SAND2012-5231C

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Simulations of Structures for Coupled Double Quantum Dots using QCAD

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INTRODUCTION

We study a number of electrostatically defined Double Quantum Dot (DQD) structures by computer simulations using the Quantum Computer Aided Design (QCAD)[1] toolkit. The intent is to improve the design of coupled, electrostatically defined, DQD structures, prior to their construction.

STRUCTURE CONSTRUCTION

Actual layouts and SEM images are used to define the structures. The shapes and locations of electrodes, contacts, and special analysis regions are defined using a customized digitizer. See Figure 1. Key information is stored in a mask file.

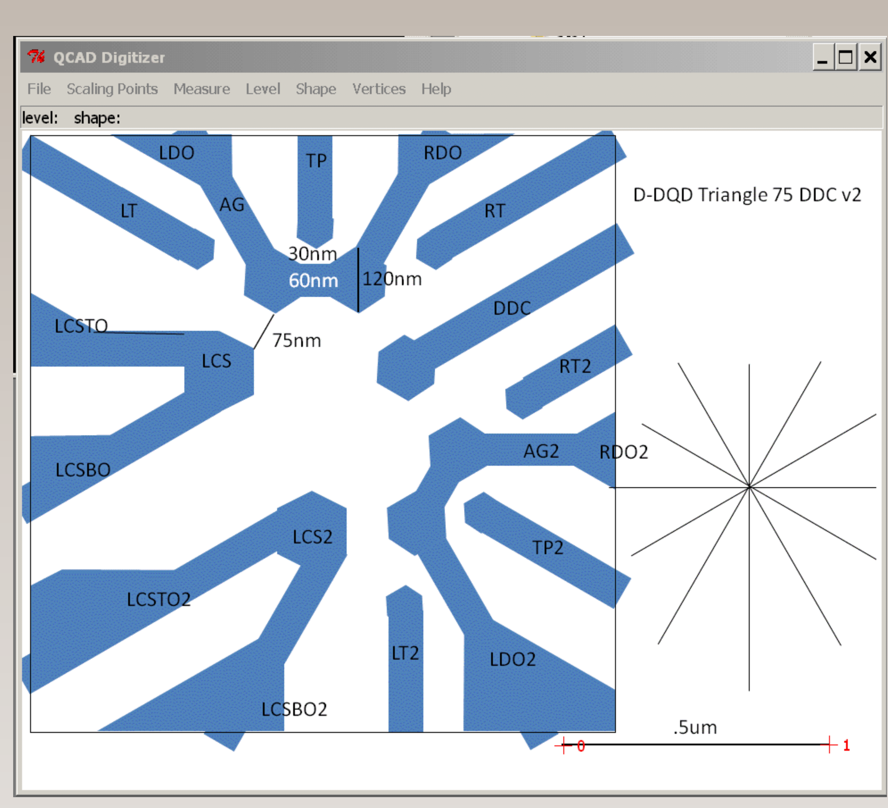

Figure 1. QCAD Digitizer showing the layout of coupled DQDs with charge sensors.

Process emulation using Sentaurus Structure Editor[2] of the actual process steps used to build the device is done to construct a solid model of the three dimensional structure. During this step, information is added to the mask file which is used later to automatically identify and locate the electrodes and material volumes in the structure.

The solid model is then meshed using the Sandia code CUBIT. Materials are properly identified and boundary conditions and analysis regions are automatically prepared as part of the meshing.

