Oxidation and Etching

1.) An arbitrary material is deposited on a silicon wafer at a thickness of 100 nm. It is then patterned with photoresist (assume 90 degree photoresist sidewall angles) and etched. What is the etch isotropic factor if the sidewall angle is:

a. 45 degrees (1 pt)
\[ A_f = 1 - \frac{r_{\text{lat}}}{r_{\text{ver}}} \]
\[ r_{\text{lat}}/r_{\text{ver}} = 1/[\tan(45^\circ)] = r_{\text{lat}}/r_{\text{ver}} = 1 \]
\[ A_f = 0 \]

b. 60 degrees (1 pt)
\[ A_f = 1 - (1/[\tan(60^\circ)]) = 0.423 \]

c. 89 degrees (1 pt)
\[ A_f = 1 - (1/[\tan(89^\circ)]) = 0.983 \]

d. For parts a-c, calculate the width at the top of the etched feature if the photoresist is patterned at a width of 200 nm. (6 pts)
\[ W_{\text{top}} = W - 2*\text{thickness}*(r_{\text{lat}}/r_{\text{vert}}) \]
\[ 45^\circ \rightarrow W_{\text{top}} = 0 \text{ nm} \]
\[ 60^\circ \rightarrow W_{\text{top}} = 84.6 \text{ nm} \]
\[ 89^\circ \rightarrow W_{\text{top}} = 196.51 \text{ nm} \]

2.) Consider a chunk of silicon, where the left half has a (100) surface and the right half has a (111) surface.

a. A wet oxidation is performed at 1050 °C for 1 hour. What is the step height between the oxides over the (100) and (111) surfaces? Draw the final cross-section of the structure and label all vertical dimensions. Oxide thicknesses must be calculated using the Deal-Grove model. (4 pts)
\[ T = 1050^\circ \text{C} = 1323 \text{ K} \Rightarrow kT = 0.114 \text{ eV} \]
\[ B_{(100)} = (386 \text{ } \mu\text{m}^2/\text{hr})*\exp(-0.78 \text{ eV}/0.114 \text{ eV}) = 0.412 \text{ } \mu\text{m}^2/\text{hr} \]
\[ B/A_{(100)} = (9.7\times10^7 \text{ } \mu\text{m}/\text{hr})*\exp(-2.05 \text{ eV}/0.114 \text{ eV}) = 1.503 \text{ } \mu\text{m}/\text{hr} \]
\[ B_{(111)} = (1.63\times10^8 \text{ } \mu\text{m}/\text{hr})*\exp(-2.05 \text{ eV}/0.114 \text{ eV}) = 2.526 \text{ } \mu\text{m}/\text{hr} \]
\[ A_{(100)} = B/[B/A] = 0.274 \text{ } \mu\text{m} \]
\[ A_{(111)} = 0.163 \text{ } \mu\text{m} \]
\[ X_i = 0 \Rightarrow \tau = 0 \]
\[ X_{\text{ox},(100)} = 0.5*(0.274)*[\sqrt{(1+4*0.412/(0.274^2))} – 1] = 0.519 \text{ } \mu\text{m} \]
\[ X_{\text{ox},(111)} = 0.5*(0.163)*[\sqrt{(1+4*0.412/(0.163^2))} – 1] = 0.566 \text{ } \mu\text{m} \]
\[ X_{\text{si},(100)} = 0.46*X_{\text{ox},(100)} = 0.239 \text{ } \mu\text{m} \]
\( X_{\text{si,(111)}} = 0.26 \, \mu m \)

**Step height** = \( (X_{\text{ox,(111)}} - X_{\text{si,(111)}}) - (X_{\text{ox,(100)}} - X_{\text{si,(100)}}) = 0.026 \, \mu m \)

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**b.** Repeat part a, except that now 20 nm of oxide is deposited and patterned over the (100) surface (i.e., the (111) surface has no oxide over it, only the (100) surface), and a dry oxidation is performed (instead of a wet oxidation as in part a). \( 4 \) pts

\[
T = 1050^\circ C = 1323 \, K \quad \Rightarrow \quad kT = 0.114 \, eV
\]

\[
B_{(100)\text{ and (111)}} = (772 \, \mu m^2/\text{hr}) \times \exp(-1.23 \, eV/0.114 \, eV) = 0.0159 \, \mu m^2/\text{hr}
\]

\[
B/A_{(100)} = (3.71 \times 10^6 \, \mu m/\text{hr}) \times \exp(-2 \, eV/0.114 \, eV) = 0.0892 \, \mu m/\text{hr}
\]

