# **SEMIDV**

A Semiconductor Device Simulator

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## Introduction

SEMIDV is a 2D semiconductor device simulator that solves Poisson-Drift-Diffusion equations using finite difference method. It contains mobility models for Phonon scattering, Coulomb scattering, high-field velocity saturation, ballistic mobility, and length dependent saturation velocity model.

### Installation

Use "**pip install semidv**" to install SEMIDV. It will also install scipy, cython, and fdint. Cython and fdint are required to compute Fermi-Dirac integral. Please visit "https://github.com/scott-maddox/fdint" for more information about fdint.

"import semidy" in Python to start using it.

## **Physics**

Most physics in SEMIDV are described in the paper "SEMIDV: A Compact Semiconductor Device Simulator with Quantum Effects". This manual will only cover the models that are not included in that paper.

## **Material**

Use **semidv.material()** to create a material object. For example, **parameters = semidv.material()**. In this class, there are built-in materials with default values.

```
"Si": { "epsilon": 11.7, "Eg": 1.12, "xi": 4.05, "Nc": 2.8e19, "Nv": 1.04e19, "un": 1400, "up": 450, "vsat_n": 1e7, "beta_n": 2, "vsat_p": 1e7, "beta_p": 2, "vt_n": 1.2e7, "vt_p": 1.2e7, "lambda_n": 7.65e-9, "lambda_p": 7.65e-9, "ua_n": 0, "eu_n": 1, "ud_n": 0, "ucs_n": 1, "nref": 1e18, "ua_p": 0, "eu_p": 1, "ud_p": 0, "ucs_p": 1, "pref": 1e18, "tau_n": 1, "tau_p": 1, "etrap": 0, }
```

"SiO2": { "epsilon": 3.9, "Eg": 8.9, "xi": 0.95, "Nc": 1e18, "Nv": 1e18, "un": 1, "up": 1, "vsat n": 1e7,

```
"beta_n": 2, "vsat_p": 1e7, "beta_p": 2, "vt_n": 1.2e7, "vt_p": 1.2e7, "lambda_n": 7.65e-9, "lambda_p": 7.65e-9, "ua_n": 0, "eu_n": 1, "ud_n": 0, "ucs_n": 1, "nref": 1e18, "ua_p": 0, "eu_p": 1, "ud_p": 0, "ucs_p": 1, "pref": 1e18, "tau_n": 1, "tau_p": 1, "etrap": 0, }
```

```
"Si3N4": { "epsilon": 3, "Eg": 5.3, "xi": 2.15, "Nc": 1e18, "Nv": 1e18, "un": 1, "up": 1, "vsat_n": 1e7, "beta_n": 2, "vsat_p": 1e7, "beta_p": 2, "vt_n": 1.2e7, "vt_p": 1.2e7, "lambda_n": 7.65e-9, "lambda_p": 7.65e-9, "ua_n": 0, "eu_n": 1, "ud_n": 0, "ucs_n": 1, "nref": 1e18, "ua_p": 0, "eu_p": 1, "ud_p": 0, "ucs_p": 1, "pref": 1e18, "tau_n": 1, "tau_p": 1, "etrap": 0, }
```

```
"HfO2": { "epsilon": 25, "Eg": 5.7, "xi": 1.2, "Nc": 1e18, "Nv": 1e18, "un": 1, "up": 1, "vsat_n": 1e7, "beta_n": 2, "vsat_p": 1e7, "beta_p": 2, "vt_n": 1.2e7, "vt_p": 1.2e7, "lambda_n": 7.65e-9, "lambda_p": 7.65e-9, "ua_n": 0, "eu_n": 1, "ud_n": 0, "ucs_n": 1, "nref": 1e18, "ua_p": 0, "eu_p": 1, "ud_p": 0, "ucs_p": 1, "pref": 1e18, "tau_n": 1, "tau_p": 1, "etrap": 0, }
```

