

## Modeling and simulation of semiconductors and semiconductor devices

### Exercise 2

# Implementation of the bulk semiconductor equations

builds on modules: 2,3,4,5

check out: **Get ready for GNU Octave**  
(exercise 1)

<https://octave.sourceforge.io/secs1d/overview.html>

# Implementation of the bulk semiconductor equations

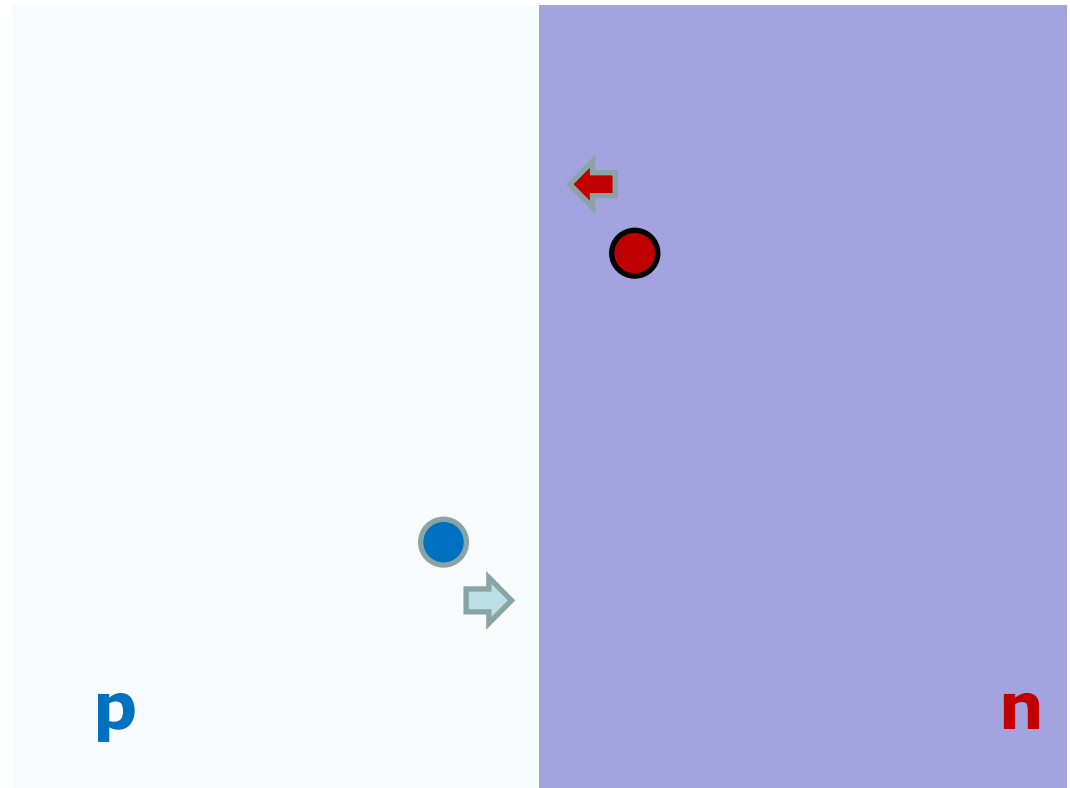
**check out:**

**Explanation of quasi-Fermi levels (TUBE SS 2020)**

- 1) .. learn to predict current densities across a pn junction for a given voltage in a self-consistent fashion
- 2) .. learn how device geometries, material properties, boundary conditions, and initial conditions are passed to a finite difference solver
- 3) .. alter the workflow of the simulation to mimic a particular experiment

