Motivation:

Diffusion is the random motion of atoms moving into other atoms. There are a variety of types based on whether it happens between the same or different species of components, happens freely or forced, is into a liquid or a solid, and more. This lab explores dopant diffusions in Si substrate through two different types: Defect Coupled Diffusion and Concentration-Dependent Diffusion. **Defect Coupled Diffusion** (Vacancy Diffusion) is where point defect (vacancies) in the host species is required for the diffusive species to diffuse. **Concentration-Dependent Diffusion** is where the concentration of the diffusive species is a factor in the rate and extent of diffusion. Developing and improving the performance of doped semiconductors is a common example of where diffusion plays a vital role. Simulating the diffusion allows for the development process to be more direct and efficient by limiting the experimental trial-and-errors that need to be done. These computational modeling labs are a form of hands-on learning that can be used in other materials engineering fields in industry and/or research.

Fick's First Law is for steady-state diffusion and describes the diffusion of particles along the concentration gradient (flux). Whereas **Fick's Second Law** is for non-steady-state and describes the rate of diffusion. In the case of this lab, the **Semi-infinite equation** can be used to represent the doping of the semi-conductive material:

$$c(x,t) = c_s \text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

- $c(x,t)$: concentration of the diffusive specie at a specific time and specific distance into the host specie from initial boundary
- c_s: concentration of diffusive specie at boundary of diffusion
- x: distance into the host specie from initial boundary
- D: material specific diffusion coefficient
- t: time in seconds since the start of diffusion

To solve for the approximate "$erfc(z)$" value:
- Solve for "z" value, $z = \frac{x}{2\sqrt{Dt}}$
- Determine "$erf(z)$" using table of predetermined data values of "$erf(z)$"
- Solve for "$erfc(z)$", $erfc(z) = 1 - erf(z)$

Simulation Tool Introduction

1) "Process Lab: Defect-coupled Diffusion"
   - **Link:** https://nanohub.org/resources/prolabdcd/about
   - **What it does:** Simulates diffusion of dopants in Si substrates with point defects.
   - **Specific Materials Used:** The tool will be used to simulate doping a semiconductor material with Phosphorus (a representative for common dopants).

2) "Process Lab: Concentration-dependent Diffusion"
- **Link:** https://nanohub.org/resources/prolabcdd
- **What it does:** Simulates standard diffusion and concentration-dependent diffusion.
- **Specific Materials Used:** The tool will simulate doping a semiconductor material with Phosphorous (a representative for common dopants).

Tools' Origin: Stanford University developed both tools to explore dopant diffusion and to understand how variables affect the diffusion (i.e. length of time, temperature, dopant species, etc).

Laboratory Overview:

**Each run will consist of comparing two simulations that vary by a single variable.
**Run time: less than a minute each

Tool 1:
- **Run 1**: Time Variation Effect on Defect Coupled Diffusion
- **Run 2**: Effect on Temperature Variation on Defect Coupled Diffusion
- **Run 3**: Time Variation Effects on Defect Independent Diffusion
- **Run 4**: Temperature Variation Effects on Defect Independent Diffusion

Tool 2:
- **Run 5**: Effect of Dopant Source Variation on Concentration-Dependent Diffusion
- **Run 6**: Effect of Dopant Dose Variation on Concentration-Dependent Diffusion
- **Run 7**: Effect of Concentration Dependence Variation on Diffusion
- **Run 8**: Effect of Variation of Dopant Element on Concentration-Dependent Diffusion

Laboratory Instructions:

Tool 1 (Process Lab: Defect Coupled Diffusion)
https://nanohub.org/resources/prolabdcd/about

- Open link, what it should look like:
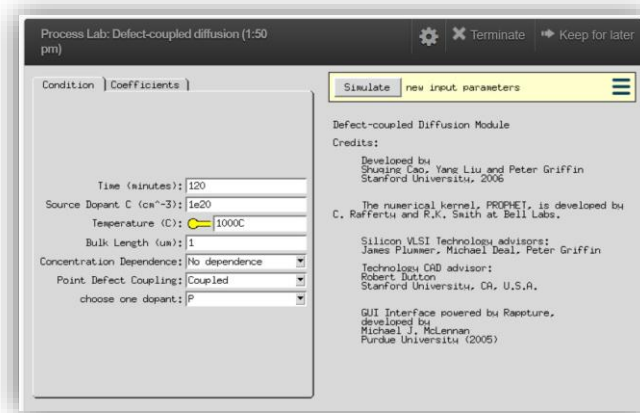
- The initial screen will show some of the input parameters of the diffusion process: time, source of the dopant, bulk length, concentration dependence, etc.

