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Random doping induced fluctuations in p-n junction diodes

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Abstract: - Random doping induced fluctuations in p-n junction diodes are analyzed by using the linearization technique. The doping concentration is considered a random variable in the transport equations and all fluctuating quantities are linearized around their average values. Numerical results for a p-n junction diode with simplified structure are presented for the fluctuations of the terminal currents and small-signal parameters.

Key-Words: - linearization technique, sensitivity analysis, random doping induced fluctuations.

1 Introduction

Dopant concentrations in semiconductor devices [1] are subject to stochastic variations due to the random nature of ion implantation and diffusion processes. Random fluctuations of doping are especially pronounced in small devices where spatial scales of these fluctuations are more or less comparable with device dimensions. The random dopant fluctuations lead to appreciable fluctuations of device parameters. For this reason, an accurate analysis of random dopant-induced effects is very important for further progress in the area of semiconductor device technology.

There are two conceptually different approaches to the analysis of random doping induced fluctuations in semiconductor devices. The first approach [2], known as the Monte Carlo approach, is based on generating numerous realizations of the doping and solving the transport equations for each of such realization. Statistics of different parameters of interest are then accumulated and used to evaluate the average values and variances of those parameters. These methods are computationally very expensive since the same device-level simulations have to be performed many times. The second approach [3]-[5], known as the linearization technique is based on linearization of the transport equations with respect to the fluctuating quantities and allows the computation of the standard deviation of intrinsic parameters of semiconductor devices, such as terminal currents and frequency characteristics. The linearization technique is much more computationally efficient than the Monte Carlo method because it circumvents computations for many devices. In addition, the linearization technique provides information on the sensitivity of parameter variances to locations of the random doping fluctuations, which makes it instrumental in the design of fluctuation resistant structures. In this article we develop a linearization technique for the analysis of fluctuations of terminal currents and small-signal parameters in p-n junction diodes.

The article is structure as follows. The transport model used in the simulations is briefly presented in Section II. In Section III we present the linearization technique and we apply it to the analysis of fluctuations of terminal currents and small-signal parameters. Numerical simulations results are presented in Section IV, which is followed by Conclusions.

2 Transport model

The electron and hole concentrations in p-n junctions can be described by using the classical drift-diffusion model [6]:

$$\nabla\cdot\left(\varepsilon\nabla\varphi\right)+q\left(p-n+D\right)=0 \quad , \tag{1}$$

$$\frac{\partial n}{\partial t}=\nabla\cdot\left(-\mu_n n\nabla\varphi+D_n\nabla n\right)-R\left(n,p,\varphi\right) \quad , \tag{2}$$

$$\frac{\partial p}{\partial t}=\nabla\cdot\left(\mu_p p\nabla\varphi+D_p\nabla p\right)-R\left(\varphi,n,p\right) \quad , \tag{3}$$

where R is the electron-hole recombination rate, φ is the electric potential, and n, μ_n, D_n and p, μ_p, D_p are the concentration, mobility, and diffusivity of the electrons and holes, respectively. In our simulations the electron and hole mobilities are described by the well-calibrated model presented in [4] and [5].

3 Analysis of fluctuations by linearization

In general, any parameter A such as terminal currents or small-signal parameters can be written as a function of doping concentration $\boldsymbol{D}$ in the diode [7]:

$$A = A(\boldsymbol{D}). \tag{4}$$

In equation (4), we have considered that the doping concentration is a function of position. Hence, if the region of the semiconductor device is spatially discretized into N cells, the doping concentration must be specified as an N-dimensional column vector whose components are the mesh-point values of the doping concentration. The doping concentration vector is as a random quantity, which can be written as the sum of its average value $\boldsymbol{D}_0$ and fluctuation $\delta\boldsymbol{D}$:

$$\boldsymbol{D} = \boldsymbol{D}_0 + \delta\boldsymbol{D}, \tag{5}$$

where by definition, the expected value of $\delta\boldsymbol{D}$ is equal to zero. In the first-order approximation, the fluctuations of parameter A can be computed by linearization:

$$\delta A = \frac{\partial A}{\partial \boldsymbol{D}}\delta\boldsymbol{D} = \sum_i \gamma_A^i \delta D_i, \tag{6}$$

where γ_A^i are called the doping superposition coefficients. These coefficients show how sensitive parameter A is to the fluctuations of doping concentration at specific locations in the device. It is customary to assume that doping densities at different locations are independent random variables. This allows us to derive the following expression for the variance of parameter A:

$$\sigma_A^2 = \sum_i \left(\gamma_A^i\right)^2 \sigma_{D_i}^2 , \tag{7}$$

where $\sigma_{D_i}^2$ represents the variance of D_i. To determine $\sigma_{D_i}^2$, we consider that the total number N_i of dopant atoms in the i th discretization cell of volume ΔV_i is a random variable with Poisson distribution. Hence, we have $\sigma_{N_i}^2 = N_{0i} = D_{0i}\Delta V_i$, where, D_{0i} is the average doping concentration in volume ΔV_i. By using this fact, we derive:

$$\sigma_{D_i}^2 = \left(\frac{1}{\Delta V_i}\right)^2 \sigma_{N_i}^2 = \frac{D_{0i}}{\Delta V_i}. \tag{8}$$

By using equations (7) and (8), the variance of parameter A can be computed as follows:

$$\sigma_A^2 = \sum_i \left(\gamma_A^i\right)^2 \frac{D_{0i}}{\Delta V_i}. \tag{9}$$

Thus, the problem of computing the variance of parameter A is reduced to the computation of superposition coefficients.

It should be noted that the superposition coefficients are mesh dependent. Therefore, it is sometimes convenient to introduce the doping "sensitivity coefficients," S_A^i, which are defined as [3]:

$$S_A^i = \left(\frac{\gamma_A^i}{\Delta V_i}\right)^2 . \tag{10}$$

With notation (10), equation (9) reads as follows:

$$\sigma_A^2 = \sum_i \left(S_A^i\right)^2 D_{0i}\Delta V_i . \tag{11}$$

3.1 Superposition coefficients of the current

The analysis of current fluctuations is extremely important for both digital and analog applications. For the sake of brevity we will consider that $\frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} = 0$ (steady state) and write the transport equations (1)-(3) in discretized form [8]:

$$\boldsymbol{F}(\boldsymbol{X}, \boldsymbol{D}) = 0, \tag{12}$$

where $\boldsymbol{F}$ is a nonlinear vector function of the unknown "state" vector $\boldsymbol{X}$ and doping vector $\boldsymbol{D}$. The state vector consist of the mesh-point values of the electrostatic potential φ, electron and hole concentration $\boldsymbol{n}$, and $\boldsymbol{p}$, and: $\boldsymbol{X} = \left[\varphi \quad \boldsymbol{n} \quad \boldsymbol{p}\right]^t$, where t denoted the transpose of the given vector. Fluctuations of the doping concentration $\delta\boldsymbol{D}$ induce fluctuations in the state vector $\delta\boldsymbol{X}$ that can be computed by solving the following linear system:

$$\hat{\boldsymbol{F}}_{\boldsymbol{X}}\delta\boldsymbol{X} + \hat{\boldsymbol{F}}_{\boldsymbol{D}}\delta\boldsymbol{D} = 0, \tag{13}$$

where $\hat{\boldsymbol{F}}_{\boldsymbol{X}}$ and $\hat{\boldsymbol{F}}_{\boldsymbol{D}}$ are the derivatives of $\boldsymbol{F}$ with respect to $\boldsymbol{X}$ and $\boldsymbol{D}$, respectively. These derivatives are computed at the given dc bias point and by assuming constant (non-fluctuating) values of the doping concentration.

