Inverse modeling for C-V profiling of modulated-doped semiconductor structures

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ABSTRACT

Inverse modeling is a way for the verification of device models and for the parameter extraction. A technique of doping profile extraction of semiconductor structures based on the capacitance-voltage measurements (or C-V profiling) is used extensively. This technique up till now has been applied in two variants: the well-known classical C-V profiling to the sufficiently smooth doping profiles and the inverse modeling technique based on the error minimization to the abrupt profiles.

The present paper describes a new method of the inverse modeling with sub-Debye resolution for arbitrary doping profiles. The calculations can be performed using a Pentium-like personal computer. For the input data obtained by forward modeling, the integral error of doping profile extraction is below 0.1 %. As an example, the doping profile determination of the GaAs modulated-doped structure is presented. The possibilities of the proposed method are discussed.

Keywords: Inverse modeling, C-V profiling, modulated-doped semiconductor structures.

1 INTRODUCTION

The capacitance-voltage (C-V) profiling is a attractive, non-destructive way of determining the doping profiles in semiconductor devices [1]. The following analytical expressions describe the classical C-V profiling:

$$N_{ap}(W) = -\frac{C(V)^3}{e\varepsilon\, dC/dV} \quad \text{and} \quad W(V) = \frac{\varepsilon}{C(V)}, \qquad (1)$$

where N_{ap} is the apparent profile, W is the depth of the depletion layer, C is the capacitance per unit area, V is the reverse bias applied to a Schottky barrier placed in space coordinate point z=0, e is the electron charge, and ε is the semiconductor permittivity.

It is known that classical C-V profiling is suitable only for the smooth doping profiles. The spatial resolution of this technique is limited by the Debye averaging [2] and, consequently, is determined by the Debye screening length λ_D:

$$\lambda_D = \left(\frac{\varepsilon kT}{e^2 N_d}\right)^{1/2}, \qquad (2)$$

where k is the Boltzmann constant, T is the absolute temperature, and N_d is the doping level.

At the same time, the typical doping profiles of modern modulated-doped structures considerable change on the distances below the Debye length. To raise the spatial resolution of C-V profiling the concept of inverse modeling has been proposed [3]. The distinctive feature of this technique consists in a combination of forward numerical modeling (solution of the nonlinear Boltzmann-Poisson equation) with the optimization driver. A choice of the approximation for the doping profile was made in advance. All computations were performed on a vector computer. So, the formal character and the considerable calculation time degrade the value of this approach.

Recently we have reported about the new efficient doping profile extraction method with the sub-Debye length resolution based on the concept of inverse modeling [4]. It includes the explicit relation between the apparent profile and the initial doping profile and does not require the preliminary choice of the profile approximation. Now we describe the inverse modeling scheme and the results of the test. As an example, a doping profile of the modulated-doped GaAs structure is used.

2 INVERSE MODELING METHOD

The algorithm of the proposed inverse modeling method is shown in Fig.1. The apparent profile $N_{ap}(W_0)$ is used as input data. The initial depth of the depletion layer W_0 and $N_{ap}(W_0)$ are obtained from measured capacitance-voltage characteristics. To test the inverse modeling method the initial apparent profile $N_{ap}(W_0)$ must be simulated from a given donor profile $N_d(z)$ using the forward modeling.

The next step is in the forward modeling. Its includes two parts. The first one is the solution of the static

