Sesame: a 2-dimensional solar cell modeling tool

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This work introduces a new software package “Sesame” for the numerical computation of classical semiconductor equations. It supports 1 and 2-dimensional systems and provides tools to easily implement extended defects such as grain boundaries or sample surfaces. Sesame has been designed to facilitate fast exploration of the system parameter space and to visualize local charge transport properties. Sesame is distributed as a Python package or as a standalone GUI application, and is available at https://pages.nist.gov/sesame/.

I. INTRODUCTION

Numerical simulations are an essential aspect of photovoltaic research and design. A number of free software packages have been developed and extensively used for solar cell modeling in 1-dimension, including AMPS [1], PC-1D [1], SCAPS [2], and wxAMPS [3]. Freely available 2-dimensional simulation tools are less common [4–6], but are necessary for describing systems with lateral inhomogeneity. A common class of such systems are polycrystalline thin film photovoltaics, such as CdTe [7], CIGS [8], and hybrid perovskites [9]. In these materials grain boundaries break the lateral symmetry of the p-n junction, leading to complex system geometries. Lateral inhomogeneity is also often encountered in nanoscale or mesoscopic measurements. The resolution of these measurements is typically achieved using an excitation source or measurement probe with nanoscale spatial extent. Examples include electron beam induced current (EBIC) or scanning Kelvin probe microscopy, which are also often surface sensitive. An appropriate model for these measurements is therefore (at least) 2-dimensional and includes localized excitation/detection sources and relevant boundary conditions.

There are numerous examples of the use of 2-dimensional solar cell modeling in the literature. For instance, the impact of grain boundaries in polycrystalline cells has been previously studied numerically [10–12] and analytically [13, 14]. Simulations have been used for interpreting experiments with localized excitations such as EBIC [15, 16], cathodoluminescence [17, 18], and two-photon photoluminescence [19]. Although these works are instructive, nonlinearities in the system response prevent a simple extrapolation of previous results to all possible system configurations of interest. Indeed there remain a number of unresolved questions of fundamental interest in polycrystalline photovoltaics, questions as basic as whether grain boundaries are harmful or beneficial to cell performance [7, 20]. It is therefore desirable for researchers to have widespread access to 2-d simulation software.

In this work we introduce Sesame, a Python package developed by the authors (B. G. and P. M. H.) which solves the drift-diffusion-Poisson equations in 1 and 2 dimensions. Sesame is open source and distributed under the BSD license. Sesame is designed to easily construct systems with planar defects, such as grain boundaries or sample surfaces, which may contain both discrete or a continuum of gap state defects. While full-featured commercial packages allow simulations of complex device configurations together with multiple physical effects, the needs of research sometimes require access to the source code and licensing that enables usage on computing clusters. The program and its code are publicly available at https://pages.nist.gov/sesame/.

FIG. 1. Coordinate system of Sesame: rectilinear geometry and contacts located at \( x = 0 \) and \( x = L \). pn junction doping is shown as an example.
The paper is organized as follows: In Sec. II we present a brief overview of the model and geometry. In Sec. III we compare the output of Sesame to established semiconductor modeling software, including SCAPS [2], Sentaurus [21], and COMSOL Semiconductor Module [22, 23]. In Sec. III we also present a hands-on tutorial script for solving a 2-dimensional system with a grain boundary, and briefly describe the functionality of the GUI. The mathematics underlying the model and technical details of the numerical implementation can be found in the Appendix.

