

BRIEF PAPER

Numerical Simulation of Single-Electron Tunneling in Random Arrays of Small Tunnel Junctions Formed by Percolation of Conductive Nanoparticles

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SUMMARY We numerically simulated electrical properties, i.e., the resistance and Coulomb blockade threshold, of randomly-placed conductive nanoparticles. In simulation, tunnel junctions were assumed to be formed between neighboring particle-particle and particle-electrode connections. On a plane of triangle 100×100 grids, three electrodes, the drain, source, and gate, were defined. After random placements of conductive particles, the connection between the drain and source electrodes were evaluated with keeping the gate electrode disconnected. The resistance was obtained by use of a SPICE-like simulator, whereas the Coulomb blockade threshold was determined from the current–voltage characteristics simulated using a Monte-Carlo simulator. Strong linear correlation between the resistance and threshold voltage was confirmed, which agreed with results for uniform one-dimensional arrays.

key words: single-electron effects, percolation, circuit simulation, Monte-Carlo simulation

1. Introduction

Single-electron (SE) devices commonly comprise arrays of small tunnel junctions [1]. The shortest array is a two-junction SE transistor [2], whereas Coulomb blockade thermometers are composed of long one- or two-dimensional junction arrays [3]. Long arrays have been so far realized using tri-layer Al tunnel junctions [4], granular films [5], conductive nanoparticles (NPs) [6], etc.

Recently, we have worked on random arrays of gold NPs, which are fabricated using dispersion of colloidal gold solution over separate electrodes [7]. Not only the Coulomb blockade but also gate responses have been confirmed [8], [9]. In this fabrication method, not precise positioning but percolation of gold NPs is employed. On the other hand, there are several important parameters that should be carefully chosen in experiments, such as diameters and densities of gold NPs, layouts of electrodes, etc. Since experiments involve a good deal of cost, numerical simulation is expected to provide useful guidelines for experimental conditions.

We therefore built out a simulation environment for our experiments of SE tunneling in random junction arrays formed by percolation of conductive NPs. In this brief paper, we describe the simulation procedure and examples of simulation results including random paths between two electrodes through conductive NPs and their current–voltage characteristics. Besides, correlations between electric resistances and Coulomb blockade voltages are demonstrated.

2. Simulation Methods

Figure 1 shows a flow-chart and a schematic illustration of triangle grids used in simulation. Three electrodes, the drain (D), source (S), and gate (G), are placed in the grid plane. Our target situation is that the only two electrodes D and S are connected by percolation of conductive NPs randomly placed on grids. The G electrode should be separated from D and S so that G is capacitively coupled to percolation paths. In this work, the dimensions of the grid plane, L , W , GW , and GD were fixed to 100×100 , 10, 24, and 16, respectively, where the definitions of L , W , GW , and GD are presented in Fig. 1 (b). The grid interval was assumed to be uniform and equal to the diameter of an NP.

Simplified illustrations of the simulation sequences are also shown in Fig. 2.

After the definition of electrodes, conductive NPs were placed on grids with the occupation probability P_{occ} .

Next, if the target situation described above was confirmed, percolation paths between D and S were converted into networks of resistors as shown in Fig. 2 (b). All resistors were assumed to have the identical resistance value of R_J . The resistance R_{total} between D and S was then simulated through the use of a SPICE-based circuit simulator [10]. (More precisely, the voltage between D and S was calculated for the constant DC current input.) If the netlist contained resistors that connected to the network with a single node, the simulator reported errors in the netlist. In such cases, unnecessary resistors were eliminated from the netlist, and then, the revised netlist was simulated. (Revisions of the netlist were repeated until the simulator succeeded calculation with no errors.) Here, R_{total} obtained by use of the circuit simulator corresponds to a resistance value for V_{DS} much higher than the Coulomb blockade threshold.