"Metal": { "epsilon": 1, "Eg": 0, "xi": 4.5, "Nc": 1e25, "Nv": 1e25, "un": 1, "up": 1, "vsat\_n": 1e7, "beta\_n": 2, "vsat\_p": 1e7, "beta\_p": 2, "vt\_n": 1.2e7, "vt\_p": 1.2e7, "lambda\_n": 7.65e-9, "lambda\_p": 7.65e-9, "ua\_n": 0, "eu\_n": 1, "ud\_n": 0, "ucs\_n": 1, "nref": 1e18, "ua\_p": 0, "eu\_p": 1, "ud\_p": 0, "ucs\_p": 1, "pref": 1e18, "tau\_n": 1, "tau\_p": 1, "etrap": 0, }

"Ge": { "epsilon": 16.0, "Eg": 0.66, "xi": 4.0, "Nc": 1.2e19, "Nv": 0.6e19, "un": 3900, "up": 1900, "vsat\_n": 6e6, "beta\_n": 2, "vsat\_p": 6e6, "beta\_p": 2, "vt\_n": 3.1e7, "vt\_p": 1.9e7, "lambda\_n": 7.65e-9, "lambda\_p": 7.65e-9, "ua\_n": 0, "eu\_n": 1, "ud\_n": 0, "ucs\_n": 1, "nref": 1e18, "ua\_p": 0, "eu\_p": 1, "ud\_p": 0, "ucs\_p": 1, "pref": 1e18, "tau\_n": 1, "tau\_p": 1, "etrap": 0, }

To add new material, please use **add\_material()** to input material properties.

```
self.properties[material] = {
    "epsilon": epsilon, # Permitivity (F/m)
"Eg": Eg, # Bandgap energy (eV)
    "xi": xi, # Electron affinity (eV)
    "Nc": Nc, # Conduction band effective density of states (cm^-3)
    "Nv": Nv, # Valence band effective density of states (cm^-3)
    "un": un, # Drift-diffusion electron mobility (cm^2/V/s)
    "up": up, # Drif-diffusion hole mobility (cm^2/V/s)
    "vsat_n": vsat_n, # Electron saturation velocity (cm/s)
"beta_n": beta_n, # Electron saturation parameter
    "vsat_p": vsat_p, # Hole saturation mobility (cm/s)
"beta_p": beta_p, # Electron saturation parameter
    "ua_n": ua_n, # Phonon scattering electron mobility degradation ((m/V)^eu n)
    "eu_n": eu_n, # Phonon scattering electron mobility degradation
    "ud_n": ud_n, # Columbic scattering electron mobility degradation
    "ucs n": ucs n, # Columbic scattering electron mobility degradation
    "nref": nref, # Columbic scattering electron mobility degradation (cm^-3)
    "ua_p": ua_p, # Phonon scattering hole mobility degradation ((m/V)^eu_p)
    "eu_p": eu_p, # Phonon scattering hole mobility degradation
    "ud p": ud p, # Columbic scattering electron mobility degradation
    "ucs_p": ucs_p, # Columbic scattering electron mobility degradation
"pref": pref, # Columbic scattering electron mobility degradation (cm^-3)
    "vth_n": vth_n, # Electron thermal velocity (cm/s)
    "vth_p": vth_p, # Hole thermal velocity (cm/s)
    "lambda_n": lambda_n,  # Effective scattering length for electron saturation velocity (m) "lambda_p": lambda_p,  # Effective scattering length for hole saturation velocity (m)
    "tau_n": tau_n, # SRH electron lifetime (s)
    "tau_p": tau_p, # SRH hole lifetime (s)
    "etrap": etrap, # Field factor (eV)
```

To change the property of existing materials, please use **update property()**.

For example, parameters.update property("Si", "un", 310).

