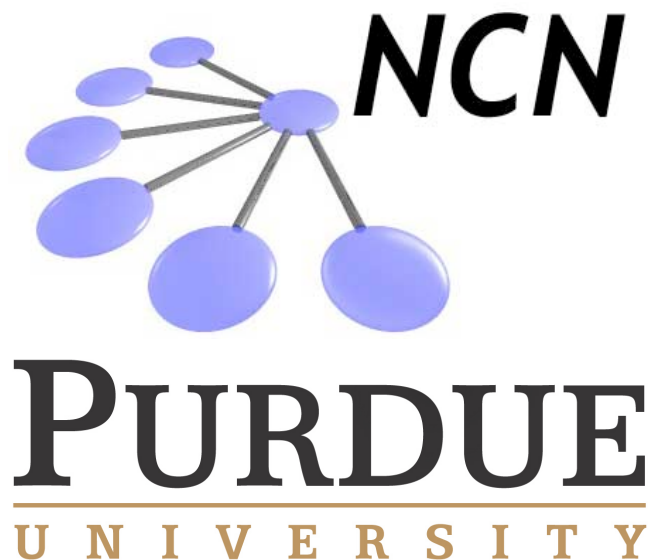


# *Network for Computational Nanotechnology (NCN)*

*UC Berkeley, Univ. of Illinois, Norfolk State, Northwestern, Purdue, UTEP*

## **First-Time User Guide Drift-Diffusion Lab v1.31**



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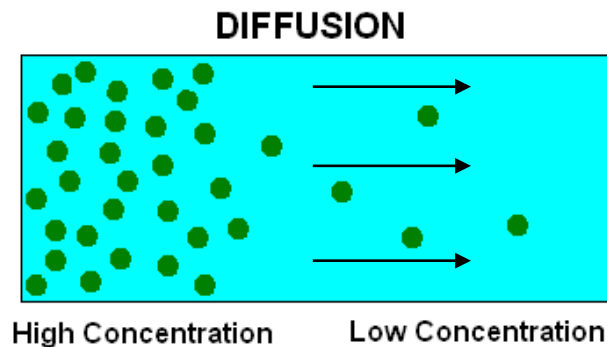
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# Introduction: What is Drift and Diffusion ?

