SIMULATION PROJECT 2

Part 2 (80 Points): Assigned *Wednesday, April 15*
Due *Friday, May 1 at 11:59 PM* on Canvas

Part 2 Objective

This simulation project asks you to use Silvaco Atlas to first understand the influence of in-gap state (trap states) distributions on device behavior and then to implement a short sweep of the geometry.

Submission Checklist:

- ☐ Section I
  - ☐ Interface trap peak density **(5 plots)**
  - ☐ Bulk shallow trap peak density **(5 plots)**
  - ☐ Bulk deep trap peak density **(5 plots)**
  - ☐ Script of ".in" file for one of the bulk trap sweeps
- ☐ Section II
  - ☐ Channel length **(4 plots)**
  - ☐ Script of ".in" file for the channel length sweep

Section I: Influence of trap density of states on device behavior

Warning! These simulations take a long time to run.
(~25 min/parameter x 3 parameters = ~75 min/sweep,
total run time for 3 sweeps is ~225 min)

Starter files:

- TFT_0.in
- TFT_InterfaceExample.in

Simulation Overview

Investigate the changes in threshold voltage (Vth) and subtheshold swing (SS) as the trap density of states is varied. The exponential-Gaussian density of states model is defined in eqn 15-1 through 15-5 in *Atlas 15.2.3, pg 817*. The following trap distribution parameters will be varied:

- Interface trap peak density [cm^{-2}]
  - Statement: `intdefect`
  - Parameter: `nta`
  - Sweep: `(0.5e12,2e12,8e12)`
- Bulk shallow trap peak density [cm^{-3}]
  - Statement: `defects`
  - Parameters: `nta` and `ntd`
  - Sweep: `(0.5e21,2e21,8e21)`

- Bulk deep trap peak density [cm^{-3}]
    - Statement: `defects`
    - Parameter: `ngd`
    - Sweep: `(0.5e16,2e16,8e16)`

Simulation Report

Report results of each trap distribution parameter. 5 plots/parameter sweep for a total of 15 plots for Section I. All plots need labels and units for both the x- and y-axis.

- (1) Plot of trap density of states, g(E), for all **3 parameters** in one sweep. These will look similar to the defect plots that were automatically plotted in TonyPlot from Project 2 Part 1.
    - g(E) defined by eqn 15-1, *At 15.2.3, pg 817*. The same equation form applies to both bulk and interface states.
    - When sweeping bulk traps, plot only the bulk traps. When sweeping interface traps, plot only the interface traps.
    - For the interface trap sweep, plot only $g_{TA}(E)$ and not the full g(E).
    - x-axis linear, from conduction band to valence band; y-axis log; key required
- (2) Plots of transfer curves for all **3 parameters** in one sweep.
    - (1) x-axis linear; y-axis linear; key required
    - (1) x-axis linear; y-axis log; key required
    - Include captions on both plots with observations on trends
- (1) Plot of threshold voltage (V_{th}) as a function of the parameter being swept
    - x-axis log; y-axis linear
    - Include caption with observations on trends
- (1) Plot of subthreshold swing (SS) as a function of the parameter being swept
    - x-axis log; y-axis linear
    - Include caption with observations on trends
- Script of ".in" file for one of the bulk trap sweeps

Additional Simulation Notes

- **"TFT_0.in"** Besides the trap distribution parameters being swept, all other parameters should be the same as the base file TFT_0.in
- **"TFT_InterfaceExampe.in"** This file demonstrates the syntax and code of how to generate a sweep over interface traps. Use this file as a template to sweep over other trap parameters. See Appendix I for a summary of key commands showcased in the starter file.
- **Folders:** It is recommended that you put each ".in" sweep file in separate folders. This will help minimize the file clutter when you're doing data analysis and also prevent accidental file overwriting and data loss.
- **Plotting trap density of states:** Trap density of states can be plotted from the ".dat" files or you can create a MATLAB (or equivalent plotting program) plot of the g(E) function defined in eqn 15-1 through 15-5 in *Atlas 15.2.3, pg 817*. However, regardless of the program you use to plot in, the plots must be a sum of all the components of g(E) unless otherwise mentioned.
- **Voltage threshold (V_{th}) and subthreshold swing (SS):** Values for both can be extracted in Deckbuild or separately through MATLAB or an equivalent data processing program. V_{th} can be found using the graphical method shown in Fig. 5.1 of Wager's paper and SS can be found in the text located right above Fig. 5.1.

