EMISSION OF QD IN ELECTROSTATIC FIELDS

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Abstract

The paper presents the wave functions ψ, probability functions $\psi\psi^*$ and the ground states energy of a nanostructure consisting of a Si QD embedded in SiO_2 dielectric medium, which is under bias of varying electrostatic field. Abrupt displacement of the peak of $\psi\psi^*$ at a certain field value is elucidated as the QD emission. The field distribution and the characteristics of the nanostructure quantum states are obtained with help of Comsol Multiphysics Poisson-Schrödinger 2D (PSM) model, developed by the authors.

Introduction

Quantum dots (QDs) are advanced semiconductor nanodevices, consisting of hundreds to hundreds of thousands atoms, produced by temporary top experimental techniques (molecular beam epitaxy, chemical vapor deposition). They are fabricated in many different shapes (cubes, spheres, discs, pyramids, cones and their combinations). The semiconductor nucleus or nanocrystal is usually embedded in a larger-bandgap semiconductor or a dielectric. Colloidal QD can be supplied in liquid suspensions or dispersed in a glass or plastic composites.

The QD application have been reported in many fields: as memory elements – in quantum informatics and computers, as efficient lasers, light-emitting diodes, solar cells – in modern electronics, as biological sensors and optical tags – in biology, detectors of explosive – in criminalistics. Promising results have been obtained in medicine with tumor targeting and others [1].

1 Quantum states of nanostructures

The behavior of QD is described by Quantum mechanics. Energy levels are discrete, strongly determined by the QD size and shape and probability of electron location is proportional to the square of the wave function amplitude. The QDs can be viewed as tunable artificial atoms.

Properties of QDs are under permanent study of researchers for several years. Numerical analysis of GaAs-InAs nanostructure with conical QD was performed by Melnik and Wilatzen in 2004 [2]. They applied FEM method available in COMSOL program. Deleruyelle et al. used COMSOL in 2007 and obtained 1D band diagram with probability function of the ground state at several biasing fields. They did not attempt to estimate the emission field value – the significant QD characteristic parameter [3]. The authors of the present paper performed numerical analysis of electron traps in paper [4].

The present paper is devoted to the numerical analysis of a circular Si QD. A 2D Poisson-Schrödinger COMSOL Multiphysics model was developed and solved. The results, including the emission bias value are presented and discussed.

1.1 Nanostructure

The nanostructure under investigation is sketched in Fig. 1. The rectangular nanostructure in *xy* plane is 12 nm long and 4 nm wide. The radius *R* of the circular Si QD is 1 nm, the centre is at 7/12 of the nanostructure length. Relative permittivity of Si is 11.9. The QD is surrounded by insulating medium SiO_2 with relative permittivity of 3.9.

The potential barrier between the QD and its surroundings is 3.2 eV. It is result of different electron affinities of Si and SiO_2. Effective electron mass is $m_{eff} = 0.9$.

1.2 Electrostatic field

Electrostatic field is applied to the nanostructure between edges **a**, **b.** It points from edge **a** (grounded) to edge **b**. The bias of the field is $V_{ab} = V_a - V_b$.

The field distribution obeys the Poisson Equation (PEq)

$$-\nabla\cdot(c\nabla u) = \rho \qquad (1)$$

Dependent variable u is electrostatic potential, $c = \varepsilon_{\mathrm{rel}} \times 8.852\times10^{-12}$ F/m and $\rho = 0$.

Boundary conditions at edges **c, d** are of the von Neumann type, indicating insulation, at edges **a**, b are of the Dirichlet type, indicating applied bias V_{ab}.

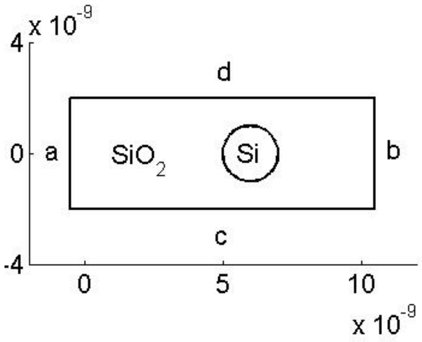
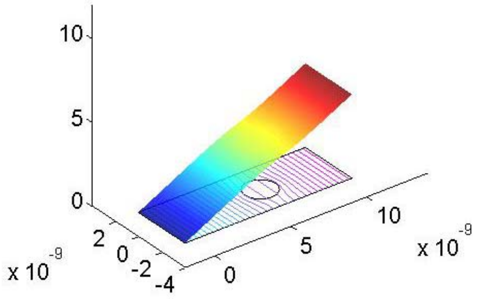


Fig.1. A sketch of the nanostructure including the Si QD. Electrostatic field points from edge **a** to edge **b.** Edges **c**, **d** are insulated. Sketch is in *xy* plane.

