

Towards "atomistic" dopant profiling using SCM measurements

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Abstract—In this article we develop a mathematical algorithm for computing the spatial locations of ionized impurities in semiconductor materials using scanning capacitance microscopy (SCM) measurements. We show that SCM measurements can in principle be used to determine the coordinates of the doping atoms in a layer of a thickness equal to the width of the depletion region if the noise in the SCM measurements is extremely low. The proposed mathematical algorithm is based on computing the doping sensitivity functions (i.e. the Gâteaux derivatives) of the differential capacitance and using a gradient-based iterative method to find the locations of the ionized impurities.

Keywords—SCM, dopant profiling, inverse methods

I. INTRODUCTION

Scanning capacitance microscopy (SCM) is often used in the semiconductor industry for dopant profiling. The conventional procedure to extract the doping concentration is to bias the semiconductor in depletion mode and measure the differential capacitance of the biasing electrode (probe) as a function of the applied voltage [1]. The differential capacitance can then be used to determine the average dopant concentration at the edge of the depletion region.

In this article we investigate the possibility to use SCM for 3-D profiling of discrete ionized impurities in semiconductor materials [2]. We show that it is in principle possible to use multiple sets of experimental C-V curves and compute the spatial coordinates (x_i, y_i, z_i) of the ionized impurities in the depletion region, where $i = 1, \dots, N$, and N is the number of ionized impurities in the depletion region. The larger the amount of experimental data the higher is the accuracy of the numerical predictions. As far as we know this is the first attempt to use SCM to compute the exact locations of the dopant atoms in semiconductor materials. All the previous attempts were limited to finding the average carrier distribution and dopant concentration inside the material, without being able to retrieve the individual locations of the impurities.

To compute the locations of the impurities we need to solve the inverse problem, in which we compute the doping concentration, $D(\mathbf{r})$, from the experimental C-V curves. This problem is particularly difficult to solve using heuristic optimization techniques because these techniques require a large number of trial-and-error simulations. For instance, let us consider the simplified case of a semiconductor material

discretized in 10^4 nodes (for example using a finite element or finite difference mesh). The total number of combinations in which N dopant atoms can be arranged in this mesh is of the order of 10^{4N} , which require a prohibitively large number of simulations even for a small number of impurities, N . For a similar reason, traditional evolutionary algorithms such as genetic algorithm are also unpractical for atomistic dopant profile. The only choice is to develop a non-heuristic algorithm, which requires a small number of device simulations. The algorithm presented in this article is based on the estimation of doping sensitivity functions and uses a gradient-based iterative method to find the locations of the dopants.

The experimental setup is relatively similar to standard scanning microscopy and is presented in Fig. 1. The probe is moving above the surface of the semiconductor and is not in direct contact with the semiconductor. The space between the probe and semiconductor can be filled with the native oxide of the semiconductor. If the measurements are made in high vacuum one can also create a small gap between the probe and the semiconductor, which separates the two materials. The small-signal capacitance is measured as a function of the bias voltage between the probe and the substrate and is used to compute to doping concentration.

II. COMPUTATION OF THE DOPING SENSITIVITY FUNCTIONS OF THE DIFFERENTIAL CAPACITANCE

The doping sensitivity function of a parameter is defined as the Gâteaux differential of that parameter in the directions of possible doping variations. If C is the differential capacitance of the probe and we consider an infinitesimally small doping variation $\delta D(\mathbf{r})$, the variation of the differential capacitance can be expressed as a function of the doping sensitivity function, $\gamma(\mathbf{r})$, by means of the Riesz representation theorem

$$\delta C = \int_{\Omega} \gamma(\mathbf{r}) \delta D(\mathbf{r}) d\mathbf{r} \quad (1)$$

where Ω denotes the region of the semiconductor material. Since $\gamma(\mathbf{r})$ measures the sensitivity of device parameters (in our case the sensitivity of the differential capacitance) to doping variations, this function is instrumental in the study of random doping fluctuations and for device optimization. Next,

we summarize the technique for the computation of $\gamma(\mathbf{r})$. For more details about the derivation of the final equations and numerical implementation we recommend reading [3].