Finally, networks of resistors were converted into those

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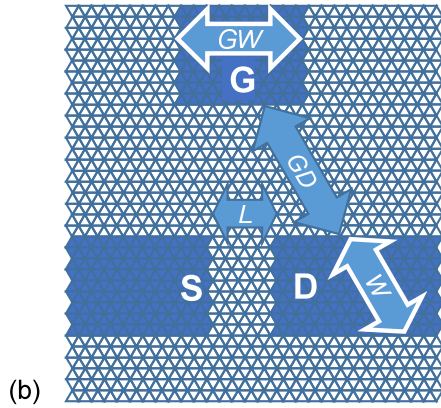
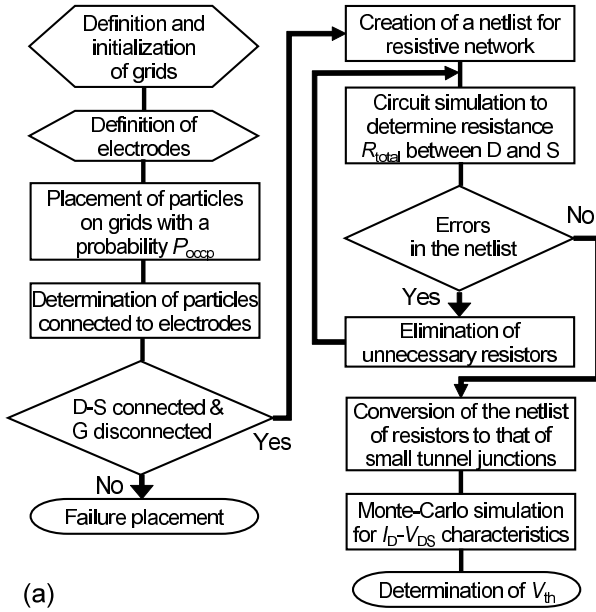


Fig. 1 (a) Simulation flow-chart. (b) Schematic illustration of triangle grids with three electrodes. Definitions of the electrode widths and gaps are also presented. Conductive NPs are assumed to be placed on grids with occupation probability P_{occ} . Tunnel junctions are assumed to be formed between neighboring NP-NP and NP-electrode connections.

of small tunnel junctions as shown in Fig. 2 (c). All tunnel junctions were assumed to have the identical junction resistance C_J and junction resistance R_J . Their I_D - V_{DS} characteristics for symmetrical voltage bias were calculated using a Monte-Carlo simulator [11]. The threshold voltage V_{th} of the Coulomb blockade was extracted from the I_D - V_{DS} characteristics.

3. Results and Discussion

An example of random NP placements for P_{occ} of 0.30 are presented in Fig. 3 (a). This NP placement realizes our target situation, although it is difficult to determine it by eye from this figure. Percolative paths from/to D and S electrodes are extracted as shown in Fig. 3 (b). The circuit simulator provided R_{total} of $10.7R_J$ after conversion to resistor networks. Next, I_D - V_{DS} characteristics were obtained by Monte-Carlo

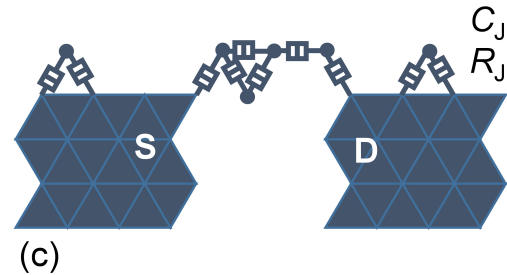
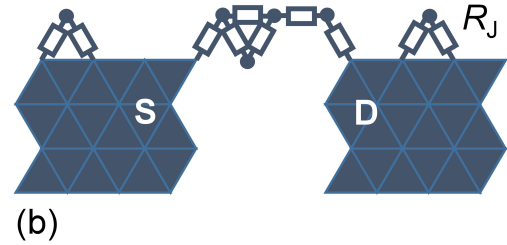
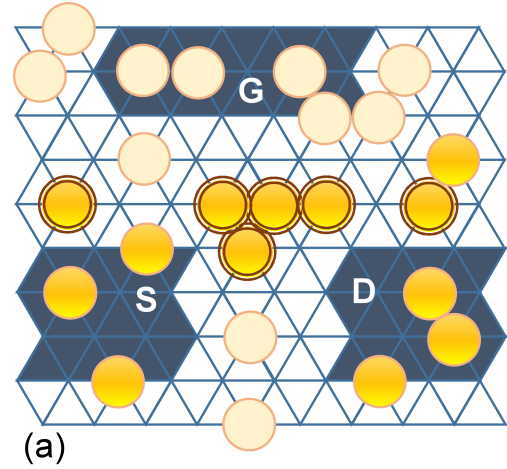