## Run 1: Time Variation Effect on Defect Coupled Diffusion

- *First Simulation:* The first simulation will use all the preset variables as is, click "Simulate" button to start the tool. The resulting graph should look like:
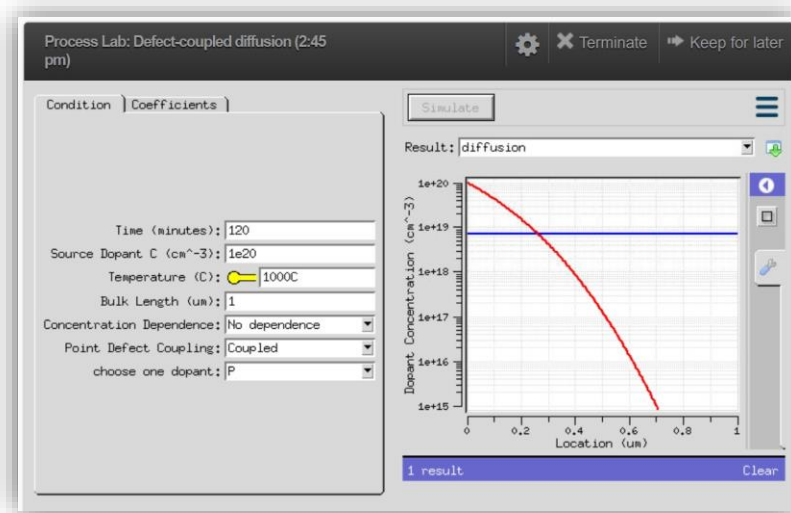

- *Second simulation:* Adjust time to 12 minutes (make sure to hit enter and you'll see a light-yellow bar appear above the graph that says "new input parameters") and hit simulate
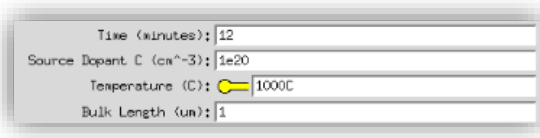

- Once finished, click the "All" button below the resultant graph to show both results next to each other to visually compare.
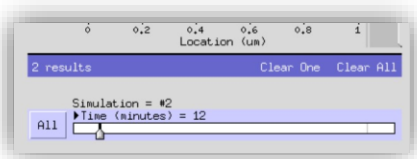

- Above the resultant graph, you will see a "Result: Diffusion" bar, click the down arrow and choose "download" from drop-down menu OR click green, downward arrow to the right of the drop-down menu.
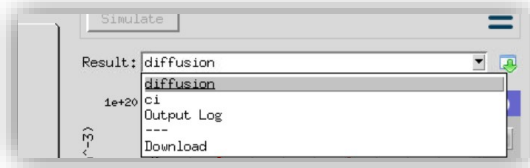
- An additional menu will pop up for options on how to download, click "Download" again to download as "Data as Comma-Separated Values".
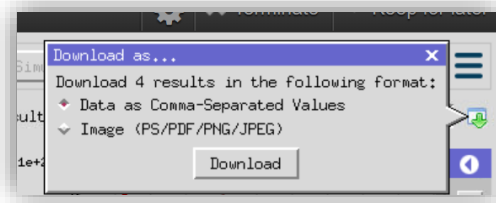
- Click "Save As…" and an additional window will pop up (might be on Notepad app). Click the in window and then "Ctrl + A" to highlight the whole data set, then right click into the highlighted portion and copy.
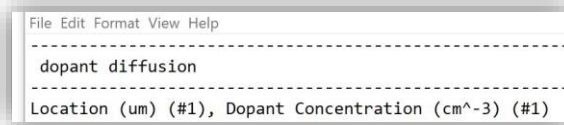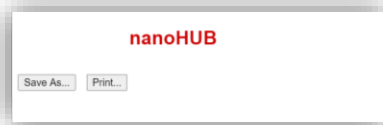
- Open Excel, right click and paste into an empty cell. From there the data will be in two separate columns (Dopant Concentration and Location).
- Graph the dopant diffusion data from both simulations in a scatter plot. Click an empty cell and then insert a scatter plot. Click the "choose data" tab on top (you will have 2 sets of data: dopant concentration from first simulation against the location and the second set being the dopant concentration from the second simulation against the location) into a single scatter plot with **axis labels, units, and legend** (location on x-axis and dopant concentration on y-axis). Cut off second simulation data as soon as it plateaus. Your graph may look slightly different from the simulation results because the tool uses a log y-axis and sometimes it does not, all the graphs you produce will not have a log axis.

