Evaluation of the effect of fabrication tolerances on the ground-state energy of electrostatically defined quantum dots

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We have investigated the precision achievable, with state-of-the-art lithography, in the fabrication of quantum dots for the realization of quantum cellular automaton cells, and we have compared it with the requirements for proper device operation. Our conclusion is that a simple 'hole-array' approach is not feasible, and that individual tuning of each dot is necessary.

Key words: quantum cellular automata, fabrication tolerances.

1. Introduction

One of the most important obstacles to the realization of large-scale circuits based on mesoscopic devices is represented by their sensitivity to fabrication tolerances and to the presence of stray charges. Precision requirements, in particular, are extremely severe for some proposed devices [1], such as those based on the quantum cellular automaton (QCA) concept [2].

We present an experimental and theoretical investigation of the precision achievable in the fabrication of 4-dot cells defined by means of openings in a metal gate evaporated on top of a GaAs/AlGaAs heterostructure. Specifically, our aim has been that of determining the dispersion of the ground-state energy of single electrons in each dot, due to tolerances in the boundaries of the gate openings. Such an investigation has been performed both for the case of single dots and for that of groups of four dots located at the vertices of a square (as in the case of a QCA cell). Gates with arrays of square openings have been fabricated by means of state-of-the-art high-resolution electron-beam lithography and scanning electron microscope (SEM) photographs of the resulting structures have been processed, extracting the contour of each opening. The confinement potential generated by such contours at a depth corresponding to that of the two-dimensional electron gas (2DEG) has then been computed, assuming Fermi level pinning at the semiconductor–air interface, and statistics about the ground-state energy for each dot have been derived and discussed.

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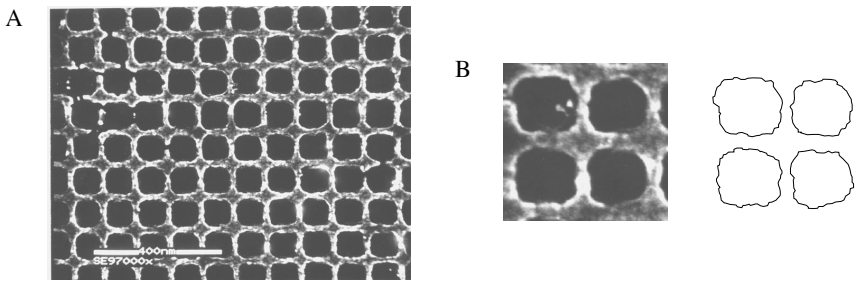

Fig. 1. A, Dot array with 60 holes, with an average hole area of 5961 nm^2 and a standard deviation of 349 nm^2. B, Comparison between the SEM image of a cell and the manually extracted contours.

2. Sample fabrication

Samples have been fabricated at L2M on a GaAs/AlGaAs heterostructure consisting of a 20 nm AlGaAs spacer layer, a delta doping layer of Si, of about 6×10^{12} cm^{-2}, an undoped 10 nm AlGaAs layer, and, on top, an undoped 5 nm GaAs cap layer. The 2DEG is therefore at a depth of 35 nm from the surface.

Since our aim was that of evaluating the minimum size fluctuations achievable with state-of-the-art technology, a very high-resolution electron-beam lithography system has been used, based on a modified Philips CM20FEG STEM (scanning transmission electron microscope). A probe size of less than 1 nm, with a current of 12 pA and an electron energy of 200 keV has been selected, and the actual linewidth on the resist has been varied between 10 nm and 25 nm by tuning the dose between 3 nC cm^{-2} and 6 nC cm^{-2}.

The sample has been first spun to deposit a 100 nm layer of PMMA resist and baked at 170 °C before exposure. After exposure, the resist has been developed in MIBK-isopropyl alcohol. A 10 nm titanium and a 20 nm gold layers have then been evaporated on the sample, and, finally, a lift-off process with trichloroethylene solvent has been performed. The main technological difficulty is that of avoiding a poor lift-off.

3. Numerical results

Let us first consider the dot array shown in Fig. 1: it contains 60 holes, whose area has an average of 5961 nm^2 and a standard deviation of 349 nm^2.

The contour of each dot has been extracted visually, by manually following the edge of the holes in the digitized SEM image shown in Fig. 1, using the 'xfig' public-domain graphic software. The xfig output file has then been processed with a purposely developed automatic procedure, in order to compute the area of each hole and, for each cell, the confinement potential acting on a 2DEG at a depth of 35 nm. The confinement potential has been obtained implementing the quasi-analytical procedure proposed by Davies and Larkin [3], which allows the determination of the potential produced by an arbitrary polygonal gate on top of a heterostructure, within the approximation of Fermi level pinning at the exposed GaAs surface. The slight variation of permittivity in the heterostructure has been neglected. The holes have been divided into groups of four (corresponding to the four openings needed to define a QCA cell) and the confining potential for each dot has been computed as a result both of all the holes defining the cell and of just the corresponding hole (as if the hole defining it were isolated from the others). Then, the single-particle Schrödinger equation has been solved for each computed confining potential, in order to obtain the ground-state energies.