\[
B/A_{(111)} = (6.23 \times 10^6 \, \mu m/\text{hr}) \times \exp(-2 \, eV/0.114 \, eV) = 0.1498 \, \mu m/\text{hr}
\]

\[
A_{(100)} = B/|B/A| = 0.1783 \, \mu m
\]

\[
A_{(111)} = 0.1061 \, \mu m
\]

\[
X_{\text{si,(100)}} = 25 \, \text{nm} + 20 \, \text{nm} \Rightarrow \tau = (X_i^2/B) + X_i/(B/A) \Rightarrow \tau_{(100)} = 0.6318 \, \text{hr}
\]

\[
X_{\text{ox,(100)}} = 0.5*(0.1783)^*\sqrt{(1+4*0.0159*1.6318/(0.1783^2)) - 1} = 94.95 \, \text{nm}
\]

\[
X_{\text{ox,(111)}} = 0.5*(0.1061)^*\sqrt{(1+4*0.0159*1.2062/(0.1061^2)) - 1} = 95.25 \, \text{nm}
\]

\[
X_{\text{si,(100)}} = 0.46*(X_{\text{ox,(100)}} - 20 \, \text{nm}) = 34.47 \, \text{nm}
\]

\[
X_{\text{si,(111)}} = 43.81 \, \text{nm}
\]

**Step height** = \( (X_{\text{ox,(111)}} - X_{\text{si,(111)}}) - (X_{\text{ox,(100)}} - X_{\text{si,(100)}}) = -9.04 \, \text{nm} \)
3.) Consider the figure below. To simplify our process flow, we will use a single RIE step to etch both the nitride and the silicon. Let’s assume the following parameters: \( A_f, \text{silicon} = 0.2929, S, \text{silicon/nitride} = 6.5, S, \text{silicon/resist} = \infty \), Etch Rate for silicon = 5 nm/sec.

a. How long would the RIE need to be to etch down to the oxide layer? (1 pt)

\[
\text{Nitride etch rate} = \frac{5 \text{ nm/sec}}{6.5} = 0.769 \text{ nm/sec} \\
\text{Nitride etch time} = \frac{10 \text{ nm}}{0.769 \text{ nm/sec}} = 13 \text{ sec.} \\
\text{Si etch time} = \frac{200 \text{ nm}}{5 \text{ nm/sec}} = 40 \text{ sec.} \\
\text{Total etch time} = 53 \text{ sec.}
\]

b. How much undercut exists between the patterned silicon and photoresist? (1 pt)

\[
A_f = 1 - r_{\text{lat}} / r_{\text{vert}} = 0.2929 \\
\Rightarrow r_{\text{lat}} / r_{\text{vert}} = 0.7071 \\
\text{Undercut} = T_{\text{si}} \times 0.7071 = 141.42 \text{ nm}
\]

c. What is the sidewall angle after etching? (1 pt)

\[
\text{Sidewall angle} = \tan^{-1} \left( \frac{r_{\text{vert}}}{r_{\text{lat}}} \right) = \tan^{-1} (0.7071) = 54.7^\circ
\]

d. After this etch is completed, the photoresist is stripped away and the wafer is cleaned. It is then placed in a furnace with dry O\(_2\) for 3 hours at 900 °C. **Draw the final structure in full detail and label all dimensions, including oxide thicknesses**, which must be calculated by hand using the Deal-Grove model. You can ignore the bird’s beaking effect and assume that the nitride layer does not oxidize. (7 pts)

54.7° sidewall angle means that the silicon sidewall is a (111) plane, with \( X_i = 25 \text{ nm.} \)

Some oxide will also grow on the substrate, with \( X_i = 25 \text{ nm} + 200 \text{ nm} = 225 \text{ nm.} \)

\[
T = 900^\circ \text{ C} = 1173 \text{ K} \Rightarrow kT = 0.1011 \text{ eV} \\
B_{(100) and (111)} = (772 \mu\text{m}^2/\text{hr}) \times \exp(-1.23 \text{ eV}/0.1011 \text{ eV}) = 0.004 \mu\text{m}^2/\text{hr} \\
B/A_{(100)} = (3.71 \times 10^6 \mu\text{m/hr}) \times \exp(-2 \text{ eV}/0.1011 \text{ eV}) = 0.0095 \mu\text{m/hr} \\
B/A_{(111)} = (6.23 \times 10^6 \mu\text{m/hr}) \times \exp(-2 \text{ eV}/0.1011 \text{ eV}) = 0.01596 \mu\text{m/hr} \\
A_{(100)} = B/(B/A) = 0.4211 \mu\text{m} \\
A_{(111)} = 0.2506 \mu\text{m} \\
X_{i,(100)} = 25 \text{ nm} + 200 \text{ nm} \Rightarrow \tau = X_i^2/B + X_i/(B/A) \Rightarrow \tau_{(100)} = 36.34 \text{ hr} \\
X_{i,(111)} = 25 \text{ nm nm} \Rightarrow \tau = X_i^2/B + X_i/(B/A) \Rightarrow \tau_{(111)} = 1.723 \text{ hr}
\]