II. OVERVIEW OF THE PHYSICAL MODEL

The system geometry consists of a semiconductor device connected to contacts at $x = 0$ and $x = L$ (see Fig. 1). Sesame describes the steady state behavior of this system, which is governed by the drift-diffusion-Poisson equations:

$$\nabla \cdot \vec{J}_n = -q(G - R) \quad (1)$$
$$\nabla \cdot \vec{J}_p = q(G - R) \quad (2)$$
$$\nabla \cdot (\epsilon \nabla \phi) = -\rho/\epsilon_0 \quad (3)$$

with the currents

$$\vec{J}_n = -q\mu_n n \nabla \phi + qD_n \nabla n \quad (4)$$
$$\vec{J}_p = -q\mu_p p \nabla \phi - qD_p \nabla p \quad (5)$$

where $n$ and $p$ are the respective electron and hole number densities, and $\phi$ is the electrostatic potential. $\vec{J}_{n(p)}$ is the charge current density of electrons (holes). Here, $q$ is the absolute value of the electron charge. $\rho$ is the local charge density, $\epsilon$ is the dielectric constant of the material, and $\epsilon_0$ is the permittivity of free space. $\mu_{n,p}$ is the electron/hole mobility, and is assumed to satisfy the Einstein relation: $D_{n,p} = k_B T \mu_{n,p}/q$. $G$ is the electron/hole pair generation rate density and $R$ is the recombination rate density.

Sesame includes Schockley-Read-Hall, radiative, and Auger recombination mechanisms. Sesame is currently limited to describing non-degenerate semiconductors with Boltzmann statistics, and does not include thermionic emission and quantum tunneling at interfaces. These can be important contributions to the transport in heterojunctions [24], so care should be exercised when using Sesame to simulate such systems. Sesame includes Ohmic and Schottky contact boundary conditions, and periodic or hardwall (infinite potential) transverse boundary conditions. Sesame uses finite differences to solve Eqs. (1-5), and the standard Scharfetter-Gummel scheme for discretizing the current [25]. Details of the implementation can be found in the Appendix.

III. BENCHMARKS AND EXAMPLES

A. Benchmarks

We first verify the consistency between Sesame and other software packages. We have compared the output of Sesame with the well-established software packages Sentaurus, COMSOL, and SCAPS for many systems, and present two illustrative examples here. We first consider a 1-d heterojunction consisting of a thin $n^+$-doped layer of CdS and a $p$-type CdTe. The material parameters are shown in Table I. Fig. 2(a) shows the computed $J-V$ curve under uniform illumination of $G = 3.3 \times 10^{20} \text{cm}^{-3} \text{s}^{-1}$. We find close agreement between Sesame, Sentaurus, and COMSOL. To quantify the comparison, we define the relative difference between two computed currents $J_1$ and $J_2$ as $|J_1 - J_2|/(J_1 + J_2)$, where $\langle \rangle$ denotes the average. The maximum relative difference between Sesame and Sentaurus is 0.2%, and between Sesame and COMSOL it is 2%. We observe a more substantial difference between Sesame and SCAPS, with a maximum value of 7%. In all cases, the maximum discrepancy occurs near $V_{oc}$, where the current is minimized so that relative differences are maximized. We attribute the larger difference between Sesame and SCAPS to the different interface recombination model used in SCAPS, in which the system variables are multi-valued at the interface and allow for recombination between layers [2].

We next consider a 2-d homojunction with a single columnar grain boundary (see inset of Fig. 3(a) for system geometry). We use the same bulk parameters as given for CdTe in Table I for both $n$ and $p$ layers, except with $\tau_e = \tau_h = 10$ ns. The thickness of the $n^+$ layer is taken to be 100 nm. The grain boundary contains a donor and an acceptor defect, both positioned at 0.4 eV above midgap, with defect density $\rho_{GB} = 10^{14} \text{cm}^{-2}$ and equal hole and electron capture cross section $\sigma_{GB} = 10^{-14} \text{cm}^2$. The grain boundary is positioned in the middle of the system, and terminates at a distance of 100 nm from either contact. For this simulation we again use a uniform gen-
TABLE I. List of parameters used for the 1-d heterojunction calculation. The label (D) and (A) for the doping value indicate donor and acceptor, respectively.

