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LOW-DIMENSIONAL SYSTEMS

Model of Multi-Island Single-Electron Arrays Based on the Monte Carlo Method

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Abstract—A two-dimensional model of multi-island single-electron arrays, based on a numerical solution to the Poisson equation and the Monte Carlo method, is suggested. The adequacy of the model is shown by comparing the *I–V* characteristics calculated for two different five-island structures with experimental data. This model was used to assess quantitatively a number of geometrical parameters of a single-electron device structure, which are difficult to determine experimentally. © *2003 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

The Monte Carlo method has become one of the principal approaches to constructing completely adequate models for describing the physical processes in a variety of device structures [1, 2]. For example, it will suffice to mention the theoretical studies [3, 4] of MOS (metal–oxide–semiconductor) transistors based on a number of semiconductors that are significant for microelectronics. It turned out that none of the semiconductor materials which have been studied offers significant advantages over silicon when transistor channels are shorter than 100 nm. Only indium phosphide is an exception. Unfortunately, a completely adequate and much needed model [3, 4] is difficult to develop and cannot be widely used. In particular, the calculation of a single point of the *I–V* characteristic of a MOS transistor using the DAMOCLES code requires from 10 to 100 h (or more!) using the high-efficiency IBM 3090S computing system. Therefore, great efforts are now being made to develop various efficient procedures for the models under consideration on the basis of physical approaches, approximations, and a fuller account of problem specific features [5].

The overall situation seams to be even more complicated for nanoelectronic device structures. Fortunately, the situation is somewhat less serious in the theoretical study of structures whose description using the semiclassical approach remains correct. Specifically such structures are single-electron devices [6, 7]. As is known, the Monte Carlo method is presently one of a few more or less efficient approaches for the theoretical analysis of multi-island single-electron one-dimensional arrays [6, 8, 9]. A popular code for Monte Carlo simulation is MOSES [9] in the case under consideration.

Nevertheless, the conventional models of multi-island single-electron one-dimensional arrays, based on the Monte Carlo method, have a significant limitation. These models rely on tunnel junction resistances and capacitances as required parameters for matching with experimental data. As a result, the relation between the model and the device design and material parameters is lost. Hence, applying the model in the course of theoretical studies and development of single-electron device structures is complicated.

This study is aimed at the development of a model of multi-island single-electron one-dimensional arrays on the basis the Monte Carlo method, devoid of the abovementioned drawback, as well as the confirmation of its adequacy by comparing it with experimental data. It is significant that the model suggested may be realized using a Pentium III computer; i.e., the model may be widely used.

2. MODEL

In [10–12], a two-dimensional numerical model of a single-electron transistor with a single island was suggested. In this model, the Poisson and master equations are solved. In [13], this approach was extended to the case of two-island single-electron one-dimensional arrays. The model described in [13] is characterized by an acceptable adequacy and high efficiency; unfortunately, the solution of the master equation becomes significantly more complicated as the number of tunnel junctions increases. Therefore, we apply this approach to single-electron structures with a large number of islands in combination with the Monte Carlo method.

Let us consider the essence of the model suggested. According to the classification [7], the device being analyzed was chosen to correspond to the principal block diagram of multi-island single-electron one-dimensional arrays (see Fig. 1). The initial parameters are the structure sizes, material properties, background

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charges at islands, and the controls: source, drain and gate voltages, and temperature *T*.

The Poisson equation in the form given in [10–12] is numerically solved in the region *ABCD* (Fig. 1). The influence of background charges at islands is taken into account using the approximation suggested in [13]. The Dirichlet boundary conditions at contacts and the Neuman conditions at free *ABCD* boundaries are chosen as boundary conditions. The numerical methods of the finite-difference approximation of the Poisson equation and the solutions of sets of linear algebraic equations are described in [10] in detail. The numerical solution of the Poisson equation yields a potential distribution in the device in relation to the geometrical and electrical parameters of the structure and control effects.

The resistances of the tunnel junctions and the probabilities of carrier transport through them are calculated by the known formulas, whose form when taking into account the role of the electrostatic potential for one-island structures is given in [10]. These formulas are easily extended to the case of multi-island structures.

