SILICON/SILICON DIOXIDE NANOSTRUCTURE IN ELECTROSTATIC FIELD

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ABSTRACT

Paper presents a numerical analysis of quantum states and probability $\psi\psi^*$ function of a Si/SiO_2 nanostructure in varying electrostatic field. The position of probability function peak x_p is traced and the bias, under which it abandons the structure (emission or discharging bias), is determined. Variations of the ground state energy with the bias is also examined. The Poisson - Schrödinger model of COMSOL Multiphysics program is devised and employed. The results would help understanding the electronic properties and behavior of ultrascaled Si/SiO_2 memory devices utilizing semiconducting quantum dots and Si single nanocrystals, to mention only one application.

Keywords: *Nanostructure, Si/SiO_2 quantum dot, Discharging bias, Poisson-Schrödinger numerical analysis, Comsol Multiphysics*

1. INTRODUCTION

Modern experimental techniques, such as molecular beam epitaxy, enable production of various semiconductor nanostructures in dielectric surroundings. Such a nanostructure represents a space confinement of free electrons, usually called the Quantum Dot (QD).

The fine structure of QDs is governed by Quantum Physics - the energy eigenstates, wave functions and related probabilities obey the Schrödinger Equation (SchE). The boundary conditions of this equation depend on electric constants of media involved and on barriers created on the QD surface and their modifications due to applied electric field. For the latter quantities, the Poisson Equation (PE) should be applied. Expected results are: variations of the ground eigenstates and variations of the probability function with applied bias. The central characteristic is the dot discharging bias, at which the electron in the QD penetrates through the dot surface barrier and jumps to the control electrode.

Properties of QDs have attracted researchers for several recent years. Numerical analysis of a GaAs – InAs – GaAs system with a conical InAs QD grown from the wetting layer was performed by Melnik and Wilatzen in 2004 [1]. They focused attention on proving that the ground state of the wetting layer affects considerably the quantum states of the entire QD. They used 2D axisymmetrical model, with support of Femlab program (Femlab was later renamed to Comsol) and submitted important E - k curves.

Deleruyelle et al. [2] analyzed numerically, using Comsol Multiphysics, a spherical Si QD in SiO2 medium in 2007. They obtained 1D band diagram with probability function of the ground energy eigenvalue at several biasing fields. They do not report getting the significant characteristic quantity – the discharging bias. In 2007, the authors of the present paper numerically analyzed, using Matlab program, electron 1D traps of arbitrary shape [3]. The present paper is devoted to a Si QD. It is analyzed using the Finite Element Method (FEM) available through Comsol program. A 1D Poisson – Schrödinger model was developed with the aim of full scale electronic characteristics evaluation, including the discharging bias. The results are presented in the paper.

2. SUBJECT OF ANALYSIS

The schematic diagram of the 1D Si nanostructure with its surroundings is given in Fig. 1.

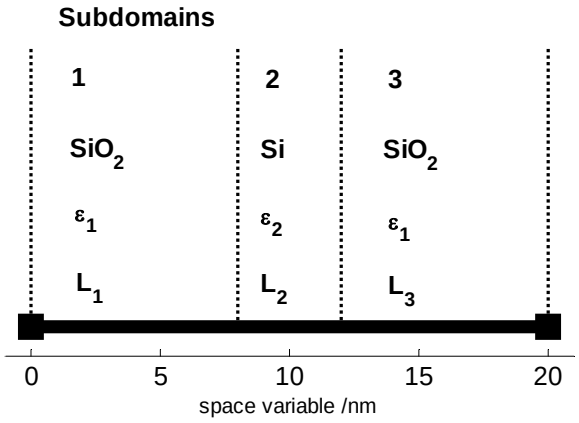

Fig. 1 Sketch of SiO_2-Si-SiO_2 system with QD. Length of the system is L = 20 nm. Varying bias between the electrodes determines the potential energy in the QD and throughout the system.

The Si nanostructure is in the subdomain 2. Its length is L_2 = 4 nm, relative permittivity ε_2 = 11.9. Subdomains 1 and 3 contain dielectric medium – the nanostructure surroundings SiO_2. Lengths L_1 and L_2 are equal, $L_1 = L_2$ = 8 nm, relative permittivity ε_1 = 3.2. The lower (left) and upper ends of the whole system are equipped with metallic electrodes. The left electrode (+) is taken as reference point. The potential barrier between Si and SiO_2, representing the electron affinity difference, is U_0 = 3.9 eV.

