LENGTH DEPENDENCE OF THE THERMALLY ACTIVATED INELASTIC AND ELASTIC TUNNEL CURRENT THROUGH A MOLECULAR WIRE

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A theoretical model of formation of the combined elastic and inelastic interelectrode current through a regular molecular wire is proposed in the case where terminal sites of the wire play a role of donor and acceptor centers. It is shown that the current is formed with two alternative mechanisms, superexchange and sequential ones. But, such an additivity is true if only a definite relation between the elementary rate constants specifying the transitions within a common system "electrode–molecular wire–electrode", exists. The analytic dependence of the current on the number of wire units is derived.

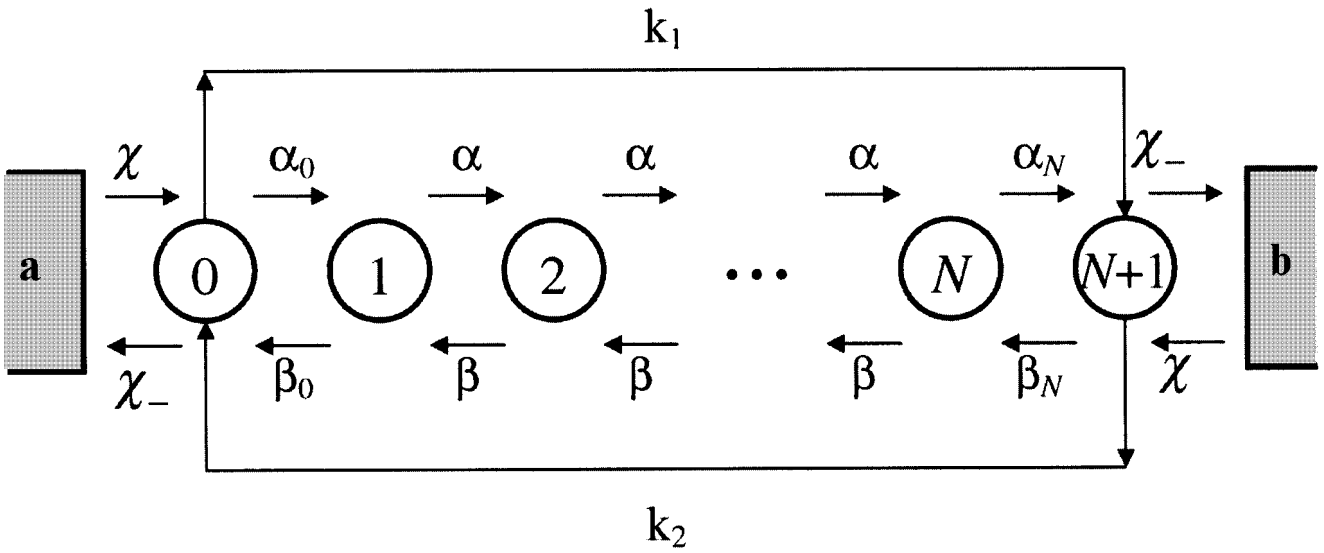
Introduction

Current-voltage (I—V) characteristics contain a rich information on physical mechanisms of charge transfer in conducting systems. Thus, a linear dependence of current I on voltage bias V reflects an Ohmic character of conductivity caused by the motion of free carriers in the conducting system. The Ohmic type of conductivity is typical of macroscopic samples of normal metals. As to a conductance of atomic and molecular chains, it can exhibit large deviations from the Ohmic type. For instance, if a chain of gold atoms is connected to two gold leaves, a linear dependence of the current through the atomic chain is observed. Another picture occurs if the same atomic chain is connected to the leaves but with reduced contact coupling. In this case, one observes nonlinear I—V characteristics of the chain [1]. Recent experiments on conductivity of separate molecules [2—5] have also detected strongly nonlinear I—V characteristics. Note that a theory predicts the appearance of a nonlinear current in a short molecular wire if only the formation of the current proceeds on the background of fast relaxation processes within the wire [6, 7]. Specific I—V characteristics appear in the case of a long regular molecular wire where the important role in formation of the current belongs to an inelastic hopping competing with an elastic tunnelling [8—11]. Each process forms the own dependence of the current on wire length and thus a specific current behavior. Therefore, the studies of a length dependence of the current is exclusively important for understanding the mechanism of formation of the wire-mediated interelectrode current, especially in the case of a regular molecular wire.

The goal of the present work is to clarify a length dependence of the current under conditions when the short-range sequential and long-range superexchange mechanisms are responsible for formation of the thermally activated current through a regular molecular wire.