The current passing through the tunnel junction is calculated by the formula (see [6, 13])

$$I = \frac{V_{\text{eff}}}{R}\left[1 - \exp\left(-\frac{eV_{\text{eff}}}{k_{\text{B}}T}\right)\right]; \quad (1)$$

$$V_{\text{eff}} = \frac{V_i + V_f}{2}, \quad (2)$$

where V_i and V_f are the voltages before and after electron tunneling, respectively; and k_{B} is the Boltzmann constant.

We now consider the procedure for calculating the *I–V* characteristic by the model suggested. The flowchart of this procedure in the case of one-point calculation is shown in Fig. 2. As an example, we explain it for the case of a five-island structure, i.e., $N = 5$.

First, the Poisson equation is solved for an initial (with the index $i = 0$) combination of excess carriers in islands, $\{n_i\} \equiv (n_1 = 0, n_2 = 0, n_3 = 0, n_4 = 0, n_5 = 0)$, and partial currents through all of the tunnel junctions are calculated by formulas (1) and (2). To save computer time, the values obtained are stored when the next combination $\{n_0\}$ arises. We note at once that the most time-consuming process is solving the Poisson equation. Therefore, this time-saving method in this model is expedient and shortens the computer time by three orders of magnitude, or even more in specific cases. Then the number *K* of tunnel events was selected. The larger the value of *K*, the more accurate the result; unfortunately, the computation time also increases. Then, according to the Monte Carlo method, the first random number $r_i \in [0, 1]$ is generated and the time t_i to the next tunnel event is determined,

$$t_i = -\frac{e\ln r_i}{\Sigma I}, \quad (3)$$

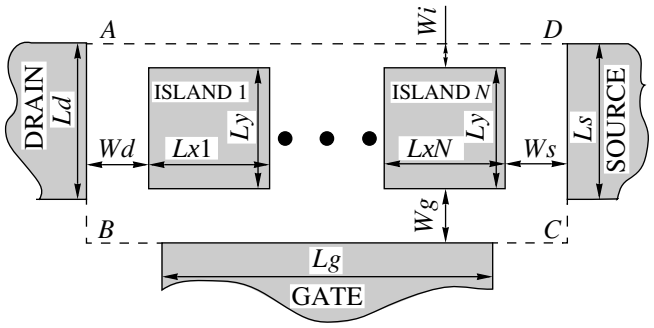

Fig. 1. Structure of the multi-island single-electron one-dimensional array.

where ΣI is the sum of partial currents for all the probable independent events, corresponding to tunneling of a carrier in two directions through either junction.

Then the next random number r_i is generated. The interval [0, 1] is partitioned into segments proportional to partial currents corresponding to tunneling of a carrier in two directions through either junction. A segment within which a given random number r_i occurs is advantageous. As a result, a new combination $\{n_i\}$ is determined. It is then checked whether this combination was found previously or not. If it was, partial currents are extracted from the computer memory; if not, the Poisson equation is solved and partial currents through all of the tunnel junctions are calculated and stored. It is then checked whether all the probable tunnel events (number *K*) were enumerated or not.

The total current *j* passing through an isolated tunnel junction is given by

$$I_j = \frac{n_j e}{t_\Sigma}, \quad (4)$$

where n_j is the number of carriers that passed through a given junction for the entire period, *e* is the elementary charge, and t_Σ is the total time of tunneling events. The validation criterion of the calculation is the equality of the currents I_j through all of the tunnel junctions within a certain accuracy.

The most significant differences between the model suggested and the models of [6, 8, 9], which are also based on the Monte Carlo method, are as follows: (i) the Poisson equation is solved in the form given in [10–12] with the aim of calculating the voltages at the tunnel junctions and (ii) the partial currents through the tunnel junctions calculated by formulas (1) and (2) are used instead of the tunneling rates. We note a number of advantages of the model suggested in comparison with the model of [13], in which the master equation is solved: (I) complex single-electron one-dimensional arrays with $N > 2$ can be calculated; (II) the procedure under consideration is based on a microscopic model of tunnel events, which more closely reflects the actual behavior of carriers in the single-electron

