Modelling of the tunnelling effect in granulated metallic nanostructures

A V Istratov and A O Kucherik

A.G and N.G. Stoletov Vladimir State University (VSU), 87 Gorki st., Vladimir, Russia, 600000

E-mail: aleksgreene@gmail.com

Abstract. Obtaining thin films of today is unthinkable without use of mathematical modeling, numerical methods and complex programs. In this regard, the practical importance of this calculations is that it can be used to investigate the conductivity of nano-sized granular structures that expands the diagnostic capabilities of thin films, opens up new perspectives in the creation of new devices based on thin-film technology, allow to predict their properties.

1. Introduction

The achievements of nanotechnologies are based on fundamentally new scientific knowledge about the nature of the structure materials, and, consequently, fundamentally new technologies and design principles. As the particle size of a substance decreases, its physical and chemical properties can change substantially.

The characteristic dimensions of semiconductor structures at the modern micro- and nanoelectronics are $10^{-7}$-$10^{-8}$ m. Such a range of linear dimensions of elements is a fundamental physical barrier behind which all the properties of a solid body, including electrical conductivity, change drastically.

Dimensional effects in solids are a phenomenon observed when the geometric dimensions of an object are comparable with one or other of the lengths that determine the course of physical processes (for example, the mean free path of the charge carrier, the de Broglie wavelength, etc.). Depending on the size of the sample being examined, classical and quantum dimensional effects are distinguished, which can affect practically any properties of the substance. As a rule, for nanometer objects, where the particle sizes are comparable with the de Broglie wavelength of an electron, the quantum size effects determine such properties of matter as heat capacity, electrical conductivity, optical properties, and the like.

The most striking representative of quantum size effects is the tunnel effect, a phenomenon that plays an important role in nanotechnology. The tunnel effect is the microparticle overcoming a potential barrier between two conductors with a small cross-section. Using this effect, you can control the movement of individual electrons. According to the basic principles of quantum mechanics, microparticles (in particular electrons) can pass through an insulator (dielectric) from one conductor to another that is a tunnel transition.

One-electron devices are promising nano electronic devices based on the effect of discrete tunneling of individual electrons and providing ultra-low levels of energy consumption at ultra-low operating voltages. The first devices based on the tunnel effect: tunnel diodes, transistors, sensors, thermometers...
for measuring ultra-low temperatures, and finally, scanning tunneling microscopes, which laid the
foundation for modern nanotechnology.
Since physical models of colored plastic balls don’t accurately reflect the real properties of
carbon-based nanoparticles, computer models are usually used in which one can set the real laws of quantum physics.
Based on a powerful mathematical apparatus, computer modeling plays a key role in the development
of nanosystems.

2. Computer modelling
Algorithm, which simulates the electrical properties of thin granular films, is realized in several stages:

2.1. Simulation of a granular film.
The sedimentation of particles on the surface of the substrate is carried out by random sedimentation
method. Random sedimentation is the simplest model of surface growth - a cellular automaton that
includes simple deterministic deposition rules. The precipitated particles fall into randomly chosen
points on the surface, are fixed there and do not have the ability to diffuse into neighboring points. A
particle that hits a certain point on the surface increases its thickness by one relative unit.
Mathematically, this model is similar to the model of Brownian motion of particles and is intensively
studied by analytical and numerical methods. The disadvantage of deterministic cellular automata is that
the state at the next instant of time is uniquely determined by the state at the previous moment of time.

![Figure 1. The random sedimentation model](image)

The proposed model for the growth of thin-film surfaces is as follows:
  a) The surface of a thin film in the model is a rectangular grid;
  b) The new particles are assumed to be identical and their sedimentation locations are chosen
     randomly, and for one relative unit of time within the given model, more than one particle does not
     precipitate into one cell of the surface;
  c) The rate of particle sedimentation is determined by the number of particles that hit the surface in
     one step of modeling the sedimentation of particles;
  d) After the step of modeling the sedimentation of film particles, a transition to the next.

2.2. Modelling tunnel effect
To simulate a metallic granular nanostructure with a potential difference applied to the ends, a one-
electron mathematical model was used in the form of a three-dimensional stochastic cellular automaton.
The metal particles are represented as spheres located on the substrate at a distance $S$ from each other.
The electric potential is applied to the ends of the film, and the charge accumulates in the particles until
its magnitude is sufficient for making the tunnel by the electrons to the subsequent particles in the
direction of the positive potential: this flow of electrons moving in the same direction is electric
amperage.

In the Euclidean metric, the distance between the pairs of neighboring particles in question is not the
same, therefore, the type of neighborhood (common face, edge or vertex) must be taken into account. A
cellular automaton, implemented in the Moore neighborhood in the three-dimensional case.
The three-dimensional Moore neighborhood in the simulated space consists of 26 neighboring cubic
cells in which the particles are located and which have a current particle with the cell: common faces (6
units) are neighbors of the first order; common ribs (8 units) - neighbors of the second order; common
vertices (8 units). Obviously, the distance between the cell centers of the particle in question and the
neighboring one, having a common edge, is $\sqrt{2}$ times larger than the distance between the centers of the cells that have a common face. If they have only a common vertex, then the distance between the centers of the given cells will increase by $\sqrt{3}$ times.

Calculation of the probability of the tunnel effect. The probability is calculated for each pair of particles: the current particle and its nearest neighbor are not more than the third order:

$$P_1 = \begin{cases} \arccotg \left( \frac{8}{\pi} \left( \sqrt{\frac{1}{n_i}} (S + 2R) - 2R - \frac{U}{\sqrt{n_i}} \left( \frac{q_i - q_0}{e_0} + 0.5 \right) \right) \right), \\
0, \text{ if } \frac{q_i}{e_0} = 1 \text{ or } \frac{q_0}{e_0} = -1 \end{cases},$$

(1)

Where $n_i$ - the order of the neighborhood of the $i$-th neighboring particles; $S$ - the distance between the nearest particles along the axes; $R$ - the radius of the deposited particles; $U$ - the voltage at the ends of the simulated thin film, collinear with the X-axis; $x_0$ - the x-coordinate of the current particle center; $x_i$ - the x-coordinate of the $i$-th neighboring particle center; $q_0$, $q_i$ - the charges of the particles under consideration; $e_0$ - the charge of the electron.

3. Computer modelling
The main quantitative morphological parameters characterizing the inhomogeneity of thin films: thickness and surface roughness film (standard deviation of the film thickness), particle size (diameter of spheres) and gap (the distance between the particles).

![Figure 2. Current-voltage characteristics of the deposited and simulated gold and silver films: 1 – a particle diameter (D) is 4nm, the distance between the particles (gap) is 2nm, the surface roughness (W) about 7nm; 2 – D is 4nm, gap is 2nm, W about 8.5nm; 3 – D is 4nm, gap is 3nm, W about 13.5nm; 4 – D is 6nm, gap is 3nm, W about 16.5nm; 5 – D is 9nm, gap is 4nm, W about 21nm; 6 – D is 10nm, gap is 10nm, W about 34nm; 7 – D is 14nm, gap is 15nm, W about 53nm.](image)

The volt-ampere characteristics of the deposited films and the results of modeling the tunnel effect using the model of a stochastic cellular automaton are shown in Figure 2.

The calculated volt-ampere characteristics are in qualitative agreement with the experimental one. The discrepancy in numerical values can be explained by the geometry of the calculation of features: in the model, the particles lie strictly on each other (because of the need to use a computational grid) and a clearly defined interval $S$. 
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