\[
X_{\text{ox,(100)}} = 0.5 \times (0.4211)^{[\sqrt{(1+4 \times 0.004^3 \times 39.34/(0.4211^2))} - 1]} = 238.6 \text{ nm} \\
X_{\text{ox,(111)}} = 0.5 \times (0.2506)^{[\sqrt{(1+4 \times 0.004^3 \times 4.723/(0.2506^2))} - 1]} = 60.6 \text{ nm} \\
X_{\text{si,(111)}} = 0.46 \times (X_{\text{ox,(111)}} - 20 \text{ nm}) = 18.68 \text{ nm} \\
X_{\text{si,(100)}} = 0.46 \times (X_{\text{ox,(100)}} - 200 \text{ nm}) = 17.76 \text{ nm}
\]

Silicon width at top = 650 nm – 2*(18.68 nm + 141.42 nm) = 329.8 nm

Silicon width at bottom = 650 nm – 2*18.68 nm = 612.64 nm

Step height between bottom of silicon and top of oxide grown over buried oxide layer = 0.54*(238.6 nm – 200 nm) = 20.84 nm

Remaining space on either side = (1000 nm – 0.54*60.6 nm) + 20.84 nm/tan(54.7°) = 982.03 nm
<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Thickness</th>
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</thead>
<tbody>
<tr>
<td>Silicon with (100) surface</td>
<td>$T_{si} = 200\text{nm}$</td>
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<tr>
<td>Nitride (10 nm thick)</td>
<td></td>
</tr>
<tr>
<td>Oxide</td>
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</tr>
<tr>
<td>Silicon substrate (100)</td>
<td></td>
</tr>
</tbody>
</table>

Initial structure:

- **Silicon with (100) surface**: $W = 650\text{nm}$
- **Nitride (10 nm thick)**: $W = 1000\text{nm}$
- **Oxide**: $W = 1000\text{nm}$
- **Silicon substrate (100)**: $W = 1000\text{nm}$

Resist: $T_{si} = 200\text{nm}$

- **Resist**: $W = 1000\text{nm}$
- **Nitride (10 nm thick)**: $W = 1000\text{nm}$
After etching and oxidation:

\[ W = 329.8 \text{nm} \]
\[ T_{ox} = 60.6 \text{nm} \]
\[ T_{step} = 20.84 \text{nm} \]
\[ X_{si,(100)} = 17.76 \text{nm} \]
Thin Film Deposition:

Figure 1

![Graph showing Phosphorus concentration vs. PH₃ partial pressure for different Ge concentrations.](image)

Figure 2

![Graph showing % Ge vs. GeH₄ partial pressure for different doping levels.](image)
The UC Berkeley Microlab has a MOS clean LPCVD reactor (Tystar 19) which is used to deposit in-situ doped silicon and silicon germanium (Si_{1-x}Ge_x). Figures 1-3 are actual SIMS (secondary ion mass spectroscopy) data collected from a series of Si_{1-x}Ge_x runs in Tystar 19, in order to characterize the tube for future experiments. All depositions in these figures were performed at 425°C at a total pressure of 400 mTorr. (note in Fig. 1 that the data for 0%, 16.3%, 22.7%, and 28.7% Ge were achieved by using SiH_6 as the Si carrier gas, while the data for 4.8%, 6.9%, and 8.8% Ge were achieved by using SiH_4 as the Si carrier gas). The available gases and maximum flow rates (limited by the mass flow controllers or MFC’s) are shown below:

Si source gas #1: SiH_4. Max flow = 200 sccm.
Si source gas #2: SiH_6. Max flow = 200 sccm.
Ge source gas #1: GeH_4. Max flow = 50 sccm (Ge LO MFC).
Ge source gas #2: GeH_4. Max flow = 200 sccm (Ge HI MFC).
B source gas: BCl_3. Max flow = 50 sccm. Diluted as 1% BCl_3, 99% He.

