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Computer Physics Communications 169 (2005) 309–312

Computer Physics Communications

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A numerical iterative method for solving Schrödinger and Poisson equations in nanoscale single, double and surrounding gate metal-oxide-semiconductor structures

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Available online 8 April 2005

Abstract

Numerical solution of the Schrödinger and Poisson equations (SPEs) plays an important role in semiconductor simulation. We in this paper present a robust iterative method to compute the self-consistent solution of the SPEs in nanoscale metal-oxide-semiconductor (MOS) structures. Based on the global convergence of the monotone iterative (MI) method in solving the quantum corrected nonlinear Poisson equation (PE), this iterative method is successfully implemented and tested on the single-, double-, and surrounding-gate (SG, DG, and AG) MOS structures. Compared with other approaches, various numerical simulations are demonstrated to show the accuracy and efficiency of the method.
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PACS: 72.15.Rn; 73.40.Ty; 73.40.Qv; 02.70.Fj; 02.70.-c

Keywords: Schrödinger and Poisson equations; Quantum corrected Poisson equation; Numerical iterative method; Monotone iterative method; Nanoscale MOS structures

1. Introduction

Advanced process technology has allowed us to fabricate diverse semiconductor devices including nanoscale MOS structures. For nanoscale SG, DG, and AG MOS structures, the displacement of the inversion carrier density away from the interface of silicon and silicon dioxide (Si/SiO_2) due to the quantum mechanical (QM) effect cannot be neglected [1–3]. Thus any accurate analysis must take the QM effect into consideration. A set of the SPEs subject to an appropriate boundary condition at the interface of materials plays an accurate way of incorporating the QM effect [1–3]. Various solution techniques have been proposed for solving only the SG MOS structures [1–3]. However, these methods may encounter divergence prob-

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doi:10.1016/j.cpc.2005.03.069

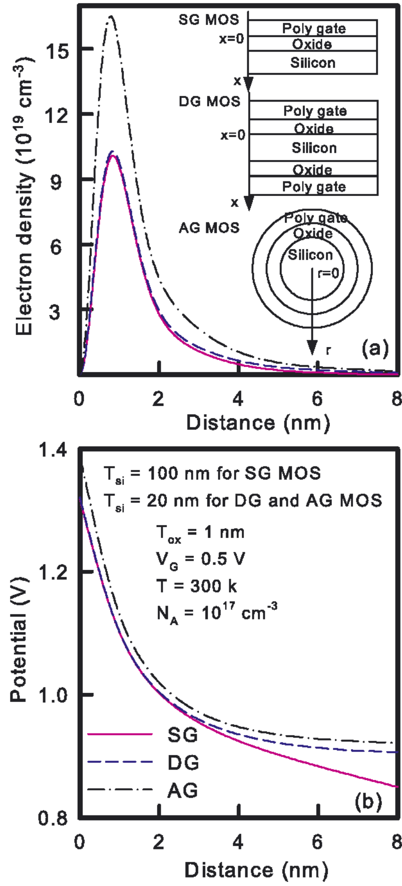

Fig. 1. (a) The computed electron density and (b) the potential of the three MOS structures. The inset figures, shown in Fig. 1(a), are the cross-sectional views of the MOS structures.

lem when applied to simulate the DG and AG MOS structures.

In this paper, we propose a robust numerical iterative method for solving the SPEs in the SG, DG, and AG MOS structures shown in the inset of Fig. 1. This unified iterative scheme successfully integrates the MI method [4] and the potential relaxation update method [1], where the effect of strong quantum correction charge density [2] is taken into consideration simultaneously. First of all the nonlinear PE is solved with the MI method instead of the Newton's iterative method [4]. The calculated potential (ϕ) energy, after a relaxation update, is used in the solution of the Schrödinger equation (SE). The calculated electron wavefunctions (ζ_{jk}) and eigenenergies (E_{jk}) are applied to estimate the electron density and its derivatives. The calculated quantum corrected electron density is feedback into the PE and we solve the PE with the MI method. Iteration is terminated when a self-consistent solution is obtained. Compared with other well known approaches [1,2], application of this method to simulate the nanoscale SG, DG, and AG MOS structures under various testing conditions has confirmed the robustness of the method. In Section 2, we state the SPEs for the SG, DG, and AG MOS structures and discuss the iterative method. In Section 3, we discuss the results. Finally, we draw conclusions.

2. The Schrödinger and Poisson equations and the iterative method

To calculate the potential distribution and electron's density in the nanoscale SG, DG, and AG MOS structures, shown in the inset of Fig. 1, we consider the following SPEs [1–3] in a unified formation

$$\frac{\mathrm{d}^2\phi(r)}{\mathrm{d}r^2}+\frac{m}{r}\frac{\mathrm{d}\phi(r)}{\mathrm{d}r}=-\frac{q}{\epsilon_{\mathrm{si}}}(p-n+N_D-N_A) \quad (1)$$

and

$$-\frac{\hbar^2}{2m_{rk}}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{m}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)\zeta_{jk}(r)+E_c(r)\zeta_{jk}(r) = E_{jk}\zeta_{jk}(r), \quad (2)$$

