Computational Microelectronics
Lecture 8 Diffusion

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Diffusion

A simple case

- Neglect the electric field dependence.
  - Also consider only one dopant.

$$\frac{C(x_i, t_k) - C(x_i, t_{k-1})}{\Delta t} \Delta x - D \frac{1}{\Delta x} [C(x_{i+1}, t_k) - C(x_i, t_k)]$$
$$+ D \frac{1}{\Delta x} [C(x_i, t_k) - C(x_{i-1}, t_k)] = 0$$

  - Now, find out entries of the Jacobian matrix. Note that there are three variables, $C(x_{i+1}, t_k)$, $C(x_i, t_k)$, and $C(x_{i-1}, t_k)$.

Jacobian

- The diagonal component, $A_{i,i}$

$$A_{i,i} = \frac{\Delta x}{\Delta t} + 2\frac{D}{\Delta x}$$

  - Positive

- Off-diagonal components, $A_{i,i+1}$ and $A_{i,i-1}$

$$A_{i,i+1} = -\frac{D}{\Delta x}$$

$$A_{i,i-1} = -\frac{D}{\Delta x}$$

  - Negative

HW#8

- Due: AM08:00, September 25
- Problem#1
  - Solve again Problem#1 of HW#5. However, in this time, implement the code with the Newton-Raphson method. Of course, since the system is linear, your update vector will become very small after the first Newton iteration.

Diffusion – Electric Field

Single dopant with electric field

- Now, consider the electric field dependence.
  - Still, consider only one dopant, which is positively charged.
  - Use the following discretized flux:

$$F_{C,i+0.5} = -\frac{D}{\Delta x}\frac{1}{\sqrt{n(x_{i+1},t_k)n(x_i,t_k)}} \times [C(x_{i+1},t_k)n(x_{i+1},t_k) - C(x_i,t_k)n(x_i,t_k)]$$

  - Confirm the correctness of the above expression.

Jacobian

- The diagonal component, $A_{i,i}$

$$A_{i,i} = \frac{\Delta x}{\Delta t} + \frac{D}{\Delta x}\sqrt{\frac{n(x_i,t_k)}{n(x_{i+1},t_k)}} + \frac{D}{\Delta x}\sqrt{\frac{n(x_i,t_k)}{n(x_{i-1},t_k)}} + \textit{terms related to } \left.\frac{dn}{dC}\right|_{C(x_i,t_k)}$$

  - We must prepare $\left.\frac{dn}{\partial C}\right|_{C(x_i,t_k)}$.
  - (Similar terms for off-diagonal components)