To check the value for a given material, please use **get\_property()**.

```
def get_property(self, materials, property_name):
    """Retrieve a specific property for a given material or array of materials."""
    if isinstance(materials, np.ndarray):
        # Process array element-wise
        return np.array(
        [
            self.properties.get(element, {}).get(property_name, None)
            for element in materials.flatten()
        ]
        ).reshape(materials.shape)
    else:
        # Handle single material name
        material_props = self.properties.get(materials, None)
        if material_props:
            return material_props.get(property_name, None)
    return None
```

## Device Structure

#### Create Device Object

To set up a device for simulation, first, create a device object with semidv.device().

For example, device = semidv.device(T=300, fermi=True, tolerance=1e-6, L=12e-9).

```
def init (self, T=300, fermi=True, tolerance=le-6, L=1):
```

T is the ambient temperature for device simulation. The default is 300K. In the current version, there is no self-heating, so T is also the device temperature.

tolerance is the convergence criteria. The default is 1e-6 V.

L is a parameter for ballistic mobility and saturation velocity calculation. The default is 1.

#### Create Device Structure

```
Build a 2D array representing the device structure with separate spatial steps for x and y.

Parameters:
- domain_size: tuple (width, height) in meters, e.g., (1e-6, 1e-6)
- spatial_steps: tuple (x_step, y_step) in meters, e.g., (1e-9, 2e-9)
- materials: list of dictionaries with material and range, e.g.,
    [{"material": "5i", "X": (1e-9, 2e-9), "y": (2e-9, 3e-9)}]
- doping_profiles: list of dictionaries with doping type, concentration (cm^-3), and range, e.g.,
    [{"type": "n-type", "concentration": 1e18, "x": (1e-9, 2e-9), "y": (2e-9, 3e-9)}]

Returns:
- A dictionary containing:
- "structure": A 2D numpy array representing the device structure materials.
- "doping": A 2D numpy array representing the doping concentrations (n-type positive, p-type negative).
"""
```

Users need to specify the simulation range in x, y axis, and the step size.

```
For example,
domain = (Thickness, Length)
steps = (dx, dy)
```

The device structure is defined by a list specifying the materials for different regions.

The default material for all regions is Silicon. Define the material by specifying the start and end point in x, y axis.

```
For example,
materials = [
    {"material": "Metal", "x": (0, Tsp-Tox-Thk), "y": (Lsd+Lsp+Thk, Length-Lsd-Lsp-Thk)},
    {"material": "Metal", "x": (Thickness-Tsp+Tox+Thk, Thickness), "v": (Lsd+Lsp+Thk,
Length-Lsd-Lsp-Thk)},
    {"material": "HfO2", "x": (Tsp-Tox-Thk, Tsp-Tox), "y": (Lsd+Lsp, Length-Lsd-Lsp)},
    {"material": "HfO2", "x": (Thickness-Tsp+Tox, Thickness-Tsp+Tox+Thk), "y": (Lsd+Lsp,
Length-Lsd-Lsp)},
    {"material": "HfO2", "x": (0, Tsp-Tox-Thk), "y": (Lsd+Lsp, Lsd+Lsp+Thk)},
    {"material": "HfO2", "x": (0, Tsp-Tox-Thk), "y": (Length-Lsd-Lsp-Thk, Length-Lsd-Lsp)},
    {"material": "HfO2", "x": (Thickness-Tsp+Tox+Thk, Thickness), "y": (Lsd+Lsp,
Lsd+Lsp+Thk)},
    {"material": "HfO2", "x": (Thickness-Tsp+Tox+Thk, Thickness), "y": (Length-Lsd-Lsp-Thk,
Length-Lsd-Lsp)},
    {"material": "SiO2", "x": (Tsp-Tox, Tsp), "y": (Lsd+Lsp, Length-Lsd-Lsp)},
    {"material": "SiO2", "x": (Thickness-Tsp, Thickness-Tsp+Tox), "y": (Lsd+Lsp, Length-Lsd-
Lsp)},
    {"material": "Si3N4", "x": (0, Tsp), "y": (Lsd, Lsd+Lsp)},
    {"material": "Si3N4", "x": (0, Tsp), "y": (Length-Lsd-Lsp, Length-Lsd)},
    {"material": "Si3N4", "x": (Thickness-Tsp, Thickness), "y": (Lsd, Lsd+Lsp)},
    {"material": "Si3N4", "x": (Thickness-Tsp, Thickness), "y": (Length-Lsd-Lsp, Length-Lsd)}
1
```