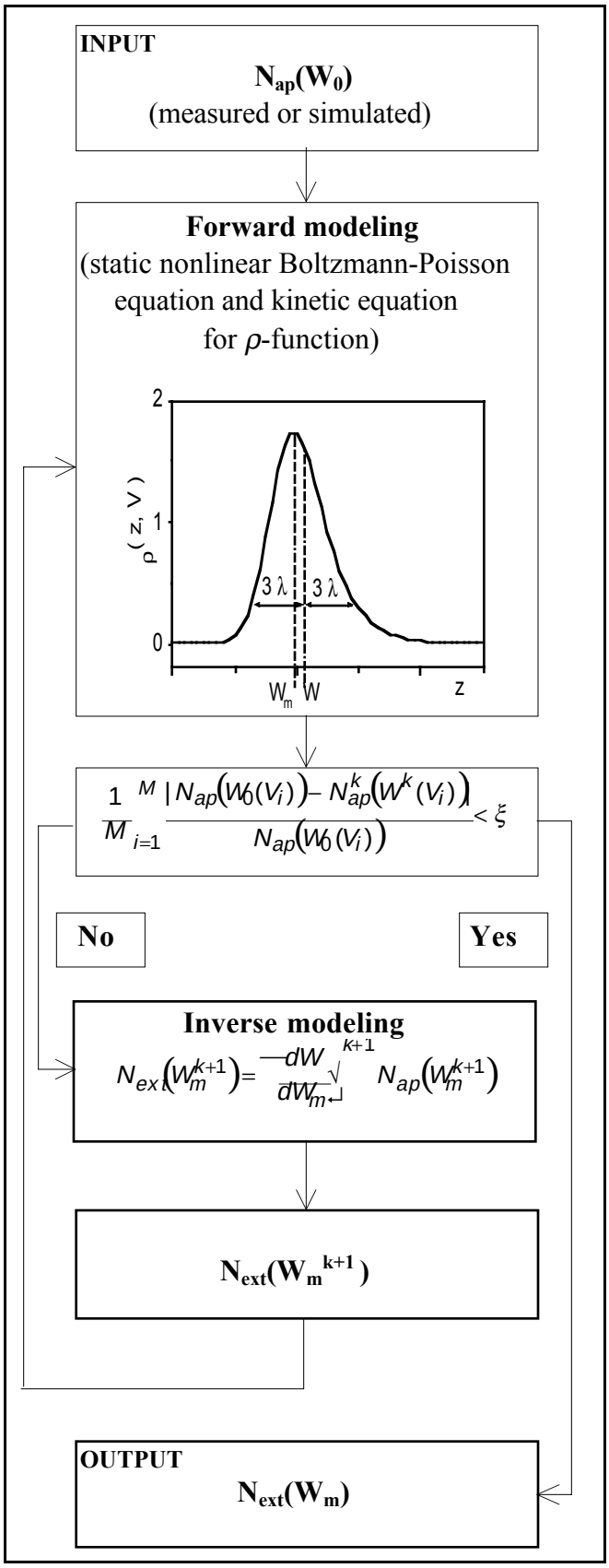

Fig.1. Inverse modeling scheme.

nonlinear Boltzmann-Poisson equation. As a result, the spatial distribution of the electron concentration $n(z,V)$ for a given donor profile and reverse bias V is obtained. The second one consists in the determination of the capacitance and the apparent profile. The capacitance is calculated as:

$$C(V)=\frac{\varepsilon}{W(V)}=\varepsilon<z>^{-1}=\varepsilon\left(\int_0^L z\rho(z,V)dz\right)^{-1}, \qquad (3)$$

where $\rho(z,V)$ is the distribution function for the perturbed space charge density (or ρ-function) and $<z>$ is the first moment [4,5]. This function obeys the condition:

$$\int_0^L \rho(z,V)dz=1 \qquad (4)$$

and describes the localization of the space charge density modulated due to the small-signal perturbation. As is seen from equation (3), W is the mean position of the modulated charge. The second central moment gives the standard deviation λ:

$$\lambda^2=\int_0^L (z-W)^2\rho(z,V)dz. \qquad (5)$$

The parameter λ defines the spatial scale of the modulated charge. For a uniform doping profile, we have:

$$\lambda=\sqrt{2}\lambda_D. \qquad (6)$$

The shape of the ρ-function (see Fig.1) is non-equilibrium (i.e. non-Gaussian) and depends on the donor profile. Note, that in the general case, W does not coincide with the position of the mode W_m (i.e. maximum). The ρ-function is calculated using a linear kinetic equation [5]. The relative error in the calculations of the capacitance is equal to $5*10^{-6}$. The capacitance derivative dC/dV is determined in a similar way as the capacitance from the ρ_v-function and the corresponding linear differential equation [5]:

$$\frac{dC(V)}{dV}=-\frac{C^2(V)}{\varepsilon}\frac{dW(V)}{dV}=-\frac{C^2(V)}{\varepsilon}\int_0^L z\rho_V(z,V)dz. \qquad (7)$$

The integral approach yields a high accuracy of the calculations. The relative error of the capacitance derivative in our simulation method is below $1*10^{-5}$. So, the relative error for the apparent profile is also less than $1*10^{-5}$. Such accuracy of the forward modeling is the necessary condition of the sub-Debye resolved doping profile extraction.