**Diffusion** – movement of carriers from a region of a higher concentration to a region of a lower concentration

$$J(x) = q.D.\frac{dn}{dx} \quad [1]$$



**$J(x)$  : Current Density (A/cm<sup>2</sup>)**

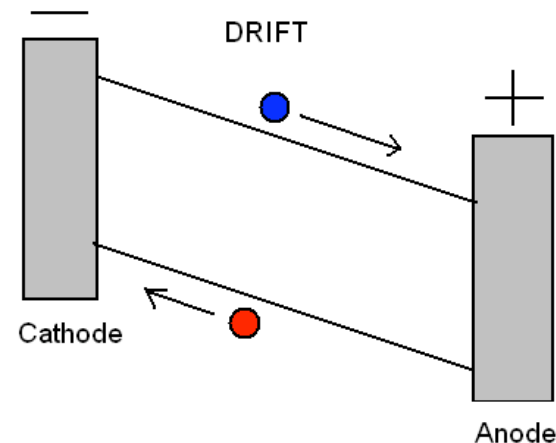
**$q$  : Charge of an Electron (C)**

**$D$  : Diffusion Constant (cm<sup>2</sup>/s)**

**$n$  : Carrier Density (cm<sup>-3</sup>)**

**Drift** –under movement of carriers application of electric field

$$J(x) = q.n\mu.E \quad [1]$$



**$J(x)$  : Current Density (A/cm<sup>2</sup>)**

**$q$  : Charge of an Electron (C)**

**$\mu$  : Carrier Mobility (cm<sup>2</sup>/V.s)**

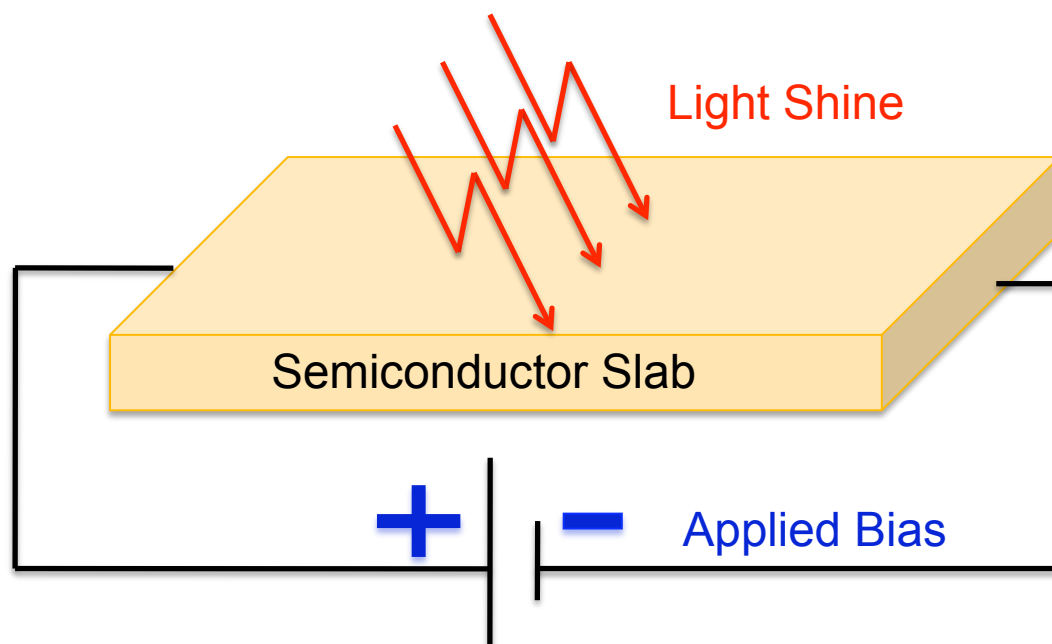
**$E$  : Electric Field (V/cm)**

## Introduction: What can be Done with the Drift-Diffusion Lab?

Simulate multiple experiments with a combination of  
**Drift** and **Diffusion** mechanisms.

simulate **drift** with applied **bias**

simulate **diffusion** by shining **light**



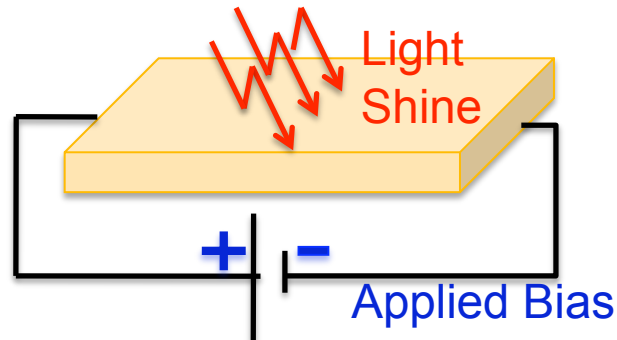
## Input Parameters for the Tool

### Simulation Setup:

- Material (Si/Ge/GaAs)
- Minority carrier lifetime (us)
- Length of slab (um)
- Type of doping (n/p type)
- Doping level (/cm<sup>3</sup>)
- Turn ON/OFF surface recombination
- Set operation temperature (K)

### Choose Experiment:

- Apply bias only
  - define bias value
- Shine light at edge
  - define generation rate (/cm<sup>3</sup>.s)
  - define depth of penetration
- Shine light at top
  - define the region at top for light shine
- Shine light at edge and apply bias
- Shine light at top and apply bias



## Example 1: A Walk-through of a 'Drift' Problem

- This tool can be used to estimate low field **electron mobilities**  $\mu_n$  for bulk Si, Ge and GaAs. Consider the following example:

Drift-Diffusion Parameters

Structure Experiment Materials

Semiconductor slab length(um): 1um

Type of doping: N-type

Doping level: 1e+15/cm3

Assume a 1  $\mu\text{m}$  long semiconductor  
N type doped at 1e15/cm3

Drift-Diffusion Parameters

Structure Experiment Materials

Type of experiment: 1. Apply bias only

Choose the Experiment:  
1. Apply bias only

## A Walk-through of a 'Drift' Problem, cont'd

Drift-Diffusion Parameters

Structure Experiment Materials Env

Material: GaAs

Minority carrier lifetimes

For electrons: 1us

For holes: 1us

Choose material – Si/Ge/  
GaAs

Drift-Diffusion Parameters

Structure Experiment Materials Environment Surface Recombination

Ambient temperature: 300K

Applied Voltage: 0.6V

Number of points: 12

Generation Rate/(cm<sup>3</sup>\*s), G = 2e+20

Penetration depth: 0.01um

Let the experiment be at  
room temperature – 300K  
and the bias ranges from  
0-0.6V.

**E=6000 V/cm**  
“0.6V applied  
across 1μm”

Set surface  
recombination velocity  
to a high value to  
obtain an ideal contact.