**pn junction**  
**thermal**  
**equilibrium**

**no net current**



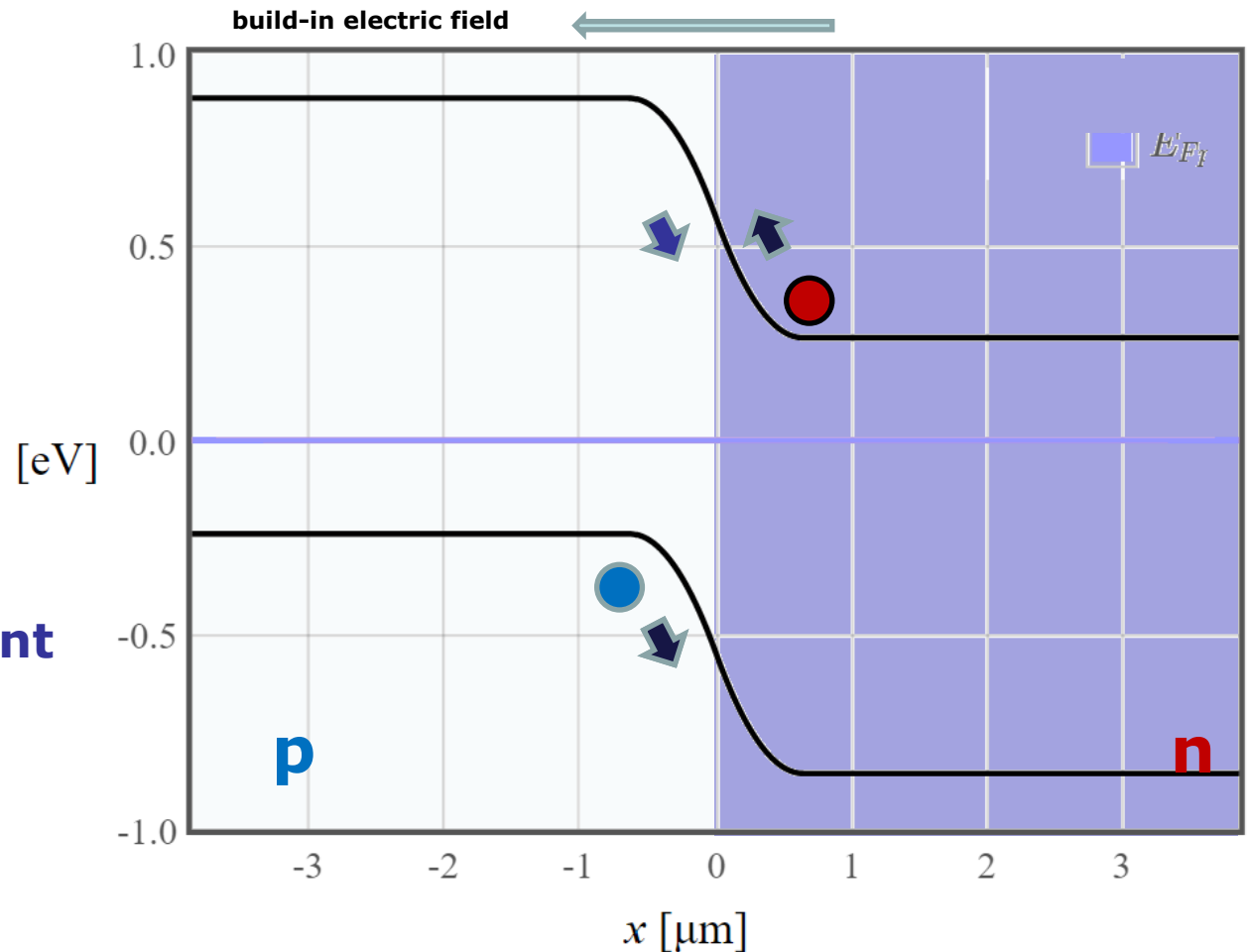
pn junction  
thermal  
equilibrium

