1. INTRODUCTION

In the past two decades, in connection with the discovery of the “Coulomb blockage” phenomenon for semiconductor quantum dots and fabrication of experimental samples of cryogenic single-electron transistors based on this phenomenon [1–5], designers started attempts to use metal nanoparticles, mainly of noble metals Ag, Pd, Ir, Pt, and Au [6, 7], in order to fabricate a single-electron transistor operating at room temperature. Their sizes can be brought to 1 or even to 0.5 nm. The corresponding Coulomb energy

\[ E_q = \frac{q^2}{2C} \]  

is of the order of 1.6–3.2 eV, which is already by approximately two orders of magnitude larger than quantity \( k_B T \) at room temperature. In formula (1), \( q \) is the absolute value of the elementary charge, \( C = 4\pi \varepsilon_0 r \), where \( r \) is the nanoparticle radius, and \( \varepsilon_0 \) is the permittivity of vacuum. Unfortunately, the task to place a single metal particle of such a size into a planar nanodimensional capacitor turned out to be too complicated. The use of the cantilever tip of the atomic tunnel microscope, which passes alternately over several metal nanoparticles lying on the oxide-covered metal surface [8] with their inevitable deformation [9] also cannot be considered a solution suitable on which to base industrial technology.

In attempts to fabricate a stationary metal nanotransistor, researchers started to use the so-called self-organizing ensembles of metal nanoparticles enveloped into ligand shells of dielectric liquids (or covered with the Langmuir–Blodgett films) and placed into planar nanocapacitors [10–14]. A series of performed experiments showed the Coulomb blockage phenomenon in such ensembles; however, new difficulties appeared here on the way of fabricating the nanotransistor. The spread of nanoparticle sizes in these ensembles turned out to be too large, 1–5 nm in the better case. In addition, the particles arranged between the capacitor plates were arranged chaotically, in several layers, rather than in one layer, and instead of simple tunneling through one layer, hopping conductivity along the layer additionally appeared [15]. Even in the case of the arrangement in one layer, the ensemble of quantum dots did not demonstrate the set of expected properties inherent to a transistor.

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**Abstract**—This work is devoted to the investigation of electron tunneling through “magical” nanoclusters Au₅₅ and Au₁₄₇. Using the quantum-chemical calculation, it is shown that the energy of the highest occupied molecular orbital (HOMO) level is \( E_{\text{HOMO}_{\text{Au}_{55}}} = -3.2 \text{ eV} \) and \( E_{\text{HOMO}_{\text{Au}_{147}}} = -4.4 \text{ eV} \), respectively. It is established that the difference between energy \( E_{\text{LUMO}} \) of the lowest unoccupied level LUMO and energy \( E_{\text{HOMO}} \) for the anions of clusters (Au⁻₅₅ and Au⁻₁₄₇) is 0.86 and 0.24 eV, respectively. Based on the results of the calculations, it is assumed that nanosandwiches W–WO₂–(Au₁₄₇)–Al₂O₃–Al can be promising structures for implementation of metal nanodiodes based on them, while nanosandwiches Nd–Nd₂O₃–(Au₅₅)–Nd₂O₃–Nd can be promising for implementation of energy filters not producing hot electrons and allowing the fabrication of the ring Aharonov–Bohm interferometers based on normal metals at liquid-helium temperatures.

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First, according to the spread of the particle sizes, the chaotic spread of the Coulomb energies in a range of 0.3–1.6 eV and corresponding peaks of differential conductivity was acquired. Characteristic peaks of the Coulomb blockade in $I–V$ characteristics were severely blurred [16, 17].

Second, as shown in [18], because of the same spread of sizes, a new phenomenon appeared. Electrons tunnel from the Fermi level of the first (left) nanocapacitor plate. At a certain specially selected bias potential they enter the $E_{\text{highest}}$ occupied molecular orbital $E_{\text{HOMO}}$ level of the anion of the metal nanocluster with the smallest size of 1 nm. In other nanoclusters having the larger size (2–5 nm), electrons during tunneling pass by several tenths of an eV above the corresponding level $E_{\text{HOMO}}$ or the Fermi level of the anion of the larger nanocluster. As a result, hot electrons are formed. Investigations show that they can considerably, up to 1000 K, heat gold nanoclusters and increasingly blur the entire pattern of ideal tunneling through the nanoparticles [19].