Electron potential energy is $\mathcal{E}_{\mathrm{pot}}$ = - e × potential. To consider the Si-SiO$_2$ potential barrier U_0, we have to use a modified potential function, where the factor in parentheses is treated by Comsol as logical function

$$uu = u - U_0/\mathrm{e}^*(1- ((x - 6\mathrm{e}\text{-}9)^2 + y^2 < R^2)) \qquad (2)$$

Graphs of potential energy distribution numerically obtained in PSM are drawn in Fig.2, and Fig.3, in terms of functions *u* and *uu,* resp.



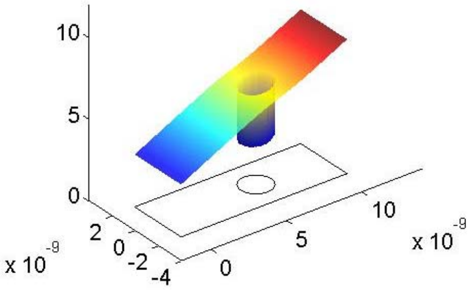


Fig.2. Product – $e\times u$ (in eV) within the nanostructure at bias V_{ab} = 5V, V_{a} = 0V. In the QD region, the effect of high relative permittivity of Si is observable.

Fig.3. Electron potential energy $E_{\mathrm{pot}} = - e\times uu$ (in eV). Bottom of the Si QD conduction band is at the bottom of protruded cylinder, indicating the potential barrier between Si and SiO$_2$.

1.3 Quantum states, wave and probability functions

Energy of the quantum states and corresponding wave functions are obtained with the use of the Schrödinger Equation (SchE).

$$\hat{H}\,\psi = \mathcal{E}\,\psi \qquad (3)$$

Quantum Hamilton's operator is $\hat{H} = -\dfrac{\hbar^2}{2m}\nabla^2 + \mathcal{E}_{\mathrm{pot}}$, $\mathcal{E}$ is total energy of the quantum state and ψ the wave function of the electron at this state.

Boundary conditions are: at **a**, **b** $\vec{n}\cdot(\nabla\psi)=0$ (von Neumann)

at **c**, **d** $\psi = 0$ (Dirichlet).

Probability d*P* of the particle location in space element d*V* is d*P* = $\psi\psi^*$ d*V*, the probability function $\psi\psi^*$ thus being the volume probability density. It is a real function. Its maximum coincides with the maximum of the wave function amplitude $|\psi|$. Displacement of this maximum may be related, in our case, to the particle displacement.

2 QD under bias of electrostatic field

Behavior of the QD was analyzed by applying potential difference V_{ab} at the nanostructure edges, as explained above. Wavefunctions at two selected electrostatic fields, 5V and 6V, respectively, are visualized in Figs. 4 and 5 along the vertical axis, with the ground energy levels (3.1573 eV and 3.4630 eV, respectively), and in terms of contours in *xy* plane. Since the figures serve only as illustration, there was no need for wavefunctions normalization. The corresponding band diagrams (slant surface with protruded cylinder indicating the electron potential energy) and the wave functions with corresponding energy of the ground states are drawn in Figs. 6 and 7.

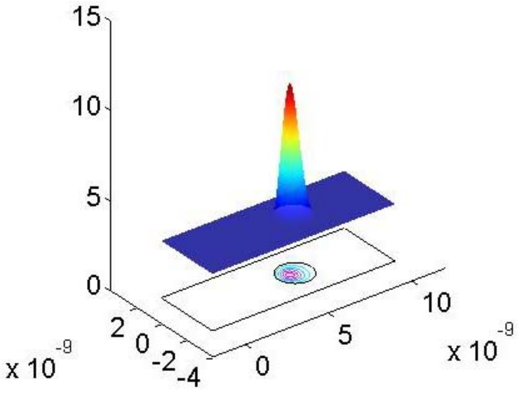


Fig.4. Energy eigenvalue E_{eig} = 3.1573 eV of the ground state and the wave function amplitude $|\psi|$ with contours. V_{ab} = 5V, not to scale.

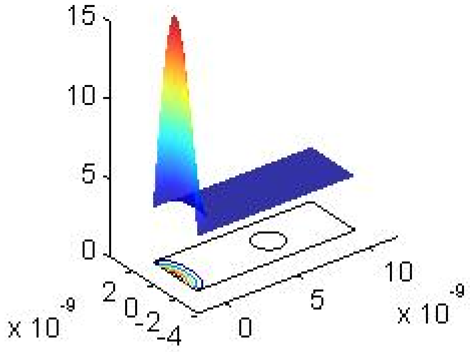


Fig.5. Energy eigenvalue E_{eig} = 3.4630 eV of the ground state and the wave function amplitude $|\psi|$ with contours, V_{ab} = 6V, not to scale.