1. General Form of the Current

In the model under consideration, relaxation processes within each site of electron localization are assumed to be much more fast than the processes responsible for electron transfer (ET) between the sites. It means that the interelectrode current is formed by electron hoppings along the wire [6, 10]. Figure manifests the scheme of kinetic processes forming the current through a regular molecular wire of $N + 2$ units. Terminal wire units, 0 and $N + 1$, make direct contact with the adjacent microelectrodes "a" and "b", and with the neighboring wire units 1 and N. The corresponding hopping ET rates are denoted via $\chi_{a(b)}$ and $\chi_{-a(-b)}$, and $\alpha_{0(N)}$ and $\beta_{0(N)}$, respectively. Rate constants α and β characterize forward and backward ET hoppings within the inner part of a regular wire. It is important to note that, due to a polarization effect of the metallic electrodes, the image forces decrease essentially (up to 1—1.5 eV) the LUMO-levels of the terminal wire units [7, 10]. Therefore, even though the wire obeys a completely regular structure,the rate constants between the $0(N + 1)$th and the $1(N)$th units differ from those of the inner units. Let, generally, $\alpha_0, \alpha_N \neq \alpha$ and $\beta_0, \beta_N \neq \beta$. The essential decrease of the energy position of the terminal LUMO-levels (0 and $N + 1$) compared to the inner LUMO-levels (1,2,...,N) brings to a specific superexchange coupling between the



Kinetic scheme of formation of an interelectrode current through a linear molecular wire

terminal units. Just LUMO-levels belonging to the inner units exhibit itself as virtual levels forming the mentioned superexchange coupling. Bearing this fact in mind, we shall consider a molecular wire where only inner wire units ($n = 1,2,...N$) have a regular structure with identical energy position of LUMO-levels. Thus, along with sequential hops, one has to consider a contribution of distant superexchange ET hops between the terminal wire units. The corresponding forward and backward rate constants are denoted through k_1 and k_2.

To derive the form of interelectrode current I, we start from the general expression

$$I = -e\dot{N}_a, \tag{1}$$

where e is the value of electron charge, and $\dot{N}_a = -\dot{N}_b$ is the time variation of the number of electrons which are capable of being transferred through a molecular wire from electrode "a" to electrode "b". Let P_n be the site population of the nth wire unit, $(n = 0,1,...,N+1)$.

In line with a kinetic scheme represented in Figure, these populations (as well as quantities $\dot{N}_a$ and $\dot{N}_b$) are found from the set of coupled kinetic equations

$$\dot{N}_a = -\chi_a + \chi_{-a}P_0\,,$$

$$\dot{P}_0 = -(\chi_{-a} + \alpha_0 + k_1)P_0 + \chi_a + \beta_0 P_1 + k_2 P_{N+1}\,,$$

$$\dot{P}_1 = -(\alpha + \beta_0)P_1 + \alpha_0 P_0 + \beta P_2\,,$$

$$\dot{P}_n = -(\alpha + \beta)P_n + \alpha P_{n-1} + \beta P_{n+1}\,,\ (n = 2,...,N-1)\,,$$

$$\dot{P}_N = -(\alpha_N + \beta)P_N + \alpha P_{N-1} + \beta_N P_{N+1}\,,$$

$$\dot{P}_{N+1} = -(\chi_{-b} + \beta_N + k_2)P_{N+1} + \chi_b + \alpha_N P_N + k_1 P_0\,,$$

$$\dot{N}_b = -\chi_b + \chi_{-b}P_{N+1}\,. \tag{2}$$

Below we consider a stationary regime of ET when $\dot{P}_n = 0$, and $\dot{N}_a = -\dot{N}_b$ =const. The above set of equations for only the site populations reduces to

$$\mathbf{P}\hat{\mathbf{A}} = \mathbf{C}\,. \tag{3}$$

Vectors $\mathbf{P}$ and $\mathbf{C}$ are defined by components P_n and $C_n = \chi_a\delta_{n,0} + \chi_b\delta_{n,N+1}$, respectively ($\delta_{n,0}$ is the Kronecker symbol). Exact solution of set (3) reads

$$P_n = (\chi_a + \chi_b)\frac{S_n}{\chi_{-a}S_0 + \chi_{-b}S_{N+1}}\,. \tag{4}$$

Here,

$$S_0 = [(\chi_a q_{N+1} + \chi_b k_2)q_1 q_N - \chi_a q_1 \alpha_N \beta_N]\,D(N-2) -$$

$$-[(\chi_a q_{N+1} + \chi_b k_2)(q_1 + q_N) - \chi_a \alpha_N \beta_N]\alpha\beta\,D(N-3) +$$

$$+(\chi_a q_{N+1} + \chi_b k_2)\alpha^2\beta^2\,D(N-4) + \chi_b\beta_0\beta_N\beta^{N-1},$$

$$S_{N+1} = [(\chi_b q_0 + \chi_a k_1)q_1 q_N - \chi_b q_N \alpha_0 \beta_0]\,D(N-2) -$$

$$-[(\chi_b q_0 + \chi_a k_1)(q_1 + q_N) - \chi_b \alpha_0 \beta_0]\alpha\beta\,D(N-3) +$$