Section II: Dynamically modifying geometry

Starter files:

- TFT_0.in

Simulation Overview

Implement a script that dynamically modifies the geometry, in this case, the channel length. No analysis required for this section, only plots.

- Channel length [µm]
  - Sweep: `(15,30,60)`

The starter file, "TFT_0.in" has a channel length of 30 um. Modify the "TFT_0.in" file to sweep over the different channel lengths. Be sure your script adjusts both the mesh definitions and the electrode definitions for the new channel lengths.

Simulation Report

- (2) Plots of transfer curves for all **3 parameters** in one sweep.
  - (1) x-axis linear; y-axis linear; key required
  - (1) x-axis linear; y-axis log; key required
- (1) Plot of threshold voltage (V_{th}) as a function of the parameter being swept
  - x-axis log; y-axis linear
- (1) Plot of subthreshold swing (SS) as a function of the parameter being swept
  - x-axis log; y-axis linear
- Script of ".in" file for the channel length sweep

Additional Simulation Notes

- For these channel length simulations, the solver takes smaller steps in order to converge. This results in different numbers of data points for the 3 different parameters. If you would like the .csv file to have only the points specified in the sweep, modify your log statement to the following:

```
log outf=${file_name}.log csvfile=${file_name}.csv no.trap
```

Note on Midterm 2 Take Home Exam

The take home part of Midterm 2 will feature Silvaco TFT design and optimization simulations. One of the key components of the simulation portion will include optimizing the device geometry. Some TFT figures of merit to optimize will include, Vth, SS, and mobility.

Appendix I: TFT_InterfaceExample.in Starter File

Below are the key features in the file that will be useful for this section:

- **Loop**: (*Db 4.8; ppg 91, mpg 88*)
  - Example initialize command
    `loop steps=5`
  - End command
    `l.end`
  - Deckbuild User Manual (Db) 4.8; pdf page (ppg) 91, manual page (mpg) 88
- **Assign**: defining global variables that can dynamically change with the loop (*Db 4.2; ppg 80, mpg 77*)
  - Index Example
    - Example initialize command
      `assign name=index print n.value = 1 delta = 1`
    - Calling variable
      `${index}`
  - Array of Values Example
    - Example initialize command
      `assign name=infF print`
      `n.value=(0.5e12,1e12,2e12,4e12,8e12)`
    - Calling variable
      ${infF}
- **Extract**: Deckbuild's in-system extraction language that allows the measurement of physical and electrical properties in a simulated device. (*Db 5.4; ppg 167*)
  - Example Command: Extract V_{th}
    ```
    extract name="vt" (xintercept(maxslope( \
    curve(abs(v."gate"),abs(i."drain")))) \
    - abs(ave(v."drain"))/2.0)
    ```
  - "\" is used to continue a command onto a new line
  - When the simulation is done running (has reached the "quit" command), Silvaco will auto generate a summary of all extracted values during the run. Otherwise the extracted values will also show up in the log.
- **How to use the Atlas User Manual**
  - Structure of an Atlas command
    `<STATEMENT> <PARAMETER>=<VALUE>`
  - Example
    `region num=1 material=igzo y.min=0  y.max=0.02`
    - Statement: `region`
    - Parameters: `num, material, y.min, y.max`
  - Go to Chapter 22 in the Atlas User Manual to look up commands by statement and its affiliated parameters. Default values and units are also listed in this chapter.