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Cross Validation of Quantum Simulations and Optical Measurements in Single Electron Memories with Silicon Nano-crystallites

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Abstract

Quantum simulations of Single Electron Memories (SEM) have been performed on single nano-crystals, axisymetrical and far enough from their neighbors to allow Poisson and Schrödinger equations to be solved in polar coordinates. The variations of the transition energies with respect to the shape of the dots is discussed , arriving to the conclusion that the major dependency is with respect to the volume of the dots, while the tunneling current depends more on their flatness. For the first time, numerical simulation results are cross checked with photoluminescence and absorption measurements in silicon quantum dots.

1 – INTRODUCTION

Due to the rapid development of nanotechnologies to explore innovative solutions for the replacement of MOS technologies, there is nowadays a strong demand to investigate quantum effects in silicon nanodevices, and to improve device simulators accordingly. Indeed, an accurate prediction of tunneling current through dielectric layers is nowadays mandatory to support the design of new memory architectures. With single electron memories using nanocrystallites, this prediction can not be achieved without an accurate simulation of quantum levels in the dots. Unfortunately, the experimental validation of simulation results is more hazardous in silicon than in III-V devices [1], mainly because of the poor photonic properties of silicon, and the spreading of dot sizes on a wafer, even with state of the art technologies. Therefore, in order to cross check numerical simulations with not too noisy measured data, we had to consider both direct and indirect gaps in silicon.

2- NUMERICAL MODEL

For solving the Schrödinger equation for electrons over an axi-symetrical structure, a special attention has to be paid to effective masses in the 3 valley pairs of silicon. Lets denote (r,θ,y) the 3 coordinates in a cylindrical coordinate system, m_l and m_t the longitudinal and transverse effective masses for electrons in silicon (m_l=0.98m_0, m_t=0.19m m_0). While one ellipsoid pair has its greater radius towards the symmetry axis (y), and therefore is seen identically whatever the θ value is, the 2 other pairs are not. However, in order to solve the equation in a 2D coordinates system (r,y), we have checked that using a unique ellipsoidal shape for these 4 valleys was valid, and that the 2 masses could be chosen as : m_y=m_t in the y direction , and $m_r = \sqrt{m_l m_t}$ in the r direction. With these assumptions, the Galerkin formulation of Schrödinger equation simply reads:

$$\iint\left(-\frac{\hbar}{2m_r}\frac{\partial\psi}{\partial r}\frac{\partial w}{\partial r}-\frac{\hbar}{2m_y}\frac{\partial\psi}{\partial y}\frac{\partial w}{\partial y}+(E-V)\cdot\psi.w\right)r\,\partial r\,\partial y$$
$$+\oint_\Gamma r\frac{\hbar}{2m_n}\frac{\partial\psi}{\partial\nu}\cdot w\cdot\partial\Gamma=0$$

for any test function w in a suitable Hilbert space, where denotes the eigen energy, Ψ the corresponding eigen vector (wave function), Γ denotes the set of boundaries and interfaces of the domain, and ν is the normal direction to Γ. Classical boundary and interface conditions, i.e. continuous or vanishing probability current towards ν lead the surface integral over Γ to vanish (so-called "natural" boundary conditions); 3-nodes triangular finite elements have been introduced in order to fit with the shape of the dots. In contrast with the finite difference method, this technique leads to an eigenvalue problem with 2 matrices. In a previous work ([2]) we used a mass lumping technique to force the second matrix to be diagonal. This is less convenient in the present situation, where polynomials up to 4th degree with respect to r have to be integrated over the elements.

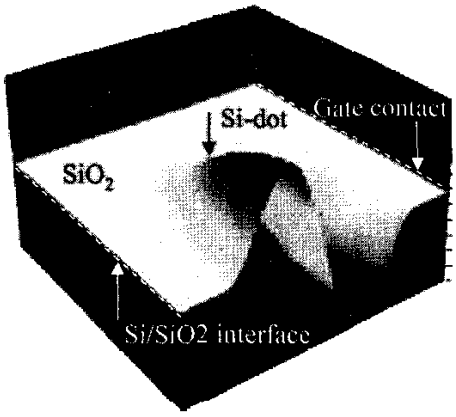

Figure 1. Exemple of wave function plotted in a meridian cross section of a spherical dot. This wave function corresponds to the 2nd eigen energy level in the valley perpendicular to the interface. Dot radius = 3nm.

3- QUANTUM LEVELS

With the numerical model described above, we carried out simulations of isolated silicon nano-crystallites of various shapes: cylinders, spheres and disks, in order to analyse the impact of the volumes and aspect ratios on the quantum band width. An example of wave function is given in figure 1, which corresponds to the second quantization level of electrons in a spherical dot with a radius equal to 3nm.

3-1 Cross checking simulation and optical measurements

The validation of quantum levels was performed on silicon dots fabricated either from re-crystallisation of SiO_x layers (sample #1, x=1.6, sample #2, x=1.8 [3]) or by silicon implantation (sample #3 [4]).