| Param. | CdS | CdTe |
|--------|-----|------|
| $L$ [nm] | 25  | 4000 |
| $\epsilon$ | 10  | 9.4  |
| $\tau_n$ [ns] | 10  | 5    |
| $\tau_p$ [ns] | $10^{-4}$ | 5    |
| $N_C$ [cm$^{-3}$] | $2.2 \times 10^{18}$ | $8 \times 10^{17}$ |
| $N_V$ [cm$^{-3}$] | $1.8 \times 10^{19}$ | $1.8 \times 10^{19}$ |
| $E_g$ [eV] | 2.4 | 1.5  |
| $\chi$ [eV] | 4.0 | 3.9  |
| $\mu_n$ [cm$^2$/(V s)] | 100 | 320  |
| $\mu_p$ [cm$^2$/(V s)] | 25  | 40   |
| doping [cm$^{-3}$] | $10^{17}$ (D) | $10^{19}$ (A) |

FIG. 3. Comparison between Sesame, COMSOL and Sentaurus for a 2-dimensional system. (a) Illuminated JV curve. Insert: schematic of the system, an n-p junction with a columnar grain boundary. (b) Band diagram along the grain boundary core under short-circuit conditions.

Next we define the grids for $x$ and $y$. We use uniform grids for this example, but generally non-uniform grids are necessary to optimize the simulation accuracy and speed (non-uniform grids are used in the simulation of Fig. 3). (Note: Sesame assumes all lengths are given in units of cm.)

```python
x = np.linspace(0, 3e-4, 100)
y = np.linspace(0, 3e-4, 100)
```

We create the system with the `Builder` function. The input to `Builder` are the $x$ and $y$ grids. The output is an object `sys` which contains all the information needed to describe the simulation.

```python
sys = sesame.Builder(x, y)
```

Additional simulation settings are set by calling various methods of `sys`, as we show below.

Next we define the material properties with a python dictionary object (called `mat` in this example). The dictionary key names correspond to standard definitions. (Note: Sesame assumes times are given in units of s, energies in units of eV, densities in units of cm$^{-3}$, and mobility in units of cm/(V s)).

```python
mat = {'Nc': 8e17, 'Nv': 1.8e19, 'Eg': 1.5, 'affinity': 4.1, 'epsilon': 9.4, 'Et': 0, 'mu_e': 320, 'mu_h': 40, 'tau_e': 1e-8, 'tau_h': 1e-8}
```

The dictionary key `Et` represents the energetic position of bulk recombination centers, as measured from the intrinsic energy level, and `tau_e/tau_h` are the electron/hole lifetimes. The dependence of the Shockley-Read-Hall recombination on these parameters can be found in the Appendix. The material is added to the system using the `add_material` function, which takes the `mat` dictionary as input. Note that `add_material` is a method of the `sys` object, and is called with the command:

```python
sys.add_material(mat)
```

To build a p-n junction we add a position-dependent doping profile to the system. We must define functions which describe the different doping regions; for this example, these functions are called `n_region` and `p_region`. They return True when the input variable `position` belongs to the region. For this example the two regions are delimited at the `junction` coordinate which corresponds to $x = 10^{-5}$ cm.

```python
junction = 1e-5
```
def n_region(position):
    x, y = position
    return x < junction

def p_region(position):
    x, y = position
    return x >= junction

Having defined the different doping regions, we add the donors and acceptors with the sys methods add_donor and add_acceptor. The input for these methods are the doping magnitude and doping region functions we just defined. Sesame currently assumes that all bulk dopants are fully ionized. (Note: Sesame assumes the units of density is cm$^{-3}$):

donorDensity = 1e17
sys.add_donor(donorDensity, n_region)
acceptorDensity = 1e15
sys.add_acceptor(acceptorDensity, p_region)

Next we specify the contact boundary conditions. For this example, we specify Ohmic contacts with the function contact_type. Note the order of input arguments is left contact ($x = 0$) type first, right contact ($x = L$) type second:

sys.contact_type('Ohmic', 'Ohmic')

We next specify the value of recombination velocity for electrons and holes at both contacts (Note: Sesame assumes the units of velocity are cm/s). For this example, both contacts only collect majority carriers. This is accomplished with the function contact_S:

Sn_L, Sp_L, Sn_R, Sp_R = 1e7, 0, 0, 1e7
sys.contact_S(Sn_L, Sp_L, Sn_R, Sp_R)

Next we add a grain boundary. We must specify the grain boundary defect energy level $E_{GB}$ (note the defect energy level is measured from the intrinsic energy level), the electron and hole capture cross sections $\sigma_{eGB}$ and $\sigma_{hGB}$, the defect density $\rho_{GB}$, and the endpoints of the line defining the grain boundary $p_1, p_2$. These are input arguments to the function add_line_defects which creates a grain boundary. We also specify the charge transition states of the defect with the function input transition. In this case the specified charge states are $(+1,-1)$, corresponding to having a donor and acceptor at the same energy level.

EGB = 0.4
sigmaeGB = 1e-15
sigmahGB = 1e-15
rhoGB = 1e14
p1 = (.1e-4, 1.5e-4)
p2 = (2.9e-4, 1.5e-4)
sys.add_line_defects([p1, p2], rhoGB,

We add illumination by defining a function illumination which returns the position-dependent intensity as a function of the input coordinate $x, y$

def illumination(x,y):
    return 2.3e21 * np.exp(-2.3e4 * x)
sys.generation(illumination)

With the system now fully defined, we specify the list of applied voltages used to compute the current-voltage relation with the IVcurve function:

voltages = np.linspace(0,1,11)
jset = sesame.IVcurve(sys, voltages,
    solution, 'GB_JV')

The function IVcurve returns an array jset containing the computed current density for each applied voltage. The IVcurve function also saves output files with seedname “GB_JV” concatenated with a suffix labeling the applied voltage index. These output files contain objects describing the simulation settings and the solution arrays. By default these files are compressed data files containing python Pickle objects (.gzip files). There is also an option to output the data in Matlab format (.mat files). Sesame includes an Analyzer object which contains several functions for computing quantities of interest from the solution, such as current densities, total recombination, carrier densities, and others. We refer the reader to the online documentation for a detailed list of all these functions.

C. GUI

Use of the standalone GUI as an alternative to scripting can be more convenient for small-scale calculations, or for those without access to a python distribution. Simulation settings can be saved and loaded, and the GUI also provides an interactive python prompt. The GUI is divided into three tabs, as shown in Fig. 4:

1. The System tab contains fields to define the system geometry and material parameters (see Fig. 5).
2. The Simulation tab lets the user specify which parameter is varied: either the voltage is swept, or a user-defined variable related to the generation rate density is swept. The boundary conditions and output file information is also set here, and the simulation is launched from this tab. The program output is provided so that the user can follow the progress of the calculations.

3. The Analysis tab enables the user to plot the output of the simulation, and to save and export plotted data (see Figs. 6 and 7).

Sesame is distributed with a number of sample input files for setting up standard PV simulations in the GUI. More detailed documentation for the GUI is included in the distribution.

IV. CONCLUSION

Modeling tools are essential for describing and understanding polycrystalline materials and nanoscale measurements. System behavior for complex, 2-dimensional geometries can be drastically different than the textbook 1-dimensional $p$-$n$ junction model. Numerical simulations provide the capability to explore and develop in-
tution about this rather unchartered territory. Our aim in releasing Sesame is to provide the research community with a free, easy-to-use resource which will enable broader use of simulation in complex photovoltaic systems. There are opportunities for additional functionalities (e.g. time-dependence, small-signal analysis, more advanced interface transport models) and further optimizations (e.g. use of Cython) of the code. Our intent in releasing the fully documented source code is to provide users the option to make these and other additions as their research needs require. An additional feature not discussed here is 3-dimensional modeling, which is included in the distribution as an untested feature which will be investigated further in future work.