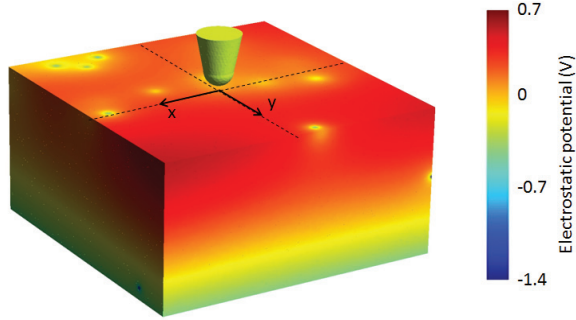


Fig. 1. Electrostatic potential in an “atomistically” generated semiconductor. The probe is scanning the surface of the semiconductor in the x and y directions.

Let us denote the discretized transport equations in the semiconductor in vector form as

$$\frac{dI^k}{dt}(x^1, \dots, x^n, D^1, \dots, D^m) + F^k(x^1, \dots, x^n, D^1, \dots, D^m, V) = 0 \quad (2)$$

where x^i and D^i denote the state variables and the doping concentration at the mesh point i , and V is the bias voltage. Superscript k denotes the index of each equation. Functions I^k come from the discretization of electron and hole concentration free terms in the continuity equations, while F^k come from the discretization of the source and divergence terms in these equations. The discretized doping sensitivity function of the differential capacitance can be computed as

$$\begin{aligned} \gamma_j = & C_i \frac{\partial x^i}{\partial G^j} \left(-\frac{\partial^2 G^l}{\partial x^m \partial x^n} \frac{\partial x^n}{\partial F^k} \frac{\partial F^k}{\partial D^j} + \frac{\partial^2 G^l}{\partial x^m \partial D^j} \right) \frac{\partial x^m}{\partial G^k} \frac{\partial F^k}{\partial V} \\ & - C_i \frac{\partial x^i}{\partial G^k} \left(-\frac{\partial^2 F^k}{\partial V \partial x^l} \frac{\partial x^l}{\partial F^l} \frac{\partial F^l}{\partial D^j} + \frac{\partial^2 F^k}{\partial V \partial D^j} \right) \end{aligned} \quad (3)$$

where $G^k = j\omega I^k + F^k$ and C_i are coefficients that can be obtained by writing the differential capacitance in differential form as $C = C_i \delta x^i / \delta V$. In the previous equation we have used the Einstein summation convention. Notice that in order to compute the doping sensitivity function of the differential capacitance one needs to evaluate the second order derivatives of the transport equations. A simplified version of eq. (3) can be found in [4, 5].

III. INVERSION ALGORITHM

In this section we summarize the inversion algorithm for computing the doping distribution from the experimental values of the differential capacitance. For this purpose let us denote the experimental values of C by $C_i^{(\text{exp})}$, where subscript

i is used to index each data point. Values $C_i^{(\text{exp})}$ can belong to the same C-V curve or to C-V curves measured with the probe situated at different locations above the surface of the semiconductor. In general, we need to have a large number of data points measured at different positions above the area where we need to estimate the doping locations. Due to symmetry considerations, in the case of 2-D simulations, one needs to measure the C-V curve in at least two different locations above the semiconductor; in the case of 3-D simulations, one needs to measure the C-V curves in at least three different locations in order to extract the 3 spatial coordinates.

To compute the doping concentration, we start with an initial doping profile $D^{(0)}(\mathbf{r})$ and update it iteratively using the following equation

$$D^{(k)}(\mathbf{r}) = D^{(k-1)}(\mathbf{r}) + \varepsilon \Delta D^{(k)}(\mathbf{r}) \quad (4)$$

where k denotes the iteration number and ε is a relaxation parameter. The optimal change in the doping concentration, $\Delta D^{(k)}(\mathbf{r})$, can be estimated from eq. (1), which implies

$$C_i^{(\text{exp})} - C_i^{(k)} \approx \int_{\Omega} \gamma_i(\mathbf{r}) \Delta D^{(k)}(\mathbf{r}) d\mathbf{r} \quad (5)$$

where $C_i^{(k)}$ is the computed value of the differential capacitance and $\gamma_i(\mathbf{r})$ is the doping sensitivity function computed under the same bias point and probe position as the experimentally measured value of $C_i^{(\text{exp})}$.