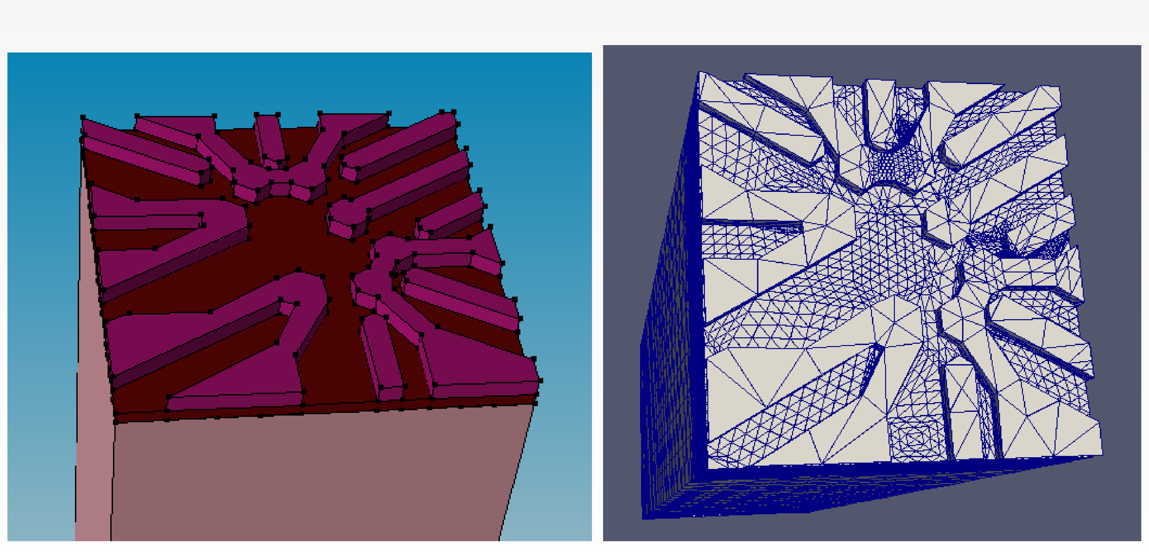

Figure 2. Left: Solid model made by process emulator. Right: CUBIT mesh.

ELECTROSTATIC SOLUTION

We use the Poisson solver in the QCAD toolkit to solve the electrostatic potential as bias voltages are applied to the contacts and electrodes. Electron density is also calculated at each node in the mesh. Structures are first made accessible to modelers and experimentalists using iQCAD, a web-based simulator. Subsequently, gate voltages are optimized using Dakota and the RedSky super computer for the formation of few electron quantum dots and the nearby potential barriers used to isolate the dots from the 2 Degree of Freedom Electron Gas (2DEG). Dot to dot and DQD to DQD coupling is also studied.

GATED WIRE STRUCTURE

Figure 3 shows how the QCAD simulations were used to improve the design of a gated wired structure of a single DQD with a charge sensor. This structure uses a positively biased polysilicon accumulation gate to create electron charge at the silicon dioxide/silicon interface. Nearby polysilicon depletion gates are biased negatively to form the charge into two isolated dots.

A possible explanation for the difficulty the experimentalists had in forming two isolated dots is illustrated in the left plot. Because of the long thin shape of the electron density in the dot regions it is difficult to separate the dots from each other and from the 2DEG. When negative biases are applied to the depletion gates (the three electrodes above the wire) the electron density in the wire is depleted too uniformly without leaving localized charge in the dot regions. To help remedy this problem widened regions were introduced in the gated wire accumulation gate where the dots are intended to form, as shown in the right plot in Figure 3. The simulation shows that wider electron charge regions form in the dot regions as intended.

