Solution of Schrödinger equation in double-gate MOSFETs using transfer matrix method

T.M. Abdolkader, H.H. Hassan, W. Fikry and O.A. Omar

The transfer matrix method (TMM) has been extensively used to investigate quantum-mechanical tunnelling through potential barriers. Reported is the application of TMM, for the first time, to solve the Schrödinger equation in double-gate MOSFETs. The method is shown to be more accurate than the conventional finite difference method, especially for high energy levels.

Introduction: Numerical simulation of nanoscale devices is basically accomplished by the self-consistent solution of Schrödinger and Poisson equations [1]. An initial guess for the potential distribution in the device is firstly assumed. According to this potential, the Schrödinger equation is solved in the direction normal to the interface (transverse direction) assuming a plane wave function in the direction parallel to the interface (longitudinal direction). The eigenenergies and eigenfunctions resulting from the solution of the Schrödinger equation are used to calculate the carrier distribution in the device, which is fed to the Poisson equation yielding new potential distribution. This process is repeated until the potential difference of two successive iterations is below a certain tolerance.

The transfer matrix method (TMM) is one of the methods used for the numerical solution of the 1D Schrödinger equation [2]. TMM was excessively used in solving tunnelling problems [3–6]. It was introduced to solve bounded problems by Kalotas and Lee [7]. In this Letter, we take a DG-MOSFET as a sample nanoscale MOS structure and apply the procedure of Kalotas to solve the Schrödinger equation in the device as a part of finding a self-consistent solution. Eigenenergies and eigenfunctions resulting from TMM are compared with that resulting from the standard finite difference method (FDM) [8].

Transfer matrix method: The 1D Schrödinger equation in the z-direction is written as:

$$\frac{-\hbar^2}{2m^*}\frac{d^2\psi}{dz^2} - (E - V(z))\psi(z) = 0 \tag{1}$$

where $\psi(z)$ is the eigenfunction, E is the eigenenergy, and $V(z)$ is the potential energy function. Referring to Fig. 1, which shows the potential energy profile across the transverse direction of a DG-MOSFET, TMM is based on breaking up the domain of the solution into N segments, where in each segment the potential energy is assumed constant. Consequently, for the nth segment, the wave function can be approximated as:

$$\psi_n(z) = A_n \exp(\alpha_n z) + B_n \exp(-\alpha_n z)$$
$$\alpha_n = \frac{\sqrt{2m^*(V_n - E)}}{\hbar} \tag{2}$$

Applying the conditions of continuity for $\psi(z)$ and $d\psi(z)/dz$ between each two successive segments, we arrive at a series of matrix equations relating A_n and B_n of any segment with those of the preceding segment A_{n-1} and B_{n-1} as follows:

$$\begin{bmatrix} A_{n-1} \\ B_{n-1} \end{bmatrix} = M^{-1}(\alpha_{n-1}, z_{n-1}) M(\alpha_n, z_{n-1}) \begin{bmatrix} A_n \\ B_n \end{bmatrix}$$
$$M(\alpha_n, z_m) = \begin{bmatrix} e^{\alpha_n z_m} & e^{-\alpha_n z_m} \\ \alpha_n e^{\alpha_n z_m} & -\alpha_n e^{-\alpha_n z_m} \end{bmatrix} \tag{3}$$

For bound states solution, A of the right boundary segment (A_R) and B for the left boundary segment (B_L) must vanish [7]. Thus, on eliminating the intermediate coefficients from (3), we obtain:

$$\begin{bmatrix} A_L \\ 0 \end{bmatrix} = M^{-1}(\alpha_L, 0)\Pi M(\alpha_R, Z_n) \begin{bmatrix} 0 \\ B_R \end{bmatrix}$$
$$\Pi = K_1 K_2 \cdots K_N \quad \text{and} \quad K_n = M(\alpha_n, z_{n-1}) M^{-1}(\alpha_n, z_n) \tag{4}$$

Applying boundary conditions and assuming nearly infinite conduction band offset, offset, $E_{C_{offset}}$, between Si and SiO_2, it is found that the matrix element Π_{12} must vanish, i.e.

$$\Pi_{12} = 0 \tag{5}$$

This condition represents an implicit equation that determines all the eigenenergies. In addition, for each eigenenergy, the corresponding eigenfunction is determined by calculating the coefficients A_n and B_n for each segment from (3).