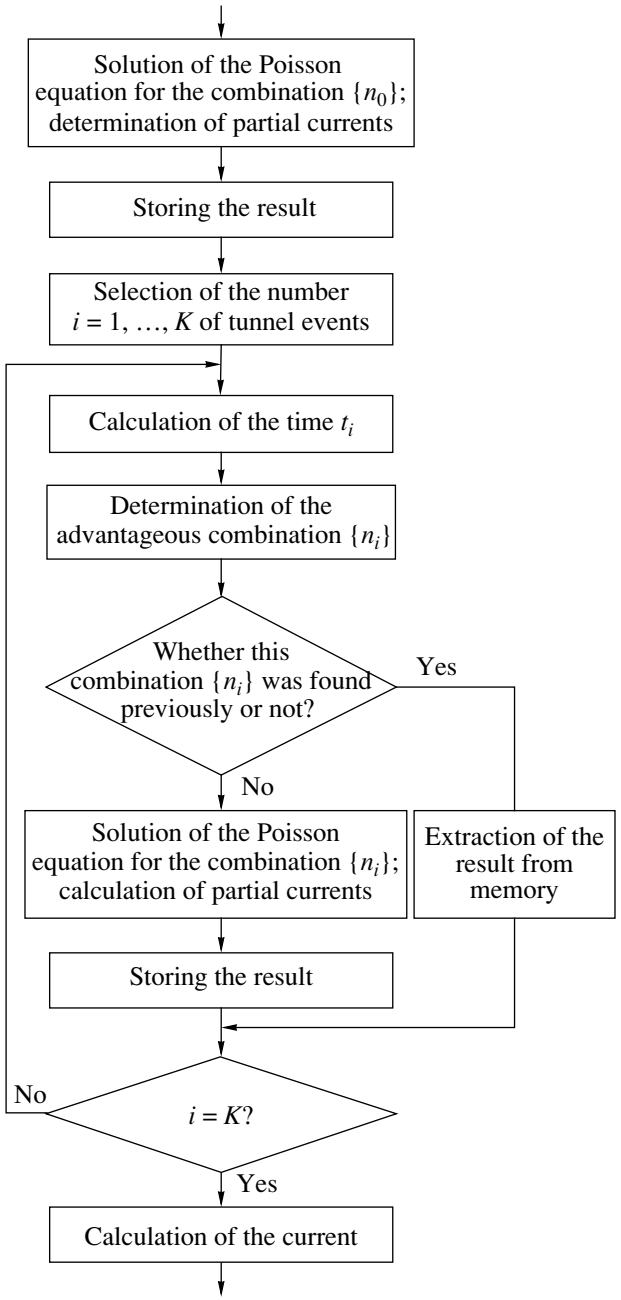

Fig. 2. Flowchart of the calculation procedure for a point of the *I–V* characteristic of single-electron one-dimensional arrays according to the model suggested.

structure; and (III) there is high stability of the computing process. The disadvantage of the model is much longer times for calculating the *I–V* characteristic at $N = 2$ in comparison with the model of [13]. Nevertheless, this time, e.g., for five-island one-dimensional arrays, is, in general, no longer than 10 h (which is acceptable) for the Pentium III computer.

The model suggested was realized in FORTRAN and incorporated in the MTJ-SET-NANODEV package for calculating multi-island single-electron one-dimensional arrays in the NANODEV software for simulating nanoelectronic devices [10]. All the results considered in Section 4 were obtained using a Pentium III computer.

3. RESULTS

As the object to be simulated, we took a single-electron transistor with five islands, i.e., $N = 5$. This choice is explained as follows. First, this number of islands allows manifestation of all the basic features of multi-island array operation, e.g., the temporal and spatial correlation of tunneling events. Second, in the case of a larger number of islands, the total resistance is high (the passing current is very small); hence, production of such structures is complicated. Therefore, data on structures with $N > 5$ are scarce in the literature. Third, the time of calculating the *I–V* characteristic unfortunately becomes longer as the number of islands increases further.

We now consider the simulation results confirming the adequacy of the model suggested. They were obtained at $K = 20000$, proceeding from the attainable equality of the currents through all the tunnel junctions within an error no larger than 0.1%.

In [14], the fabrication of a single-electron transistor with five islands is described, as are experimental data and results calculated by the MOSES code. We note that the structure is produced artificially and controlled using the SECO (step-edge cutoff) method. Titanium and *p*-type silicon are used as the island and tunnel junction materials, respectively. Figure 3 shows the experimental characteristic for the drain current I_d versus the drain voltage V_d (curve *1*), as well as the results calculated by the MOSES code (curve *2*) and the model suggested (curve *3*). One can see that both models satisfactorily fit the experimental data.