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Appendix A  MODEL DETAILS

A  Mathematical Description

In this section we provide a full description of the equations solved by Sesame. These are fairly standard and can be found in textbooks [26–29], but we include them here for the sake of completeness and to specify notation and conventions used in the code. We first write densities in terms of quasi-Fermi levels, denoted by \( E_{F_n} \) and \( E_{F_p} \) for electrons and holes, respectively. Since we assume Boltzmann statistics (i.e., a non-degenerate semiconductor), the carrier densities are related to quasi-Fermi levels by:

\[
n = N_C \exp \left( \frac{E_{F_n} + \chi + q\phi}{k_B T} \right) \tag{6}
\]

\[
p = N_V \exp \left( \frac{-E_{F_p} - \chi - E_g - q\phi}{k_B T} \right). \tag{7}
\]

where \( E_g \) is the material band gap, \( \chi \) is the electron affinity, and \( N_{C,V} \) are the conduction, valence band effective density of states, respectively. All quantities except temperature can vary with position.

The electron and hole current can be expressed in terms of the spatial gradient of the quasi-Fermi levels [30]:

\[
\vec{J}_n = q\mu_n n \mathbf{\nabla} E_{F_n} \tag{8}
\]

\[
\vec{J}_p = q\mu_p p \mathbf{\nabla} E_{F_p}. \tag{9}
\]

1  Recombination

Sesame includes Shockley-Read-Hall, radiative and Auger recombination. The steady-state Shockley-Read-Hall recombination rate density is given by:

\[
R_{SRH} = \frac{np - n_i^2}{\tau_p (n + n_1) + \tau_n (p + p_1)} \tag{10}
\]

where \( n_i \) is the material intrinsic carrier density, given by \( n_i = \sqrt{N_C N_V} \exp (-E_g/(2k_B T)) \). The equilibrium Fermi energy at which \( n = p = n_1 \) is the intrinsic energy level \( E_i \). We specify the defect energy level \( E_T \) relative to \( E_i \) (see Fig. 8), so that the expressions for \( n_1 \) and \( p_1 \) in Eq. 10 are given by:

\[
n_1 = n_i \exp \left( \frac{E_T}{k_B T} \right), \tag{11}
\]

\[
p_1 = n_i \exp \left( -\frac{E_T}{k_B T} \right). \tag{12}
\]

\( \tau_{n,(p)} \) is the bulk lifetime for electrons, holes. It is given by

\[
\tau_{n,p} = \frac{1}{N_T v_{n,p}^{\text{th}} \sigma_{n,p}} \tag{13}
\]

The electron and hole current can be expressed in terms of the spatial gradient of the quasi-Fermi levels:

\[
\vec{J}_n = q\mu_n n \mathbf{\nabla} E_{F_n} \tag{8}
\]

\[
\vec{J}_p = q\mu_p p \mathbf{\nabla} E_{F_p}. \tag{9}
\]

where \( N_T \) is the three-dimensional trap density, \( n_i^{\text{th}} \) is the thermal velocity of carriers (\( v_{n,p}^{\text{th}} = \sqrt{3k_B T/m_{n,p}} \) with \( m_{n,p} \) the electron/hole effective mass), and \( \sigma_{n,p} \) is the capture cross-section for electrons, holes.

The radiative recombination has the form

\[
R_{\text{rad}} = B(n p - n_i^2) \tag{14}
\]

where \( B \) is the radiative recombination coefficient of the material. The Auger mechanism has the form

\[
R_A = (C_n n + C_p p)(n p - n_i^2) \tag{15}
\]

where \( C_n \) (\( C_p \)) is the electron (hole) Auger coefficient.

2  Planar defects

Sesame has been created with the intent of studying extended defects in solar cells, such as grain boundaries and sample surfaces. These extended planar defects are represented by a point in a 1-d model, a line in a 2-d model, and a plane in a 3-d model. The extended defect energy level spectrum can be discrete or continuous. For a discrete spectrum, we label the defect with the subscript \( d \). The occupancy of the defect level \( f_d \) is given by

\[
f_d = \frac{S_n n + S_p p_d}{S_n (n + n_d) + S_p (p + p_d)} \tag{16}
\]

where \( n (p) \) is the electron (hole) density at the spatial location of the defect, \( S_n, S_p \) are recombination velocity parameters for electrons and holes respectively. \( n_d \) and \( p_d \) are

\[
n_d = n_i \exp \left( \frac{E_d}{k_B T} \right) \tag{17}
\]

\[
p_d = n_i \exp \left( -\frac{E_d}{k_B T} \right) \tag{18}
\]
where $E_d$ is calculated from the intrinsic level $E_i$.