It was also revealed that the location of the Fermi level ($E_{\text{HOMO}}$) of the nanocluster strongly depends not only on the sizes but also on the variation of the shape (ball-like, ellipsoidal, or flat nanoclusters) [20].

Thus, modern failures with the development of a metal nanotransistor are mainly explained by a large spread of geometry and, as a consequence, energy parameters of nanoparticles in the used ensembles.

In parallel with this technology of obtaining the ensembles of nanoclusters of an indefinite shape and size, the direction of obtaining and isolating the so-called “magical” (odd, in contrast with nuclear physics, where even–even nuclei are referred to as magical) gold nanoclusters by means of colloid chemistry and liquid chromatography [21–30]. These nanoclusters are of a rigorously definite size, structure, and shape. They comprise a series of regular polyhedrons packed around the common symmetry center—icosahedra; or semiregular polyhedrons—cuboctahedra: Au$_{13}$ (one layer), Au$_{55}$ (2 layers), Au$_{147}$ (3 layers), Au$_{309}$ (4 layers), etc. Until now, only the spectral and chemical–catalytic properties of magical gold nanoclusters have been studied in this direction [21–30].

The goal of this work is to theoretically investigate the possibilities of using the magical nanoclusters of one definite type (Au$_{55}$ or Au$_{147}$) as the main elements of metal quantum nanodiodes and in prospective nanotransistors with high reproducible standard characteristics and a high switching frequency of $\sim 10^{10}–10^{12}$ Hz.

We evaluated the spectrum width of electrons tunneling through the system metal–dielectric–gold nanocluster–dielectric–metal occurring in nanodiode, which suggest the experiment with the ring Aharonov–Bohm interferometer [31] using the magical nanocluster as a monochromator of the electron spectrum, and also suggest the hypothetic schematic of a high-frequency “cold” (not producing “hot” electrons) single-electron multichannel metal nanotransistor.

2. STATEMENT OF THE PROBLEM AND THE METHOD

Let us investigate electron tunneling through nanostructures metal1–oxide1–(Au$_{147}$ or Au$_{55}$)–oxide2–metal2 depicted in Figs. 1 and 2 (on the top) according to the following schematics of calculations.

(i) Derivation of the condition of the energy balance providing the possibility of electron tunneling from the left electrode through the nanocluster into the right electrode.

(ii) Quantum-chemical calculation of molecular orbitals and corresponding energies of nanocluster and selection of metals, for which the balance condition of point (i) of this schematic is fulfilled.

(iii) Quasi-classical evaluation of partial resistances of elements of the tunnel nanostructure constructed from selected metals.

(iv) Calculation of atomic potentials of metals forming the walls of potential barriers in the 1D projection of the potential of the 3D nanostructure (Fig. 1 at the bottom).

(v) Construction of the 1D projection for the 3D potential well of the nanocluster.

(vi) Construction of dielectric potential barriers of the tunnel nanostructure.

(vii) Construction of the potential of “imaging forces” and potential of the nanocapacitor formed by the external electrodes of the nanostructure.

(viii) Calculation of tunneling coefficients, $I–V$ characteristics, and the spectrum width of the electrons passing through the nanocluster.

Let us start implementation of the above-presented schematic of actions.

2.1. Derivation of the Balance Condition of Energy Providing the Possibility of Electron Tunneling from the Left Electrode through the Nanocluster into the Right Electrode

The condition of electron passage through the tunnel structure under consideration from the left to the right is the simultaneous fulfillment of two inequalities:

$$\mu_{\text{Left}} + \Delta U_{\text{Left}} q_e \geq E_{\text{HOMO}}$$

and

$$E_{\text{HOMO}} \geq \Delta U_{\text{Right}} q_e + \mu_{\text{Right}}$$

where $E_{\text{HOMO}}$ is the HOMO level of the nanocluster anion, $q_e$ is the elementary charge, $\mu_{\text{Left}}$ is the level of the chemical potential of the left electrode, $\Delta U_{\text{Left}}$ is the bias potential between the left electrode and nanocluster, $\mu_{\text{Right}}$ is the chemical potential of the right electrode, and $\Delta U_{\text{Right}}$ is the bias potential between the right electrode and nanocluster. We assume that the