Numerical solution of space charge density and field in arbitrarily doped diode structures

Peter Fischer, ZITI, Heidelberg University

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1 Device description

We consider a silicon structure with a thickness D. The doping is a function of the depth x in the device, with $0 \leq x \leq D$. We can merge the donor doping $N_D(x)$ and the acceptor doping $N_A(x)$ into an effective doping

$$N(x) := N_D(x) - N_A(x), \tag{1}$$

because opposite dopings compensate each other. $N(x)$ shall be positive for n-doped and negative for p-doped regions, respectively. The built-in potential V_{bi} of this structure is given by the dopings at the surfaces to

$$V_{bi} = U_T \ln\left(-\frac{N(0)}{n_i}\frac{N(D)}{n_i}\right) \tag{2}$$

where n_i is the intrinsic carrier concentration and $U_T = kT/q$ is the thermal voltage[1].

In the following, we will calculate the electrostatic potential $\Phi(x)$ (and also the field $E(x)$) numerically for an *arbitrary* doping profile $N(x)$. We will first write down a (nearly) exact differential equation for $\Phi(x)$, then define an iterative procedure to successively improve an initial guess and carry out the procedure numerically by discretization of the space coordinate.

2 Differential equation

The position dependent density of mobile electrons/holes shall be given by $n(x)$ and $p(x)$. The electrostatic potential $\Phi(x)$ follows from the one-dimensional Poisson equation

$$\frac{d^2\Phi(x)}{dx^2} = \Phi''(x) = -\frac{\rho(x)}{\epsilon\,\epsilon_0} \tag{3}$$

where ϵ is the semiconductor dielectric constant, ϵ_0 is the permittivity of free space and $\rho(x)$ is the charge density given by

$$\rho(x) = q\,\left[p(x) - n(x) + N(x)\right]. \tag{4}$$

In this 'depletion approximation' we have assumed that *all* doping atoms are activated (donors have lost their electron, acceptors have catched an electron), which is basically fulfilled in the *depletion regions*, which we are interested in. n-doped regions are positively charged when depleted, so that we need a '+' sign for $N(x)$ in (4). In equilibrium, electron and hole densities are functions of the potential only[2]:

$$p(x) = n_i \exp\left(-\frac{\Phi(x)}{U_T}\right) \tag{5}$$

$$n(x) = n_i \exp\left(+\frac{\Phi(x)}{U_T}\right), \tag{6}$$

[1] The device can be considered as a series connection of many pn-structures where built-in voltages just add up

[2] Understanding this needs a bit of solid state physics...

where the potential $\Phi(x)$ is relative to the *Fermi potential* Φ_F which we arbitrarily fix to zero and $U_T = kT/q$ is the thermal voltage. Note that these expressions fulfill the mass action law $n(x) \cdot p(x) = {n_i}^2$. The two expressions can be injected into (4) so that we get

$$\rho(x) = q\,N(x) - 2\,q\,n_i\,\sinh\frac{\Phi(x)}{U_T}. \tag{7}$$

The Poisson equation (3) becomes

$$\Phi''(x) = D(x) + C\sinh\frac{\Phi(x)}{U_T} \tag{8}$$

with the *known* quantities

$$D(x) := -\frac{qN(x)}{\epsilon\,\epsilon_0} \tag{9}$$

$$C := \frac{2qn_i}{\epsilon\,\epsilon_0}. \tag{10}$$

The task is therefore to solve (8) for $\Phi(x)$ for a $D(x)$ given by the doping profile.

3 Iterative Solution (Newton - Raphson Method)

We use an iterative procedure to solve (8). In the i-th iteration, we assume that the exact solution $\Phi(x)$ is given by an approximative solution $\Phi^i(x)$ and a (small) error term $\Lambda^i(x)$, i.e.

$$\Phi(x) = \Phi^i(x) + \Lambda^i(x), \qquad \text{with} \qquad i = 0...\infty. \tag{11}$$

In each iteration, we determine an *approximative* solution $\lambda^i(x)$ for $\Lambda^i(x)$ and then use this result to get a *better* solution $\Phi^{i+1}(x) = \Phi^i(x) + \lambda^i(x)$. In the following, we omit the (upper) iteration index i for better readability. Injecting (11) into (8) leads to

$$\Phi''(x) + \lambda''(x) = D(x) + C\sinh\left(\frac{\Phi(x)}{U_T} + \frac{\lambda(x)}{U_T}\right) \tag{12}$$