As discussed in [2], one could in principle solve integral equation (5) for $\Delta D^{(k)}$ and, then, replace it in eq. (4) to update the doping concentration. However, in order to improve the convergence rate of the algorithm as well as the robustness of the algorithm under experimental noise, it is better to expand $\Delta D^{(k)}(\mathbf{r})$ as a linear superposition of a given set of basis functions $\Gamma_i(\mathbf{r})$ and look for solutions of (5) in the form

$$\Delta D^{(k)}(\mathbf{r}) = \sum_{i=1}^M \alpha_i^{(k)} \Gamma_i(\mathbf{r}) \quad (6)$$

where M is the number of basis functions and α_i are the superposition coefficients. These coefficients can be computed by solving the following system of equations using linear least squares technique

$$\sum_{i=1}^M \alpha_i \gamma_{i,j} = \Delta C_j^{(k)} \quad (7)$$

where $\gamma_{i,j} = \int_{\Omega} \Gamma_i(\mathbf{r}) \gamma_j(\mathbf{r}) d\mathbf{r}$. In the case of “atomistic” doping profiling it is convenient to choose $\Gamma_i(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_i)$, where δ is the Dirac-delta function. In this case $\gamma_{i,j} = \gamma_j(\mathbf{r}_i)$ and coefficients α_i can be computed by solving $\sum_{i=1}^M \alpha_i \gamma_j(\mathbf{r}_i) = \Delta C_j^{(k)}$.

IV. NUMERICAL EXAMPLES

To test the inversion algorithm presented in the previous section we have implemented the algorithm numerically in RandFlux, which is a device simulator specifically designed for finite element optimizations using adjoint space techniques. In order to avoid numerical problems related to the dynamic mesh generation when the probe is moving on the surface of the semiconductor, we consider a set of three metallic probes situated at approximately 17.5 nm from each other and 1 nm above the semiconductor surface. The movement of the SCM tip is modeled by applying different potentials on the probes. To compute the complex impedance, Z , we superimpose a small-signal a.c. voltage, v , on the d.c. bias and compute the a.c. current, i , using perturbation theory. The differential capacitance is computed as $C = \text{Im}(Z)/\omega$. The way in which the differential capacitance is defined does not change the numerical algorithm as long as both the "experimental" procedure and the computer simulations use the same method.

The semiconductor material was modeled by placing p-type impurities at random locations inside the simulation domain. Once the material was generated, the "experimental" C-V curves were determined by applying a d.c. bias on each probe and keeping the other probes at zero potential. The three "experimental" C-V curves generated in this way are represented by continuous lines in Figs. 2(a)-(c), respectively. The initial placement of the impurities is shown in Fig. 3(i). The iterations were started by starting with an undoped semiconductor, see Fig. 3(a). The doping sensitivity functions for each probe is represented in Figs. 3(b)-(d) at a bias of -1 V. Due to the symmetry of the system, the doping sensitivity functions are symmetrical for Probe 1 and Probe 3. The most sensitive regions to doping variations are the regions under the probes. For this reason, the SCM technique presented in this work is able to find the ionized impurities only in the proximity of the metallic probes (i.e. in the depletion region).

The values of the differential capacitance used in solving the inversion problem, $C_i^{(\text{exp})}$, are denoted by symbols on the continuous lines presented in Fig. 2. Only 24 such points have been used in the inversion. Using more "experimental" points from the same C-V curve makes the equations in system (7) to become almost linearly dependent and increases the numerical instability of the algorithm. In practice, one should collect data from a larger number of "experimental" C-V curves and use it when solving the inversion problem. To update the doping concentration we consider a set of 15 Dirac-delta functions distributed approximately uniformly throughout the semiconductor (notice that the number of base functions should be smaller or equal to the number of "experimental" points, so system (7) has unique solution).

The C-V curves computed for the undoped semiconductor are represented with dash line "Initial guess" in Figs. 2(a)-(c) for each probe, respectively. The computed differential capacitance at different iterations is represented in Figs. 2(a)-(c) with dash lines. After 39 iterations the algorithm converged to the "experimental" values of the capacitance. The total number of iterations depends on the initial guess, the relaxation parameter (ϵ), and the number and distribution of impurities

in the semiconductor. Figs. 3(f)-(h) present the doping sensitivity functions after iteration 13, while Figs. 3(j)-(l) present the sensitivity functions after iteration 39, when convergence was obtained. In both cases, since the doping configuration is not symmetric with respect to the vertical axis, the doping sensitivity functions for Probes 1 and 3 are also asymmetric.

