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Solving Schrodinger Equation with Non-Uniform Grids by Scale Transformation Method

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Abstract: A new scale transformation method is used in solving the Schrodinger equation. With it, the uniform grids in the discretization in conventional method are changed into non-uniform grids. Consequently, in some cases, the computing quantity will be greatly reduced at keeping the required accuracy. The calculation of the quantized inversion layer in MOS structure is used to demonstrate the efficiency of the new method.

Key words: Schrodinger equation; non-uniform grids; scale transformation method
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1 Introduction

Quantum Mechanical Effects (QMEs) in MOS structures are well-known in the deep-submicron ULSI device characterization[1—3]. Rigorous study of QMEs in the MOS inversion and accumulation layer requires self-consistent solution to Schrodinger and Poisson equations[3,4]. Further more, due to the technical advance and the application technique, more and more attention has been paid to the alternative structures and devices rather than the conventional MOSFET, such as quantum wire, quantum dot devices[5,6] and resonant tunneling devices[7]. Generally speaking, studying the physics and behavior of these devices needs a full quantum mechanical approach, so it is inevitable to solve the Schrodinger equations. However, since solving Schrodinger equations is an eigenvalue problem, and in most cases, iteration procedure is necessary to find the self-consistent results, this approach is a time-consuming process. The required accuracy is always in contradiction with the computing budget in such problems. In this letter, a new scale transform method is developed to partially overcome the difficulty, whose principle is stated below, the application of the method to the MOS inversion and accumulation layer is indicated as well. The comparison between the results from the new method and the conventional one is also given and discussed in this paper.

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2 Method Description

In many cases, due to the requirement of boundary conditions, the domain of the Schrodinger equation being solved is much wider than the relevant region (namely, the active device region concerned), such as the accumulation layer in MOS structure[8] and the device region in the resonant tunneling diode[7]. Usually, Schrodinger equation is discretized by finite differential method and then results in an eigenvalue problem of a three-diagonal matrix. This approach requires that the discretization be based on a set of uniform grids. Therefore, a small part of the grids are allocated in the important device region while a larger part are in the relatively less important region. Consequently, in order to get the accuracy, much more grids are needed than the necessary. Most computing time is wasted in those less important grids. However, the solving domain can be transformed nonlinearly into a new scale, within which the relevant region is a larger part of the transformed domain but the less important one is the smaller part. And if the boundary conditions can meet the requirements at the same time, the efficiency of the solution would be greatly improved.

The new method is implemented in a MOS (Metal-Oxide-Semiconductor) structure as an example. In MOS structure, the voltage drop between the gate (metal) and the substrate (semiconductor) leads to a potential well in the semiconductor region near the oxide-semiconductor interface. Carriers in inversion and in accumulation layer are quantized into subbands and described by a self-consistent model with effective-mass Schrodinger and Poisson equations[1]. The Schrodinger equation is given by Ref. [1]:

$$-\frac{\hbar^2}{2m_3}\frac{d^2\Psi}{dx^2}+V(x)\Psi=E\Psi \tag{1}$$

The scale transformation function is chosen to be the inverse hyperbolic tangent:

$$x=x_0\operatorname{arctanh}(\xi) \tag{2}$$

ξ in (2) is the new scale variable and is a scale coefficient as 2.76×10^{-8}cm. The value of x_0 has been determined so as to fulfil the relations of $\frac{\hbar^2}{m_0x_0^2}=1$eV. Thus, eq. (1) can be converted into:

$$(pu'(\xi))'-qu(\xi)=-Eru(\xi) \tag{3}$$

in which

$$p(\xi)=(1-\xi^2)/x_0 \tag{4}$$

$$q(\xi)=\frac{2m_3x_0V(x_0\operatorname{arctanh}(\xi))}{\hbar^2(1-\xi^2)} \tag{5}$$

and

$$r(\xi)=2m_3x_0/\hbar^3(1-\xi^2) \tag{6}$$

In eq. (3), $u(\xi)=\Psi(x_0\operatorname{arctanh}(\xi))=\Psi(x)$. Thus, Schrodinger eq(1) is converted to another equivalent equation, and then the discrete energy levels in subbands and the carrier density can be calculated by self-consistent solution of eq. (3) and Poisson equation. Equation (3) is solved by finite difference method. While eq. (1) is transformed into eq. (3), the boundary condition of Schrodinger equation keeps unchanged, i. e., the boundary condition of eq. (1) is $\Psi(x) = 0$ at the point of $x = 0$ and $x = \infty$, while the boundary of eq. (3) is $u(\xi) = 0$ at the points of $\xi = 0$ and $\xi = 1$. Note that if the grids for eq. (1) and eq. (3) are in the same amount, the calculations for both equations are also the same. It has been shown that the results from the new method with half amount of the grids have the same accuracy with those from the conventional method . So, the calculation is reduced substantially due to its rapid increase with the amount of grids. The solving region is also transformed non-linearly (e. g. from [0, 1] to [0, ∞].). The inverse hyperbolic tangent function has been plotted in Fig. 1. The inset of Fig. 1 is the transformed nonuniform grid space. The space of the uniform grid is a unity before the transformation. Obviously, in the lower part of the grids, the space is almost unchanged, being as approximate unity. However, in the upper part of grids, the space between grids can be significantly larger. It is necessary to note that since in both methods the equations have been discretized, the solving region in the new method can not reach the infinity. In the new method, because of the application of non-uniform grids, the minimum amount of the necessary grids can be reduced greatly and keep the required accuracy as well.