drift current

=

- diffusion current

no net current



# pn junction thermal equilibrium

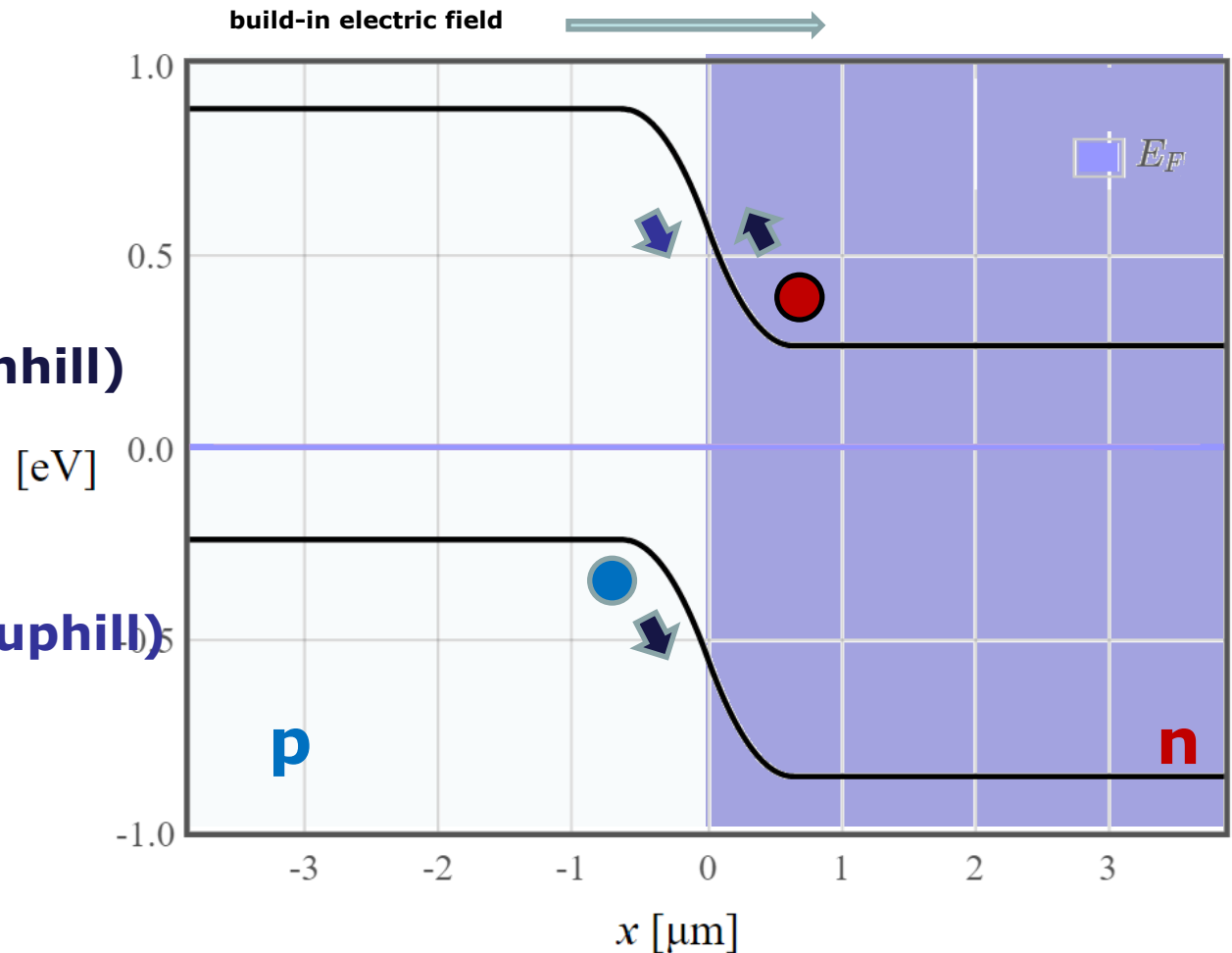
## drift current (downhill)