In Fig. 2, we show the scatter plot of the dot ground-state energy versus the reciprocal of the area, for a dot in a cell (open circles) and for single isolated dots (full circles). In both cases a very good linear fit is obtained: the correlation coefficient is 0.998 for isolated dots, and 0.927 for dots in a cell. In the latter case the ground state energy is lower and more randomized, because of the effect of the holes defining the

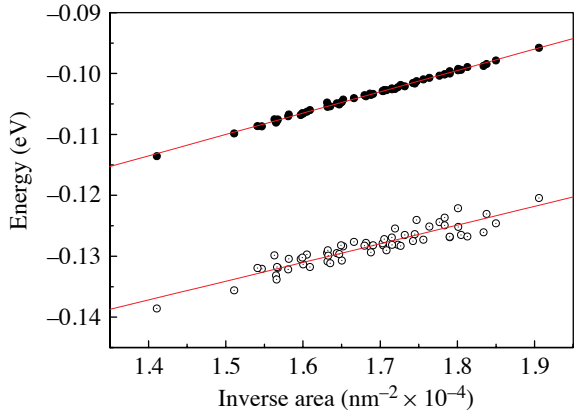

Fig. 2. Ground-state energy versus inverse area for single dots (full circles) and for dots in a cell (open circles), relative to the sample shown in Fig. 1.

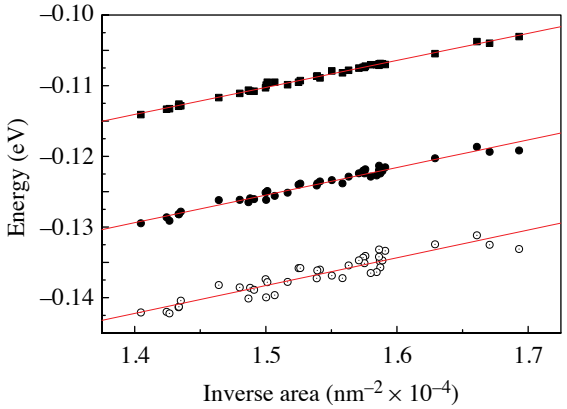

Fig. 3. Ground-state energy versus inverse area of for the dots in a cell with a pitch of 100 nm (open circles), for the dots in a cell with a pitch of 200 nm (full circles), and for single dots (full squares), relative to the second hole-array sample.

rest of the cell, whose area fluctuates independently of that of the hole relative to the dot being considered. The second set of samples is a similar dot array of 40 holes, whose area has an average of 6520 nm^2 and a standard deviation of 295 nm^2.

In Fig. 3 the ground-state energy is plotted versus the inverse area for the second sample. Results are reported for a cell with an interdot distance (measured between the centers of adjacent dots) of 100 nm (open circles), for an enlarged cell obtained spreading the dots apart so that the interdot distance becomes 200 nm (full circles), and for isolated dots (full squares). Also, in this case the average energy decreases and randomization increases as the interaction between adjacent holes is incremented.

As far as the statistics of ground-state energies are concerned, the standard deviation is about 3% of the average value, i.e. about 4 meV, for both sets of data. The operation of a QCA cell will be disrupted if the fluctuation of the ground-state energy in one of the dots is comparable to or larger than the energy splitting between the two configurations [1]. For cells with an interdot separation of 100 nm, obtained in a 2DEG at a depth of 35 nm, and considering a separation between cell centers of 150 nm, we obtain a splitting of only

0.022 meV (the situation would somewhat improve for a heterostructure with a deeper 2DEG: 0.065 meV for a depth of 100 nm). In order to obtain a reasonably reliable QCA array, the standard deviation of the ground-state energy should be no more than one-tenth of the splitting, i.e. 0.0022 meV. It is therefore apparent that the achievable precision is three orders of magnitude less than what would be required, and that, even allowing for technological improvements, a 'hole-array' approach cannot realistically lead to a working QCA circuit. Furthermore, even larger fluctuations of the confinement potential may result from the random distribution of dopants and impurities, particularly in the case of heterostructures in which the delta doping layer is close to the 2DEG. At this stage a tunable design, such as that with several split gates proposed in [1], is better suited to demonstrate the principle of QCA operation.

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