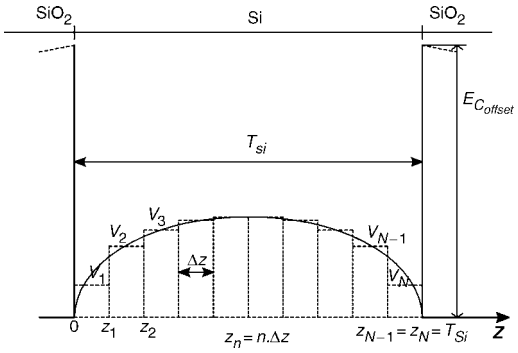

Fig. 1 *Conduction band edge across transverse direction (normal to interface) of DG-nMOSFET*
Domain divided into N segments, each with width Δz

Results: A DG-MOSFET of Si-film thickness $T_{si} = 5$ nm, oxide thickness $T_{ox} = 1.5$ nm, and with Al gate is used as a sample nanoscale MOS structure. Results are drawn for an acceptor doping in the channel $N_A = 1 \times 10^{17}$ cm^{-3}, and at gate voltage $V_G = 1.5$ V. For ⟨100⟩ Si, there are two groups of subbands (known as two ladders) corresponding to the six ellipsoidal constant energy surfaces. One of the ladders has an effective mass $m_l = 0.92m_o$ (with energies designated as E_{11}, E_{12}, E_{13}, ...), and the other has an effective mass $m_t = 0.19m_o$ (with energies designated as E_{21}, E_{22}, E_{23}, ...).

For the purpose of assessment of the results of FDM and TMM, reference values for the eigenvalues and eigenfunctions are found first using the shooting method [9]. In this method, we seek an energy E such that, when (1) is integrated from 0 to T_{si}, two function nodes ($\psi = 0$) are produced at both interfaces $z = 0$ and $z = T_{si}$. The integration was carried out using an efficient Runge-Kutta engine and the solution obtained this way is considered 'exact' for the purpose of comparing the TMM and FDM methods.

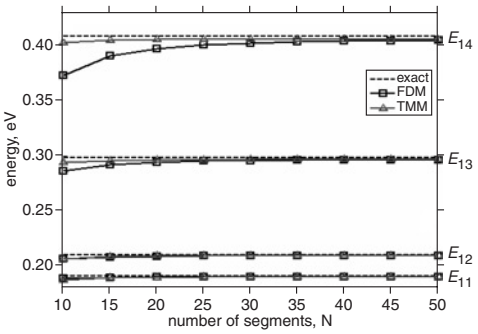

Fig. 2 *Lowest four eigenenergies of first ladder of ⟨100⟩ Si calculated in Si-film of DG-nMOSFET with $T_{si} = 5$ nm, $T_{ox} = 1.5$ nm, $N_A = 1 \times 10^{17}$ cm^{-3}, $V_G = 1.5$ V, using both FDM and TMM at different number of segments N*
Dashed horizontal lines indicate 'exact' eigenenergies

Fig. 2 shows the first four eigenvalues of the first ladder calculated using both FDM and TMM at different values of the number of segments N along with the exact values calculated by the shooting method. At the same number of segments N, it is evident from Fig. 2 that the results of TMM are generally more accurate than those of FDM, and the difference in accuracy increases for higher levels. More specifically, the error in calculating E_{12}, E_{14} is drawn against N for the two methods (see Fig. 3), where it is noted that for small N the error in calculating E_{14} by TMM is less than that of FDM by ~ 0.03 eV. Turning to the assessment of eigenfunctions, the eigenfunctions of the first and fourth levels of the first ladder (ψ_{11} and ψ_{14}) calculated by the two methods at $N = 10$ are compared to exact ones as shown in Figs. 4 and 5. It is observed that, even for this very rough mesh size, TMM continues to do well when it comes to calculating eigenfunctions. While results of TMM match well with the exact solution, those of FDM look

unrealistic, especially for ψ_{14} (see Fig. 5). Generally, the superiority of TMM is more evident for higher levels than for lower levels. This is explained by the rapid change of the eigenfunctions of higher levels for which the assumption of linear variation of ψ within each segment supposed by FDM is fairly poor, while exponential (or sinusoidal) variation assumed by TMM is more suitable.