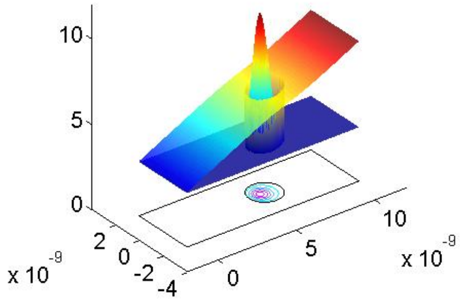


Fig.6. Band diagram of the nanostructure with energy eigenvalue and amplitude $|\psi|$ at V_{ab} = 5V, not to scale. Conduction electron resides at the QD.

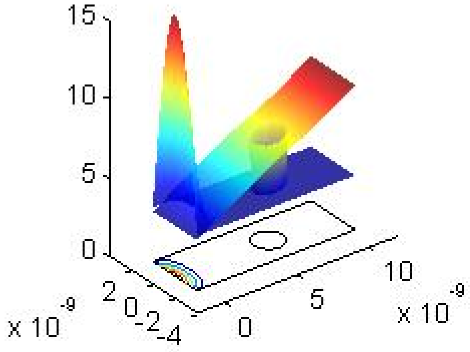


Fig.7. Band diagram of the nanostructure with energy eigenvalue and amplitude $|\psi|$ at V_{ab} = 6V, not to scale. Conduction electron has abandoned the QD.

The QD is occupied by conduction electron at 5V, Figs. 4, 6, while at 6V there is *no conduction electron* within the QD. Other electrons, if any, were emitted at bias below 5.493V.

3 Results and discussion

Electrostatic fields of varying potential bias were applied to the nanostructure, thus the potential energy function of SchE varied. It significantly affected the nanostructure parameters. The ground state and excited states energies of the nanostructure were calculated, together with the wave and probability functions. The wave function ψ or its amplitude $|\psi|$ and probability function $\psi\psi^*$ provide full information on the conduction electron location. Observing variations of the nanostructure quantum parameters versus applied bias, we were able to register miscellaneous features of the QD behavior in the electrostatic field.

Dependence of $|\psi|$ contours in jet color map versus V_{ab} bias is presented for several selected bias values in Fig.8. Another view on the maxima displacements under the bias of the field is available in Fig. 9.

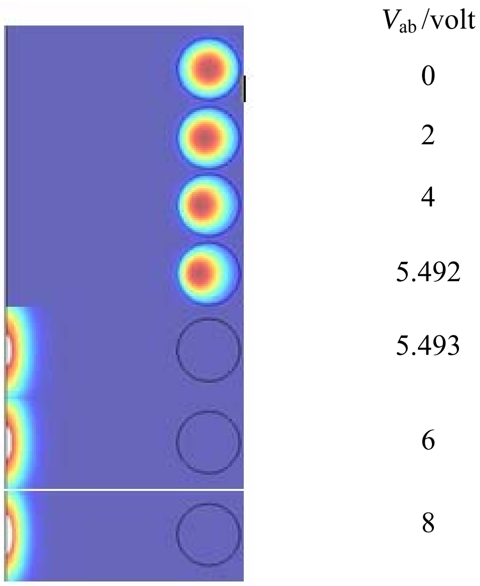


Fig.8. Projection of $|\psi|$ to x-y plane at varying field bias. A distinct change of the wave function amplitude at 5.493 V is observed.

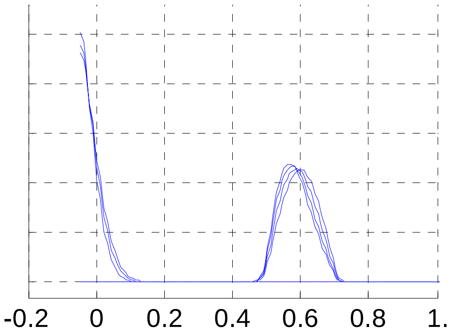


Fig.9. Cross-section of a series of functions $|\psi|$ at varying bias, V_{ab} = 0, 2, 4, 5.492, 5.493, 6 and 8V – displacement towards left.

The shape and the location of the wave function amplitude $|\psi|$ dramatically changed within (5.492V and 5.493V) bias interval. We denote $V_{emission}$ = 5.493V as the *Emission bias*.

The displacement of the peak of the wave function amplitude is indicated in Fig.10. The graph serves as a basis for the statement that the QD can occupy only one of two stable quantum states, either that for $V_{ab} < V_{emission}$ or that for $V_{ab} > V_{emission}$ (switching). In applications, it is possible to distinguish the two states with photoluminescence [6].

Very interesting results offers the set of 30 lowest energy values at eight distinct fields, drawn in Fig.11. The energy levels are discrete below U_0 = 3.2 eV, while quasi-continuous above the potential barrier. This characteristic feature reminds the energy spectra of finite quantum wells, or the Hydrogen atom, as presented in Quantum Mechanics textbooks.