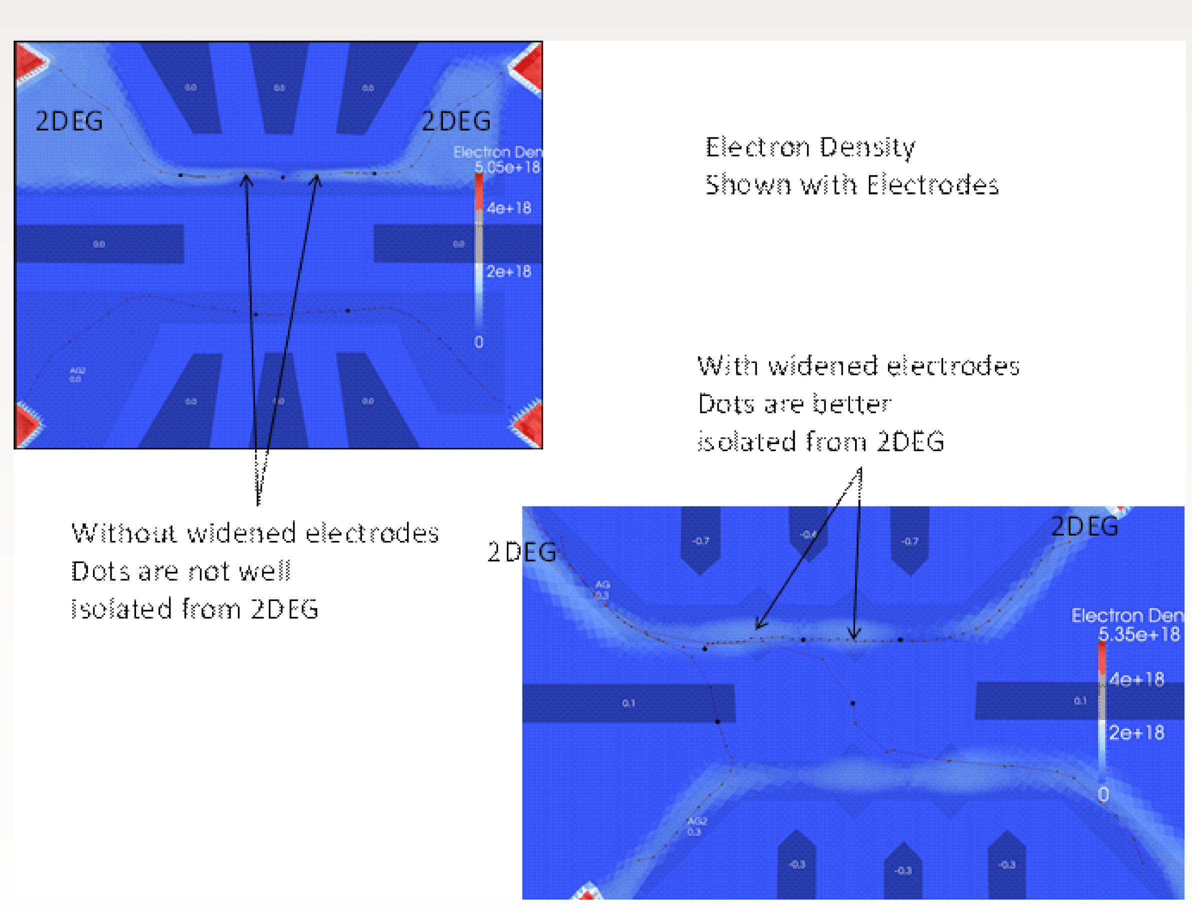

Figure 3. Simulations of a gated wire structure. Left: Simulation explains difficulty forming 2 isolated dots. Right: Simulation proposing widened dots.

Based on these simulations a number of electron beam defined patterns were designed and fabricated in a short loop experiment. The most promising of these is shown in Figure 4. A full structure with this pattern is under construction.

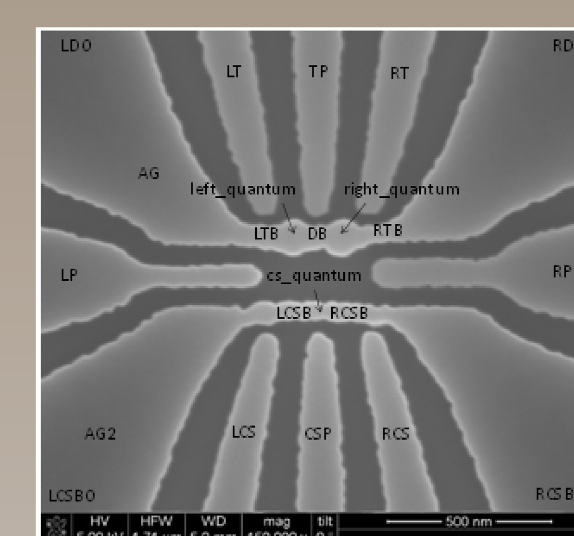

Figure 4. SEM of the gated wire structure with widened dots.