motion without energy barrier

## diffusion current (uphill)

motion against energy barrier

## key to current control: alter balance



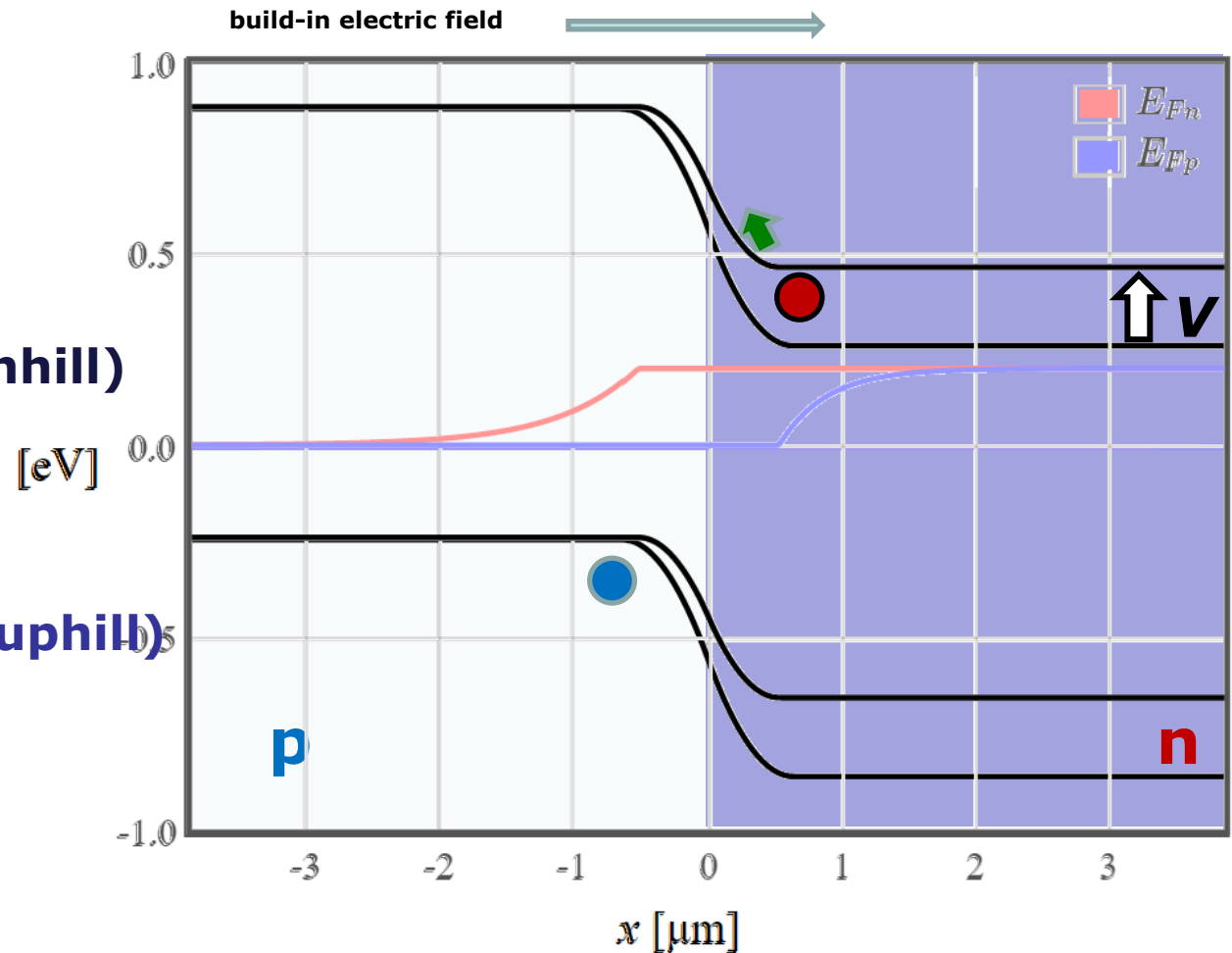
## pn junction with voltage

### drift current (downhill)

motion without energy barrier

### diffusion current (uphill)

barrier reduced: motion activated  
with **bias** or **enlarged**  
**temperature**

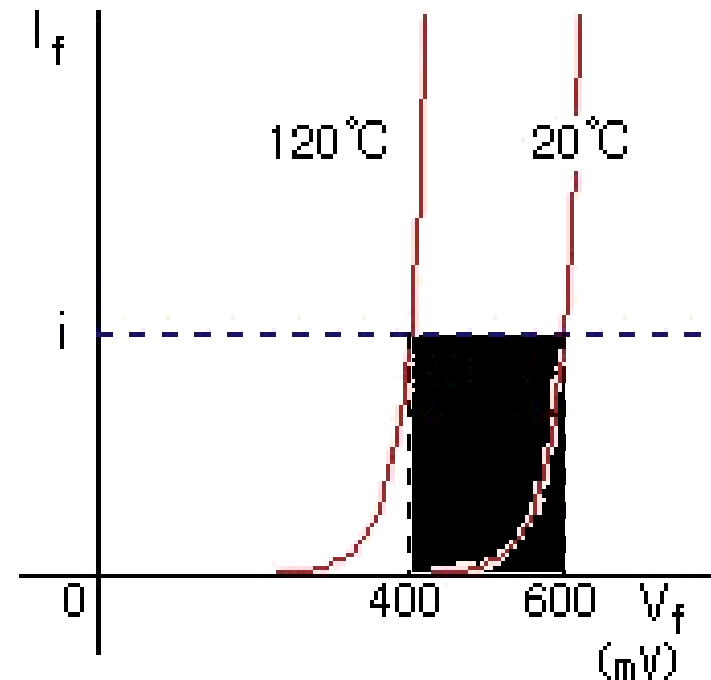
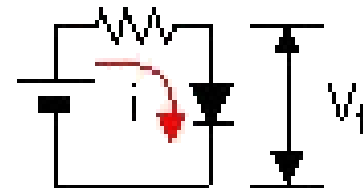