On the right hand side, we exploit that λ is small compared to Φ so that we can use the first order Taylor approximation $\sinh(x+\epsilon) \approx \sinh(x) + \epsilon \cdot \cosh(x)$. Equation 12 becomes

$$\Phi''(x) + \lambda''(x) \approx D(x) + C\sinh\frac{\Phi(x)}{U_T} + \frac{C}{U_T}\lambda(x)\cosh\frac{\Phi(x)}{U_T}.$$

Bringing all λ-terms to the left leads to

$$\frac{C}{U_T}\cosh\frac{\Phi(x)}{U_T}\tilde{\lambda}(x) - \lambda''(x) = \Phi''(x) - D(x) - C\sinh\frac{\Phi(x)}{U_T}$$

or

$$A(x)\,\lambda(x) - \lambda''(x) = B(x). \tag{13}$$

with

$$A(x) = \frac{C}{U_T}\cosh\frac{\Phi(x)}{U_T} \tag{14}$$

$$B(x) = \Phi''(x) - D(x) - C\sinh\frac{\Phi(x)}{U_T} \tag{15}$$

Equation 13 is linear in λ and therefore much simpler than the initial equation (8). The values of $A(x)$ and $B(x)$ can be calculated from the doping profile and the approximative solution of the i-th iteration $\Phi^{(i)}(x)$. Note that $B(x)$ is the difference of both sides in (8). It vanishes when $\Phi(x)$ is the exact solution, so that $\lambda(x)$ becomes zero.

4 Discretization

We must solve (13) for $\lambda(x)$ to get an improved solution. This can be done numerically by discretization of all functions. We subdivide $x = 0 \dots D$ into N equal intervals of length $\Delta := D/N$. The j-th grid point is at $x_j = j \cdot \Delta$, the grid points at the boundaries $x_0 = 0$ and $x_N = D$ having indices 0 and N, respectively. All functions are now evaluated at discrete positions only, i.e. we use now a vector f_j instead of a function $f(x)$. The second derivative of λ at an *inner* grid point j is

$$\lambda_j'' = \frac{\lambda_{j+1} + \lambda_{j-1} - 2\lambda_j}{\Delta^2} \qquad \text{for} \qquad j = 1 \dots N-1.$$

Using this, (13) becomes

$$A_j \; \lambda_j + \alpha \, (\lambda_{j+1} + \lambda_{j-1} - 2\lambda_j) = B_j \qquad \text{for} \qquad j = 1 \dots N-1 \tag{16}$$

with

$$\alpha := -\frac{1}{\Delta^2} = -\frac{N^2}{D^2}$$

For now, we fix the voltage at the diode to V_{bi} (i.e. we apply no additional bias voltage). This fixes the values of Φ_0 and Φ_N and we have $\lambda_0 = \lambda_N = 0$. We therefore only need to calculate indices $j = 1 \dots N-1$. Equation 16 can be rearranged as

$$\alpha\lambda_{j-1} + (A_j - 2\alpha)\lambda_j + \alpha\lambda_{j+1} = B_j$$

which can be written in matrix form as

$$\begin{pmatrix} A_1 - 2\alpha & \alpha & 0 & \cdots & 0 \\ \alpha & A_2 - 2\alpha & \alpha & 0 & \cdots \\ 0 & \alpha & A_3 - 2\alpha & \alpha & \cdots \\ \vdots & 0 & \alpha & \ddots & \alpha \\ 0 & \cdots & \cdots & \alpha & A_{N-1} - 2\alpha \end{pmatrix} \cdot \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \cdots \\ \lambda_{N-1} \end{pmatrix} = \begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ \cdots \\ B_{N-1} \end{pmatrix}$$

or

$$\begin{pmatrix} X_1 & \alpha & 0 & \cdots & 0 \\ \alpha & X_2 & \alpha & 0 & \cdots \\ 0 & \alpha & X_3 & \alpha & \cdots \\ \vdots & 0 & \alpha & \ddots & \alpha \\ 0 & \cdots & \cdots & \alpha & X_{N-1} \end{pmatrix} \cdot \vec{\lambda} = \begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ \cdots \\ B_{N-1} \end{pmatrix} \tag{17}$$

with

$$X_i := A_i - 2\alpha = \frac{C}{U_T} \cosh \frac{\Phi_i}{U_T} - 2\alpha \tag{18}$$

This equation is of a simple form as only the first off-diagonal elements are non-zero. It can be solved by Gauss elimination. We first subtract an α/X_1-fold multiple of the first row from the second row in order to eliminate the α in the first column. This gives

$$\begin{pmatrix} X_1 & \alpha & 0 & \cdots & 0 \\ \mathbf{0} & X_2 - \frac{\alpha^2}{X_1} & \alpha & 0 & \cdots \\ 0 & \alpha & X_3 & \alpha & \cdots \\ \vdots & 0 & \alpha & \ddots & \alpha \\ 0 & \cdots & \cdots & \alpha & X_{N-1} \end{pmatrix} \cdot \vec{\lambda} = \begin{pmatrix} B_1 \\ B_2 - \alpha\frac{B_1}{X_1} \\ B_3 \\ \cdots \\ B_{N-1} \end{pmatrix} \tag{19}$$