In order to cross check simulation results with optical measurements, i.e. photon absorption and photo-luminescence, both direct and indirect gaps have been considered. Indeed, measured absorption profiles are very noisy in the indirect gap of silicon (fig. 2). Following Nakajima [5], the absorption of photons can be related to the quantum gap E_g by the expression: $\alpha h\nu \sim (h\nu - E_g)^{\gamma}$ where α is the measured absorption ratio, h is the Planck constant, ν is the wave number, $\gamma=1/2$ in the direct gap and $\gamma=2$ in the indirect gap.

Simulations in the direct gap were performed by introducing one single equivalent valley for electrons with a unique effective mass equal to 0.2. Hole parameters were kept unchanged.

According to absorption profiles, larger oxygen ratio in the deposited SiO_x material leads to higher transition energy (i.e. distance between the higher sub-band for holes and the lower sub-band for electrons). This is consistent with the assumption that dot size is smaller and therefore quantum confinement is stronger for larger oxygen ratios in SiO_x.

Figure 3 depicts comparisons between the transition energies obtained after

(i) 2D axi-symetrical Poisson-Schrödinger simulations,

(ii) linear fits on absorption curves, and

(iii) photoluminescence spectra.

For both direct and indirect gaps, an overall agreement was achieved between the different data : the mean dot sizes extracted from TEM : 4nm for sample #1 (σ=0.7nm) and 3nm for sample #3 (σ=1.7nm), are consistent with simulation results.

When a SiO_x layer is annealed to form nanocrystals, the available silicon volume is twice larger with $SiO_{1.6}$ than with $SiO_{1.8}$. Assuming that the number of nanocrystals does not depends on x , it can be expected that, accordingly, the radius of Si-dots is 26% larger with $SiO_{1.6}$. A reduction of the direct gap has been obtained from both absorption measurement (fig. 2) and simulations (fig. 3), with consistent values around 0.2 eV. It means that this reduction can definitely be attributed to quantum confinement rather than eventual traps in the dielectric layer or at Si/SiO_2 interface. On the other hand, the absorption profiles in the indirect gap look inconsistent with other results. This is explained by the weakness of the optical signal which can not to be used seriously in this case for the determination of the transition energies.

3-2 Impact of the shape of nano-crystals

Simulations were performed with spherical dots and cylindrical dots having either an equal radius (2nm in fig. 4), or an equal volume ($50nm^3$ in fig. 5), but different aspect ratios. It comes out that the quantum confinement in a cylinder reaches its minimum when the aspect ratio value (diameter/height) is 1; confinement is even weaker for spheres. Fig. 5 provides quantitative information on the band widening resulting from high aspect ratios. A 0.1eV shift is observed for a ratio equal to ¼ or 4,

meaning that the aspect ratio has a weaker impact on transition energy than the size.

The impact of the number of stored charges in the dot on the gap width has been also carefully checked : both electron and hole quantum levels are shifted together, that makes the gap very weakly sensitive to this number.

4- TUNNELING CURRENTS

In the present work, a very simple expression of discharge current has been used: the tunneling current was integrated along each mesh line perpendicular to the collecting surface (supposed to be flat) by using the 1D WKB model introduced by Register [6]. This is obviously a very rough approximation in the case of spherical dots, but the results show that the current decreases so quickly apart from the symmetry axis that it remains valid as far as we just need orders of magnitude. In the case of cylinders or flat disks, this model is obviously much more appropriate, the misfit arriving only from the defocusing current lines at the periphery of the dots. Simulation results depicted in fig. 6, with minimum thicknesses of the tunnelling layers equal to 0.5nm and 2nm, predict a much higher discharge current in cylindrical dots that in spherical dots, in agreement with results published elsewhere [7]. In spherical dots, and with respect to cylindrical dots, the tunneling current has been found all together smaller on the symmetry axis and dropping down more quickly apart from this axis. This smaller current on the axis is mainly caused by a smaller electric field (factor 4 in the example depicted here).

5- CONCLUSION

The impact of shape and size in quantum dots on transition energies as well as on tunnelling currents has been highlighted thanks to 2D axisymmetrical self consistent Poisson-Schrödinger simulations. Both direct and indirect gaps in silicon have been considered in order to carry out a better comparison between simulations and optical measurements.