From a practical standpoint, it is preferred to keep the gas flows for a given recipe within 5% of the maximum (or minimum) gas flows that the MFC can handle. This minimizes fluctuations in gas flow rates over the course of the deposition. It is also preferred to use a MFC with as little maximum gas flow as possible, since these MFC’s have better control over gas flow.

1.) Now, let’s have some fun…
   a. Suppose we want to deposit 100 nm of n-type Si (at 425°C, 400 mT), and the target dopant concentration is 1x10^{20} cm^{-3}. Design two recipes for this (gas flows, partial pressures, and deposition time). For one recipe, the total gas flow must be 75 sccm.
(2.5 pts), while for the other recipe, the total gas flow is 200 sccm (2.5 pts). Are both recipes possible in Tystar 19 (1 pt)? Explain why or why not.

First recipe: 75 sccm total flow.
Dep. Rate ~0.7 nm/min \( \rightarrow \) deposition time = 142.85 min or 2 hr, 22 min, 51 sec.
1x10^{20} \text{ cm}^{-3} \text{ for pure Si} \rightarrow \text{PH}_3 \text{ partial pressure} = 22.5 \text{ mT}, \text{ but remember PH}_3 \text{ is diluted 50\%}. 
(\text{PH}_3 + \text{SiH}_4) \text{ partial pressure} = 45 \text{ mT} \rightarrow \text{PH}_3 \text{ flow rate} = 75 \text{ sccm} \times (45 \text{ mT}/400 \text{ mT}) = 8.44 \text{ sccm}. \ \text{Si}_2\text{H}_6 \text{ flow rate} = 75 \text{ sccm} - 8.44 \text{ sccm} = 66.56 \text{ sccm} (\text{partial pressure} = 400 \text{ mT} - 45 \text{ mT} = 355 \text{ mT}).

Second recipe: 200 sccm total flow.
Dep. Rate ~0.5 nm/min \( \rightarrow \) deposition time = 200 min or 3 hr, 20 min.
\text{PH}_3 \text{ partial pressure} = 22.5 \text{ mT} \rightarrow (\text{PH}_3 + \text{SiH}_4) = 45 \text{ mT}.
200 \text{ sccm} \times (45 \text{ mT}/400 \text{ mT}) = 22.5 \text{ sccm}.
\text{Si}_2\text{H}_6 \text{ partial pressure} = 355 \text{ mT} \rightarrow \text{flow rate} = 200 \times 355/400 = 177.5 \text{ sccm}.

The first recipe is possible, but the second recipe is not. This is because, for the second recipe, the PH\textsubscript{3} flow rate must be 22.5 sccm, but the MFC only goes up to 9 sccm.

b. Repeat for Si\textsubscript{1-x}Ge\textsubscript{x} with 28.7\% Ge content and a target dopant concentration of 5x10^{20} \text{ cm}^{-3}. 75 sccm total gas flow only. (3.5 pts)
Deposition rate at 28.7\%, 75 sccm total ~ 1.15 nm/min \( \rightarrow \) deposition time = 86.96 min or 1 hr, 26 min, 58 sec.
\text{GeH}_4 \text{ partial pressure} = 200 \text{ mT} \rightarrow \text{GeH}_4 \text{ flow rate} = 75 \text{ sccm} \times (200 \text{ mT}/400 \text{ mT}) = 37.5 \text{ sccm} (\text{use the Ge LO MFC}).
\text{PH}_3 \text{ partial pressure} = 20 \text{ mT} \rightarrow \text{PH}_3 \text{ flow rate} = 75 \text{ sccm} \times ([20 \text{ mT} \times 2]/400 \text{ mT}) = 7.5 \text{ sccm}.
\text{Si}_2\text{H}_6 \text{ partial pressure} = 400 \text{ mT} - (200 + 20 \times 2) \text{ mT} = 160 \text{ mT} \rightarrow \text{Si}_2\text{H}_6 \text{ flow rate} = 75 \text{ sccm} \times (160 \text{ mT}/400 \text{ mT}) = 30 \text{ sccm}.

c. It was noted earlier that Si\textsubscript{2}H\textsubscript{6} was used to achieve high phosphorus concentration in the Si and Si\textsubscript{1-x}Ge\textsubscript{x} films, which is not achievable by using SiH\textsubscript{4}. Explain why this is true, and cite references (2 maximum) to support your answer. (3 pts)