The electron/hole recombination velocity is related to the electron/hole capture cross section and the defect density $\rho_d$ according to:

$$S_{n,p} = \rho_d \sigma_{n,p} n_{th}.$$  \hfill (19)

The defect recombination is of Shockley-Read-Hall form:

$$R_d = \frac{S_n S_p (n p - n_d^2)}{S_n (n + n_d) + S_p (p + p_d)}.$$  \hfill (20)

The charge density given of a single defect depends on the defect type (acceptor vs. donor)

$$Q = q \rho_d \times \begin{cases} (1 - f_d) & \text{donor} \\ (-f_d) & \text{acceptor} \end{cases}$$  \hfill (21)

where $\rho_d$ is the defect density of state at energy $E_d$. Multiple defects are described by summing over defect label $d$, or performing an integral over a continuous defect spectrum.

## B Boundary conditions at the contacts

For a given system definition, Sesame first solves the equilibrium problem. In equilibrium, the quasi-Fermi level of electrons and holes levels are equal and spatially constant. We choose an energy reference such that in equilibrium, $E_{F_n} = E_{F_p} = 0$. The equilibrium problem is therefore reduced to a single variable $\phi^{eq}(r)$. Sesame employs both Dirichlet and von Neumann equilibrium boundary conditions for $\phi^{eq}$, which we discuss next.

### 1 System in thermal equilibrium

Sesame uses Dirichlet boundary conditions as the default. This is the appropriate choice apply when the equilibrium charge density at the contacts is known a priori. This applies for Ohmic and ideal Schottky contacts. For Ohmic boundary conditions, the carrier density is assumed to be equal and opposite to the ionized dopant density at the contact. For an $n$-type contact with $N_D$ ionized donors at the $x = 0$ contact (i.e. no free excess carriers at the contact), Eq. (6) yields the expression for $\phi^{eq}(x = 0)$:

$$q \phi^{eq}(0, y, z) = k_B T \ln \left( \frac{N_D}{N_C} \right) - \chi(0, y, z)$$  \hfill (22)

Similar reasoning yields expressions for $q \phi^{eq}$ for $p$-type doping and at the $x = L$ contact.

For Schottky contacts, we assume that the Fermi level at the contact is equal to the Fermi level of the metal. This implies that the equilibrium electron density is $N_C \exp[-(\Phi_M - \chi)/k_B T]$, where $\Phi_M$ is the work function of the metal contact. Eq. (9) then yields the expression for $\phi^{eq}$ (shown here for the $x = 0$ contact):

$$q \phi^{eq}(0, y, z) = -\Phi_M |_{x=0} \text{ contact} \hfill (23)$$

An identical expression applies for the $x = L$ contact.

Sesame also has an option for von Neumann boundary conditions, where it’s assumed that the electrostatic field at the contact vanishes:

$$\frac{\partial \phi^{eq}}{\partial x}(0, y, z) = \frac{\partial \phi^{eq}}{\partial x}(L, y, z) = 0.$$  \hfill (24)

The equilibrium potential $\phi^{eq}$ determines the equilibrium densities $n^{eq}$, $p^{eq}$ according to Eqs. (6) and (7) with $E_{F_n} = E_{F_p} = 0$.

### 2 System out of thermal equilibrium

Out of thermal equilibrium, Dirichlet boundary conditions are imposed on the electrostatic potential. For example, in the presence of an applied bias $V$ at $x = L$, the boundary conditions are

$$\phi(0, y, z) = \phi^{eq}(0, y, z)$$  \hfill (25)

$$\phi(L, y, z) = \phi^{eq}(L, y, z) + qV$$  \hfill (26)

where $\phi^{eq}$ is the equilibrium electrostatic potential.