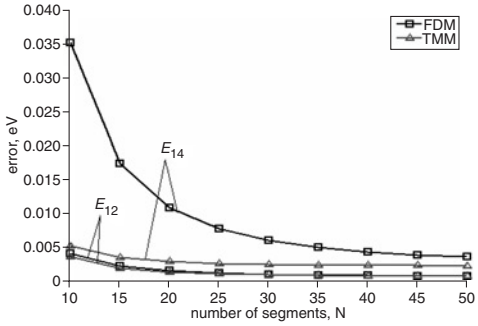

Fig. 3 *Comparison of errors in calculating eigenenergies E_{12}, E_{14} by both FDM and TMM in same device of Fig. 2*

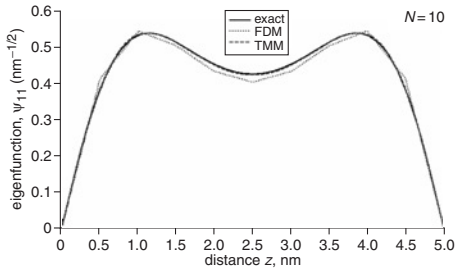

Fig. 4 *Eigenfunction of ground level of first ladder ψ_{11} calculated using both FDM and TMM*

Domain of solution in either case divided into 10 segments ($N = 10$)

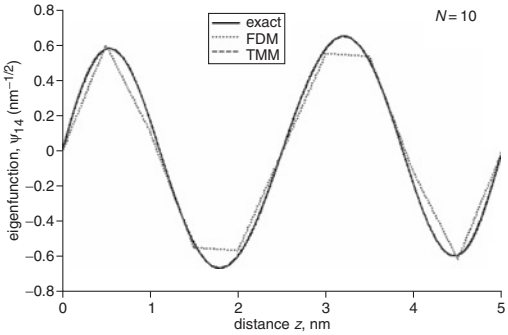

Fig. 5 *Eigenfunction of fourth level of first ladder ψ_{14} calculated using both FDM and TMM*

Domain of solution in either case divided into 10 segments ($N = 10$)

Conclusions: The transfer matrix method (TMM) is successfully used to solve the 1D Schrödinger equation in a DG-MOSFET. The method is based on dividing the Si-film region into small segments and assuming constant potential energy in each segment, then an implicit equation is numerically solved to find energy eigenvalues, and thus, for each eigenenergy, the eigenfunction is found in terms of a series of coefficients each corresponding to one of the segments. The TMM is proven to be more accurate than the conventional finite difference method (FDM), especially for high-order levels. The method can be extended to simulate other similar MOS structures such as bulk-MOSFET, PD-SOI and FD-SOI.

11 June 2004
Electronics Letters online no: 20045595
doi: 10.1049/el:20045595

T.M. Abdolkader and H.H. Hassan (*Department of Basic Sciences, Benha Higher Institute of Technology, Benha, Egypt*)

W. Fikry (*Mentor Graphics, Egypt*)

O.A. Omar (*Department of Engineering Physics and Mathematics, Faculty of Engineering, Ain Shams university, Cairo, Egypt*)

References

1 Ohkura, Y.: 'Quantum effects in Si in n-MOS inversion layer at high substrate concentration', *Solid-State Electron.*, 1990, **33**, (12), pp. 1581–1585
2 Gilfoyle, G.P.: 'A new teaching approach to quantum mechanical tunneling' (Computer Based Learning Unit, University of Richmond, Virginia, USA)
3 Kalotas, T.M., and Lee, A.R.: 'A new approach to one-dimensional scattering', *Am. J. Phys.*, 1991, **59**, pp. 48–52
4 Vatannia, S., and Gildenblat, G.: 'Airy's functions implementation of the transfer-matrix method for resonant tunneling in variably spaced finite superlattices', *IEEE J. Quantum Electron.*, 1996, **32**, pp. 1093–1105
5 Gehring, A., *et al.*: 'Design optimization of multi-barrier tunnelling devices using the transfer-matrix method'. Int. Semiconductor Device Research Symp., December 2001, pp. 260–263
6 Govoreanu, B., *et al.*: 'An investigation of the electron tunnelling leakage current through ultrathin oxides/high-k gate stacks at inversion conditions'. SISPAD, September 2003, pp. 287–290
7 Kalotas, T.M., and Lee, A.R.: 'The bound states of a segmented potential', *Am. J. Phys.*, 1991, **59**, (11), pp. 1036–1038
8 Ferry, D.K.: 'Quantum mechanics' (Institute of Physics Publishing, Bristol and Philadelphia, 2001)
9 Press, W.H., *et al.*: Numerical recipes in FORTRAN, the art of scientific computing (Cambridge University Press, Cambridge, 1992, 2nd edn.), p. 749