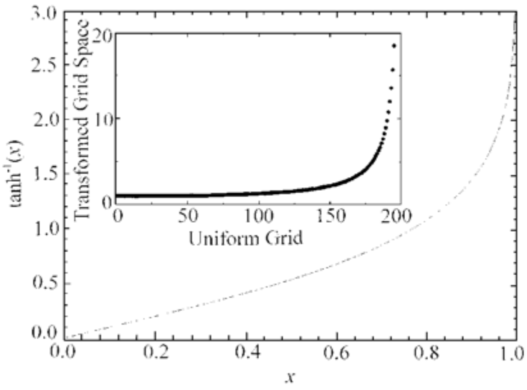

FIG. 1　Inverse Hyperbolic Tangent Function
The inset is the transformed non-uniform grid. The horizontal axis of the inset is the grid number and the longitudinal axis is the transformed grid space at each grid.

3　Results and Discussions

The calculation results are compared with the conventional uniform grids, as shown in Fig. 2 and Fig. 3. Figure 2 gives the comparison between the carrier sheet density in the inversion layer calculated by the conventional uniform grids method and the transformed non-uniform grids method with different amount of grids. The lines represent the results from the conventional method while the symbols from the new method. Different line and symbol stand are for different grid amount as illustrated in the caption. It can be seen that the accuracy of the new method with 10 grids is the same as that of the conventional method with 20 grids. The new method with 20 grids has negligible errors while the conventional method with 30 grids has still significant errors. Figure 3 gives the results of gate capacitance. Similar conclusion can be drawn on the gate capacitance.

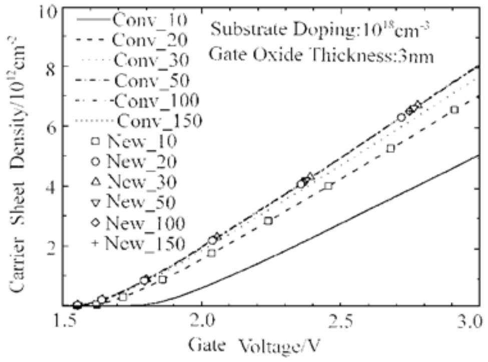

FIG. 2 Inversion Layer Carrier Sheet Density in MOS Structure Calculated by Two Methods (The number of grids in the legend).

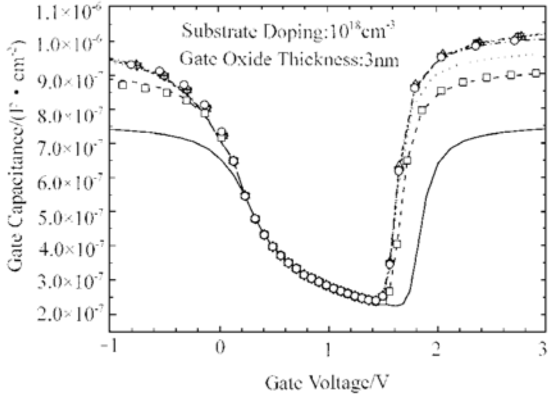

FIG. 3 Gate Capacitance Results, Conditions for Calculation.

4 Conclusion

In conclusion, a scale transform method is used to solve the Schrodinger equation, and thus the conventional uniform grid discretization is changed into non-uniform grids. Consequently, the calculation budget will be greatly reduced if we keep the required accuracy constant. The carrier sheet density and the gate capacitance in MOS structure with a quantized inversion layer are calculated with the two methods (conventional uniform grids method and new non-uniform grids method) and the comparison between the results demonstrates the high efficiency of the new method.

Appendix: Verification of the Equivalence of Eq. (1) and Eq. (3)

From eq. (2), it can be obtained that:

$$\frac{\mathrm{d}x}{\mathrm{d}\xi} = x_0 \frac{1}{1-\xi^2} \tag{A.1}$$

Thus:

$$\frac{\mathrm{d}\xi}{\mathrm{d}x} = \frac{1-\xi^2}{x_0} \tag{A.2}$$

So:

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}\Psi}{\mathrm{d}x}\right) = \frac{\mathrm{d}\xi}{\mathrm{d}x}\left(\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}u}{\mathrm{d}\xi}\right)\right) = \frac{1-\xi^2}{x_0}\left(\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{1-\xi^2}{x_0}\frac{\mathrm{d}u}{\mathrm{d}\xi}\right)\right) \tag{A.3}$$

Substitute eq. (A.3) into eq. (1) can directly result in eq. (3).

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