# FULLERENE-BASED SYSTEMS AS COMPONENTS OF NANOELECTRONIC DEVICES

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***Abstract*** –The electric conduction of a single fullerene molecule and chains of fullerenes placed between two metal electrodes was simulated. The electric current was calculated as a function of the bias voltage using the Landauer approach, which connects charge transport with the transmission of electrons. To obtain the transmission function, the supplementary problem of the electron tunneling coupled with its scattering by the fullerenes was solved. It has been shown that the current - voltage characteristics of such structures can have negative-conductance regions that makes it possible to use them as active components of nanoelectronic devices. As an example, the operation of the oscillator including the single fullerene-based component has been demonstrated. The interpretation of the phenomenon has been discussed.

The current–voltage characteristics of systems including fullerenes (the single fullerene molecule or small clusters of fullerenes placed in a gap between two metal electrodes), as it has been shown in [1], have negative-conductance regions. This makes it possible to use them as active components for nanoelectronic devices.

We extend this study to consider similar problem for chains of fullerenes and the influence of the electrode material on the phenomenon. Distances between fullerenes and between a fullerene and an electrode surface were taken to be equal to 0.3 nm, which approximately corresponds to configurations stabilized by week van der Waals interactions. The molecular dynamics simulation confirms the stability of such chains. Due to polarization of fullerenes, the stability of the chains increases when an electric field is applied.

The electric current as a function of the bias voltage was calculated using the Landauer approach, which connects charge transport with the transmission of electrons [2]:

$$I = (q/h) \int_{-\infty}^{\infty} \overline{T}(E)[f_0(E-\mu_1) - f_0(E-\mu_2)]dE\,, \tag{1}$$

where $f_0(E) = (\exp(E/k_B T) + 1)^{-1}$ is Fermi function, $\mu_1$ and $\mu_2$ are the electrochemical potentials of the electrodes, $(\mu_2 - \mu_1) = -qV$, $q$ is the absolute value of the electron's charge, $V$ is the bias voltage.
A gap between electrodes is considered as a tunneling barrier that separates two reservoirs of electrons on each side of it, at different electrochemical potentials $\mu_1$ and $\mu_2$. To obtain the transmission function $\overline{T}(E)$, a supplementary problem of the electron tunneling coupled with its scattering by the fullerenes was considered based on the solution of Schrödinger equation with appropriate Hamiltonian [1].
The results of calculations show that in all the cases the current–voltage characteristics demonstrate nonmonotonic behavior and exhibit sharp jump of current followed by a region of negative differential resistance (Figs. 1 and 2).

The reason of such a behavior is that the transmission function $\overline{T}(E)$ has a peak, the position of which correlates with the energy level of the fullerene, working as a quantum dot (the resonance phenomenon). When $V$ is increased, the peak in the $\overline{T}(E)$ is shifted to the lower values of energy because of the lowering of the resonance energy level in accordance with the lowering of the potential at the center of fullerene. The sharp jump in $I(V)$ occurs when the peak of $\overline{T}(E)$ enters the "window" of the electron's energy with nonzero contribution to the total current (as follows from formula (1)). Further increase of $V$ leads to the decrease of the peak in $\overline{T}(E)$, because it shifts to the more low values of energy of the electron, and hence to the low probability for tunneling. That leads to the decrease in $I$ with the increase in $V$.

In a case of fullerene chains this region is shifted to the higher values of the bias voltage when a chain length is increased.

Due to the specific current–voltage characteristics revealed, the fullerene-based systems, similar to the tunnel diode, can be used as active components for electronic devices.

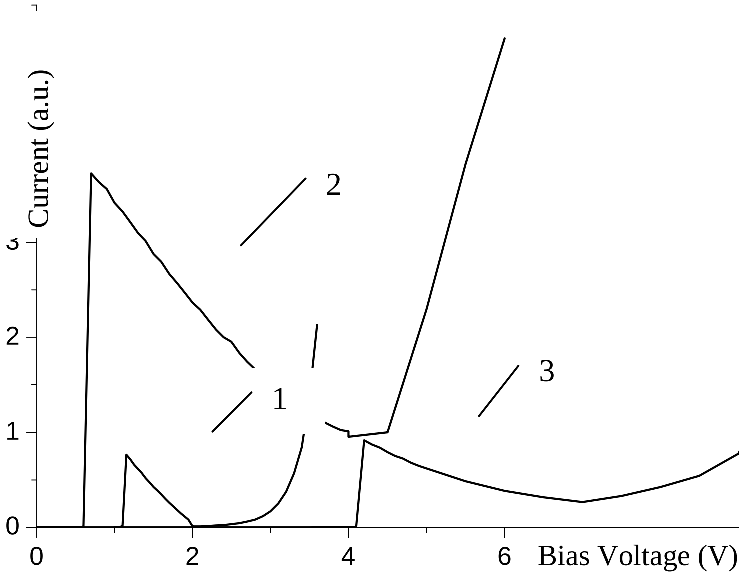


Figure 1 – Current–voltage characteristics corresponding to the different materials of the electrodes: (1) caesium, (2) magnesium, (3) chromium.

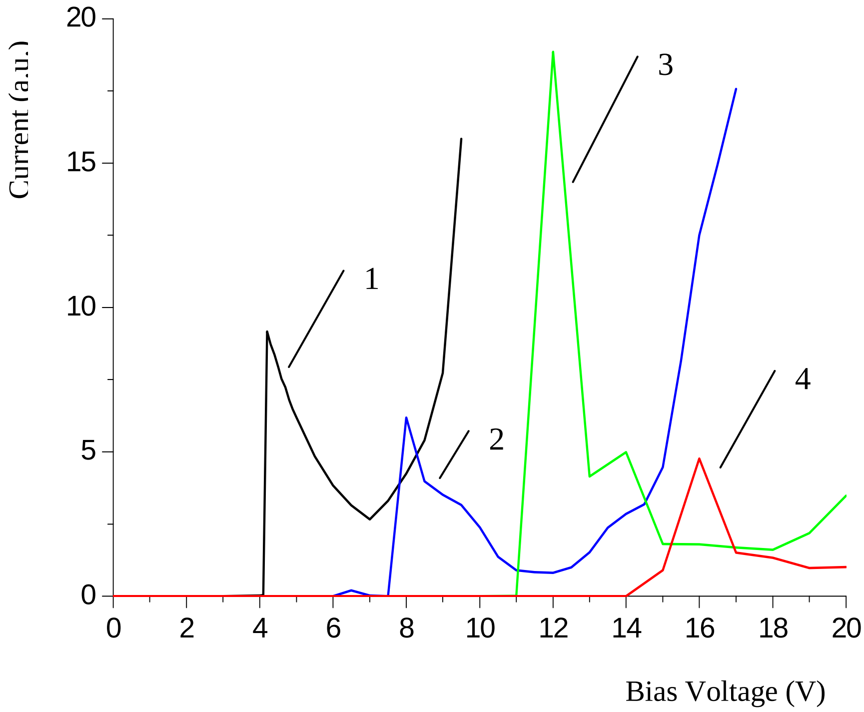


Figure 2 – (1) to (4): current–voltage characteristics corresponding to the fullerene chains consisting of 1 to 4 molecules.

## References

[1] M.A. Britch, K.V. Dobrego, L.I. Krasovskaya, "Numerical analysis of the electrical conduction in carbon nanostructures", *J. Nanophotonics*, vol. 7, 073098, Jan. 2013.
[2] S. Datta, *Quantum Transport*: *Atom to Transistor*. Cambridge University Press, Cambridge, 2005.