PN Diode Exercise: Graded Junction

Dragica Vasileska and Gerhard Klimeck
(ASU, Purdue)

This example is a demonstration of the fact that explicit numerical integration methods are incapable of solving even the problem of linearly-graded junctions in thermal equilibrium, for which $N_D - N_A = mx$, where a is the edge of the depletion region. To demonstrate this, calculate the following:

(a) Establish the boundary conditions for the electrostatic potential [$\psi(-a)$ and $\psi(a)$] by taking into account the free carrier terms in the equilibrium 1D Poisson equation:

(b) Solve analytically the 1D Poisson equation for $\psi(x)$ within the depletion approximation (no free carriers) and calculate a using this result as well as the boundary conditions found in (a). What is the expression for the absolute value of the maximum electric field?

(c) Apply the explicit integration method for the numerical solution of the 1D Poisson equation (that includes the free carriers) by following the steps outlined below:

- Write a Taylor series expansion for $\psi(x)$ around x=0, keeping the terms up to the fifth order.
- Starting from the equilibrium Poisson equation, analytically calculate

$$\psi^{''}(0),\ \psi^{(3)}(0),\ \psi^{(4)}(0)\ \text{and}\ \psi^{(5)}(0)$$

- Use the maximum value of the electric field derived in (b) to determine from the Taylor series expansion for $\psi(x)$, the terms $\psi(h)$, $\psi(2h)$ and $\psi(3h)$.
- Compute $\psi(x)$ at x=4h,5h,6h, …, up to x_{max}=0.5um, using the predictor-corrector method in which the predictor formula:

$$\psi_{i+1} = 2\psi_{i-1} - \psi_{i-3} + 4h^2\left(\psi_{i-1}^{''} + \frac{\psi_i^{''} - 2\psi_{i-1}^{''} + \psi_{i-2}^{''}}{3}\right)$$

is applied to predict ψ_{i+1}, which is then corrected by the corrector formula:

$$\psi_{i+1} = 2\psi_i - \psi_{i-1} + h^2\left(\psi_i^{''} + \frac{\psi_{i+1}^{''} - 2\psi_i^{''} + \psi_{i-1}^{''}}{12}\right)$$

In both, the predictor and the corrector formulas, the second derivatives are obtained from the Poisson's equation. The role of the predictor is to provide ψ_{i+1}" that appears in the corrector formula.

- Repeat the above procedure for the following values of the first derivative:
  - Trial 1: $\psi'(0)_1 = \psi'(0)$,
  - Trial 2: $\psi'(0)_2 = \psi'(0)_1/2$
  - Trial 3: $\psi'(0)_3 = 0.5[\psi'(0)_1 + \psi'(0)_2]$.

Repeat the above-described process for several iteration numbers, say up to n=22. Comment on the behavior of this explicit integration scheme. Use the following parameters in the numerical integration:

$e=1.602\times10^{-19}$ C, $\varepsilon=12\varepsilon_0=1.064\times10^{-12}$ F/cm, T=300K,
$n_i=1.4\times10^{10}$ cm^{-3}, $m=10^{21}$ cm^{-4}, $h=2\times10^{-7}$ cm.