PH\textsubscript{3} tends to “poison” the silicon surface during Si LPCVD, an effect quite literally known as “phosphorus poisoning.” This happens because PH\textsubscript{3} has a higher reactive sticking coefficient (RSC) than SiH\textsubscript{4}. In other words, for the same flow rates of PH\textsubscript{3} and SiH\textsubscript{4}, more PH\textsubscript{3} will adsorb to the Si surface than will SiH\textsubscript{4}. For high enough PH\textsubscript{3} flow rates, we end up with complete surface coverage of phosphorus, which leaves zero available adsorption sites for SiH\textsubscript{4} and the deposition ceases. By using Si\textsubscript{2}H\textsubscript{6} (which has a higher RSC than SiH\textsubscript{4}), the Si deposition rate increases, and so the “race condition” between P and Si deposition gets pushed out to higher P concentrations before P-poisoning takes place.
2.) Suppose we want to sputter an alloy. This alloy is a combination of Pt, Al, Cr, Ti and, because we’re endlessly obsessed with bling, Au.
   
a. The sputtering ion bombardment energy is 1000 eV. Determine the requirements for Pt, Al, Cr, Ti, and Au % concentrations in the sputtering target if we want the deposited film to have 20% concentration of each of these metals. From the notes, the following sputter yields (approx.) result at 1000 eV: Ti (0.83), Cr (1.61), Pt (2.42), Al (1.92), Au, (3.14). (2.5 pts)

Ti has the lowest sputter yield, so it must have the highest alloy concentration in the sputter target. Thus, we normalize everything against Ti.

\[
\frac{S_{Ti}}{S_{Cr}} = 0.5155 \\
\frac{S_{Ti}}{S_{Pt}} = 0.3430 \\
\frac{S_{Ti}}{S_{Al}} = 0.4323 \\
\frac{S_{Ti}}{S_{Au}} = 0.2643 \\
\frac{S_{Ti}}{S_{Ti}} = 1
\]

Adding these up gives us the total normalized sputter yield, a number equivalent to “total pressure” in LPCVD recipes: 2.5551

Now we take the “partial pressure” of each metal relative to this “total pressure” to determine the alloy concentration in the sputter target to achieve equal parts in the deposited film.

\[
\text{Ti} = 100\% \times \frac{1}{2.5551} = 39.14\% \\
\text{Cr} = 100\% \times \frac{0.5155}{2.5551} = 20.18\% \\
\text{Pt} = 100\% \times \frac{0.3430}{2.5551} = 13.42\% \\
\text{Al} = 100\% \times \frac{0.4323}{2.5551} = 16.92\% \\
\text{Au} = 100\% \times \frac{0.2643}{2.5551} = 10.35\%
\]

b. Suppose the deposition rate at 1000 eV bombardment energy is 10 nm/sec. If we want to deposit a film that is 10 nm thick, would it be a good idea to use 1000 eV? Why or why not? Give two reasons. (3 pts)

This would not be a good idea. First, the variation in film thickness may be large, since the deposition is so short. Second, the alloy concentration on the wafer will likely be different than what we designed for, since the sputtering process has not yet reached a steady state.

c. Suppose we keep the sputtering target that we’ve designed in part A, but we reduce the bombardment energy to 400 eV. Determine the resulting alloy concentrations in the deposited film (2.5 pts). Also, if the deposited film thickness from part A was 100 nm, what would the film thickness be for the same sputter time at 400 eV (1 pt)? From the notes, the following sputter yields (approx.) result at 400 eV: Ti (0.45), Cr (1.07), Pt (1.46), Al (1.0), Au, (1.85).

The answer is more complex than just multiplying the sputter yield by the alloy content in the sputter target from part A, which would give:
Ti = 0.45*39.14% = 17.61%
Cr = 1.07*20.18% = 21.59%
Pt = 1.46*13.42% = 19.6%
Al = 1.0*16.92% = 16.92%
Au = 1.85*10.35% = 19.14%

Note that the sum of percentages from what is shown above adds up to 94.85%. Multiplying these values by 100/94.85 gives the correct answer, where the percentages now add up to 100:

Ti = 18.57%
Cr = 22.76%
Pt = 20.66%
Al = 17.84%
Au = 20.18%

For the 100 nm film, thickness, we take the alloy concentrations in the target and multiply by the corresponding sputter yields at (A) 1000 eV. Then we do the same for the sputter yields at (B) 400 eV, take the ratio, and multiply by 100 nm film thickness:

A = (0.3914)*0.83 + (0.2018)*1.61 + (0.1342)*2.42 + (0.1692)*1.92 + (0.1035)*3.14 = 1.6244

B = (0.3914)*0.45 + (0.2018)*1.07 + (0.1342)*1.46 + (0.1692)*1.0 + (0.1035)*1.85 = 0.9487

100*B/A = 58.4 nm