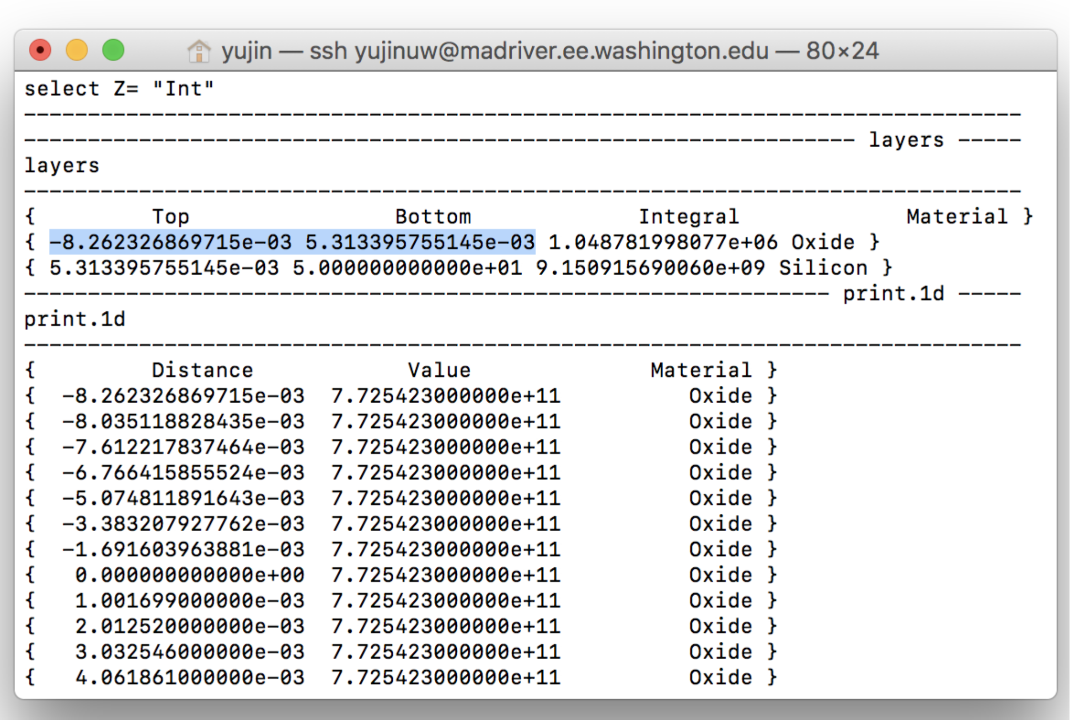
```
line x location=0 spacing= 0.001 tag=SiDevTop
line x location=1 spacing=0.01
line x location=5 spacing=0.1  tag=SiDevBot
region silicon xlo=SiDevTop xhi=SiDevBot
init concentration=5e16<cm-3> field=Phosphorus wafer.orient=100
```

diffuse pO2=0.2 temperature=1000<C> time=0.5<hr>
grid remesh

struct tdr=d4

layers

The output of “layers” command is shown in the following figure:



```
select Z= "Int"
------------------------------------------------------------------------------
----------------------------------------------------------------- layers -----
layers
------------------------------------------------------------------------------
{          Top                  Bottom                 Integral           Material }
{ -8.262326869715e-03 5.313395755145e-03 1.048781998077e+06 Oxide }
{ 5.313395755145e-03 5.000000000000e+01 9.150915690060e+09 Silicon }
--------------------------------------------------------------- print.1d -----
print.1d
------------------------------------------------------------------------------
{          Distance            Value                Material }
{   -8.262326869715e-03  7.725423000000e+11          Oxide }
{   -8.035118828435e-03  7.725423000000e+11          Oxide }
{   -7.612217837464e-03  7.725423000000e+11          Oxide }
{   -6.766415855524e-03  7.725423000000e+11          Oxide }
{   -5.074811891643e-03  7.725423000000e+11          Oxide }
{   -3.383207927762e-03  7.725423000000e+11          Oxide }
{   -1.691603963881e-03  7.725423000000e+11          Oxide }
{    0.000000000000e+00  7.725423000000e+11          Oxide }
{    1.001699000000e-03  7.725423000000e+11          Oxide }
{    2.012520000000e-03  7.725423000000e+11          Oxide }
{    3.032546000000e-03  7.725423000000e+11          Oxide }
{    4.061861000000e-03  7.725423000000e+11          Oxide }
```

The oxide layer thickness after 0.5-hour oxidation is 8.3nm+5.3nm=13.6nm.
Similarly, we can get the oxide layer thickness for 2-hour oxidation from Sprocess, which is 31.6nm.
The simulated thickness is larger than the hand calculation due to:

1) Initial thickness about 2 nm is assumed;
2) Thin oxides grow faster than the linear-parabolic model initially as observed experimentally.