Drift-Diffusion Parameters

Structure Experiment Materials Environment Surface Recombination

Surface Recombination on left contact: ☒ yes

Left Contact Electron surface recombination velocity: 1e+07cm/s

Left Contact Hole surface recombination velocity: 1e+07cm/s

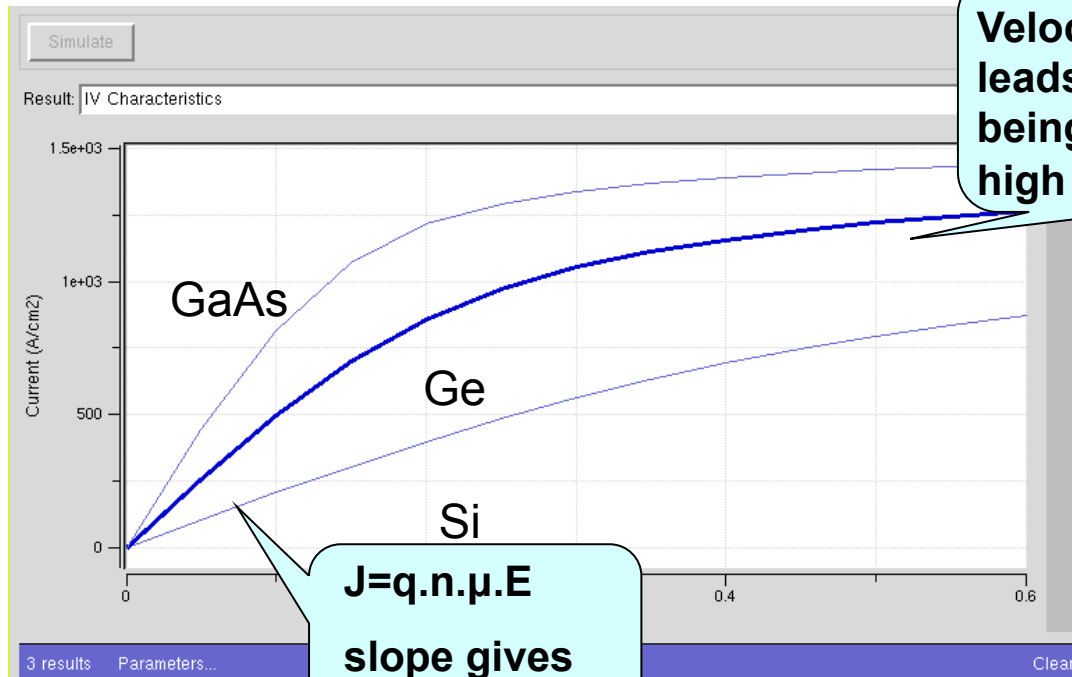
Surface Recombination on right contact: ☒ yes

Right Contact Electron surface recombination velocity: 1e+07cm/s

Right Contact Hole surface recombination velocity: 1e+07cm/s



# A Walk-through of a 'Drift' Problem, cont'd



Velocity saturation leads to the current being saturated at a high electric field

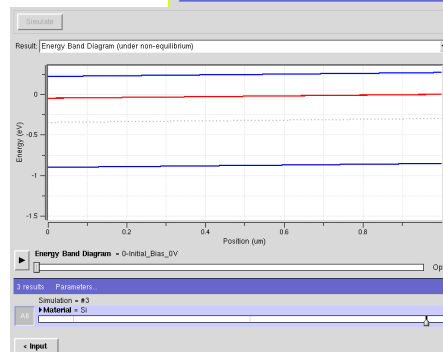
$J = q \cdot n \cdot \mu \cdot E$   
slope gives us  $\mu$

Calculated **electron mobilities** at 300K for  $N_d = 1e15/cm^3$  doping level:

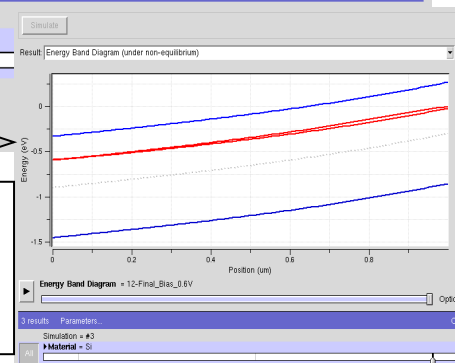
Si - 1281  $cm^2 / V \cdot s$

Ge - 3100  $cm^2 / V \cdot s$

GaAs - 5093  $cm^2 / V \cdot s$



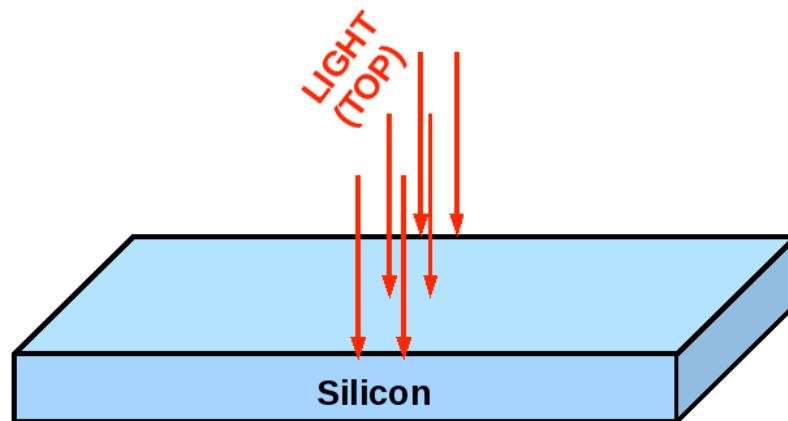
Energy band at equilibrium and at high bias