Now, let us denote the current through the diode by I. In order to compute the superposition coefficients of I it is convenient to write I as a explicit functions of state vector $\boldsymbol{X}$ and doping concentration $\boldsymbol{D}$:

$$I_{Diode} = I(\boldsymbol{X}, \boldsymbol{D}). \tag{14}$$

The fluctuations of terminal current can be found by linearizing (14) with respect to the fluctuating quantities:

$$\delta I = \left(I_{\boldsymbol{X}}\right)^t \delta\boldsymbol{X} + \left(I_{\boldsymbol{D}}\right)^t \delta\boldsymbol{D}, \tag{15}$$

where $I_{\boldsymbol{X}}$ and $I_{\boldsymbol{D}}$ are the derivatives of I with

respect to the state variable and doping concentration. By solving equations (13) and (15) for the fluctuations of the terminal current, one gets:

$$\delta I = -\left[\boldsymbol{g}^t \cdot \hat{\boldsymbol{F}}_{\boldsymbol{D}} - \left(I_{\boldsymbol{D}} \right)^t \right] \cdot \delta \boldsymbol{D}, \qquad (16)$$

where $\boldsymbol{g}^t$ is the transpose of column vector $\boldsymbol{g}$, which is the solution of the following linear system of equations:

$$\hat{\boldsymbol{F}}_{\boldsymbol{X}}^t \boldsymbol{g} = I_{\boldsymbol{X}}, \qquad (17)$$

where $\hat{\boldsymbol{F}}_{\boldsymbol{X}}^t$ denotes the transpose of matrix $\hat{\boldsymbol{F}}_{\boldsymbol{X}}$. By comparing (6) and (16), it can be inferred that the superposition coefficients of the terminal current are given by the following formula:

$$\gamma_{I_\alpha}^i = -\left(\boldsymbol{g}^t \cdot \hat{\boldsymbol{F}}_{\boldsymbol{D}} \right)_i + \left(I_{\boldsymbol{D}} \right)_i^t. \qquad (18)$$

The standard deviation of terminal currents can be calculated now by using: $\sigma_I^2 = \sum_i \left(\gamma_I^i \right)^2 \frac{D_{0i}}{\Delta V_i}$. The most expensive computational task related to the calculation of these coefficients is to solve linear system (17). For 2-dimensional simulations this system can be solved numerically by using the classical Gauss-Seidel method. However, for 3-dimensional simulations the computation time and memory requirements increase considerably if the Gauss-Seidel method is used, so other procedures are needed to solve (17). In our simulations, we took advantage of the diagonal dominance of matrix $\hat{\boldsymbol{F}}_{\boldsymbol{X}}$ and solved it efficiently by using the Successive Over-Relaxation (SOR) method.

3.2 Superposition coefficients of the small-signal parameters

In this section we introduce the technique for the calculation of variances of admittance matrix elements (i.e. variances of y-parameters). We suppose that one of the terminals of the diode is grounded, while a small-signal ac potential v is applied on the other terminal. The admittance is defined as:

$$y = \frac{i}{v}, \qquad (19)$$

where i small-signal phasor current through the terminals of the diode. The variance of parameter y can be computed in three steps:

1. First, we solve the transport equations and find the dc bias point.
2. Then, we solve the linearized transport equations and find the values of y-parameters.
3. Finally, we find the superposition coefficients and the variances of y-parameters.

Each of these steps is discussed below.