In the next step, we subtract a $\frac{\alpha}{(X_2 - \alpha^2/X_1)}$-fold multiple of the second row from the third row and get

$$\begin{pmatrix} X_1 & \alpha & 0 & \cdots & 0 \\ 0 & X_2 - \frac{\alpha^2}{X_1} & \alpha & 0 & \cdots \\ 0 & \mathbf{0} & X_3 - \frac{\alpha^2}{X_2 - \frac{\alpha^2}{X_1}} & \alpha & \cdots \\ \vdots & 0 & \alpha & \ddots & \alpha \\ 0 & \cdots & \cdots & \alpha & X_{N-1} \end{pmatrix} \cdot \vec{\lambda} = \begin{pmatrix} B_1 \\ B_2 - \alpha\frac{B_1}{X_1} \\ B_3 - \alpha\frac{B_2 - \alpha\frac{B_1}{X_1}}{X_2 - \frac{\alpha^2}{X_1}} \\ \cdots \\ B_{N-1} \end{pmatrix} \tag{20}$$

We proceed with the following rows until all αs below the diagonal are eliminated. We then eliminate the remaining αs *above* the diagonal in a similar way, starting at the lowermost row. The resulting matrix has only diagonal elements so that the λs can be extracted directly.

5 Applying an External Reverse Bias Voltage

If we apply an external voltage V (in reverse bias), the structure is no longer in equilibrium and the Fermi level is not constant any more: the levels at the p- and n-side are offset by $q \cdot V$. Electron and hole densities can be determined by using *effective Fermi energies*, one for each carrier type. Figure 1 shows the band structure of a pn-junction with reverse bias voltage V. Equations (5) and (6) must be replaced by

$$\begin{aligned} p(x) &= n_i \exp\left(\frac{E_{Fi}(x) - E_{Fp}}{kT}\right) = n_i \exp\left(\frac{E_{Fi}(x) - E_{Fp}}{q\,U_T}\right) \\ n(x) &= n_i \exp\left(\frac{E_{Fn} - E_{Fi}(x)}{kT}\right) = n_i \exp\left(\frac{E_{Fn} - E_{Fi}(x)}{q\,U_T}\right). \end{aligned}$$

We arbitrarily fix the reference of all potentials in the middle between the effective Fermi level for holes, E_{Fp}, and the effective Fermi level for electrons, E_{Fn}. These are therefore located at $\pm V/2 \cdot (-q)$, if we refer them to electrons with a charge of $-q$. The mid band gap Fermi level E_{Fi} is equivalent to the potential, i.e. $E_{Fi} = -q\Phi$. Putting this together, we get

$$p(x) = n_i \exp\left(\frac{-\Phi(x) - V/2}{U_T}\right) = n_i e^{-\frac{\Phi(x)}{U_T}} e^{-\frac{V}{2U_T}} \tag{21}$$

$$n(x) = n_i \exp\left(\frac{+\Phi(x) - V/2}{U_T}\right) = n_i e^{+\frac{\Phi(x)}{U_T}} e^{-\frac{V}{2U_T}}. \tag{22}$$

Using these more general expressions for the carrier densities, the charge density (7) becomes

$$\rho(x) = q\,[p(x) - n(x) + N(x)] = q\,N(x) - 2\,q\,n_i \cdot e^{-\frac{V}{2U_T}} \sinh\frac{\Phi(x)}{U_T}. \tag{23}$$

We see that the only consequence of an externally applied voltage V is a change of the constant C in (10).

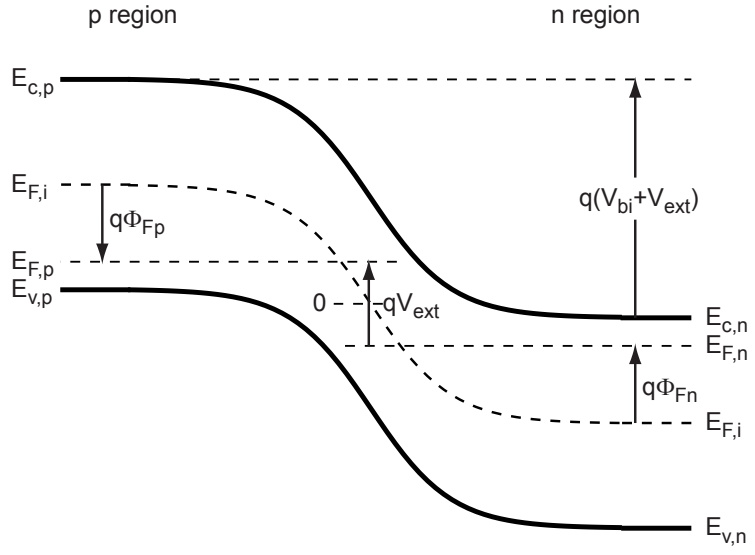

Figure 1: Band diagram of pn-structure with applied reverse bias.