2.1. Physics

Potential distribution $V(x)$ in the system is governed by the PE:

$$\nabla \cdot (c \nabla V) = \rho \,, \tag{1}$$

with $c = \varepsilon_{rel}\, \varepsilon_0$ and $\rho = 0$.

The boundary conditions are $V_1 - V_2 = V_{appl}$, where $V_1 = V(x=0)$ and $V_2 = V(x=L)$ are the electrode potentials; V_{appl} is the varying applied bias.

The potential distribution and the QD surface barrier determine the potential energy of an electron throughout the entire system and thus the band diagram.

The quantum properties of the system are governed by the SchE:

$$-\frac{\hbar^2}{2m}\Delta\psi + U\psi = E\psi \tag{2}$$

where m is mass of the electron, in Si including its effective mass. The potential energy of an electron, $U = qV(x) + U_0$ is obtained with help of (1). The potential barrier is equal to zero inside the QD (subdomain 2). The boundary conditions are $\psi(x=0) = \psi(x=L) = 0$. The model with the two differential equations, PE and SchE, and their boundary conditions is referred to as Poisson-Schrödinger 1D model. In this manner, Physics has introduced a Math problem.

2.2. Numerical

The Math problem has been solved using FEM method. The meshing process and matrices manipulation are performed smoothly in Comsol Multiphysics program. Number of mesh elements used for each applied bias is 120, degrees of freedom are 241. We have chosen the direct Choleski solver, time required for six energy eigenvalues and corresponding number of eigenfunctions determination is less than 0.1 s.

The numerical part of our problem seems to be straightforward and relatively simple. Solutions of more sophisticated nanostructures of higher dimensions will probably require more laborious approach. In the analysis, there is no need for the wave function normalization, since only the peak of probability function position, x_p, is traced. Selected results are shown in Fig. 2 below.

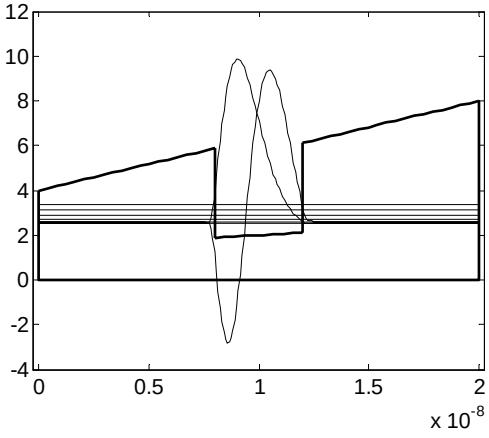

Fig. 2 The band diagram of the nanostructure. The potential energy is drawn in a thick line. Six lowest energy levels are indicated by fine horizontal lines. Wave functions ψ_1 and ψ_2 are attached to levels E_1 and E_2. Energy scale is given in eV units; wave functions are given in arbitrary scale. External bias is 4 V.

3. RESULTS

The results of numerical evaluation are used to visualize the evolution of the band diagram, the ground energy state and the probability function with increasing electric bias. At a characteristic bias the probability function distinctly changes its space location, "jumps" to the control electrode. It indicates that the electron, its location being described by the probability function, has abandoned the QD. We can say, that the DQ changed its state from occupied (charged) to empty (discharged). The characteristic bias is the emission (discharge) bias. The process has a potential application in quantum computing.

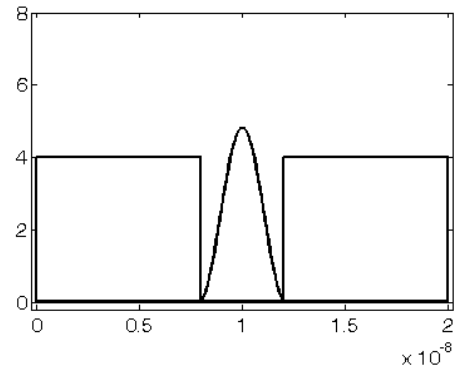

Fig. 3 Band diagram of the QD without external bias. Ground state energy E_1 = 23.66 meV, maximum of probability function $\psi\psi^*$ at x_p = 10.0 nm.