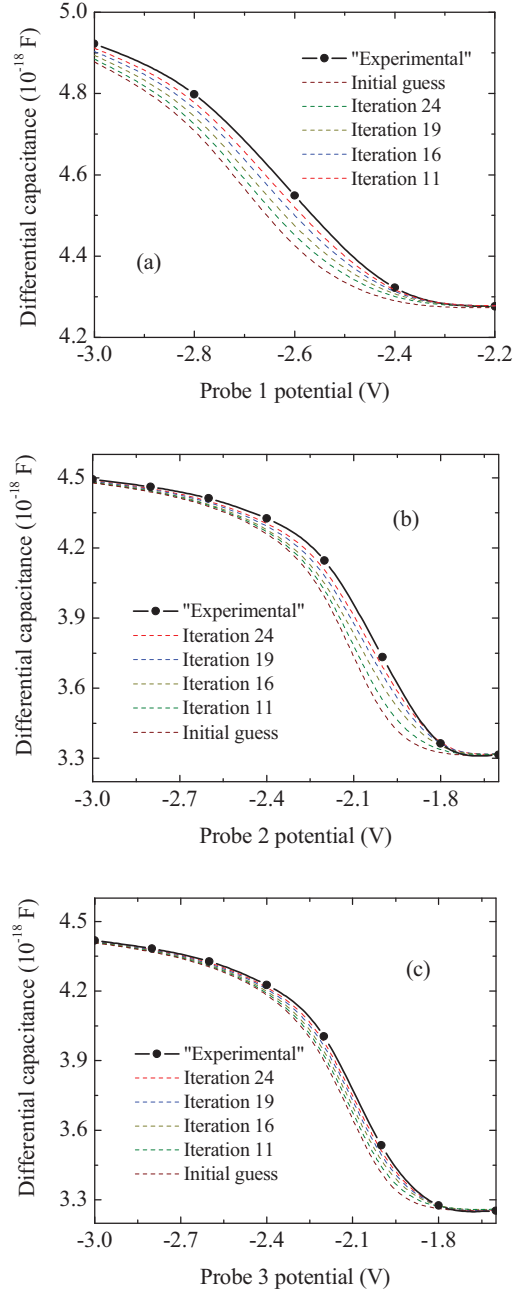


Fig. 2. Differential capacitance of the three probes computed at different iterations. The continuous lines show the "experimental" values of the differential capacitance. The iterations converge after 39 iterations to the doping configuration shown in Fig. 3(i).