6 Implementation

In order to avoid permanent unit conversion, you should stay with a consistent set of units. A suggestions is to use μm for x. The required numerical constants are then

$$\begin{aligned} q &= 1.60217646 \times 10^{-19} C \\ k &= 1.3806503 \times 10^{-23} J/K \\ \epsilon_0 &= 8.8541878176 \times 10^{-18} F/\,\mu\mathrm{m} \\ n_i &= 1.01 \times 10^{-2}\,\mu\mathrm{m}^{-3} \\ \epsilon_{Si} &= 11.9 \\ T &= 300K \end{aligned}$$

The algorithm is as follows:

1. Choose the number of discretization steps N, for instance $N = 400$.
2. Prepare an array $D[i]$ with the doping profile. n-doped regions are positive. Use the correct unit of, for instance, atoms per μm^3!
3. Initialize an array Φ with a start potential. A reasonable approach is to require charge neutrality everywhere by setting ρ to zero in (23), so that we get $\Phi(x) = U_T \operatorname{arcsinh}\left(\frac{N(x)}{2n_i} e^{\frac{V}{2U_T}}\right)$.
4. Calculate X and B according to (18) and (15). The external voltage comes in through C in (13).
5. Process X and simultaneously B twice to solve the matrix equation. This is a bit tricky. This code perform the required operation:

```
// Eliminate the elements below the diagonal
// Process the matrix elements. S[i] is the resulting factor
S[1] = X[1];
for (int j=2; j<=N; j++) S[j] = X[j] - a * a / S[j-1];
// Process the B-vector. U[] contains the intermediate result
U[1] = B[1];
for (int j=2; j<=N; j++) U[j] = B[j] - a * U[j-1] / S[j-1];
// Eliminate the elements above the diagonal. Start at the bottom!
// Y[] is the result of the second step
Y[N] = U[N];
for (int j=N-1; j>=1; j--) Y[j] = U[j] - a * U[j+1] / S[j+1];
// Calculate Lambda from Y[] and S[]
Lambda[0] = 0;
for (int j=1; j<=N; j++) Lambda[j] = Y[j] / S[j];
```

6. Calculate λ from X and B (see code above)
7. add this λ to Φ
8. Start over with step 4.

6.1 Numerical Issues

For large bias voltages V, the straight forward implementation of (23) leads to problems because two very large numbers (the exponential of V and the sinh of the potential) must be calculated and subtracted. This problem can easily be solved by writing down the definition of the sinh and pulling V into the exponent there.

7 Addendum: Why Fermi level must be constant

In *equilibrium*, the current in the device must vanish. This is why diffusion and field currents (shown here for holes) must be equal:

$$q\,D_p\frac{dp}{dx} = q\,p\,\mu_p\,E. \tag{24}$$

The hole density p and its derivative are given by

$$p = n_i \exp\frac{E_i - E_F}{kT} \rightarrow \frac{dp}{dx} = \frac{p}{kT}\left(\frac{dE_i}{dx} - \frac{dE_F}{dx}\right) \tag{25}$$

Using $D_p = \mu_p\,kT/q$ and $q\,E = -dE_i/dx$ (this is not so obvious!), (24) becomes

$$q\,\mu_p\frac{kT}{q}\frac{p}{kT}\left(\frac{dE_i}{dx} - \frac{dE_F}{dx}\right) = -p\,\mu_p\,\frac{dE_i}{dx} \rightarrow \frac{dE_F}{dx} = 0. \tag{26}$$

Therefore, the Fermi level is constant in x.

8 References

1. D. A. Neaman: *Semiconductor Physics and Devices: Basic Principles*, The McGraw-Hill COmpanies 1992, ISBN 0-256-20869-7. (p. 221: Band Diagram with reverse bias, p. 269: electron/hole densities with pseudo Fermi Level

2. F. R. Shapiro: *The numerical solution of Poisson's equation in a pn diode using a spreadsheet*, IEEE Trans. Educ., 38 (1995), 380-384.

3. S. M. Sze: *Semiconductor Devices Physics and Technology*, John Wiley, New York, 2002, 2nd edition.