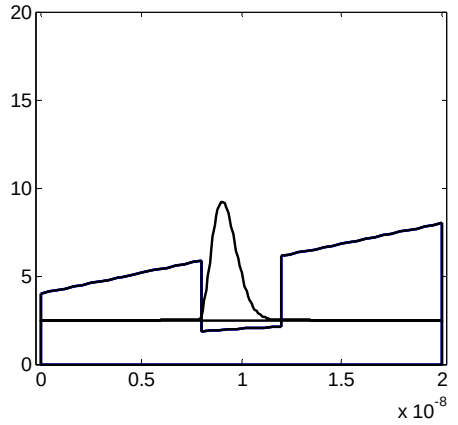

Fig. 4 Band diagram and probability function of the QD. External bias V_0 = 4 V. E_1 = 2.5 eV, x_p = 9.083 nm. Vertical (energy) axis is in eV units.

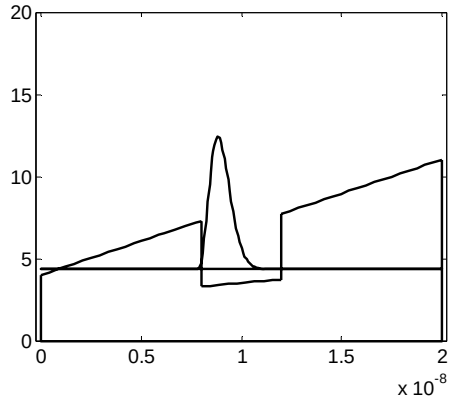

Fig. 5 Band diagram and probability function of the QD. External bias V_0 = 7.02 V. E_1 = 4.347 eV, x_p = 8.833 nm.

Remarkable displacement of the probability function takes place as the bias slightly increases:

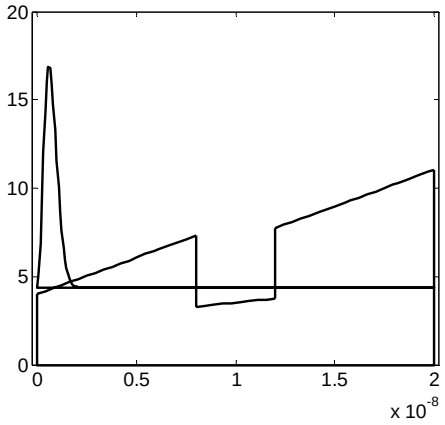

Fig. 6 Band diagram and probability function of the QD. V_0 = 7.04 V. E_1 = 4.3514 eV, x_p = 0.5833 nm. Electron has abandoned the dot region and reached the electrode.

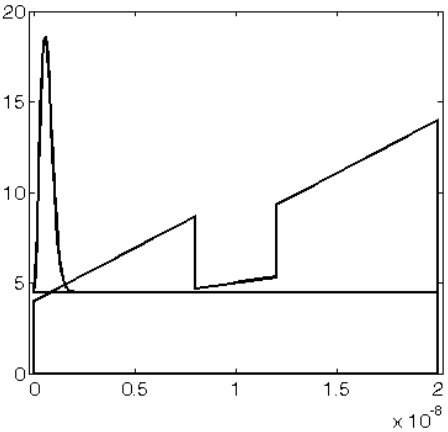

Fig. 7 Band diagram and probability function of the QD. V_0 = 10 V. E_1 = 4.4707 eV, x_p = 0.583 nm. Electron has reached the electrode.

To summarize data, obtained in Poisson-Schrödinger 1D analysis of a nanostructure with a Si QD, we present graphs, describing the variations of main parameters of the QD with applied bias – the ground state energy E_1 and the location of the peak of probability function x_p. An overview of the probability function variations with bias is shown, too.

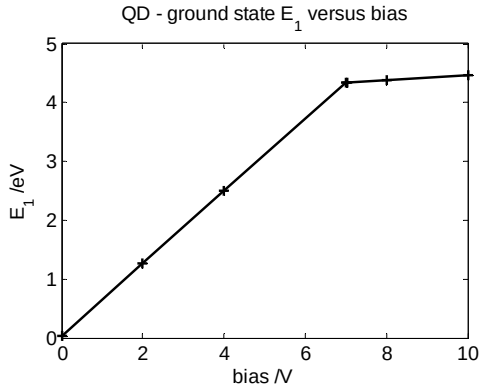

Fig. 8 Ground state energy E_1 versus applied bias.