## pn-diode as a thermometer

voltage offset  
at reference  
current  $i$

proportional to  
temperature



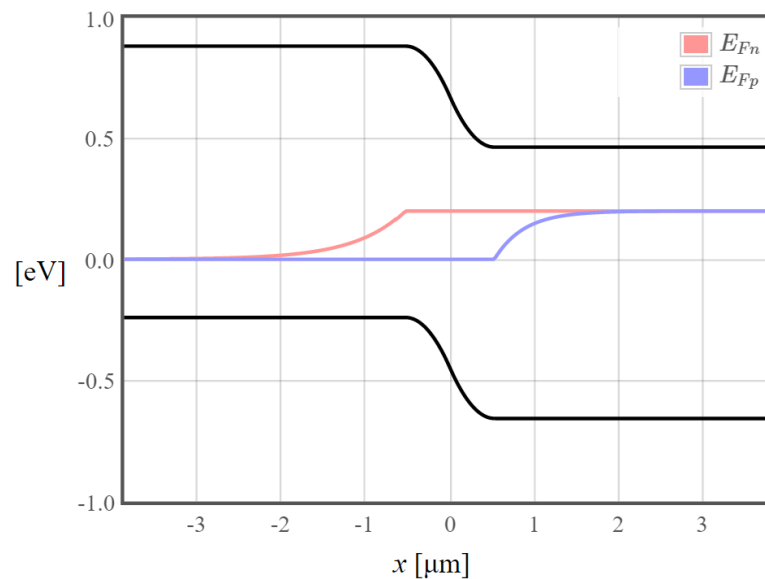
Si diode with predefined doping concentrations and geometry

simulation script

1) Get **current density  $j$  – voltage  $V$  curves**

**for different charge carrier lifetimes**

➤ **What shapes the  $j$ - $V$  curves?**



Si diode with predefined doping concentrations and geometry

simulation script

2) Get **current density  $j$  – voltage  $V$  curves**

**for different acceptor doping densities**

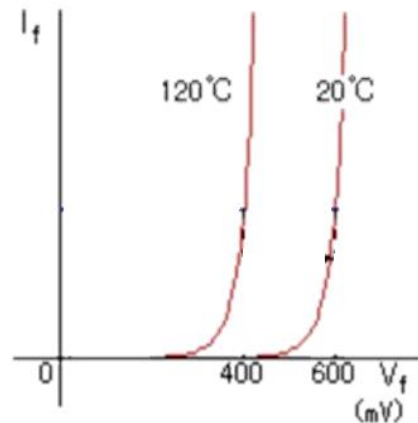
➤ **Which conditions are challenging for the solver?**

Si diode with predefined doping concentrations and geometry

simulation script

3) Get **current density – voltage curves** for different temperatures for fixed doping densities

➤ Which regions of the **j-V** curves are reasonably ideal?



Get **voltage-temperature curve** for preselected reference currents

$$\frac{\partial n}{\partial t} = \frac{1}{e} \frac{\partial \vec{j}_n}{\partial \vec{r}} + G_n(I, \vec{r}, \vec{E}, T) - R(n, p)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{e} \frac{\partial \vec{j}_p}{\partial \vec{r}} + G_p(I, \vec{r}, \vec{E}, T) - R(n, p)$$

$$0 = \frac{1}{e} \frac{\partial \vec{j}_{\textcolor{red}{n}}}{\partial \vec{r}} + G_{\textcolor{red}{n}}(I, \vec{r}, \vec{E}, T) - R(\textcolor{red}{n}, \textcolor{blue}{p})$$

$$0 = -\frac{1}{e} \frac{\partial \vec{j}_{\textcolor{blue}{p}}}{\partial \vec{r}} + G_{\textcolor{blue}{p}}(I, \vec{r}, \vec{E}, T) - R(\textcolor{red}{n}, \textcolor{blue}{p})$$