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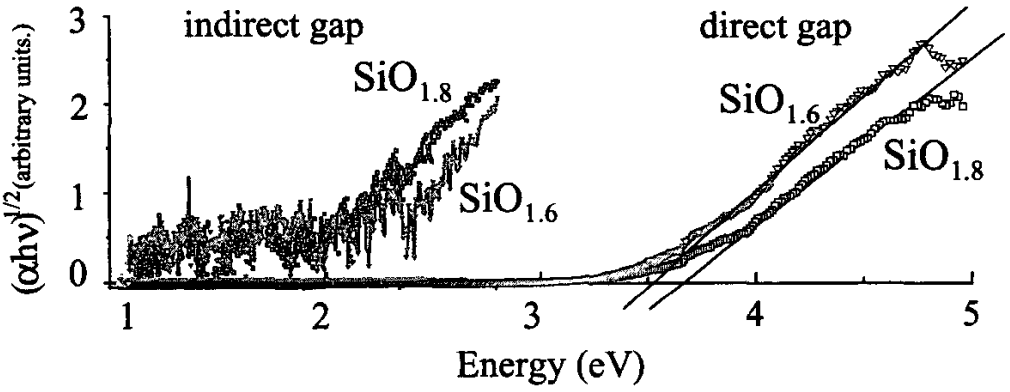

Figure 2.

Measured absorption curves in the direct and indirect gap of silicon from which transition energies are extracted.

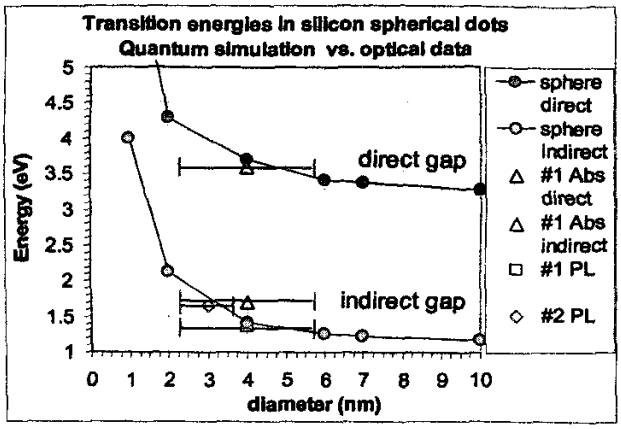

Figure 3. Simulated transition energies for spherical quantum dots, in both direct and indirect gap, compared with experimental data: absorption curves (Abs) and Photoluminescence spectra (PL). Mean size of measured dots extracted from TEM pictures.

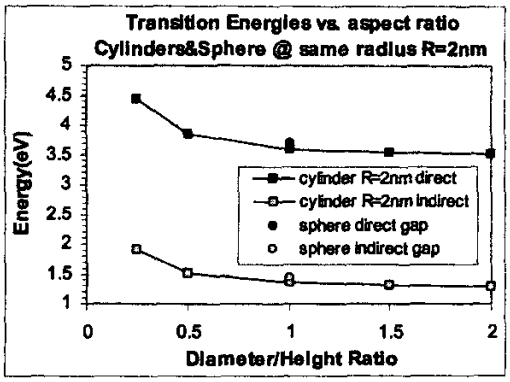

Figure 4. Simulated transition energies for cylindrical quantum dots with various heights but a fixed radius=2nm, in both direct and indirect gap. Comparison with spherical dot of same radius

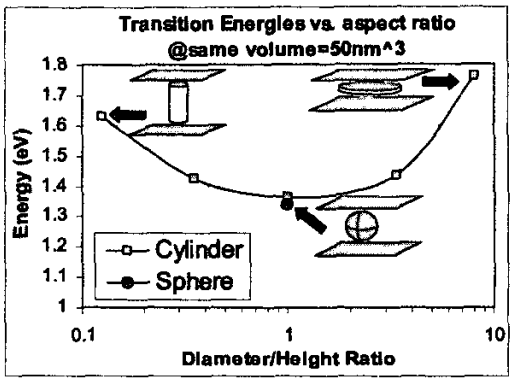

Figure 5. Simulated transition energies for cylindrical quantum dots with various radius/height ratios, but a fixed volume=50nm^3. Comparison with spherical dot of same volume

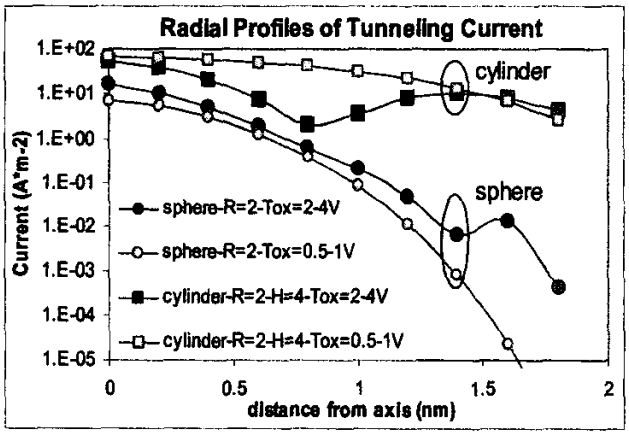

Figure 6. Tunneling current profile along radius for spheres and cylinders. Diameter=height=4nm Tox=Minimum oxide thicknesses, Vg=Gate voltage. Dark symbols : (Tox,Vg)= (2nm,4V), open symbols : (Tox,Vg)= (0.5nm, 1V)