Two values of bias (7.02 V and 7.04 V) in Fig. 8, near the line breakpoint, are the lower and upper limits of the discharging bias value. These two values also separate the regions of a curve in Fig. 9 that relates probability function peak position x_p and bias V_0.

The set of curves in Fig. 10 is obtained when calculating the probability function $\psi\psi^*$ as the bias increases from zero value by steps of one volt to ten volts. The gap between 7 and 8 volts is then recalculated with the bias step of 0.02 V. Discharging bias is thus assigned to interval (7.02, 7.04) V. The two curves are also included in the set.

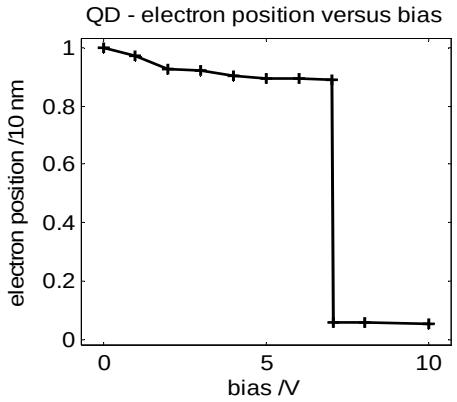

Fig. 9 Probability function peak position x_p versus applied bias V_0.

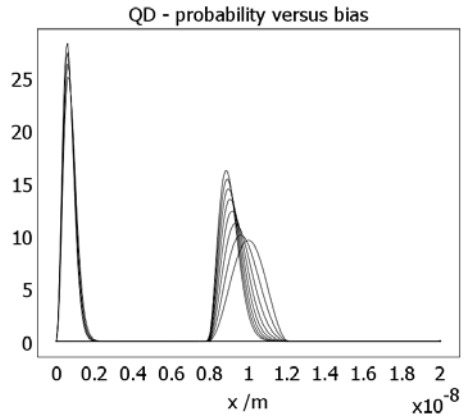

Fig. 10 Set of probability curves $\psi\psi^*$. Parameter of the set is biasing voltage V_0. It varies from zero by one to ten volts, the curve for V_0 = 7.04 V is added. Curve for V_0 = 7.02 coincides in the figure with that of V_0 = 7. 00 V.

4. CONCLUSIONS

Numerical analysis of behavior of Si QD in SiO_2 surroundings based on Poisson-Schrödinger 1D Comsol model yields extensive data. Based on the data, one can fully describe variations of the main parameters of the QD in external electric field – the ground and excited state energies and the electron probability function. The emission or discharge bias comes naturally from the data.

The original contribution of the paper is the description of behavior of the QD in electric fields and fixing the QD discharge bias value. The method applied proved to be highly efficient for this kind of QD characterization.

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BIOGRAPHIES

Pavel Hruska was born in 1937. He graduated (MSc in General Physics) at the Faculty of Science, the Masaryk University of Brno in 1960. PhD thesis "Physical Foundations of High Frequency Parameters of Tunnel Diode" defended at Faculty of Electroengineering, TU Brno in 1969. He worked as Research Technologist in Tesla-Rožnov Development Centrum. Since 1964 he is lecturer at Dept of Physics, Faculty of Electroengineering, TU Brno. He lectured and supervised laboratories at College of Sciences, Baghdad University (1975-1979). He was senior lecturer at Science Faculty, University of Addis Ababa (1984-1991). He is author and co-author of 50 Research Papers, Patents, Scientific Reports, and a series of Students' Teaching texts. Engaged in research of transport in submicron semiconductor devices, Optics and simulations of Physics phenomena.

Lubomir Grmela was born in 1958, graduated in Radio Engineering at Brno UT in 1982. PhD thesis “Stochastic processes in GaAlAs diodes” in the field of Physics of condensed materials and acoustics defended in 1988. Since 1985 he is lecturer at the Department of Physics, since 2002 Associate Professor. From 1989 to 1991 he worked as researcher with Institute of Scientific Instrument Brno, Academy of CR. He is author or co-author of 60 journal titles and 24 research reports. He is engaged in non-destructive diagnostics of semiconductor devices, being the area supervisor of research plan MIKROSYN. He participated in several EU and Czech Grants. He is Head of Department of Physics since 2002.