where Eq. (1) is the PE and Eq. (2) is the SE in the effective mass approximation. The PE is solved in whole MOS structure and the SE is only solved in the region of the silicon films. $m=0$ is for the SG and DG MOS structures in the Cartesian coordinate and $m=1$ is for the AG MOS structure in the cylindrical coordinate. $n=n_{cl}+n_{qm}$, where for n_{cl}, we consider the Feri–Dirac distribution and a two-dimensional electron gas approximation is used to calculate the quantum electron density n_{qm}. Eq. (1) is with the Dirichlet type boundary condition on the boundary of the simulated structures. For Eq. (2), the electron wavefunction is assumed to be vanished on the interface of Si/SiO_2. All notations used in Eqs. (1) and (2) are having their conventional physical meaning [1–4]. We briefly outline the proposed iterative method as follows:

(1) Solve Eq. (1) using the MI method,
(2) Solve Eq. (2),
(3) Estimate the derivative of n,

(4) Solve Eq. (1) with the MI method,
(5) The computed potential is relaxing updated, and
(6) Return to the step (2).

Iteration is terminated when the solution converges. We note the MI method converges monotonically when solves the nonlinear PE [4].

3. Results and discussion

Fig. 1 shows the computed potential distribution and electron's density from the interface of Si/SiO_2 for the three MOS structures, respectively. In our calculation, eight subbands are computed in solving Eq. (2). As shown in the figure, the oxide thickness T_{ox}, the substrate doping N_A, temperature T, and gate voltage V_G are with the same settings for all structures. The thickness of the silicon film T_{si} for SG is equal to 100 nm and $T_{\mathrm{si}} = 20$ nm for both the DG and AG MOS structures. Fig. 1(a) shows the superiority of the AG MOS among the MOS structures. The higher electron, is due to good channel controllability in AG MOS structure. To verify the robustness of the iterative method, we have studied the convergence of our method and compare with other two well known algorithms: the first algorithm (Algorithm 1) updates the computed potential using an explicit relaxation method [1] and the second one (Algorithm 2) calculates the derivative of n_{qm} by evaluating its previous computed quantities [2]. Comparison is subject to the same device configurations and settings. We have examined the convergence behavior of these three algorithms in terms of T_{ox}, N_A, T, V_G, and T_{si}. Shown in Fig. 2, it is found that our method converges for all cases of simulation. However, Algorithms 1 and 2 have suffered different divergent problems, shown in Fig. 2(a)–(d), when solving the SPEs in the SG, DG, and AG MOS structures under $T = 300$ K and $T = 77$ K, respectively.

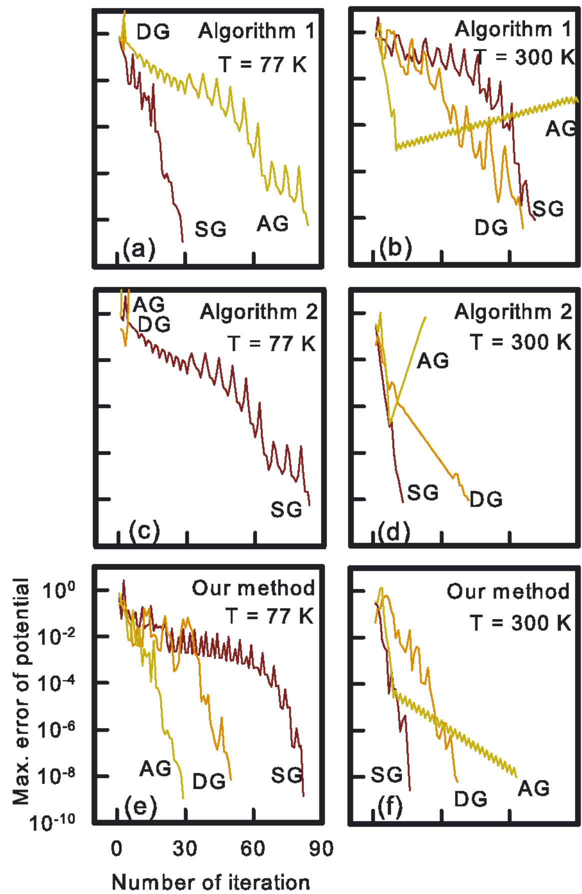

Fig. 2. The maximum norm errors of the computed potential versus the number of iteration for the three algorithms applied to SG, DG, and AG MOS structures, respectively.

4. Conclusions

We have present an effective iterative method for the self-consistent solution of the SPEs in nanoscale SG, DG, and AG MOS structures. Our method successfully integrates the MI method and the potential relaxation update method, where the effect of strong quantum correction charge density was taken into consideration simultaneously. The solution method has shown good numerical stability and robust convergence for different simulation cases.

Acknowledgements

This work is supported in part by the National Science Council of Taiwan under contracts NSC-93-2215-E-429-008 and NSC 93-2752-E-009-002-PAE, the grant of the Ministry of Economic Affairs, Taiwan under contract No. 93-EC-17-A-07-S1-0011, and the grant from Taiwan Semiconductor Manufacturing Company, Hsinchu, Taiwan in 2004–2005.

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