Fig. 2 (a) Schematic illustration of randomly-placed conductive NPs on the triangle grids. Rich-yellow and straw circles represent connected and unconnected NPs to D or S electrodes, respectively. Double contour NPs are used to simulate electrical properties. (b) Networks of resistors representing conductive paths through NPs. Each resistance is R_J . (c) Conversion into networks of small tunnel junctions. Each junction has the junction capacitance C_J and resistance R_J .

simulation as shown in Fig. 3 (c), where the absolute zero temperature was assumed. V_{th} was determined as $4.89e/C_J$.

By using this simulation environment, we executed 200 simulations for each P_{occ} of 0.25, 0.30, 0.35, 0.40, 0.45, and 0.50 to obtain some statistical results. The yields for our target situation were 0.01, 0.03, 0.10, 0.30, 0.27, and 0.02, respectively. (Since the G electrode should not be connected, P_{occ} values larger than 0.50 were unsuitable for this electrode layout.)

Among 1,200 executions of simulation, 146 placements satisfied our target situation. We extracted R_{total} and V_{th} values from the successful 146 placements, and plotted them on the R_{total} - V_{th} plane as shown in Fig. 4.

It is found that there are two types of correlation between R_{total} and V_{th} .

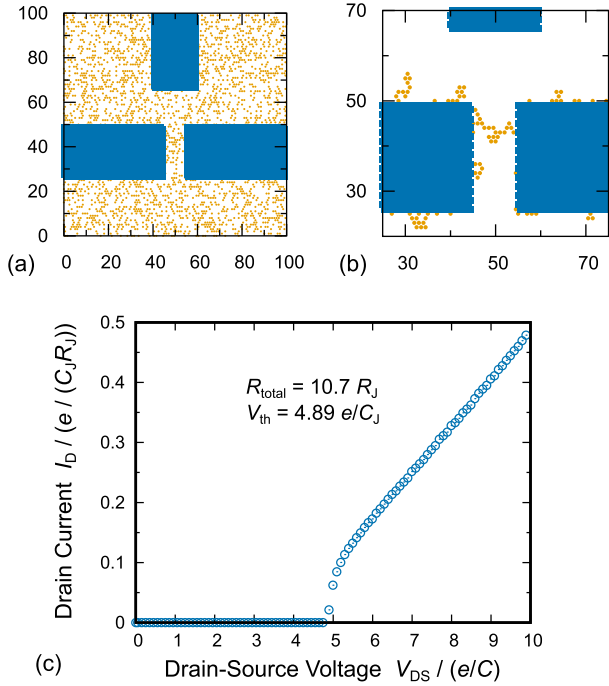


Fig. 3 Example of simulation results. (a) Particle placement on grids with P_{occ} of 0.30. (b) Extraction of percolative paths connected to D and/or S electrodes. (c) Numerical I_D - V_{DS} characteristics at the absolute zero temperature. R_{total} and V_{th} are $10.7 R_J$ and $4.82 e / C_J$, respectively.