3.2.1 Finding dc bias point

The first step in the evaluation of the variance of y-parameter is to solve the transport equations and to find the dc bias point of the device. To this end, transport equations (1)-(3) can be written in discretized form as follows:

$$\frac{d}{dt} \boldsymbol{J}(\boldsymbol{X}) + \boldsymbol{F}(\boldsymbol{X}, \boldsymbol{D}, V) = 0, \qquad (20)$$

where V is the voltage across the diode and $\boldsymbol{J}$ is a vector function which depends on $\boldsymbol{X}$ only. In equation (20), we have separated the explicit time-dependent part of the transport equations (which comes from the terms $\partial n/\partial t$ and $\partial p/\partial t$ in the current continuity equations) from the time-independent part $\boldsymbol{F}$. At dc bias conditions, equation (20) is reduced to:

$$\boldsymbol{F}(\boldsymbol{X_0}, \boldsymbol{D_0}, V_0) = 0. \qquad (21)$$

Given some doping distribution $\boldsymbol{D_0}$ and bias voltage V_0, equation (21) can be solved for state vector $\boldsymbol{X_0}$.

3.2.2 Finding the value of the admittance

The second step is to find the values of the admittance. It is customary to assume that a sinusoidal voltage of infinitesimal amplitude v is superimposes over the dc value V_0:

$$V = V_0 + v e^{j\omega t}. \qquad (22)$$

This will induce ac perturbations in the state variable:

$$\boldsymbol{X} = \boldsymbol{X}_0 + \boldsymbol{x} e^{j\omega t}, \qquad (23)$$

The governing equations for the ac component of the state variable $\boldsymbol{x}$ can be found by linearizing equation (20) around the dc bias values $\boldsymbol{X}_0$ and V_0:

$$\left(j\omega \hat{\boldsymbol{J}}_{\boldsymbol{X}} + \hat{\boldsymbol{F}}_{\boldsymbol{X}} \right) \boldsymbol{x} + \boldsymbol{F}_V v = 0, \qquad (24)$$

In this equation, $\hat{\boldsymbol{J}}_{\boldsymbol{X}}$ and $\hat{\boldsymbol{F}}_{\boldsymbol{X}}$ are the Jacobian matrices of $\boldsymbol{J}$ and $\boldsymbol{F}$ computed with respect to variable $\boldsymbol{X}$ (and evaluated at the dc bias point), while $\boldsymbol{F}_V = \frac{\partial \boldsymbol{F}}{\partial V}$. In general, $\hat{\boldsymbol{J}}_{\boldsymbol{X}}$ and $\hat{\boldsymbol{F}}_{\boldsymbol{X}}$ are $3N \times 3N$ sparse matrices, where N is the total number of mesh points.

The current through the diode can be written as a function $I(\boldsymbol{X})$. In the first-order approximation, the ac component of the current is:

$$i = I_{\boldsymbol{X}} \cdot \boldsymbol{x}, \qquad (25)$$

The admittance can now be computed by using:

$$y = \frac{I_X \cdot \boldsymbol{x}}{v}. \tag{26}$$

3.2.3 Finding the variance of admittance

The random doping fluctuations $\boldsymbol{D}$ induce fluctuations $\boldsymbol{X}_0$ and $\boldsymbol{x}$ in the dc and ac components of the state variables, respectively. By using the linearization technique, one can show that:

$$\begin{cases} \hat{\boldsymbol{F}}_X \boldsymbol{X}_0 = -\hat{\boldsymbol{F}}_D \boldsymbol{D}, \\ \hat{\boldsymbol{A}}\boldsymbol{x} + \hat{\boldsymbol{B}}\boldsymbol{X}_0 = 0, \end{cases} \tag{27}$$

where the following matrix notations have been adopted:

$$\hat{\boldsymbol{A}} = j\omega\hat{\boldsymbol{J}}_X + \hat{\boldsymbol{F}}_X, \tag{28}$$

$$\hat{\boldsymbol{B}} = \sum_{i=1}^{3N}\left(j\omega\hat{\boldsymbol{J}}_{X,X_i} + \hat{\boldsymbol{F}}_{X,X_i} \right) x_i . \tag{29}$$

Here: $\hat{\boldsymbol{J}}_{X,X_i} = \dfrac{\partial \hat{\boldsymbol{J}}_X}{\partial X_i}$, $\hat{\boldsymbol{F}}_{X,X_i} = \dfrac{\partial \hat{\boldsymbol{F}}_X}{\partial X_i}$, while X_i and x_i denote the ith component of vectors $\boldsymbol{X}$ and $\boldsymbol{x}$, respectively. Both matrices $\hat{\boldsymbol{A}}$ and $\hat{\boldsymbol{B}}$ are computed at the dc bias point $\left(\boldsymbol{X_0}, \boldsymbol{D_0}, V_0\right)$.

