A Comparison of Electrostatic Simulations to Measurements of Quantum Dot Structures

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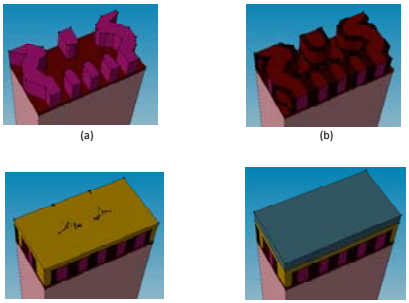
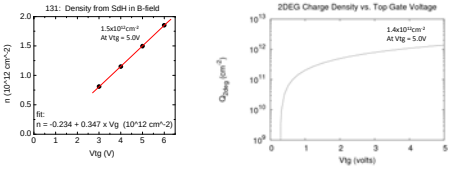
We compare measurements with electrostatic simulations of the double quantum dot structure shown below: (a) poly depletion gates, (b) poly reoxidation, (c) Al2O3 deposition, (d) Al top gate deposition

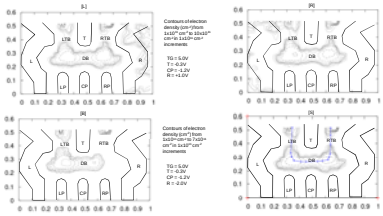


(a) (b) (c) (d)

The simulated 2DEG charge density is compared to measurements below. Good agreement is observed.



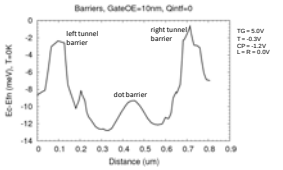
The following bias conditions were used for capacitance comparisons. [L] is designed to favor the left dot, [R] the right dot, and [B] was an empirical attempt to balance the conduction at the left and right tunnel barriers. Note that [B] is not symmetric suggesting that the actual device has a built in asymmetry.



gate - dot	Cmeas	CFD-Ace	Sentaurus	Sentaurus	
	aF	aF	aF	electrons	
LD				283	[L]
TG-LD	27	22.4	14.5		[L]
T-LD	8	8	9.2		[L]
L-LD	17.3	17.2	34.4		[B]
LP-LD	8.1	8	9.4		[B]
CP-LD	6	5.9	6.1		[L]
RP-LD	1.5	1.6	1.6		[B]
R-LD			0.3		[L]
RD				252	[R]
TG-RD	18	18.9	12.9		[R]
T-RD	7	7	8.8		[R]
L-RD			0.1		[R]
LP-RD	1.6	1.2	0.7		[B]
CP-RD	5	4.9	5.3		[R]
RP-RD	5.3	5.5	3.3		[B]
R-RD	11.6	11.5	4.6		[B]
	B: Double dot transport: TG=5.0, T=-0.3, CP=-1.2, R=-2.0V				
	L: TG=5.0, T=-0.3, CP=-1.2, R=+1.0V				
	R: TG=5.0, T=-0.3, CP=-1.2, L=+1.0V				

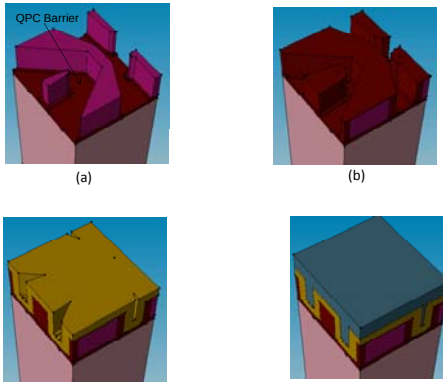
The Sentaurus columns above are electrostatic simulations solving Poisson's equation with no adjustable parameters. CFD-Ace results are solutions of Laplace's equation where the dot shapes are adjusted to make the capacitances agree with the measured values. The discrepancies between Sentaurus and measurements are indicative of the local variations which caused the asymmetry previously noted.

Figure [S] above is similar to [B] but with symmetric biasing. The figure below is a cut along the blue line in [S] showing the conduction band shape in the region of the three barriers.



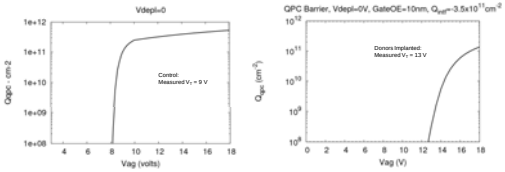
$$E_C = E_{Fn} - (.025852eV)\left(\frac{n}{2.42\times10^{19}cm^{-3}}\right)^{\frac{2}{3}}$$

The second structure we examined is shown next. Only the west half of the structure is shown in the figure. In this case we focused on the QPC barrier position. 10-20 donors were implanted at the QPC barrier position on the west side of the structure, while no donors were implanted at the QPC barrier position on the east side of the structure.