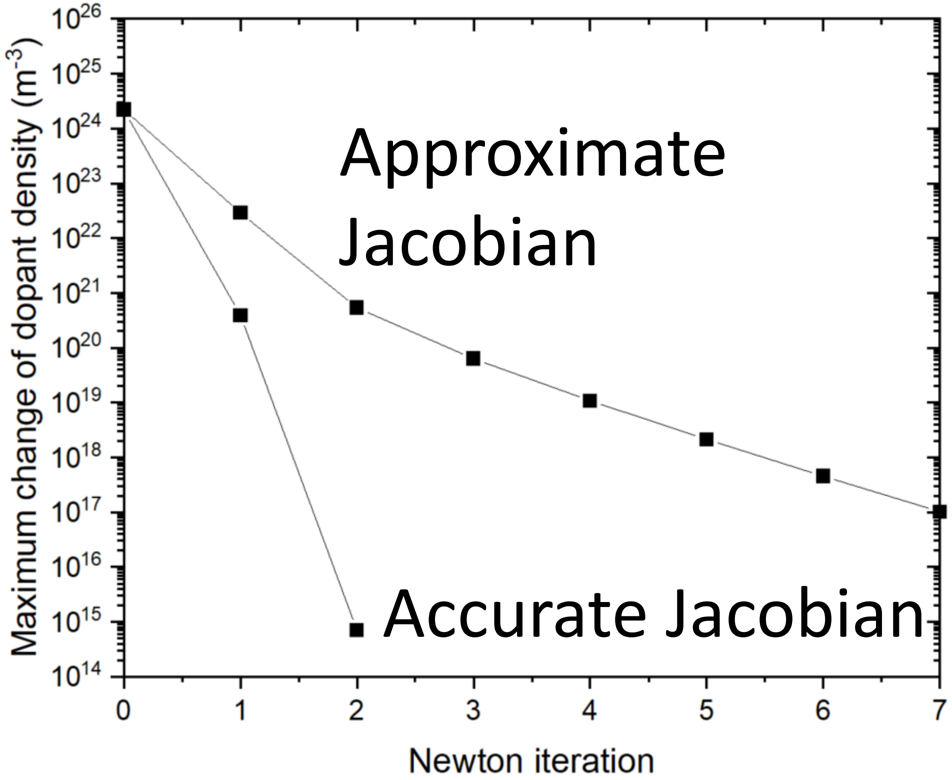
Note

- Linear case
  - Every time instance, t_k, takes only one $Ax = b$.
  - A is time-independent.
  - C's are calculated directly.
- Nonlinear case
  - Several iterations at every time instance
  - The Jacobian matrix depends on the solution. (We must re-calculate it at every iteration.)
  - δC's are calculated and C's are updated.

Number of iterations

- For a given transient simulation, it takes
  - An accurate Jacobian matrix: 137 iterations
  - A Jacobian matrix without $\frac{dn}{\partial C}$ terms: 526 iterations

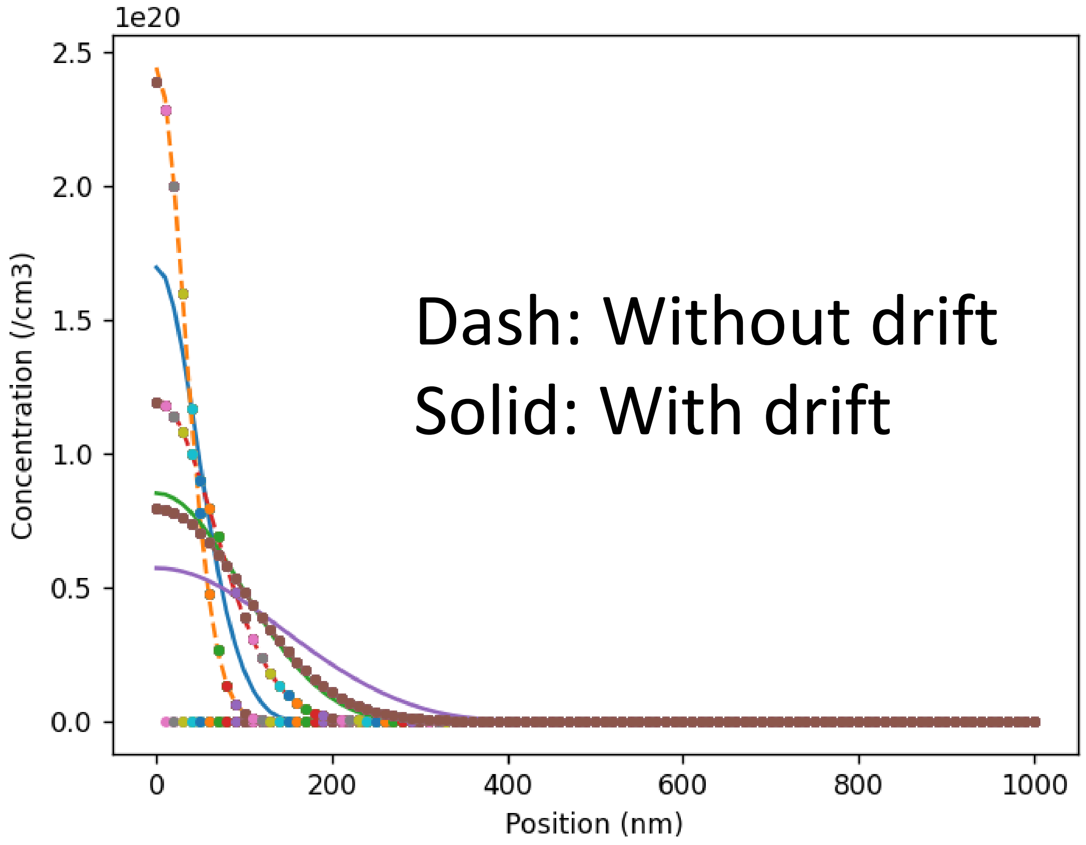
```
0 2.169197554059118e+24
1 3.900680956190052e+20
2 692935559081258.4
```