Once system (27) is solved for $\boldsymbol{x}$, we can find the fluctuations of admittance by using the formula:

$$y = \frac{I_X \cdot \boldsymbol{x} + I_{XX}\boldsymbol{X}_0 \cdot \boldsymbol{x}}{v}, \tag{30}$$

where I_{XX} is the Hessian matrix of the current through the diode. The last equation is linear with respect to $\boldsymbol{X}_0$ and $\boldsymbol{x}$ while, according to equations (27), $\boldsymbol{X}_0$ and $\boldsymbol{x}$ are linear with respect to $\boldsymbol{D}$. This means that y can also be evaluated as a linear combination of the fluctuations of doping at different mesh-points:

$$y = \sum_{i=1}^{N} \gamma_y^i D_i, \tag{31}$$

where γ_y^i are the superposition coefficients of y. By rearranging the terms in equations (27)-(29) it can be shown that the superposition coefficients can be compute by using the following equation:

$$\gamma_y^i = \boldsymbol{f} \cdot \left(\hat{\boldsymbol{F}}_D \boldsymbol{\delta}^{(i)} \right), \tag{32}$$

where, by definition, $\boldsymbol{\delta}^{(i)}$ is a vector whose ith component is one while all other components are equal to zero and $\boldsymbol{f}$ is the solution of the following system of linear equations:

$$\begin{cases} \hat{\boldsymbol{A}}^t \boldsymbol{g} = I_X, \\ \hat{\boldsymbol{F}}_X^t \boldsymbol{f} = \hat{\boldsymbol{B}}^t \boldsymbol{g} - I_{XX}\boldsymbol{x}. \end{cases} \tag{33}$$

The first equation in (33) must be solved for $\boldsymbol{g}$ and the second equation for $\boldsymbol{f}$. Then, the values of the superposition coefficients can be computed by using formula (32).

The algorithm for the calculation of admittance matrix variances can be summarized as follows:

(1) First, the nonlinear equations (21) are solved to find the dc bias conditions throughout the device.
(2) Second, equations (24) are solved and formula (26) is used to find the values of the admittance.
(3) Then, matrices $\hat{\boldsymbol{A}}$ and $\hat{\boldsymbol{B}}$ are constructed by using formulas (28) and (29), respectively, and equations (33) are solved for $\boldsymbol{g}$ and $\boldsymbol{f}$.
(4) Then, formula (32) is used to find the values of the superposition coefficients.
(5) Finally, the variances of the admittance elements are found from equation (9).

It is worth noting that the most computationally expensive steps in the algorithm are (1) and (2), which take about 90% of the total computation time. Steps (3), (4), and (5) take about 10% of the total computation time.

4 Numerical results

The techniques presented in the previous section was numerically implemented and used to compute the fluctuations of terminal currents and admittance in p-n junction diodes induced by random doping fluctuations. We have considered a p-n silicon diode with simplified architecture. Unless otherwise mentioned the doping concentration is assumed constant and equal to $N_a = 10^{17}$ cm^{-3} and $N_d = 10^{16}$ cm^{-3} in the two sides of the junction, respectively. The diode extends for about 1 μm in the x-direction and the cross-sectional area of the diode is 1 μm^2. As a consequence, the results presented in this section should be scaled accordingly for other dimensions than those indicated above.