Users can define doping profiles by creating a doping list.

```
For example,
doping = [
    {"type": "n-type", "concentration": 2e20, "x": (0, Thickness), "y": (0, Lsd)},
    {"type": "n-type", "concentration": 2e20, "x": (0, Thickness), "y": (Length-Lsd, Length)},
    {"type": "n-type", "concentration": "2e20*10**(-2*((y-"+str(Lsd)+")/"+str(Lsp)+")**2)",
"x": (Tsp, Tsp+Tch), "y": (Lsd, Length)},
    {"tvpe":
                     "n-type",
                                      "concentration":
                                                               "2e20*10**(-2*((v-"+str(Length-
Lsd)+")/"+str(Lsp)+")**2)", "x": (Tsp, Tsp+Tch), "y": (0, Length-Lsd)},
    {"type": "p-type", "concentration": 1e15, "x": (Tsp, Tsp+Tch), "y": (Lsd+Lsp, Length-Lsd-
Lsp)}
Doping can be constant.
{"type": "n-type", "concentration": 2e20, "x": (0, Thickness), "y": (0, Lsd)}
It can also be a function by a string.
{"type": "n-type", "concentration": "2e20*10**(-2*((y-"+str(Lsd)+")/"+str(Lsp)+")**2)", "x": (Tsp,
Tsp+Tch), "y": (Lsd, Length)}
Then, use build device structure() to build the device.
def build device structure(
      self, domain size, spatial steps, materials, doping profiles=None
):
```

For example, device.build device structure(domain, steps, materials, doping).

Then, input the material parameters by **device.materialproperties()**.

For example, device.materialproperties(parameters).

#### Contacts and Boundary Conditions

```
Assign boundary conditions to the device structure.

Parameters:
- boundary_conditions: list of dictionaries specifying boundary conditions, e.g.,

[{"name": "V1", "contact": "yes", "type": "Dirichlet", "value": 1.0, "barrier_height": 0.5, "x": (0, 1e-9), "y": (0, 2e-9)},

{"name": "V2", "contact": "no", "type": "Neumann", "x": (1e-9, 2e-9), "y": (0, 1e-9)}]

Returns:
- A dictionary containing:
- "boundary_containing:
- "boundary_array": A 2D numpy array with boundary values (without barrier height).
- "boundary_array_with_barrier": A 2D numpy array with boundary values (including barrier height).
- "dirichlet_positions": A dictionary with keys like "contact_1", "contact_2", etc., each containing the positions for a specific Dirichlet boundary.
```

If contact is "yes", it means the boundary is connected to electrode. It can be either **Dirichlet** or **Neumann** boundary. For **Dirichlet boundary**, a value for contact barrier in eV is required. For **Neumann boundary**, the "value" is ignored.

If contact is "no", it will automatically be Neumann boundary.

Please create a boundary list and use assign boundary conditions() to assign boundaries.

#### **Charge Integration**

SEMIDV calculates charges by specifying the region to integrate charges. Define a directory and use add\_charge\_region() to specify the charge integration region.

```
For example, channel = {"name": "channel", "x": (Tsp, Tsp+Tch), "y": (Lsd+Lsp, Length-Lsd-Lsp)} device.add charge region(channel)
```

## **Device Simulation**

#### Initialize

First, initialize device with equilibrium condition using Initialize()

For example, **Device.Initialize()** 

#### Solve Poisson-Drift-Diffusion

Use getmatrix() to get a iteration-independent Poisson finite difference matrix. Users only need to do this

once.

