EE669: Simulation Exercise
Oxidation of silicon
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Credits: First version of this exercise, Soumyadip Chatterjee

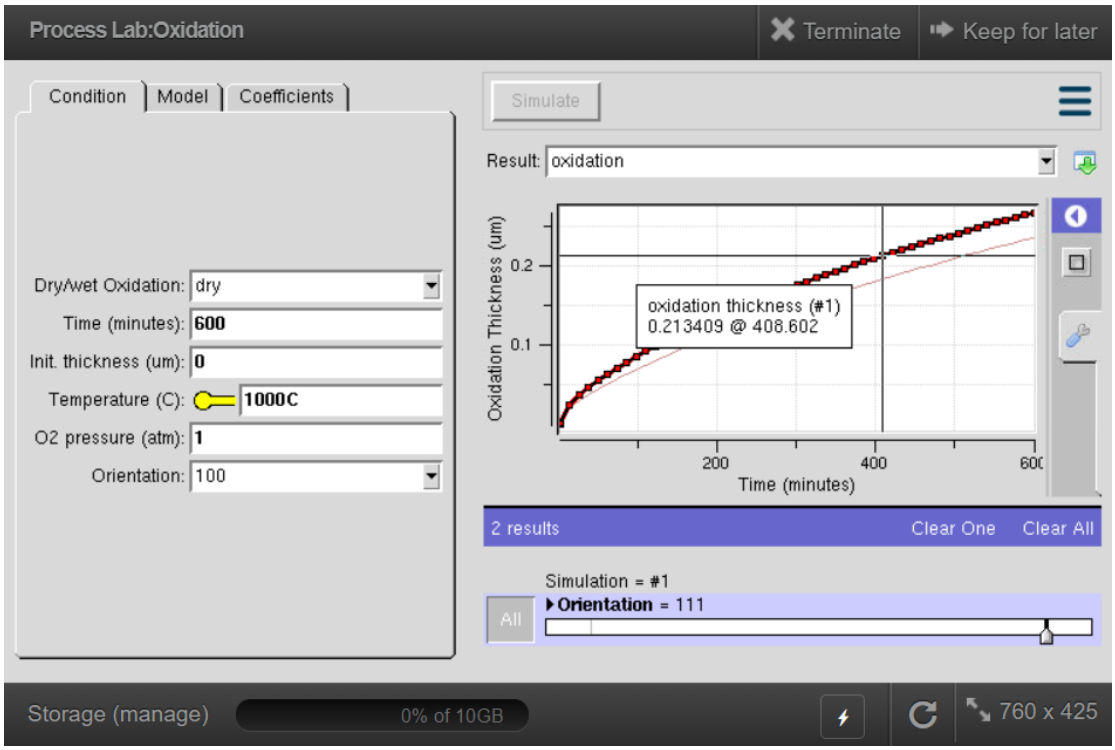
Introduction

Oxidation of silicon is an important process in silicon device fabrication. We can use two nanolab tools to develop an understanding of the process. The 'Process Lab:Oxidation' tool can be used to visualize the variation of oxide thickness or oxidation rate as a function of oxidation time. Various process and substrate conditions like, dry/wet oxidation, temperature, pressure of the oxidant, silicon surface orientation can be chosen. The oxidation is simulated using the Deal-Grove model and Massoud models of oxidation. It is possible to select "only Deal-Grove model", or "only the Massoud term" or the complete model.
The tool includes basic plotting features, and download of the results in CSV format to creat nicer plots.

You may also have a look at the 'Process Lab:Oxidation Flux' tool (https://nanohub.org/resources/prolaboxflux) which provides information about concentration of the oxidant species along the thickness of the oxide.

How to use the tool?

- Create an account in nanohub
- Open the link: https://nanohub.org/resources/prolabox and launch the 'ProcessLab:Oxidation' tool. The tool window looks something like below



- Play with the process parameters on the left hand side to understand their significance in the oxidation process
- Hovering on the graph, you can get individual data points
- You can also select oxidation rate from the ***Result*** drop down menu to check how oxidation rate evolves with time
- When the simulation is run multiple times, an ***All*** button appears below the graph, using which we can see all the plots on the same graph. The graph to be highlighted can be moving the *slider* on the right of ***All***.
- Simulation results can be downloaded in *comma-separated values (CSV)* by clicking on the green down arrow on the right side of ***Result***.

Exercise

1. For all the questions below, download the CSV files for the simulations, and make plots in Origin (IITB has license – please visit cc.iitb.ac.in to know how to use it) or Matplotlib (visualization with Python) or Matlab or Octave or Igor or …. *Do not use MS Excel*.
2. Applicability of the Deal-Grove model:
    a. Simulate dry oxidation of {100} oriented silicon wafer at a pressure of 1 atmosphere at 1000°C and 850°C for 600 minutes by using the 3 models available, namely
        i. Deal-Grove model
        ii. Massoud term only
        iii. Both

        For which of these two temperatures, Deal-Grove model alone is sufficient to predict the oxide growth?
    b. Repeat the above for wet oxidation. Comment on the results.
3. Compare the oxidation rates at 1000°C for dry and wet oxidation
4. Crystal surface orientation dependence: Simulate wet oxidation at 1100°C for 250 minutes for {100} and {111} surface orientations. Comment on the orientation dependence.
5. The orientation dependence can be partly explained by the density of silicon atoms on the {111} and {100} planes. Visualizing the unit cell using VESTA determine the arial density of silicon atoms on the {111} and {100} planes.
6. Dependence on gas pressure: Simulate dry oxidation at 1100°C for 250 minutes for {100} surface orientation at oxygen pressures of 1 atmosphere and 0.1 atmosphere. Comment on the pressure dependence of oxidation.