Problem 4

We will perform the calculation for <111> silicon wafers. For <100> wafers, the linear rate constant should be divided by 1.68.

At 1000˚C, in H_2O

$$B = 3.86 \times 10^{2} \exp\left(-\frac{0.78}{kT}\right) = 0.316\ \mu m^{2}/hr$$

$$\frac{B}{A} = 1.63 \times 10^8 \exp\left(-\frac{2.05}{kT}\right) = 1.255\ \mu m / hr$$

$$A = 0.252\ \mu m$$

The time to grow $0.2\ \mu m$ is then

$$\tau = \frac{x_i^2 + Ax_i}{B} = \frac{(0.2)^2 + (0.252)(0.2)}{0.316} = 0.286\ hr$$

The time to grow the initial $0.4\ \mu m$ was

$$\tau = \frac{x_i^2 + Ax_i}{B} = \frac{(0.4)^2 + (0.252)(0.4)}{0.316} = 0.825\ hr$$

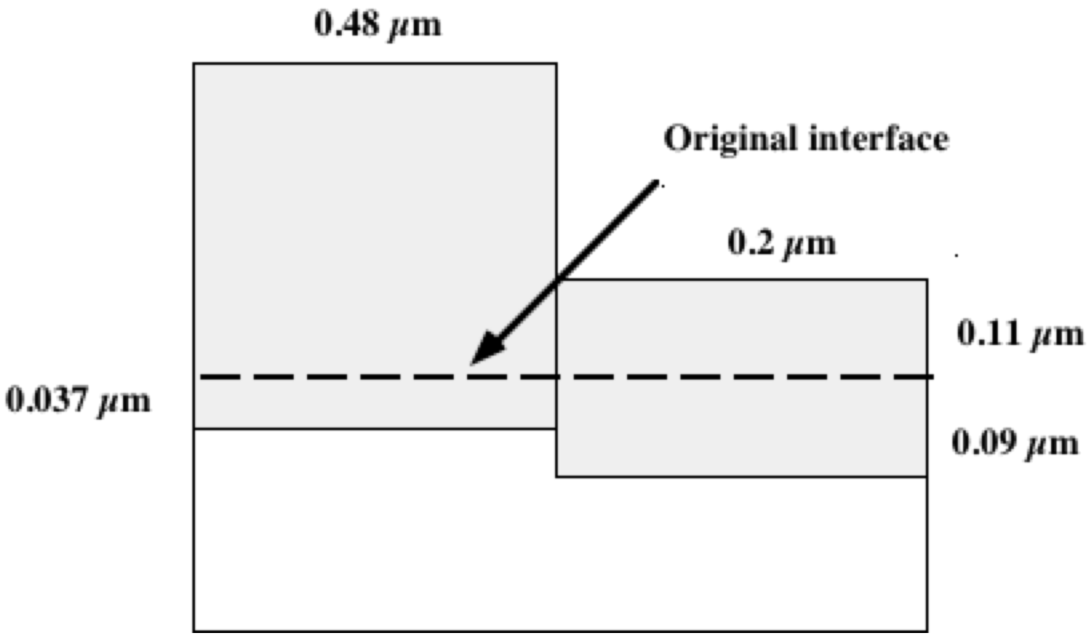
The extra time to grow $0.2\ \mu m$ in the bare areas will grow some extra oxide where the initial $0.4\ \mu m$ oxide existed

$$x_O = \frac{A}{2}\left\{\sqrt{1 + \frac{t + \tau}{A^2 / 4B}} - 1\right\} = \frac{0.252}{2}\left\{\sqrt{1 + \frac{0.286 + 0.825}{(0.252)^2 / 4(0.316)}} - 1\right\} = 0.480\ \mu m$$

The growth of the extra $0.080\ \mu m$ will consume $0.46 \times 0.080 = 0.037\ \mu m$ of silicon under the thick oxide.

The growth of $0.2\ \mu m$ of oxide will consume $0.46 \times 0.2 = 0.092\ \mu m$ of silicon.

Thus, a sketch of the old and new oxide-silicon interface is shown below:


0.48 μm
Original interface
0.2 μm
0.11 μm
0.037 μm
0.09 μm