The model developed also fits well the experimental data on single-electron multi-island one-dimensional arrays based on other materials at various operating temperatures. Furthermore, the model suggested allows reconstruction of the basic sizes of the structures under study. To illustrate this, we now consider a very complex case.

In [15], a multi-island one-dimensional array is described in which AuPd nanoparticles are used as islands. The structure is rather complex (see Fig. 5 in [15]). As the author of [15] reports, it was possible to determine only the following initial parameters of the structure: (i) the number of tunnel junctions along the shortest drain–source distance was found to be six; (ii) the island sizes were from 2 to 3 nm; (iii) the source–drain distance was 20–30 nm. Thus, the available information is very ambiguous.

Figures 4a and 4b display the experimental data and the results calculated by the suggested model, respectively. One can see that, in general, the experiment and model agree satisfactorily at $T = 300$ and 77 K. The data

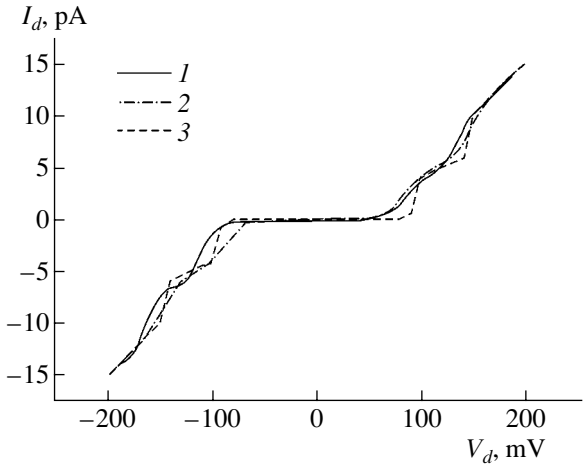

Fig. 3. *I–V* characteristics of the single-electron transistor with five islands: (*1*) experimental data, (*2*) calculation by the MOSES code, and (*3*) calculation by the model developed.

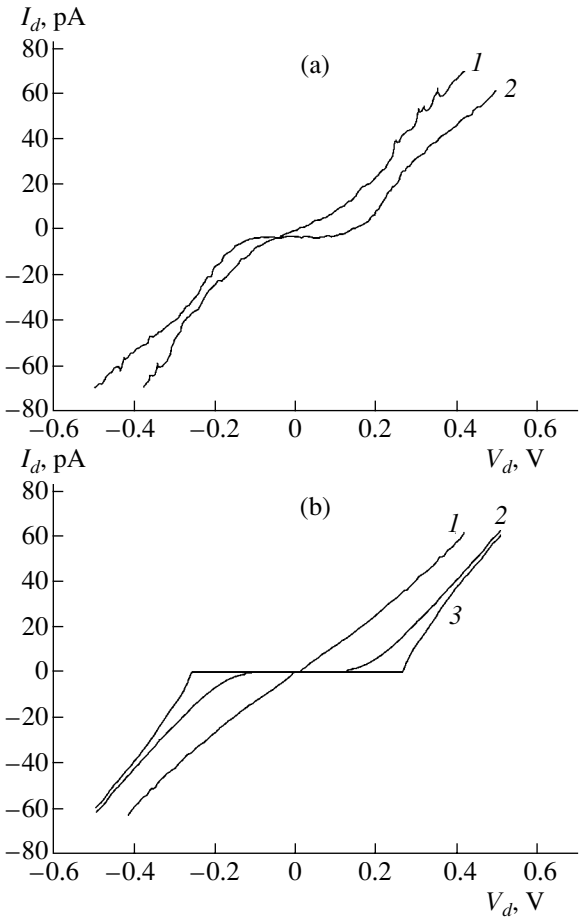

Fig. 4. *I–V* characteristics of the multi-island structure: (a) experimental data and the (b) the results of simulation according to the model developed; T = 300 (*1*), 77 (*2*), and 0.01 K (*3*).

in Fig. 4b were obtained with the following basic initial parameters of the structure: $N = 5$; the distance between islands is 1.5 nm; and the islands are of the same size (2.5×2.5 nm^2). Thus, the source–drain distance was taken as 21.5 nm ($6 \times 1.5 + 5 \times 2.5$). It is significant that all of these reconstructed initial parameters lie within the numerical range indicated by the author of [15] (see above). The results shown in Fig. 4b allow determination of the Coulomb blockade region in this structure at a very low temperature (T = 0.01 K), in particular [–0.25 V, +0.25 V]. Comparing curves *1–3* in Fig. 4b, one can ascertain that the Coulomb blockade effect is "destroyed" as the temperature increases to 300 K in the structure under study, which is fully confirmed by the experimental data in Fig. 4a.