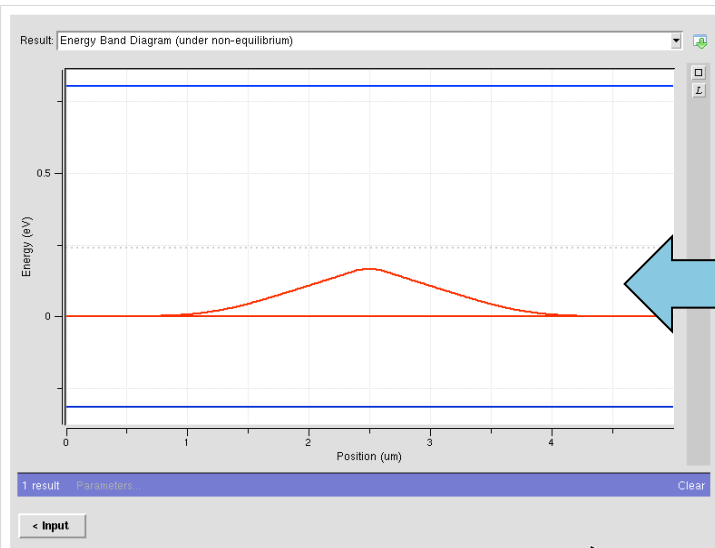
## Example 2: A Walk-through of a 'Diffusion' Problem

- This tool can be used to calculate the coefficient of diffusion for electrons  $D_n$  in Silicon.
- You would perform the experiment on a P type doped at  $1e14/cm^3$ , 5  $\mu m$  long Si bar.
- Set minority carrier lifetimes as  $\tau = 10$  ps for electrons and holes.
- Set generation rate,  $G = 2e20 /cm^3s$  and shine between 2.4~2.6  $\mu m$ .
- Set ON recombination velocity on both contacts.

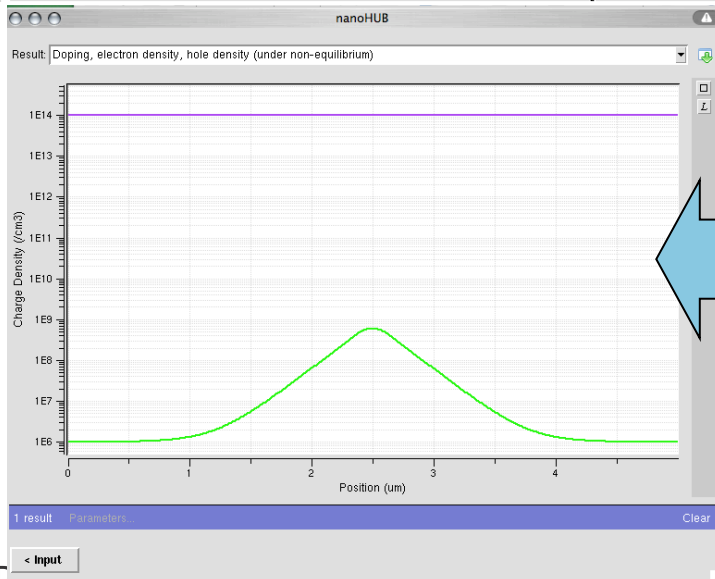


*We can now simulate the way excess electrons, generated at the left edge, would diffuse to the right!*

## A Walk-through of a 'Diffusion' Problem, cont'd



**Quasi fermi level** for electrons shift up because of extra minority carriers!



**Electron** and **hole** carriers are shown to the left.

The extra electrons generated at the center diffuse on either side.

Diffusion Length,  $L = (D_n \cdot \tau)^{1/2}$   
Estimated here  $D_n \sim 40 \text{ cm}^2/\text{s}$  [1]

## Final Comments

- More can be studied about drift and diffusion through using different experiments.
- Semiconductor slabs longer than 10  $\mu\text{m}$  would take longer to generate results, and in some cases, would lead to a convergence error.
- Minority carrier lifetimes might need to be tweaked to shorten the diffusion length and so that the whole device might visualize.
- A high surface recombination velocity defines an ideal contact.

## Reference

### [1] Semiconductor Device Fundamentals by Robert F. Pierret

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This tool is powered by PADRE (Pisces And Device Replacement) and developed by Mark Pinto & Kent Smith at AT&T Bell Labs.