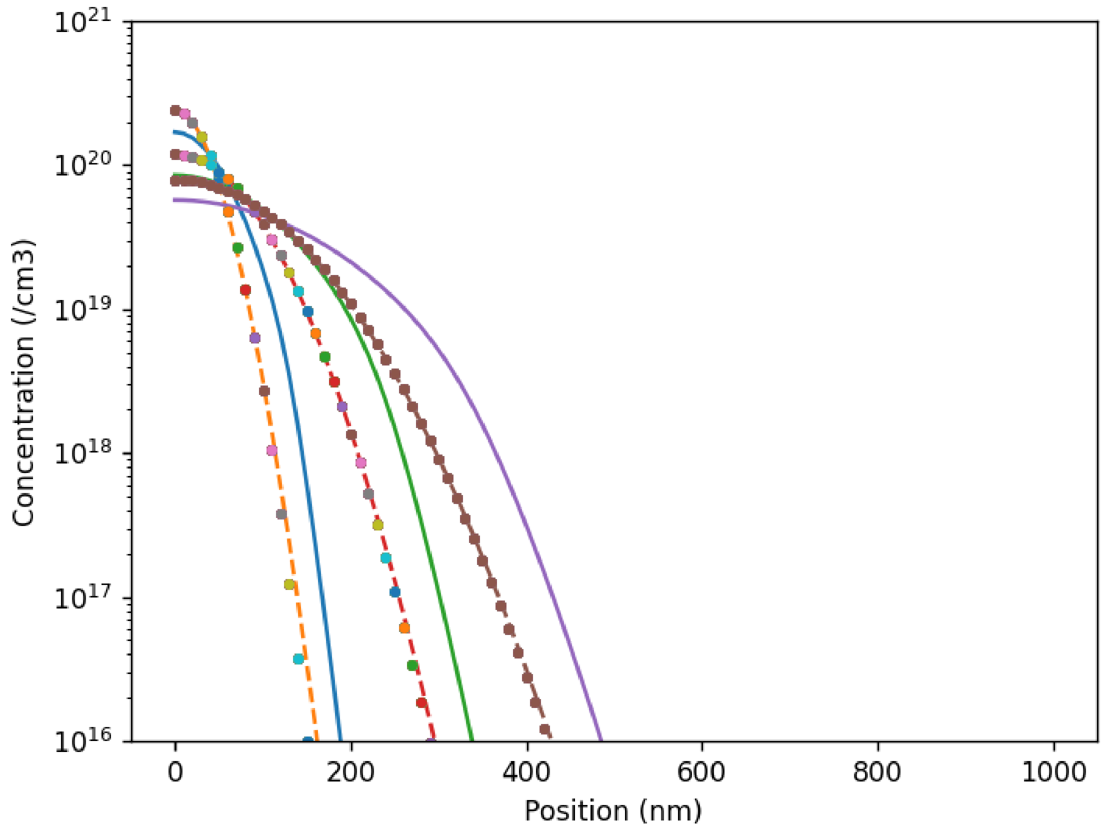



```
0 2.1978298208828112e+24
1 2.9053050667858773e+22
2 5.346531455478733e+20
3 6.31481868904466e+19
4 1.0742905060590954e+19
5 2.1224080530933048e+18
6 4.538011714971787e+17
7 1.0180945920086405e+17
```

Simulation results @ 1000 °C

- Observe the impact of drift term. (Delta-like dose, $2X10^{15}$ cm^{-2})
  - Three time instances, 400 sec, 1600 sec, and 3600 sec





HW#8

- Problem#2
  - Reproduce the last graphs.

Thank you!