Question 1: What is different between the two sets of data visually. Why do they look the way they do? Focus on how time is related to diffusion. (1-2 sentences)

Question 2: Solve Fick's 2nd law using data from the first run to solve for D and C_s.

Question 3: Display a polynomial trendline on the graph for both sets of data. What is the R^2 value? What does the slope of the trendline represent?

Question 4: How deep into the material will the diffusive specie need to go until it plateaus for the first simulation of Run 1?

- Clear all results and reset preliminary parameters again (will have to do manually or terminate tool and re-launch it)
- *Simulation 1:* Run simulation with preliminary parameters.
- *Simulation 2:* Change temperature from "1000 °C" to "1500 °C", run simulation.
- Click "All" to visually compare both results together.
- Produce an Excel graph with the data from first (**dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend**). Refer to previous instructions for more details on how to download data if needed.

Question 5: What variable needs to be adjusted for the second simulation to produce a similar trend to the first (without changing the dopant species)?

- Produce a graph with data from a run with 1500 °C as a temperature parameter after adjusting a variable to produce a similar trend to the first simulation (**dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend**). When downloading data, you can clear a couple results that will not be used (if you have extra results from adjusting a variable), so that the data you download will not have an abundance of info you will not use.

Question 6: Include a polynomial trendline and R^2 value on both of your graphs. How does the R^2 value compare to the previous run?

Question 7: Explain the effect of temperature on atoms during diffusion either physically or mathematically (2-3 sentences). For extra credit, explain the effect in both terms.

- Clear all previous results and reset preliminary parameters (will have to do manually, or terminate tool and re-launch it).
- *First simulation:* Change "Point-defect Coupling" from "Coupling" to "No coupling", then simulate.
- *Second simulation:* Change time to 12 minutes and keep the "No coupling" parameter, then simulate.
- Click "All" to visually compare both results together.
- Produce a single graph with the data from first and second simulation (**dopant concentration on y-axis, depth into host specie on x-axis, units, legend**). Refer to previous instructions for more details on how to download data if needed.

Question 8: Display a trendline and R^2 value as well? How does it compare to previous R^2 values? What could these variations mean?

Question 9: What effect did time variance have on the results between the first and second simulation?

Question 10: How does "Coupling" compare to "No coupling" dependence between Run 1 and 3?

**Run 4: Temperature Variation on Defect Independent Diffusion**

- Clear all previous results, reset original parameters (will have to do manually, or terminate tool and re-launch it).
- *First simulation:* Change "Point-defect Coupling" from "Coupling" to "No coupling", hit simulate.
- *Second simulation:* Change temperature from "1000 °C" to "1500 °C" and keep the "No coupling" parameter, run simulation.
- Click "All" to view both results to visually compare.
- Produce a graph with the data from first simulation (dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend). Refer to previous instructions for more details on how to download data if needed.

Question 11: Is the difference between the first and second simulation results comparable to those in Run 2?

- Adjust the same variable you adjusted in Run 2 to produce a similar diffusive trend for the 1500 °C parameter. Once you have a simulation trend result that is like the first simulation, produce a second graph for this run from that data. You can clear a couple results that will not be used (if you have extra results from adjusting a variable), so that the data you download will not have an abundance of info you will not use.
- Produce a graph from Excel with data from the second simulation that had a similar diffusive trend to the first. Make sure to include appropriate axis labels and units and a legend.

Tool 2: "Process Lab: Concentration-dependent Diffusion"
(https://nanohub.org/resources/prolabcdd)