After the forward modeling (as it is shown in Fig.1) the new approximations of W and $N_{ap}(W)$ are obtained. This new approximation of apparent profile is compared with the initial apparent profile. When the difference becomes less

than a given value of error ξ, the extraction procedure is ended. Otherwise, the transition to the inverse modeling follows.

The essential peculiarity of our inverse modeling method can be expressed by the relation:

$$N_{ext}(W_d) = \frac{dW}{dW_d} N_{ap}(W_d) , \qquad (8)$$

where N_{ext} is the extracted doping profile, W_d is the depth of the depletion layer. Equation (8) defines the transformation from the coordinate W to the coordinate W_d.

So, contrary to the classical C-V profiling we assume that W is not the depth of the depletion layer. The computer simulation demonstrates that the thermal motion of free carriers shifts the point W with respect to the true edge of the depletion layer W_d. The coordinate W (the mean position of the modulated charge) can be called as *apparent* whereas coordinate W_d can be considered as *true*.

The above-mentioned kinetic approach to capacitance calculation gives the possibility to determine the true coordinate W_d as the mode W_m of the ρ-function. As already noted, the distance between W and W_m is very sensitive to the variations of the doping profile. In the uniformly doped regions (when W_m is situated from a interface at the distance more 3λ) the difference W - W_m is constant. The derivative in equation (8) is equal to unity and the extracted profile faithfully reproduces the apparent profile. The effect of the change of W - W_m is the most pronounced when W_m coincides with the interfaces between doped layers. In this case the transformation coefficient in equation (8) differs from unity and initiates the change of the extracted profile.

By this means, equation (8) gives the explicit relation between apparent and extracted profiles. It eliminates the necessity to use the preliminary profile approximation and the minimization as in Ref.[3]. Hence, the inverse modeling procedure becomes more physically meaningful and universal.

3 RESULTS AND DISCUTION

To study the possibilities of the proposed method, the GaAs modulated-doped structure has been chosen. The doping profile is typical for the molecular beam epitaxy grown FET structures. The input data (the initial apparent profile) were obtained by forward modeling for given doping profile at T=300K in 35 points (from V=0.3V to V=8.8V). Such approach permits us to compare the output data of the inverse modeling with the input data of the forward modeling.

The process of the profile extraction is presented in Fig.2. The initial doping profile is marked by spheres with

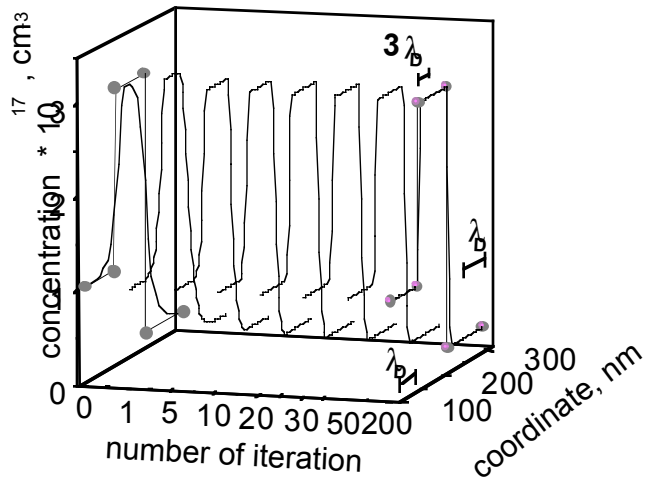

Fig.2. Process of the profile extraction.

the Debye lengths given for every layer. The thicknesses of the interface layers Δ are equal to the grid step h and are less than the Debye length of the central layer (h=2.67 nm, λ_D=7.9 nm). The CPU time on a Pentium-233 computer for 100 iterations is equal to 5 min. The quality of the profile extraction can be illustrated in Fig.3. The zero iteration corresponds to the classical C-V profiling. As it is seen, the error is concentrated in the interface

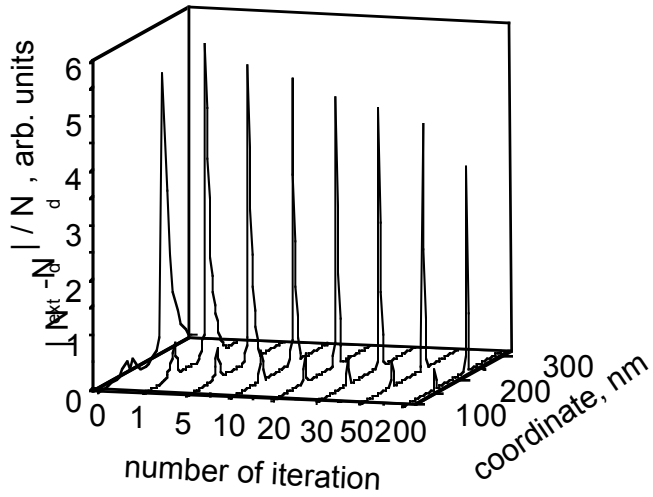

Fig.3. Spatial distributions of the error.