COUPLED DQDS WITH CHARGE SENSORS

The challenging goal of designing two coupled DQDs with charge sensors was undertaken. In order to facilitate routing of all the necessary connections to a small area, a triangular design was proposed. Each of the two DQDs occupies one side of a triangle. The third side is taken up by the two charge sensors. Widened regions in the accumulation gates are used to form the four quantum dots and the two charge sensor dots. We hope to do without extra depletion gates which might be used to isolate the charge sensor dots by careful design of the shape of the charge sensor accumulation gates.

An example of the triangular design is shown in Figure 5. The DDC gate can be used to turn the inter DQD coupling on (positive bias) or off (zero bias).

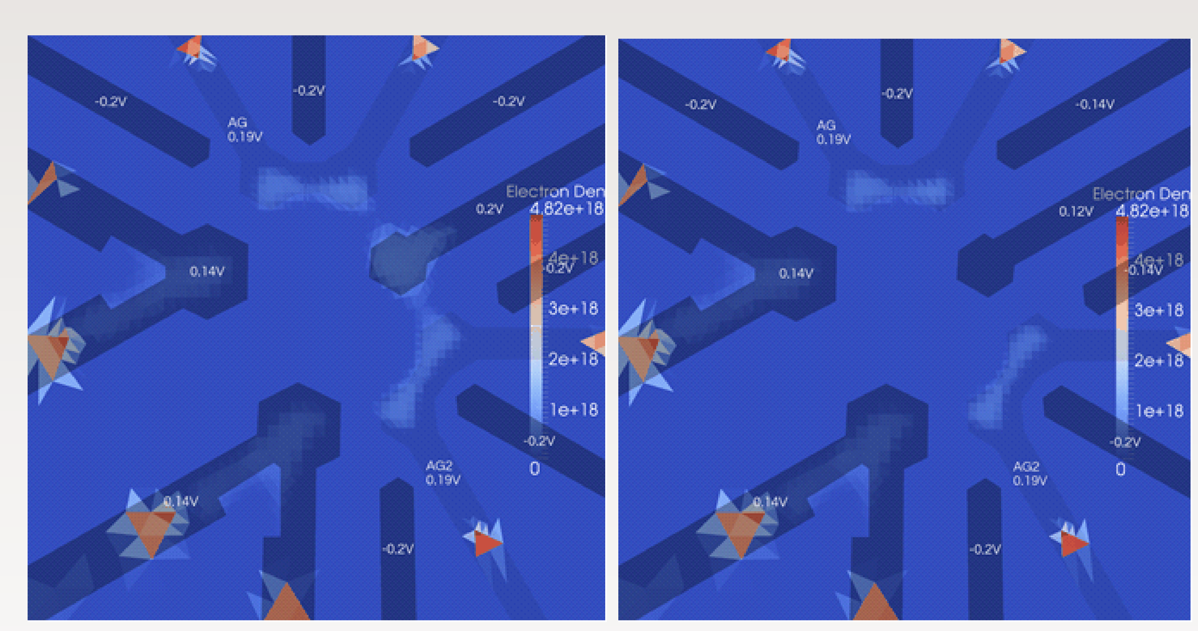

Figure 5. Simulation of two coupled DQDs with charge sensors. Left: DQD to DQD coupling on. Right: DQD to DQD coupling off.

Simulations of improvements in the charge sensor design are underway.

[1] S. Gao, E. Nielsen, R. Muller, R. Young, A. Salinger, and M. Carroll, "The QCAD Framework for Quantum Device Modeling," *15th International Workshop on computational Electronics*, poster, (2012).

[2] Synopsys, Inc.

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Adiabatic quantum architectures in ultracold systems