Charge Injection Project

The project

This project involves solving the Poisson equation and the drift diffusion equation to find the electric field pattern and current flow paths occurring when charges are injected into a semiconducting film from a small electrode like an AFM tip. Solving the equations gives the electrostatic potential $\psi$ and charge density $p$ as a function of position in the film. In your report you should provide plots of electric field and current patterns at specific applied voltage conditions. You should also give an I-V curve showing the transition to space charge limited current flow where $I \propto V^2$.

Background

Continuum device models are the basis of most modeling of semiconductor devices, including transistors, light emitting diodes, solar cells and sensors. Below is a fairly general introduction, but you only have to consider the Poisson equation and the equation for the positive charges (holes) for the case where charge is injected from the top electrode that is held at voltage $V_a$ and collected at a bottom electrode that is grounded. There are no source terms in this injection geometry.

In the standard models, the electrostatic potential, $\psi$, is found from the Poisson equation,

$$\nabla^2 \psi = \frac{q}{\epsilon} (n - p),$$

where $p$ is the hole density and $n$ is the electron density with units $1/m^3$.

The positive charge (hole) current obeys the continuity equation,

$$\frac{\partial (qp)}{\partial t} + \nabla \cdot j_p = qg$$

where $g$, with units $1/(m^3 s)$, is the generation rate and $q = e = 1.6 \times 10^{-19}$C is the elementary charge. Here we take $g = 0$ as there is no charge generation in the interior of the film. If photoactivation occurs, then $g$ is related to the local radiation intensity. A similar expression applies to the electron current, but here we assume that the holes dominate the transport so we ignore the electrons and set $n = 0$.

The drift diffusion equation treats the hole current as a sum of two terms, a drift term due to
the local electric field and a diffusion term due to random Brownian motion.

\[ j_p = q\mu_p p F - q D_p \nabla p = q\mu_p p F - q\mu_p V_t \nabla p \]  

(3)

where \( \mu_p \) is the electron mobility and \( V_t = kT/q \) is the thermal voltage. The Einstein relation relates the diffusion constant, \( D_p \), and the mobility through \( D_p = \mu_p V_t \). Combining the continuity equation with the drift-diffusion current, along with \( F = -\nabla \psi \) yields,

\[ -\nabla \cdot [\mu_p (p \nabla \psi + V_t \nabla p)] = 0 \]  

(4)

This equation and Poisson’s equation (with \( n = 0 \)) are solved to find \( p, \psi \) and \( F \). The parameters in the model are \( V_a, N_c \), the cell geometry and the mobilities.

**Formulation of the discretized equations**

Here we discuss the general case and specialize to the hole injection case in the next section.

We seek solutions to the three variables \( \psi, n \) and \( p \), that are described by Poisson’s equation (1) and the two drift-diffusion equations (11) and (12). It is convenient to define reduced variables \( n' = n/N_c \) and \( \psi' = \psi/V_t \). We work in Cartesian co-ordinates so we can discuss the method in one direction with the generalization to the other two directions being trivial. For the case of hole injection, the collecting electrode is placed at a location \( z \leq 0 \), and the injecting electrode is placed at \( z > 0 \). Both the injecting and/or collecting electrode may have a complex geometry, and the case of double injection may also be treated.

Simple central difference discretization of Eq. (1) and Eqs. (11,12) yields,

\[ \epsilon_{i+1}(\psi'_{i+1} - \psi'_i) - \epsilon_i(\psi'_i - \psi'_{i-1}) = \frac{qN_c\delta x^2}{V_t} (n'_i - p'_i), \]  

(5)

\[ \mu_{i+1}'' n'_{i+1}[(\psi'_{i+1} - \psi'_i) - 2(n'_{i+1} - n'_i)] - \mu'' n'_{i-1}[(\psi'_i - \psi'_{i-1}) - 2(n'_i - n'_{i-1})] = \frac{2\delta x^2 g_i}{N_c V_t}, \]  

(6)
and,

\[
\mu_p p'_{i+1} \left[ (\psi'_{i+1} - \psi'_i) - 2(p'_{i+1} - p'_i) \right] - \mu_p p'_{i-1} \left[ (\psi'_i - \psi'_{i-1}) - 2(p'_i - p'_{i-1}) \right] = -\frac{2\delta x^2 g_i}{N_c V_t}, \tag{7}
\]

We consider a cell of thickness \(L\) and take \(m\) mesh intervals, so that the size of a mesh is \(L/m\). The mesh points then run from \(1..m + 1\) and the boundary conditions are then,

\[
n'_1 = p'_{m+1} = 1; \quad n'_{m+1} = p'_1 = e^{-E_g/qV_t} \quad ; \quad \psi'_1 = \frac{E_g - qV_a}{qV_t}; \quad \psi'_{m+1} = 0, \tag{8}
\]

where \(V_a\) is the applied voltage.