For the drift-diffusion equations, the boundary conditions for carriers at charge-collecting contacts are parameterized with the surface recombination velocities for electrons and holes at the contacts, denoted respectively by $S_{c_n}$ and $S_{c_p}$:

$$J_n^x(0, y, z) = q S_{c_n}^0 (n(0, y, z) - n^{eq}(0, y, z))$$  \hfill (27)

$$J_p^x(0, y, z) = -q S_{c_p}^0 (p(0, y, z) - p^{eq}(0, y, z))$$  \hfill (28)

$$J_n^x(L, y, z) = -q S_{c_n}^L (n(L, y, z) - n^{eq}(L, y, z))$$  \hfill (29)

$$J_p^x(L, y, z) = q S_{c_p}^L (p(L, y, z) - p^{eq}(L, y, z))$$  \hfill (30)

## C Numerical implementation

In this section we review the set of equations solved by Sesame and provide some details of their implementation in the one-dimensional case.

### 1 Scharfetter-Gummel scheme

Sesame uses finite differences to solve the drift-diffusion-Poisson equations on a nonuniform grid. Fig. 9 shows our index-labeling convention for sites and links: link $i$ connects site $i$ and site $i+1$. Site-defined quantities (such as density and electrostatic potential) are labeled with a subscript denoting the site number. Link-defined
We consider a one-dimensional system to illustrate the model discretization. First, we rewrite the current on link \( i \) in semi-discretized form:

\[
J^i_n = q \mu_{n,i} n_i \frac{dE_{F_n}}{dx} \bigg|_i 
\]

\[
J^i_p = q \mu_{p,i} p_i \frac{dE_{F_p}}{dx} \bigg|_i 
\]

A key step to ensure numerical stability is to integrate Eqs. (31) and (32) in order to get a completely discretized version of the current \( J^i_{n,p} \). This discretization is known as the Scharfetter-Gummel scheme [25]. Here we give the final expressions for the hole current \( J^i_p \) between sites \( i \) and \( i + 1 \):

\[
J^i_p = q \frac{\psi_{p,i+1} - \psi_{p,i}}{\Delta x^i} \times \mu_{p,i} \left[ \exp \left( -\frac{E_{F_{p,i+1}}}{k_BT} \right) - \exp \left( \frac{-E_{F_{p,i}}}{k_BT} \right) \right].
\]

(33)

where \( \psi_p = q\phi + \chi + E_p - k_BT \ln(N_V) \) is the effective potential. The electron current \( J^i_n \) is given by:

\[
J^i_n = -q \frac{\psi_{n,i+1} - \psi_{n,i}}{\Delta x^i} \times \mu_{n,i} \left[ \exp \left( \frac{E_{F_{n,i+1}}}{k_BT} \right) - \exp \left( \frac{-E_{F_{n,i}}}{k_BT} \right) \right].
\]

(34)

where \( \psi_n = q\phi + \chi + k_BT \ln(N_C) \).

In the limit where either \( \delta\psi_{n(p)} \equiv -q(\psi_{n(p),i+1} - \psi_{n(p),i})/k_BT \) or \( \delta E_{F_{n(p)}} \equiv (E_{F_{n(p),i+1}} - E_{F_{n(p),i}})/k_BT \) are smaller than \( 10^{-5} \) and \( 10^{-9} \), respectively, we replace the expressions for the current with a Taylor series expansion of the small parameter. In the expansion, we evaluate the current up to second order in \( \delta\psi_{n(p)} \) and up to first order in \( \delta E_{F_{n(p)}} \).

Embedding a two-dimensional density into the three-dimensional model is formally accomplished with the use of a delta function. Numerically, the two-dimensional defect densities of states and the surface recombination velocities are divided by the size of the discretized grid at the position of the plane, and along the direction normal to the plane.