- Open link, what it should look like:
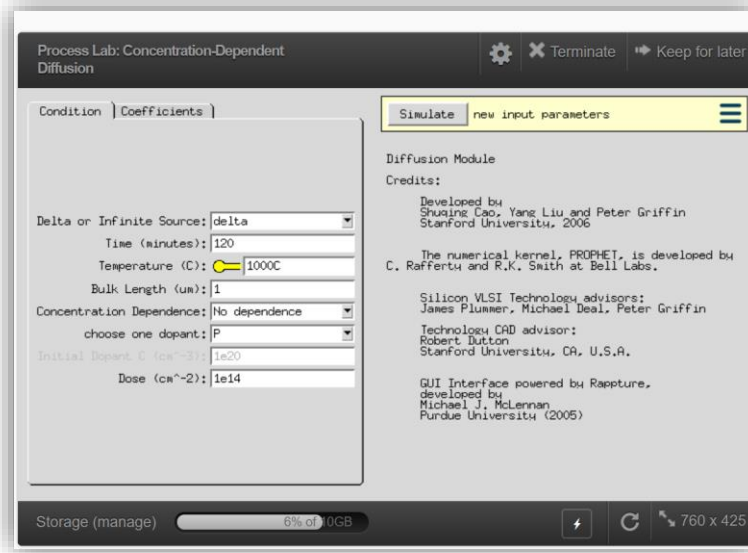
Run 5: Effect of Dopant Source Variation on Concentration-Dependent Diffusion

- First simulation: Run using preliminary parameters (Note parameters for later reference)
- Second Simulation: Change "Dopant Source" from "delta" to "infinite", run simulation.
- Click "All" to view both results to visually compare.
- Produce a single graph with the data from first and second simulation (**dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend**). Refer to previous instructions for more details on how to download data if needed.
- Download data from simulations following instructions from Run 1.
- Create a single Excel graph from the location (x-axis) versus dopant concentration (y-axis) of both simulation 1 and 2.
- On the graph, include: **axis labels and units, legend, and trendline** for both data sets.

Question 12: What is the flux of the first and second simulation (should only need graph)? How did changing the dopant source affect the results? Why?

Question 13: Solve Fick's 2nd law for preliminary parameters of Tool 2 using the data to solve for D and C_s.

Run 6: Effect of Dopant Dose Variation on Concentration-Dependent Diffusion

- Clear all previous results and reset preliminary parameters (will have to do manually, or terminate tool and re-launch it).

- First simulation: Run simulation with preliminary parameters.
- Second simulation: Change "Dose" from "1e14" to "1e15"
- Click "All" to view both results to visually compare.
- Produce a single graph with the data from first and second simulation (dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend). Refer to previous instructions for more details on how to download data if needed.

Question 14: Explain the effect of the dopant dose variation on the diffusive results between the different simulations. (2-3 sentences)

Question 15: Predict what would happen if the dopant dose were changed to "1e13", a value below the original dopant dose. Run a simulation to verify prediction.

Run 7: Effect of Concentration Dependence Variation on Diffusion

- Clear all previous results and reset preliminary parameters (will have to do manually, or terminate tool and re-launch it).
- First simulation: Run simulation with preliminary parameters.
- Second simulation: Change "Concentration Dependence" from "No dependence" to "C dependent".
- Click "All" to view both results to visually compare.
- Produce a single graph with the data from first and second simulation (**dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend**). Refer to previous instructions for more details on how to download data if needed.

Question 16: Explain effect of changing concentration dependence. (1-2 sentences)

Run 8: Effect of Variation of Dopant Element on Concentration-Dependent Diffusion

- Clear all previous results and reset preliminary parameters (will have to do manually, or terminate tool and re-launch it).
- First simulation: Run simulation with preliminary parameters.
- Second simulation: Change dopant to "As" for Arsenic
- Click "All" to view both results to visually compare.
- Produce a single graph with the data from first and second simulation (**dopant concentration on y-axis, depth into host specie on x-axis, labels, units, legend**). Refer to previous instructions for more details on how to download data if needed.

Question 17: Did changing the dopant element have a noticeable effect on the diffusion pattern? If yes, why? If no, do you think another element would?

Formatting Notes:
- Questions answered in complete sentences
  - Those with numbers, emphasize answer with box/underline
- Graphs have axis titles with units, legend, polynomial trendline, and R^2 value

Deliverables

1) All questions answered (Total of 17)
2) Graphs made from Runs 1-8

Tips for Using Tool in nanoHUB
- Can look at different ways to manipulate the results graph and see how they were plotted

Tool Citations:

1) Shuqing (Victor) Cao, Yang Liu, Peter Griffin (2019), "Process Lab: Defect-coupled diffusion," https://nanohub.org/resources/prolabdcd. (DOI: 10.21981/4TB9-S464)

2) Shuqing (Victor) Cao, Yang Liu, Peter Griffin (2019), "Process Lab: Concentration-Dependent Diffusion," https://nanohub.org/resources/prolabcdd. (DOI: 10.21981/DJ6J-7953)