The simple discretization above works for the Poisson Eq. but not for the continuity equations, as the carrier densities in the continuity equations vary rapidly in the double layer regions leading to numerical instabilities. Scharfetter and Gummel introduced a procedure to mitigate this effect. Their method is based on assuming that both \(E\) and \(J\) are constant on a mesh, so that we may solve the equation (where the factor of \(q\) is absorbed into \(F\) and into \(V_t\)),

\[
J = \mu F n + \mu V_t \frac{dn}{dx} \tag{9}
\]

by making the substitution, \(n(x) = a + be^{cx}\), to find that \(a = J/\mu F, C = -F/V_t\) and hence,

\[
n(x) = \frac{J}{\mu F} + be^{-Fx/V_t}. \tag{10}
\]

We evaluate this expression at the ends of the mesh, so that,

\[
n_i = \frac{J}{\mu F} + be^{-Fx_i/V_t}; \quad n_{i+1} = \frac{J}{\mu F} + be^{-Fx_{i+1}/V_t}. \tag{11}
\]

Solving the second of these equations for \(b\) yields,

\[
b = \frac{n_{i+1} - J/\mu F}{e^{-Fx_{i+1}/V_t}}. \tag{12}
\]

Substituting this equation into the first of Eqs. (39), yields,

\[
n_i = \frac{J}{\mu F} + \frac{n_{i+1} - J/\mu F}{e^{-Fx_{i+1}/V_t}} e^{-Fx_i/V_t}. \tag{13}
\]
Solving this equation to find the current and using \( F \delta x = -\delta \psi \) yields,

\[
J_{i+1/2} = \mu \left( \frac{-\delta \psi}{\delta x} \right) \frac{n_i - n_{i+1} e^{-\delta \psi/V_i}}{1 - e^{-\delta \psi/V_i}},
\]

(14)

or,

\[
J_{i+1/2} = \mu \left( \frac{\delta \psi}{\delta x} \right) \left[ \frac{n_{i+1}}{e^{\delta \psi/V_i} - 1} + \frac{n_i}{e^{-\delta \psi/V_i} - 1} \right].
\]

(15)

Using the Bernoulli function \( B(x) = x/(e^x - 1) \), this reduces to,

\[
J_{i+1/2} = \frac{V_i \mu}{\delta x} \left[ n_{i+1} B(\delta \psi/V_i) - n_i B(-\delta \psi/V_i) \right]
\]

(16)

We discretize the continuity equation using a simple central difference,

\[
\frac{\partial J_n}{\partial x} \approx \frac{J_{i+1/2} - J_{i-1/2}}{\delta x}
\]

(17)

yielding,

\[
\frac{\partial J_n}{\partial x} = \frac{V_i}{\delta x^2} \left[ \mu_{n+1}^{i+1} (B(\delta \psi_{i+1}) n_{i+1} - B(-\delta \psi_{i+1}) n_i) - \mu_{n-1}^{i} (B(\delta \psi_i) n_{i-1} - B(-\delta \psi_i) n_i) \right]
\]

(18)

where \( \delta \psi_{i+1} = (\psi_{i+1} - \psi_i)/V_i \). In scaled units \( g' = g \delta x^2 / V_i \mu_n N_c \). Carrying through the analysis for \( J_p \) yields,

\[
\frac{\partial J_p}{\partial x} = \frac{V_i}{\delta x^2} \left[ \mu_{p+1}^{i+1} (B(-\delta \psi_{i+1}) p_{i+1} - B(\delta \psi_{i+1}) p_i) - \mu_{p-1}^{i} (B(-\delta \psi_i) p_{i-1} - B(\delta \psi_i) p_i) \right]
\]