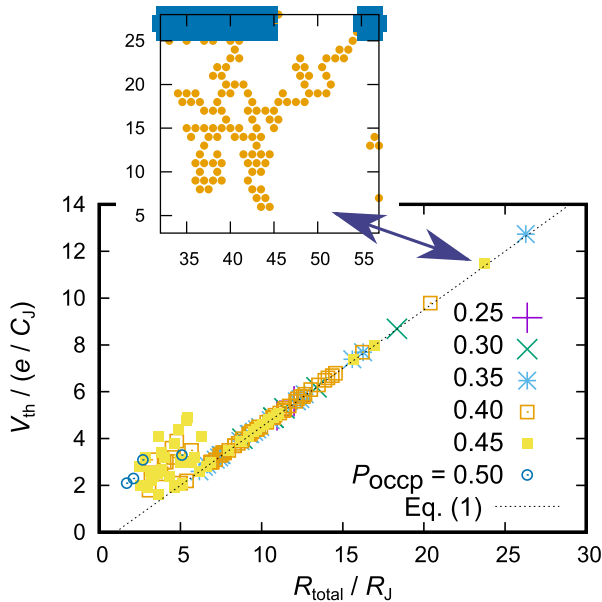


Fig. 4 Correlation between R_{total} and V_{th} . Percolative conduction paths for R_{total} of $23.7 R_J$ and V_{th} of $11.5 e / C_J$ are also presented as an example of long paths.

The first one is the linear relationship expanding from (R_{total}, V_{th}) of $(3.6 R_J, 1.3 e / C_J)$ to $(26 R_J, 13 e / C_J)$. This is interpreted as a sign that simple one-dimensional (1D) arrays are dominant for their electric properties. For a uniform 1D array of small tunnel junctions, the relationship between V_{th} and the number of islands N_{isld} is expressed as

$V_{th} = e N_{isld} / (2 C_J)$ [12], whereas that between R_{total} and N_{isld} is $R_{total} = (N_{isld} + 1) R_J$. We thus obtain the relationship between V_{th} and R_{total} as

$$V_{th} / (e / C_J) = (R_{total} / R_J - 1) / 2, \quad (1)$$

which is also plotted in Fig. 4 as a dotted line. It is clearly demonstrated that the linear correlation agrees with the results of uniform 1D arrays.

In more detail, an example of NP placements for P_{occ} of 0.45 is also shown in Fig. 4. A long path can be found between D and S electrodes. It should be noted that one of the end points of the path is not on the facing edge of the electrodes but the side edge. Such situation was different from the traditional studies on conductive percolation. All results for $P_{occ} \leq 0.35$ exhibited this correlation, whereas no results for P_{occ} of 0.50 did.

The second correlation is rather weak, found at $1.7 R_J \leq R_{total} \leq 6.3 R_J$ and $1.8 e / C_J \leq V_{th} \leq 4.9 e / C_J$. Besides all results for P_{occ} of 0.50, some of the results for P_{occ} of 0.40 and 0.45 were categorized into this correlation. Paths were found to be rather complicated (not shown here). The origin of this correlation would be attributed to the reduction of resistance due to non-negligible parallel paths.

As we demonstrated, this simulation environment is effective to simulate electric characteristics of our experimental samples, that is, percolative current transports in random arrays of gold NPs. It should be noted, however, that the capacitive coupling between G and NPs were not explicitly implemented in this environment. Because straightforward calculation of capacitances among many electrodes is a difficult challenge, it would be necessary to find a simple and efficient calculation model.

4. Conclusion

We built out a simulation environment and demonstrated numerical properties of random arrays of small tunnel junctions. The calculation model simulated our recent experiments on SE devices fabricated using dispersion of gold NPs over separated electrodes. Percolative connection among three electrodes was checked for several P_{occ} values. For placements realizing the target situation, electric properties of R_{total} and V_{th} were respectively determined by use of the SPICE-like simulator and Monte-Carlo simulator. Statistical results were also obtained by simulating 1,200 situations, among which 146 satisfied our target situation (S and D were connected, while G was disconnected.) Strong linear correlation between R_{total} and V_{th} was confirmed, which agreed with the relationship in uniform 1D arrays.

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