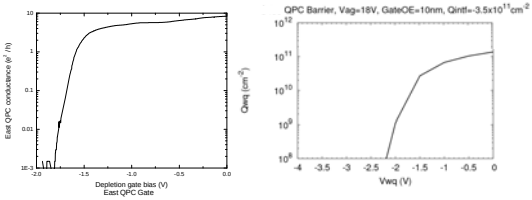


(a) (b) (c) (d)

The top gate threshold voltage for conduction through the east QPC barrier (no implant) was simulated and compared to the measurement with good agreement. See the left figure below. However, on the west (implanted) side, the conduction threshold was measured to be around 13 V. An interface charge of 3.5×10^{11} cm^{-2} had to be introduced in order to approximate this threshold shift (right figure below). It is not expected that the implant itself could cause this shift. As in the previous structure, an unexplained variation from one side of the structure to the other is apparent.



The east QPC conductance vs. the bias on the east QPC gate was measured and is shown below on the left. The simulation shown below on the right also shows that a bias of -2V turns off the conduction.



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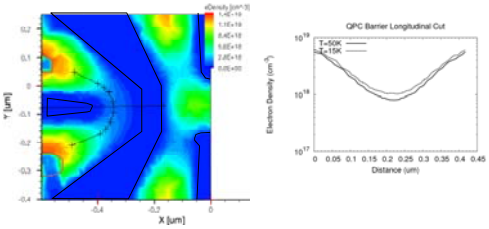
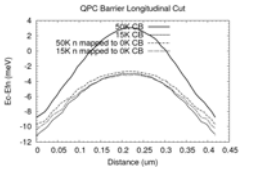
APPROXIMATION OF 0 KELVIN BARRIER SHAPE

One of the concerns with the electrostatic simulations is that a temperature in the range of 1 Kelvin or below, where the measurements are done, cannot be simulated using the commercial software. 50 Kelvin can be routinely simulated, and we were able to simulate as low as 15 Kelvin using extended precision. We did a simulation study to understand the error due to the difference between the simulated and measured temperatures. Taking a cut through the QPC barrier shown below on the left, we plotted electron density and conduction band simulated at 50K and at 15K. It was seen that the charge does not change much as the temperature is lowered. See below on the right.



However, the conduction band, shown below , does change appreciably as the temperature is decreased.



$$E_C = E_{Fn} - (.025852eV)\left(\frac{n}{2.42\times10^{19}cm^{-3}}\right)^{\frac{2}{3}}$$

To approximate the low temperature conduction band we use a 0 Kelvin Fermi-Dirac distribution, which is a step function.

$$n = N_C(T)\frac{2}{\sqrt{\pi}}F_{\frac{1}{2}}\left(\frac{E_F - E_C(T)}{kT}\right)$$

For $T \to 0$

$$F_{\frac{1}{2}}(\eta_F) = \int_0^\infty \eta^{\frac{1}{2}}\left[1 - H(\eta - \eta_F)\right]d\eta$$

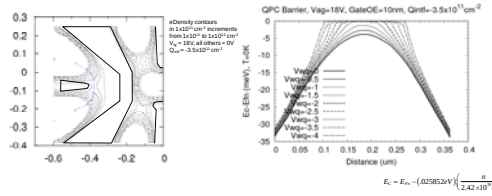
$$F_{\frac{1}{2}}(\eta_F) = \int_0^{\eta_F} \eta^{\frac{1}{2}}d\eta = \frac{2}{3}\eta_F^{\frac{3}{2}}$$

$$n = 2.42\times10^{19}cm^{-3}\left(\frac{E_F - E_C}{.025852eV}\right)^{\frac{3}{2}}$$

$$E_C = E_{Fn} - (.025852eV)\left(\frac{n}{2.42\times10^{19}cm^{-3}}\right)^{\frac{2}{3}}$$

The conduction band simulated at 15 Kelvin and the estimates calculated from the the expression above using the charge densities simulated at 50 Kelvin and at 15 Kelvin are very close to one another. This is the justification for using the above expression with 50 Kelvin simulations of the charge density to estimate the low temperature conduction band.

The plot below on the right shows the 0 Kelvin conduction band from the cut shown on the left vs. QPC gate voltage.



$$E_C = E_{Fn} - (.025852eV)\left(\frac{n}{2.42\times10^{19}cm^{-3}}\right)^{\frac{2}{3}}$$

The authors wish to acknowledge many useful discussions with Wayne Witzel, Erik Nielsen, and Rajib Rahman