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MODEL ANALYSIS AND PARAMETER EXTRACTION FOR MOS CAPACITOR INCLUDING QUANTUM MECHANICAL EFFECTS *1)

Hai-yan Jiang Ping-wen Zhang
(*LMAM, CCSE and School of Mathematical Sciences, Peking University, Beijing 100871, China*)

Dedicated to the 70th birthday of Professor Lin Qun

Abstract

The high frequency CV curves of MOS capacitor have been studied. It is shown that semiclassical model is a good approximation to quantum model and approaches to classical model when the oxide layer is thick. This conclusion provides us an efficient (semiclassical) model including quantum mechanical effects to do parameter extraction for ultrathin oxide device. Here the effective extracting strategy is designed and numerical experiments demonstrate the validity of the strategy.

Mathematics subject classification: 81V10, 65M32.
Key words: Poisson Equation, Schrödinger Equation, MOS Capacitor, Quantum Effect, Sensitivity, Parameter Extraction.

1. Introduction

Metal-Oxide-Semiconductor (MOS) structure is the core of MOS technology. This structure becomes a capacitor with one side relating to the metal and the other side to semiconductor. Its capacity depends on the gate voltage. This structure is very important for the building technique of MOS integrated circuits. In fact CV(capacity and gate voltage) curve is often measured to estimate the performance of the integrated circuits. The important parameters, such as the thickness of the oxide layer, the doping profile of the substrate is determined by fitting CV curve. Due to the high nonlinearity of the mathematical model, it is difficult to obtain an analytical solution. So we have to resort to numerical method.

For large scale MOS structure, much work about the classical model has been described in [1, 12]. As MOS devices are scaled to deep sub-micro dimensions, aggressive scaling of gate dielectric thickness has continued. According to the National Technological Roadmap for semiconductor (NTRS) [2], the scaling trend for gate dielectrics is such that for sub-100 nm generation device, an equivalent gate oxide thickness of less than 3.0 nm will be required [10]. The combination of thin gate dielectrics and high level gate bias results in deep submicron ($< 0.25\mu m$) MOS device in large transverse electric fields at the interface. When the transverse electric fields become large enough to cause the formation of a 2-D electron (or hole) gas, the modelling of quantum mechanical (QM) effects in inversion and accumulation layers becomes very important. QM effects result in decreased inversion layer charge density in the inversion layer at a given gate voltage (compared to classical calculations which ignore QM effects) [5]. An accurate model should be the completely coupled Poisson equation and Schrödinger equation. The electrostatic potential and quantum energy levels of an accumulated n-type semiconductor is fully self-consistently calculated in [9]. According to physical characteristic, additional boundary condition is set to Poisson equation and shooting method is applied the initial problem. Schrödinger equation is solved by shifting energy to make sure the wave function

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not to distort physical properties in oxide layer. Finite difference method is used to solve Poisson and Schrödinger equations self-consistently for accumulated layers [7] and applied to the calculation of tunnelling current. The fully self-consistent QM treatment of the inversion layer and accumulation layer is time-consuming and too cumbersome for practical device simulation. To do parameter extraction for ultrathin oxide gate device, it is important to choose an efficient model including QM effects. QM effects is obvious only in the potential well at the interface of oxide layer and Si layer, so it is not necessary to include QM effect in the global region. In this paper, the semiclassical model is presented, quantum region is located at the beginning of the Si layer, which is set large enough to include QM effects and other regions are considered classically.

The main purpose of this paper is to analyze the different scale mathematical models and extract important parameters. The physical model and mathematical models are introduced in section 2. Numerical method is presented and which is used to identify the phenomena for different models in section 3. In section 4, inverse strategy is designed and inverse result is given. Finally, we draw the conclusion in section 5.

2. Physical and Mathematical Model of 1-D MOS Capacitor

1-D MOS capacitor consists of three layers: Poly-Si (metal), Sio_2 layer (oxide) and Si layer from the left to the right as shown in figure 1. QM effects are obvious at the beginning of the Si layer. As we mentioned in the previous section, our approach aims at self-consistently solving the Schrödinger and Poisson equations. Although the same procedure is applicable to any semiconductor-insulator combination, as an example of illustration, we shall consider the case of n-type Si/Sio_2/Poly-Si structure.

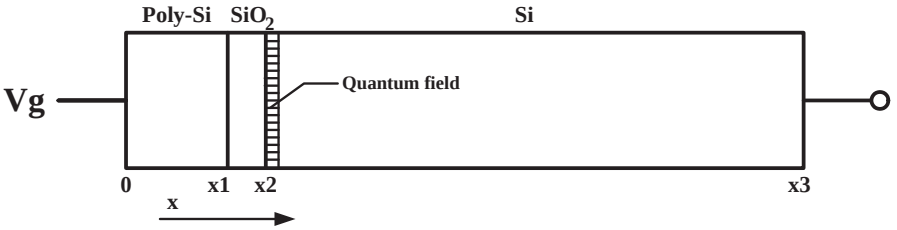

Figure 1: The structure of MOS capacitor

The following is a list of physical parameters to be used in our MOS capacitor model.

- k is Boltzman constant $\quad k = 1.38066 \times 10^{-23} J/K$
- $\hbar$ is Plank constant $\quad \hbar = 1.05457266 \times 10^{-34} J.s$
- m_0 is electron mass $\quad m_0 = 9.109 \times 10^{-31} kg$
- E_g is the length of band gap in Si $\quad E_g = 1.12ev$
- q is electron charge $\quad q = 1.60218 \times 10^{-19} C$
- T is room temperature $\quad T = 300K$
- Q_{it} is the interface-trapped charge density; $\quad Q_{it} = 3 \times 10^{10} cm^{-2}$
- n_i is intrinsic carrier concentration; $\quad n_i = 1.45 \times 10^{10} cm^{-3}$
- t_{poly} is thickness of Poly-Si layer $\quad t_{poly} = 0.01\mu m = 10nm$
- t_{si} are thickness of Si layers. $\quad t_{si} = 0.2\mu m = 200nm.$

2.1. Poisson Equation

Poisson Equation is the fundamental equation which governs the electrostatic potential and the charge distribution:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\varepsilon(x)\frac{\mathrm{d}\phi(x)}{\mathrm{d}x}\right) = \rho(\phi(x), x) = q(p(x) - n(x) + N_d(x)) \tag{1}$$