Then, use **Poisson(damping=1)** to solve the Poisson equation.

damping can control how fast the simulator updates the solution. Smaller damping value can improve convergence but increase the iteration steps.

To call the error in the Poisson equation, use call the error variable in the device object.

For example, **device.error**. It will return an error in volts.

After solving the Poisson equation, E<sub>C</sub> and E<sub>V</sub> will be updated in the object.

Use **DriftDiffusion(recombination=False)** to solve Drift-Diffusion equations.

Users can turn on the recombination module. The default is False.

SEMIDV only has Shockley-Read-Hall (SRH) recombination model now.

 $SRH = (n * p - ni^2) / (tau_p * n + ni * exp(etrap / kbT)) + tau_n * (p + ni * exp(-etrap / kbT)))$ 

Drift-Diffusion equations will update Efn and Efp in the object.

Users need to create a loop to do Gummel iteration till simulation converges.

```
For example,
device.getmatrix()
error = 1
while error > device.tolerance:
device.Poisson()
device.DriftDiffusion()
error = device.error
```

#### Solve Quantum-Poisson-Drift-Diffusion

To include quantum correction from the Localization Landscape Theory, users need to use **quantum\_getmatrix()** to obtain the iteration-independent part of the Hamiltonian first.

Then, users can choose to use either electron or hole to calculate quantum potential.

To use electron, use equantum(Kq=0).

To use hole, use hquantum(Kq=0).

Only one of them can be used not both.

Kq is a parameter for the strength of quantum correction. The default is 0. The larger the Kq, the weaker the quantum effect is.

Quantum will update quantum potential corrections QCn and QCp in the object.

To solve the device with quantum correction, users need to add **device.quantum\_getmatrix()** into the iteration.

```
For example,
device.getmatrix()
device.quantum_getmatrix()
error = 1
```

```
while error > device.tolerance:
device.Poisson()
device.equantum()
device.DriftDiffusion()
error = device.error
```

#### **Currents and Charges**

After simulation, users can use **getcurrent()** and **getcharge()** to calculate current at each contact, and charge in given integration region.

The currents and charges are stored in **current** and **charge**. Both of them are lists. Users can obtain the current or charge at different place with the "contact name" or "charge region name".

```
For example,
device.current["drain"]
device.charge["gate"]
```

#### **Initial Guess**

Users can use **update** initial **guess(Ec, Efn, Efp)** to assign Ec, Efn, and Efp at the beginning of iterations.

#### **Built-in Solver**

SEMIDV also provides a solver with predefined loops for easy use.

This solver can do double voltage sweeps and extrapolate previous solutions as initial guess.

Users need to define voltages, boundaries, and use semidv.solve().IVsweep() do the sweep.

```
def init (self, device, boundary, damping=1, recombination=False, quantum=False, Kq=0):
IVsweep(self, V1 contact name, V1 sweep, V2 contact name, V2 sweep, results):
```

This solver can recognize the name of each contact and update the electrode voltage based on the contact name.

Results will be stored in a directory using voltages as keys. It contains objects, currents, and charges for each bias.

```
results[(V1, V2)] = {
    "model": deepcopy(self.device),
    "current": self.device.current.copy(),
    "charge": self.device.charge.copy(),
}
```

## Visualization

init (self, device):

SEMIDV provides a visualizer that can generate device plots for different quantities.

First, users need to create a visual object using semidv.visual() by input a device object.