In Figure 1 we present the current through the diode by using continuous line and the standard deviation of the current by using vertical bars. The values of the standard deviations are multiplied by a factor of 10 in order to make the error bars visible on the figure. In the inset of Figure 1 we have represented the standard deviation of the current divided by the current through the diode. One can observe that between 1-2% of the total current represent fluctuations.

In Figures 2 and 3 we represent the standard

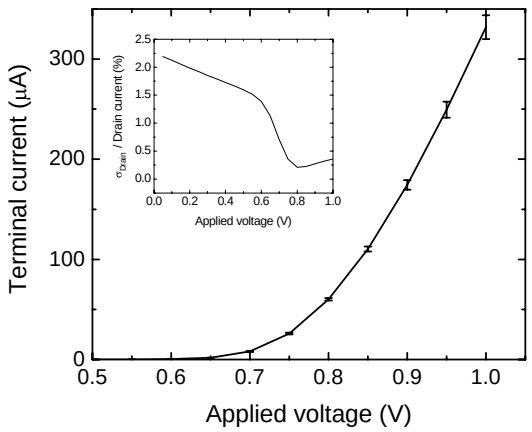

Fig. 1. Terminal current (continuous line) and standard deviation of the current (vertical bars) through the diode.

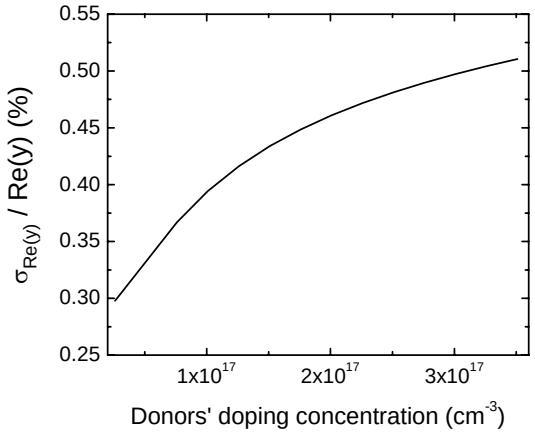

Fig. 2. Standard deviation of the real part of y-parameter divided by the real part of y-parameter.

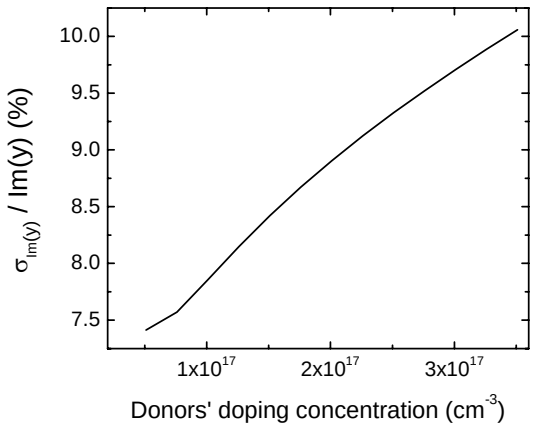

Fig. 3. Standard deviation of the imaginary part of y-parameter divided by the imaginary part of y-parameter.

deviations of the real and imaginary parts of the y-parameter divided by the value of that parameter. In both figures the doping concentration of the acceptor atoms is kept constant $N_a = 10^{16}$ cm^{-3}, while the doping concentration of the donor atoms is varied. It is important to note that the fluctuations of y-parameter increase with the doping concentration of the junction. Similar observations have been drawn for the standard deviations of threshold voltages and terminal currents in MOSFET devices [7].

5 Conclusion

Random doping induced fluctuations are becoming increasingly important in ultra small semiconductor devices, where the spatial scales of these fluctuations are comparable with the device dimensions. Significant deviations from the average values have been found for both the terminal current and the y-parameter. For a $1\mu m^2$ diode with doping concentration of the order of 10^{16} the fluctuations represent between 1% and 10% of the average values of these parameters. However, the fluctuations increase considerable for smaller device dimensions.

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