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MULTI-SCALE METHODS FOR INVERSE MODELING IN 1-D MOS CAPACITOR*[1]

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Dedicated to the 80th birthday of Professor Zhou Yulin

Abstract

In this paper, we investigate multi-scale methods for the inverse modeling in 1-D Metal-Oxide-Silicon (MOS) capacitor. First, the mathematical model of the device is given and the numerical simulation for the forward problem of the model is implemented using finite element method with adaptive moving mesh. Then numerical analysis of these parameters in the model for the inverse problem is presented. Some matrix analysis tools are applied to explore the parameters' sensitivities. And third, the parameters are extracted using Levenberg-Marquardt optimization method. The essential difficulty arises from the effect of multi-scale physical difference of the parameters. We explore the relationship between the parameters' sensitivities and the sequence for optimization, which can seriously affect the final inverse modeling results. An optimal sequence can efficiently overcome the multi-scale problem of these parameters. Numerical experiments show the efficiency of the proposed methods.

Key words: Inverse problem, MOS capacitor model, Finite element method, Adaptive moving mesh, Levenberg-Marquardt method, Sequence for optimization, Multi-scale methods.

1. Introduction

Metal Oxide Silicon (MOS) transistors are the basic building block of MOS integrated circuits. Very Large Scale Integrated (VLSI) circuits using MOS technology have emerged as the dominant technology in semiconductor industry. The direct techniques for determining the two-dimensional doping profiles, such as scanning capacitance microscopy and dopant selective etching followed by atomic force microscopy (DSE/AFM), however, are less mature at the moment. The device have to be destroyed in these direct techniques. In mathematical theory, present implementation of technique does not determine unique physical solution and requires excessive intervention to achieve acceptable results because of the high nonlinear character of the mathematical model. Therefore much work for the design and analysis of circuits focuses on scientific computing of the numerical simulation and the inverse modeling.

Since the accuracy of a device model in predicting device characteristics is fully dependent on the accuracy of the model parameter values being used, *parameters extraction*, an electronics inverse problem, is one of most important aspects of the semiconductor industry. It

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is to characterize the complicated doping profiles inside the device by curve fitting the model equations to a set of the data measured on its surface, such as the capacitance-voltage (C-V) and/or current-voltage (I-V) data using nonlinear least square optimization techniques. This is still a very challenging problem because of the lack of effective optimization methods or ideas. Especially in practical problems, with ever decreasing device dimensions, the complexity of the models used in circuit simulators have increased significantly and the physical scales of these parameters often are various. Moreover, the effect of multi-scale physical difference of the parameters is so serious that we usually can extract only part of the parameters.

The main purpose of this paper is to propose some numerical methods or strategies for solving the inverse problem of parameters extraction in 1-D MOS capacitor using C-V technique, particularly the difficulty in the multi-scale problem, based on our sensitivity analysis of the parameters.

In section 2, we will formulate the mathematical model of 1-D MOS capacitor. The model is a nonlinear two-point boundary value problem. In section 3 we use finite element method with adaptive moving mesh in the discretization of the forward problem. Then sensitivity analysis of the parameters is given in section 4. And section 5 outlines the algorithm used to solve the inverse problem. Section 6 and 7 present the results and concluding remarks. Furthermore, we will give different results based on two kinds of physical MOS models: *low-frequency capacitance* model and *deep depletion* model.

2. The Mathematical Model of 1-D MOS Capacitor

Figure 1 represents a simple structure of 1-D MOS capacitor, which consists of *Poly-Si* layer (metal), SiO_2 layer (oxide) and *Si* layer (silicon) from the left to the right.

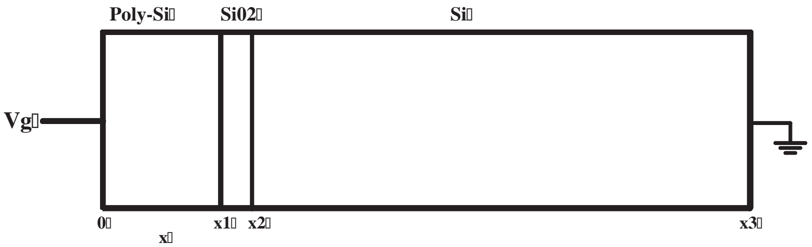

Figure 1: The structure of MOS capacitor.

A fundamental equation in MOS structure is Possion's equation, which relates the charge density ρ to the electrical potential ϕ. The formulation is

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\varepsilon(x)\frac{\mathrm{d}\phi(x)}{\mathrm{d}x}\right) = -\rho(\phi(x), x), \tag{2.1}$$

where x is the depth from the left boundary of the device, $\phi(x)$ is the electrical potential at x, $\rho(x)$ is the charge density, $\varepsilon(x)$ is the material's dielectric number. And $\varepsilon(x)$ in the three layers are constants $\varepsilon_{\mathrm{si}}$, $\varepsilon_{\mathrm{ox}}$ and $\varepsilon_{\mathrm{si}}$ respectively. And the boundary conditions

$$\begin{cases} \phi|_{x=0} = \phi_0 + \phi_{Bpoly} = \phi_0 + \dfrac{\mathrm{kT}}{\mathrm{q}}\ln\big(\dfrac{N_{0poly}}{\mathrm{n_i}}\big) \\ \phi|_{x=x_3} = \phi_B = -\dfrac{\mathrm{kT}}{\mathrm{q}}\ln\big(\dfrac{N_{const}}{\mathrm{n_i}}\big). \end{cases} \tag{2.2}$$