(19)

The equations to be solved (see Gavin A Buxton and Nigel Clarke 2007 Modelling Simul. Mater. Sci. Eng. 15 13)

Extending these expressions to all three directions, the equations that need to be solved are then,

\[
epsilon_{i+1,j,k}^{'} (\psi_{i+1,j,k}^{'} - \psi_{j,k}^{'} ) - e_{i,j,k}^{'} (\psi_{j,k}^{'} - \psi_{i-1,j,k}^{'} )
\]
\[ + \epsilon'_{ij+1k}(\psi'_{ij+1k} - \psi'_{ijk}) - \epsilon'_{ijk}(\psi'_{ijk} - \psi'_{ij-1k}) \]

\[ + \epsilon'_{ijk+1}(\psi'_{ijk+1} - \psi'_{ijk}) - \epsilon'_{ijk}(\psi'_{ijk} - \psi'_{ijk-1}) \]

\[ = C_1 a^2 (n'_{ijk} - p'_{ijk}), \quad (20) \]

where \( C_1 = \frac{qN_e \times 10^{-18}}{\varepsilon_0 V_i} \), \( a \) is the mesh size in nanometers and \( \epsilon' \) is the relative dielectric constant. Koster et al. take \( a = 1.3 \) and using the values of the constants from that paper \( C_1 = \). The drift diffusion equations become,

\[ \mu_n'_{ij+1k}[B(\delta \psi'_{ij+1k})n_{ij+1k} - B(-\delta \psi'_{ij+1k})n_{ijk}] - \mu_n'_{ijk}[B(\delta \psi'_{ijk})n_{ijk} - B(-\delta \psi'_{ijk})n_{i-1jk}] \]

\[ + \mu_n'_{ij+1k}[B(\delta \psi'_{ij+1k})n_{ij+1k} - B(-\delta \psi'_{ij+1k})n_{ijk}] - \mu_n'_{ijk}[B(\delta \psi'_{ijk})n_{ijk} - B(-\delta \psi'_{ijk})n_{i-1jk}] \]

\[ + \mu_n'_{ijk+1}[B(\delta \psi'_{ijk+1})n_{ijk+1} - B(-\delta \psi'_{ijk+1})n_{ijk}] - \mu_n'_{ijk}[B(\delta \psi'_{ijk})n_{ijk} - B(-\delta \psi'_{ijk})n_{ijk-1}] \]

\[ = -a^2[C_2^n P - C_3^n (1 - P)(n'_{ijk}p'_{ijk} - e^{-E_k/V_i})] \quad (21) \]

and

\[ \mu_p'_{ij+1k}[B(-\delta \psi'_{ij+1k})p_{ij+1k} - B(\delta \psi'_{ij+1k})p_{ijk}] - \mu_p'_{ijk}[B(-\delta \psi'_{ijk})p_{ijk} - B(\delta \psi'_{ijk})p_{i-1jk}] \]

\[ + \mu_p'_{ij+1k}[B(-\delta \psi'_{ij+1k})p_{ij+1k} - B(\delta \psi'_{ij+1k})p_{ijk}] - \mu_p'_{ijk}[B(-\delta \psi'_{ijk})p_{ijk} - B(\delta \psi'_{ijk})p_{ij-1k}] \]

\[ + \mu_p'_{ijk+1}[B(-\delta \psi'_{ijk+1})p_{ijk+1} - B(\delta \psi'_{ijk+1})p_{ijk}] - \mu_p'_{ijk}[B(-\delta \psi'_{ijk})p_{ijk} - B(\delta \psi'_{ijk})p_{ijk-1}] \]
\[
= -a^2 [C_2^\alpha P - C_3^\alpha (1 - P) (n'_{ijk} p'_{ijk} - e^{-E_g/V_i})]
\]

(22)

where \(\mu'_\alpha = \mu_\alpha / <\mu>\) and \(C_2^\alpha, C_3^\alpha\) are given by the expressions

\[
C_2^\alpha = \frac{10^{-18} G}{V_i <\mu> N_c}; \quad \text{and} \quad C_3^\alpha = \frac{10^{-18} N_c \gamma}{V_i <\mu>}. \quad \text{(23)}
\]