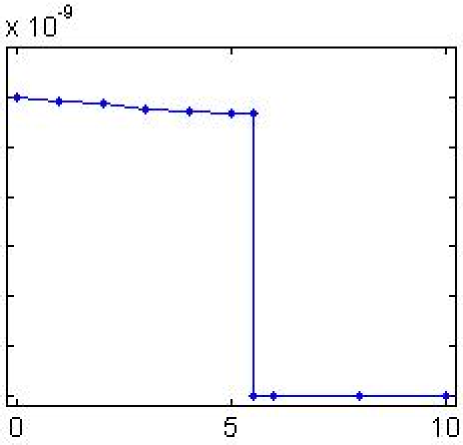


Fig.10. Location of the maximum of $|\psi|$ versus V_{ab}. Emission takes place within bias interval of (5.492V, 5.493V). $V_{emission}$ = 5.493V.

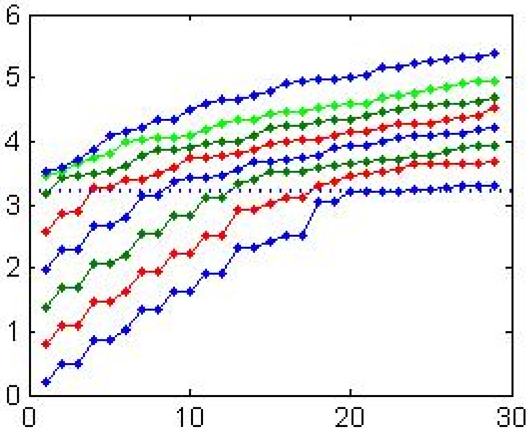


Fig.11. Eigenvalues of the Hamilton quantum operator $\hat{H}$ at V_{ab} = 0V, 1V, 2V, 3V, 4V, 5V, 6V and 6V (from bottom up). Discrete spectrum below U_0 converts into continuous one.

The following graphs are instructive for better phenomenon understanding. The band diagrams of the nanostructure at 3V and 6V are presented in Figs. 12 and 13. The conduction electron at the ground state at 3V can reside only within the QD, while at 6V it can abandon the QD by tunneling, thus be emitted to the edge **a** of the nanostructure. If electrodes are attached, it can leave the nanostructure behind.

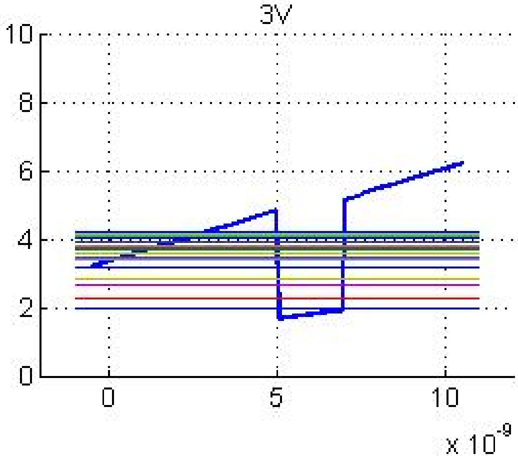


Fig.12. The band diagram of the nanostructure at bias 3V. 30 lowest energy states are indicated. The ground state can be occupied only within the QD.

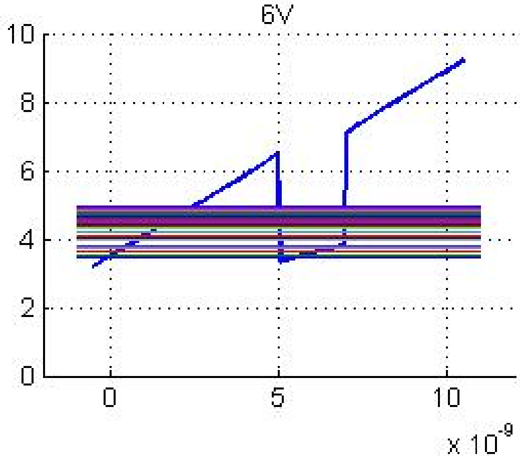


Fig.13. The band diagram of the nanostructure at bias 6V. 30 lowest energy states are indicated. The electron at the ground state can be easily emitted by the tunnel effect.

4 Conclusion

The paper deals with behavior of Quantum Dot in electrostatic fields. The authors solved the problem with application Comsol Multiphysics program. They developed 2D Poisson-Schrödinger model, performed numerical calculation and obtained a series of QD parameters dependencies on applied bias, presented mainly in graphical form with comments. Among other parameters, the emission field bias was determined. It sharply separates two stable quantum states of the QD - with and without conduction electron.

Acknowledgments

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BIOGRAPHIES

P. 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.

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