Each plot function has a save option. The default is False. If enter True, it will save the figure into "figure.png". Users can enter a figure name, and it will save the figure with that name.

```
def plot structure(self, save=False):

For example,
deviceplot = semidv.visual(device)
deviceplot.plot_structure(save="structure.tif")

SEMIDV visual provides several 2D contour plots.

plot_structure(): plot the device structure with materials
plot_potential(): plot 2D electrostatic potential
plot_efermi(): plot 2D electron quasi-fermi level Efn
plot_hfermi(): plot 2D hole quasi-fermi level Efp
plot_doping(): plot 2D doping distribution
plot_n(): plot 2D electron distribution
plot_p(): plot 2D hole distribution
plot_Efield(): plot 2D vector plot of electric field
plot_Jn(): plot 2D vector plot of electron current
plot Jp(): plot 2D vector plot of hole current
```

**SEMIDV visual** also provides 1D cut line plot for several quantities. Users will need to specify x or y coordinate for each plot.

```
def plot band xcut(self, x coord=0, save=False):
def plot band ycut(self, y coord=0, save=False):
For example.
deviceplot.plot band xcut(6e-9, save="band.tif")
Here are the available 1D plots.
plot band xcut(): Band diagram along the y axis
plot band ycut(): Band diagram along the x axis
plot efield xcut(): Electric field along the y axis
plot efield ycut(): Electric field along the x axis
plot q xcut(): n and p along the y axis
plot q ycut(): n and p along the x axis
plot J xcut(): Jn and Jp along the y axis
plot J ycut(): Jn and Jp along the x axis
plot vn xcut(): Electron velocity along the y axis
plot vn ycut(): Electron velocity along the x axis
plot vp xcut(): Hole velocity along the y axis
plot vp ycut(): Hole velocity along the x axis
```

## Physical Quantities

This section lists the accessible physical variables in the device object.

Ec: Conduction band energy
Ev: Valence band energy
Efn: Electron quasi-fermi level
Efp Hole quasi-fermi level
n: Electron concentration
p: Hole concentration

NB: Net doping concentration QCn: Electron quantum potential QCp: Hole quantum potential

vnx: Component of electron velocity in the x-direction vny: Component of electron velocity in the y-direction vpx: Component of hole velocity in the x-direction vpy: Component of hole velocity in the y-direction

Jnx: Component of electron current density in the x-direction Jny: Component of electron current density in the y-direction Jpx: Component of hole current density in the x-direction Jpy: Component of hole current density in the y-direction

current: A directory of currents charge: A directory of charges

**T:** Ambient temperature

Nc: Conduction band effective density of states Nv: Valence band effective density of states

me: Electron effective mass (self.h\*\*2 / 2 / np.pi / self.kbT \* (self.Nc / 2.0) \*\* (2.0 / 3.0)) mh: Hole effective mass (self.h\*\*2 / 2 / np.pi / self.kbT \* (self.Nv / 2.0) \*\* (2.0 / 3.0))

epsilon: Permittivity

Eg: Bandgap

xi: Electron affinity

un: low-field drift-diffusion electron mobility up: low-field drift-diffusion hole mobility

lambda\_n: Effective scattering length for electron saturation velocity lambda p: Effective scattering length for hole saturation velocity

vsat\_n: Electron saturation velocity vsat\_p: Hole saturation velocity vt\_n: Electron thermal velocity

vt\_p: Hole thermal velocity ub\_n: Electron ballistic mobility ub\_p: Hole ballistic mobility

beta\_n: Electron velocity saturation parameter beta\_p: Hole velocity saturation parameter ua\_n: Electron Phonon scattering parameter

ua\_p: Hole Phonon scattering parameter

eu\_n: Electron Phonon scattering parameter

eu\_p: Hole Phonon scattering parameter

ud\_n: Electron Coulomb scattering parameter ud\_p: Hole Coulomb scattering parameter ucs\_n: Electron Coulomb scattering parameter ucs\_p: Hole Coulomb scattering parameter

nref: Electron Coulomb scattering parameter pref: Hole Coulomb scattering parameter

ni: Intrinsic carrier concentration

tau\_n: Electron SRH recombination lifetime tau\_p: Hole SRH recombination lifetime

etrap: SRH Trap energy