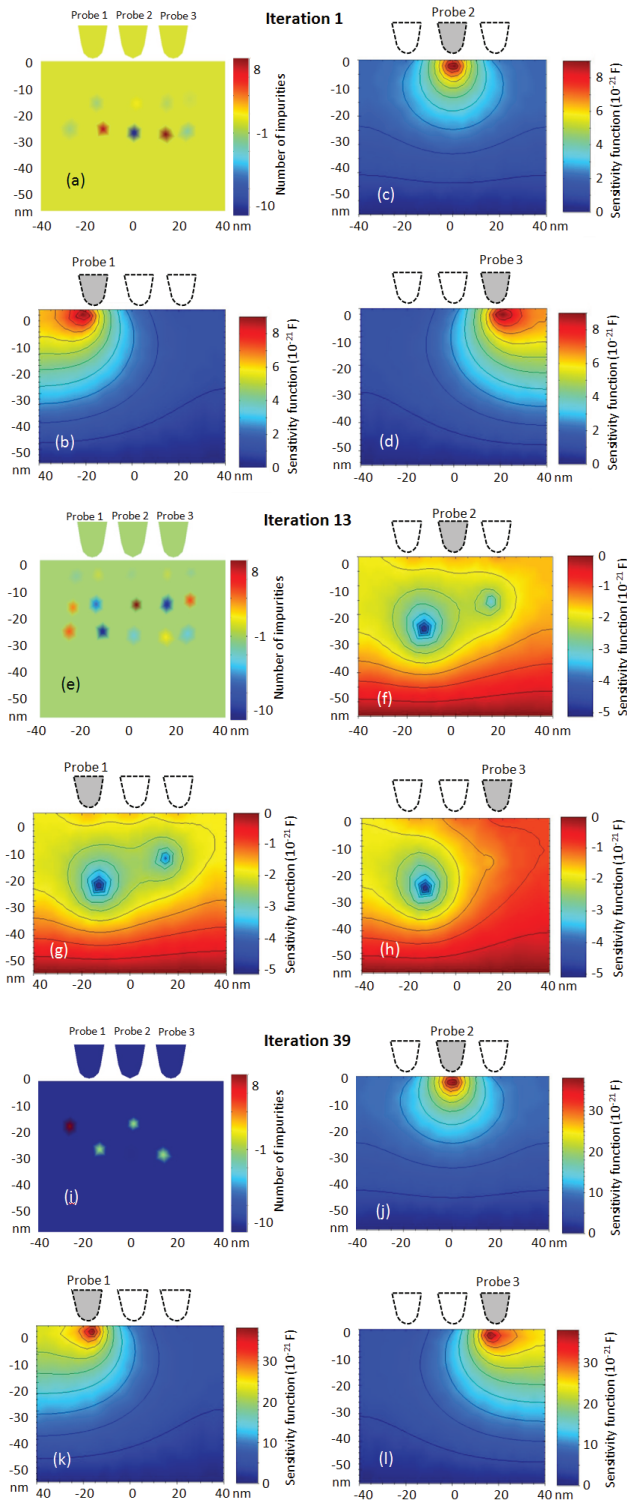


Fig. 3. Doping profiles and doping sensitivity functions computed after the first iteration (a)-(d), after iteration 13 (e)-(h), and after iteration 39 (i)-(l). The initial guess for the doping profile was an undoped structure (a). The algorithm converged towards the doping profile shown in (k) after 39 iterations. The probe for which the sensitivity function is plotted is indicated in each figure.

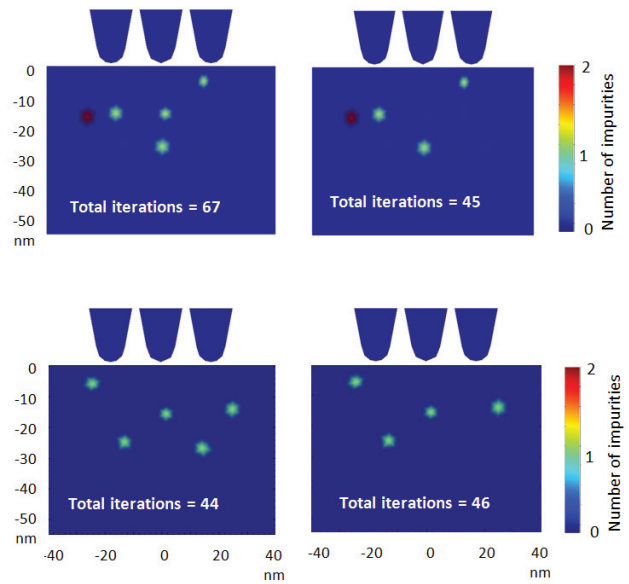


Fig. 4. Examples of simulations for different atomic profiles. The inversion algorithm converged in each case to the dopant distribution shown in each figure.

We have also tested our inversion algorithm using different doping configurations with different ionization charges (in multiples of q). Fig. 4 shows a few examples that we have tested. The number of iterations after which the original doping configuration is obtained is shown on each figure.

V. CONCLUSION

We have developed a numerical algorithm to extract the 3-D coordinates of ionized impurities in semiconductor materials using SCM measurements. The algorithm was verified numerically using a modified 2-D setup, in which the C-V curves are measured at 3 different locations on the surface of the semiconductor. Although the cases studied in this article was much idealized and, in reality, the C-V measurements are subject to noise and other experimental errors, it is shown that if the differential capacitance is measured precisely, these measurements can be potentially used for the "atomistic" profiling of ionized impurities in doped semiconductors.

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