Using the values from the paper of Koster et al: \(q = 1.6 \times 10^{-19} C, N_c = 2.5 \times 10^{25} / m^3, \epsilon = 3 \times 10^{-11} F/m, V_i = 0.025V, G = 2.7 \times 10^{27} / (m^3 s), \mu_n = 2.5 \times 10^{-7} m^2 / (Vs), \mu_p = 3.0 \times 10^{-8} m^2 / (Vs)\) leading to the values,

\[
C_1 = 5.33; \quad C_2^n = 1.73 \times 10^{-8}; \quad C_2^p = 1.44 \times 10^{-7}; \quad C_3^n = 2.987; \quad C_3^p = 24.89 \quad \text{(24)}
\]

These equations need to be solved with the boundary conditions given in Eq. (14), where \(V_a\) is the applied voltage and we take \(E_g = 1.34eV\).


We solve these equations using the following procedure: Start with Poisson’s equation and a guess for \(n', p'\). Write Poisson’s equation in the matrix form \(A_\psi \psi = b_\psi\). The matrix \(A_\psi\) is tridiagonal. Solve for \(\psi = A_\psi^{-1} b_\psi\). Use this solution to generate a matrix form of the equations for \(n', A_n n = b_n\). Here we use the old values of \(p'\). \(A_n\) is again tridiagonal. We find \(n = A_n^{-1} b_n\). Finally we do the same thing for the \(p'\) equations, but now we can use either the old values of \(n'\) or the new values of \(n'\). Check to see which is better. Once the new values of \(p'\) are found, we go back to Poisson’s equation and repeat the process until convergence. The key numerical procedure is then the solution to a tridiagonal set of equations. This can be done efficiently in many ways, for example by inverting the tridiagonal matrix.

There are only a couple of model parameters in the program, namely \(a \sim 1nm\) the mesh size in nanometers, \(L\) the size of the solar cell and \(V_a\) the applied voltage.

Appendix: Mott-Gurney limit - Physical origin of \(I \propto V^2\)

The Mott-Gurney model ignores the diffusion term, so in general the potential in the Mott-
Gurney limit is found from,
\[
\nabla \cdot j_p = \nabla (\cdot q \mu_p p F) = \nabla \cdot (\epsilon \mu_p \nabla \cdot F) = 0. 
\] (25)

If \( \epsilon \mu \) is uniform, this reduces to,
\[
\nabla^2[(\nabla \psi)^2] = \nabla^2(F^2) = 0. 
\] (26)

The square magnitude of the electric field then obeys Laplace’s equation and provides a useful approach to finding analytic solutions, as illustrated below.

Assuming that \( \epsilon \mu \) is uniform, and considering variation only in the \( x \)-direction, integration of Eq. (6) has the solution for Laplace’s equation in one dimension \( F^2 = a + bx \), so the electric field is given by,
\[
F = (ax + b)^{1/2}. 
\] (27)

From Poisson’s equation the charge density is then
\[
p = \frac{\epsilon}{q} \frac{\partial F}{\partial x} = \frac{ae}{2q} (ax + b)^{-1/2}. 
\] (28)

The potential across the film is found by integration,
\[
\psi = -\int Fdx = -\frac{2}{3a} [(ax + b)^{3/2}] + c 
\] (29)

For the boundary conditions \( \psi(0) = V, \psi(L) = 0 \), we find the solutions,
\[
F = \frac{3V}{2L} \left( \frac{x}{L} \right)^{1/2}; \quad \psi = V \left[ 1 - \left( \frac{x}{L} \right)^{3/2} \right]; \quad p = \frac{3eV}{4qL^2} \left( \frac{x}{L} \right)^{-1/2}. 
\] (30)

At the injecting electrode, the charge density diverges and the electric field goes to zero. The electric field grows with a square root dependence as we move away from the injecting electrode and is largest at the collecting electrode, \( x = L \). In this solution, the carrier density is not zero at
the \( x = L \) electrode, but is instead set by the applied voltage. The current density is given by,

\[
j = q\mu_p p F = \frac{9}{8} \mu \epsilon \frac{V^2}{L^3},
\]

(31)
or in terms of current,

\[
I = q\mu_p p W^2 F = \frac{9}{8} \mu \epsilon W^2 \frac{V^2}{L^3},
\]

(32)

which is the Mott-Gurney result in a planar geometry.