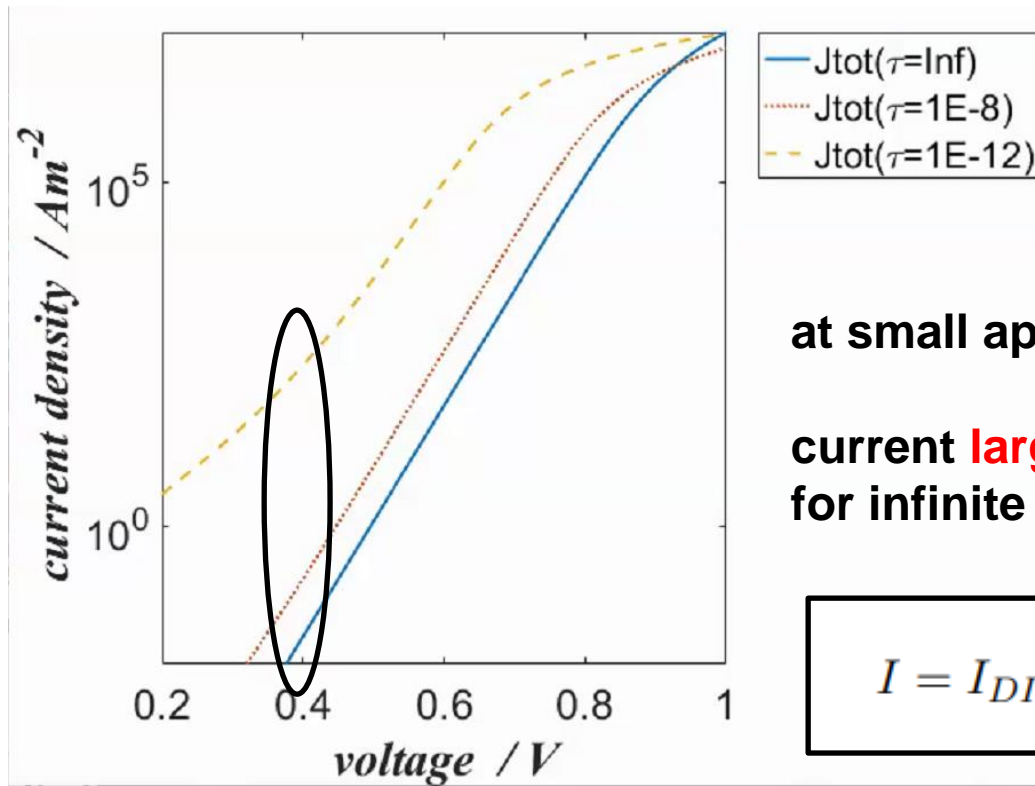
Assumes Boltzmann statistics:

Connects charge density with electrostatic potential

$$n = \eta e^{\frac{\psi}{k_B T}} = e^{\frac{\psi - \xi_p}{k_B T}}$$

quasi-Fermilevels

$$p = \rho e^{-\frac{\psi}{k_B T}} = e^{\frac{\xi_p - \psi}{k_B T}}$$



at small applied voltages:

current **larger** than expected  
for infinite carrier lifetimes

$$I = I_{\text{DIFF}} + I_{\text{R-G}}$$

**additional current contribution:** thermal carrier generation and recombination



**forward bias:** carrier concentrations increase in the depletion region  
leads to the carrier recombination

**model? Shockley Read Hall recombination**

$$I_{R-G} = -2eA \int_{-x_p}^{x_n} \frac{\partial n}{\partial t} dx$$

$$= -2eA \int_{-x_p}^{x_n} \frac{n_i^2 - np}{\tau_p(n + n_T) + \tau_n(p + p_T)} dx$$

$$n_T = n_i e^{\frac{E_T - E_i}{k_b T}}$$

$$p_T = n_i e^{\frac{E_i - E_T}{k_b T}}$$

$$I_{R-G} = \frac{-2eAn_i^2}{\tau_p n_T + \tau_n p_T} \sqrt{\frac{2\epsilon_s (\phi_{bi} + V_R)}{eN}} \frac{1 - e^{\frac{eV_A}{k_b T}}}{1 + \frac{e(\phi_{bi} - V_A)}{k_b T} \frac{\sqrt{\tau_n \tau_p}}{2\tau_0} e^{\frac{eV_A}{2k_b T}}}$$