### 2 Newton-Raphson algorithm

The discretization of Eqs. (1)–(3) leads to the system of three equations for all sites of the discretized space (except boundary sites):

\[
0 = \frac{2}{\Delta x^i + \Delta x^{i-1}} \left( J^i_p - J^{i-1}_p \right) + G_i - R_i 
\]

(35)

\[
0 = \frac{2}{\Delta x^i + \Delta x^{i-1}} \left( J^i_n - J^{i-1}_n \right) - G_i + R_i 
\]

(36)

\[
0 = \rho_i + \frac{2}{\Delta x^i + \Delta x^{i-1}} \left[ \left( \frac{\epsilon_{i+1} + \epsilon_i}{2} \right) \left( \frac{\phi_{i+1} - \phi_i}{\Delta x^i} \right) - \left( \frac{\epsilon_i + \epsilon_{i-1}}{2} \right) \left( \frac{\phi_i - \phi_{i-1}}{\Delta x^{i-1}} \right) \right]
\]

(37)

Because we exchanged the carrier densities for the quasi-Fermi levels as the unknowns of the problem, we are therefore looking for the sets \( E_{F_{n}}, E_{F_{p}} \), \( \phi \) at every grid point.

We use the Newton-Raphson method to solve the above set of equations: Given a general nonlinear function \( f(x) \), we want to find its root \( x : f(x) = 0 \). Given an initial guess \( x_1 \), one can estimate the error \( \delta x \) in this guess, assuming that the function varies linearly all the way to its root

\[
\delta x = \left( \frac{df}{dx}(x_1) \right)^{-1} f(x_1).
\]

(38)

An updated guess is provided by \( x_2 = x_1 - \delta x \). The assumption of linear variation is key here, as if the guess \( x_1 \) is too far from the root, the convergence of the algorithm is very uncertain.

In multiple dimensions the derivative in Eq. (38) is replaced by the Jacobian. In this case, Eq. (38) is a matrix equation of the form

\[
\delta x = A^{-1} F(x)
\]

(39)

### TABLE II. Quantities used to scale variables to dimensionless form.

| Quantity          | Expression | Value       |
|-------------------|------------|-------------|
| Density           | \( N_0 \)  | \( 10^{27} \text{ m}^{-3} \) |
| Mobility          | \( \mu_0 \) | \( 10^{-4} \text{ cm}^2/(\text{V} \cdot \text{s}) \) |
| Temperature       | \( T_0 \)  | \( 300 \text{ K} \) |
| Energy            | \( k_B T_0 \) | \( 0.0258 \text{ eV} \) |
| Length            | \( \sqrt{\epsilon_0 k_B T/(q^2 N_0)} \) | \( 3.78 \times 10^{-10} \text{ m} \) |
| Time              | \( \epsilon_0/(q \mu_0 N_0) \) | \( 5.5 \times 10^{-14} \text{ s} \) |
| Gen. rate density | \( N_\mu E_0/x_0^2 \) | \( 1.81 \times 10^{12} \text{ 1/(m}^2 \cdot \text{s}) \) |
| Current           | \( \mu_0 N_0 k_B T/x_0 \) | \( 1.10 \times 10^{10} \text{ A/m}^2 \) |
where $\mathbf{F}$ is a vector function of the unknowns of the problem on all sites of the discretized space, and $A$ is the Jacobian matrix given by

$$A_{ij} = \frac{\partial F_i}{\partial x_j}. \quad (40)$$

We find that convergence of the Newton-Raphson algorithm for this problem requires exact (analytically computed) values for the Jacobian.

In case the guess is far from the root we are looking for, the correction given by Eq. (38) can overshoot the solution. A simple way to improve the convergence is to damp the corrections $\delta \mathbf{x}$ given by Eq. (39). Inspired by an earlier work [32], we found that the following procedure gives good results. For $\delta x_i > 1$, we replace $\delta x_i$ by

$$\delta \bar{x}_i = \text{sgn}(\delta x_i) \log \left(1 + 1.72|\delta x_i|\right). \quad (41)$$