regions. After 10 iterations, the error within the most part of the central layer becomes less than 10^{-4}. The spatial resolution of the interfaces comes close to the Debye length of the central layer. The next iterations narrow the error domain to the sub-Debye scale. To characterize more clear the quality of the interface reconstruction, the distributions of extracted profile derivative are presented in Fig.4. For the zero and last iterations the derivatives of

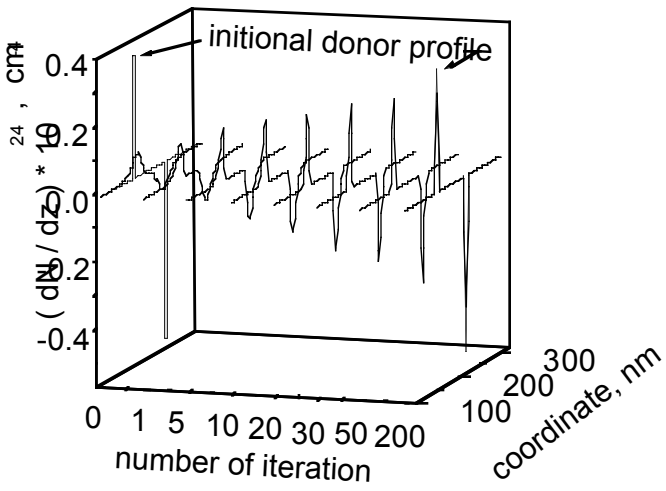

Fig.4. Distributions of the extracted profile derivative.

the initial donor profile are shown. After 200 iterations, the derivative values in the extrema comprise 80% of the initial donor profile derivatives. For the first interface the left point has the zero shift and the right point is displaced by two grid steps. For the second interface the shifts are equal to h and to $2h$, respectively. The decrease of the grid step brings into better coincidence. So, the indeterminacy of the interface position is less than the Debye length of

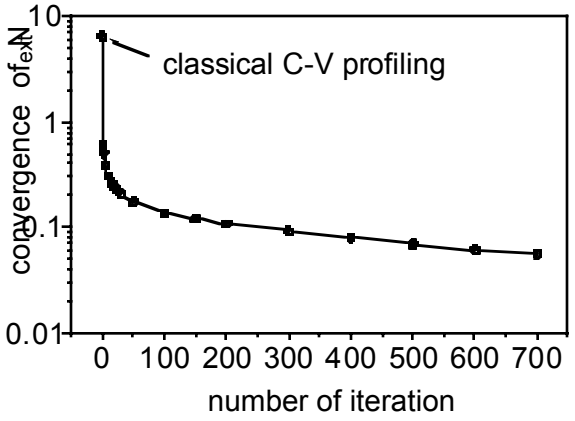

Fig.5. Convergence of the inverse modeling.

the heavily-doped layer. As it is seen in Fig.3 and Fig.4, this indeterminacy depends not only on the doping level of the heavily-doped layer [3] but on the doping levels of the neighboring layers.

Next, Fig.5 characterizes the convergence of the inverse modeling estimated as the integral error. The slowing-down of the convergence is associated with the transfer to the sub-Debye scales. It is evident, that to attain this accuracy for the output data the accuracy for the initial and simulated apparent profiles must be at the same level.

4 CONCLUSION

We have described the new universal inverse modeling method for C-V profiling with sub-Debye-length resolution. The essential feature of this method consists in using of the explicit relation between the extracted doping profile and initial apparent profile. The high accuracy of the forward modeling permits to attain the good quality of doping profile reconstruction. The integral error depends of the quantity of iterations and can be below 0.1%.

The application of this method to the modulated-doped structure demonstrates that the error is concentrated in the interface regions. The error within the most part of the layers is less than 10^{-4}. The spatial resolution is determined by the relation between the doping levels of the neighboring layers and the value of the grid step.

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