The results obtained, in addition to confirming the conclusion on the adequacy of the model, also allow the following comments. First, the model suggested can be applied to reconstruct some of the initial parameters of multi-island single-electron one-dimensional arrays, e.g., their sizes. This seems to be of crucial importance in view of the likely problems in determining them experimentally, as in the case under consideration. Second, notwithstanding the seemingly high complexity of the single-electron structure being analyzed, it is possible to simulate it using the flowchart shown in Fig. 1. Thus, the basic physical principles of the operation of multi-island single-electron one-dimensional arrays are adequately described within the model suggested, which is based on a rather simple flowchart (Fig. 1). We note that this is also important, since the use of a practical structure configuration, in many cases, will cause significant additional problems in the numerical simulation of this type of single-electron structures. As a result, it would, in fact, become impossible to study theoretically the influence of the design and material parameters on electrical characteristics of these structures.

4. CONCLUSION

A two-dimensional model of multi-island single-electron one-dimensional arrays was developed on the basis of a numerical solution of the Poisson equation in combination with the Monte Carlo method. This model was shown to be reasonably adequate and efficient. The model may also be used to reconstruct some initial parameters that are difficult to determine from experimental data.

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REFERENCES

1. R. Hockney and J. Eastwood, *Computer Simulation Using Particles* (McGraw-Hill, New York, 1984; Mir, Moscow, 1987).
2. Yu. K. Pozhela, *Physics of High-Speed Transistors* (Mokslas, Vilnius, 1989).
3. M. V. Fishetti and S. E. Laux, Phys. Rev. B **38**, 9721 (1988).
4. M. V. Fishetti and S. E. Laux, IEEE Trans. Electron Devices **38**, 650 (1991).
5. H. Kosina, M. Nedjalkov, and S. Selberherr, IEEE Trans. Electron Devices **47**, 1898 (2000).
6. *Single Charge Tunneling: Coulomb Blockade Phenomena in Nanostructures*, Ed. by H. Grabert and M. H. Devoret (Plenum, New York, 1992); NATO ASI Ser., Ser. B **294** (1992).
7. I. I. Abramov and E. G. Novik, Fiz. Tekh. Poluprovodn. (St. Petersburg) **33**, 1388 (1999) [Semiconductors **33**, 1254 (1999)].
8. N. S. Bakhvalov, G. S. Kazacha, K. K. Likharev, and S. I. Serdyukova, Zh. Éksp. Teor. Fiz. **95**, 1010 (1989) [Sov. Phys. JETP **68**, 581 (1989)].
9. R. H. Chen, A. N. Korotkov, and K. K. Likharev, Appl. Phys. Lett. **68**, 1954 (1996).
10. I. I. Abramov and E. G. Novik, *Numerical Simulation of Metallic Single-Electron Transistors* (Bestprint, Minsk, 2000).
11. I. I. Abramov and E. G. Novik, Fiz. Tekh. Poluprovodn. (St. Petersburg) **34**, 1014 (2000) [Semiconductors **34**, 975 (2000)].
12. I. I. Abramov and E. G. Novik, Fiz. Tekh. Poluprovodn. (St. Petersburg) **35**, 489 (2001) [Semiconductors **35**, 474 (2001)].
13. I. I. Abramov, S. A. Ignatenko, and E. G. Novik, Fiz. Tekh. Poluprovodn. (St. Petersburg) **36**, 1272 (2002) [Semiconductors **36**, 1192 (2002)].
14. S. Altmeyer, A. Hamidi, B. Spangenberg, and H. Kurz, J. Appl. Phys. **81**, 8118 (1997).
15. H. Ahmed, J. Vac. Sci. Technol. B **15**, 2101 (1997).

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