$$+(\chi_b q_0 + \chi_a k_1)\alpha^2\beta^2\,D(N-4) + \chi_a\alpha_0\alpha_N\alpha^{N-1}, \tag{5}$$

and $(n = 1, 2, ..., N)$

$$S_n = \chi_a\{\alpha_0\alpha^{n-1}[q_{N+1}(q_N\, D(N-n-1)-$$
$$\alpha\beta\, D(N-n-2)) - \alpha_N\beta_N\, D(N-n-1)]+$$
$$+k_1\beta_N\beta^{N-n}(q_1 D(n-2) - \alpha\beta\, D(n-3))\}+$$
$$+\chi_b\{\beta_N\beta^{N-n}[q_0(q_1 D(n-2) - \alpha\beta\, D(n-3))-$$
$$-\alpha_0\beta_0\, D(n-2)] + +k_2\alpha_0\alpha^{n-1}(q_N\, D(N-n-1)-$$
$$-\alpha\beta\, D(N-n-2))\}\,, \qquad (6)$$

where

$$D(M) \equiv (\alpha\beta)^{M/2}\frac{\sinh\Lambda(M+1)}{\sinh\Lambda}\,, \quad \left(e^{\Lambda} = \sqrt{\alpha/\beta}\right). \qquad (7)$$

In Eqs. (5) and (6), the following abbreviation has been utilized:

$$q_0 \equiv \chi_{-a} + \alpha_0 + k_1\,, \quad q_1 \equiv \alpha + \beta_0\,,$$
$$q_N \equiv \alpha_N + \beta\,, \quad q_{N+1} \equiv \chi_{-b} + \beta_N + k_2\,. \qquad (8)$$

After the substitution of the reading form of P_0 in the first equation of set (2), Eq. (1) is transformed to

$$I = e\frac{\chi_a\chi_{-b}A_{N+1} - \chi_b\chi_{-a}A_0}{\chi_{-a}A_0 + \chi_{-b}A_{N+1}}, \qquad (9)$$

where

$$A_0 = (\chi_a + \chi_b)\{k_2[(\alpha\alpha_N + \beta\beta_0 + \alpha_N\beta_0)\, D(N-2)-$$
$$-(\alpha_N + \beta_0)\alpha\beta\, D(N-3)] + \beta_0\beta_N\beta^{N-1}\}+$$
$$+\chi_a\chi_{-b}[(\alpha\alpha_N + \beta\beta_0 + \alpha_N\beta_0)\, D(N-2)-$$
$$-(\alpha_N + \beta_0)\alpha\beta\, D(N-3)]\,, \qquad (10)$$

and

$$A_{N+1} = (\chi_a + \chi_b)\{k_1[(\alpha\alpha_N + \beta\beta_0 + \alpha_N\beta_0)\, D(N-2)-$$
$$-(\alpha_N + \beta_0)\alpha\beta\, D(N-3)] + \alpha_0\alpha_N\alpha^{N-1}\}+$$
$$+\chi_b\chi_{-a}[(\alpha\alpha_N + \beta\beta_0 + \alpha_N\beta_0)\, D(N-2)-$$
$$-(\alpha_N + \beta_0)\alpha\beta\, D(N-3)]\,. \qquad (11)$$

Eqs. (9), (10), and (11) allows us to evaluate the I—V characteristics of an inelastic interelectrode current at different relations between the rate constants. Note, however, that form (9) is correct if only a tunnel regime for ET between the terminal units 0 and $N+1$ occurs. Physically, it means a small population of wire sites 1,2,...,N. Besides, we restrict ourself by consideration of thermally activated tunnel processes only, when $\chi_{a(b)} \ll \chi_{-a(-b)}$. Just these conditions guarantee the validity of a linear form of set (2).

2. Length Dependence of the Current

To derive a reading form of the current which can be employed for the analyses of a length dependence, we have to specify both a relation between the rate constants and the distances between the sites of electron localization within the wire. Here we utilize the simplest model where each site of electron localization coincides with the center of the corresponding wire unit. It allows us to determine the dependence of local electronic energies E_n $(n = 0, 1, ...N+1)$ on the voltage bias V. For the sake of definiteness, we assume electrode "a" be supported under a zero voltage. In this case,

$$E_0 = E_0^0 - (eV/L)l_a\,, \quad E_{N+1} = E_{N+1}^0 + (eV/L)l_b - eV\,,$$

$$E_n = E^0 - (eV/L)l_a - (eV/L)l_1 - (eV/L)(n-1)l\,, \qquad (12)$$

where E_0^0, E_{N+1}^0 and $E^0 = E_n^0$, $(n = 1, 2, ...N)$, are the electronic energies of two terminal wire units and any nth unit of a regular part of the wire, respectively; $l_{a(b)}$ and $l_{1(N)}$ are the distances from the $0(N+1)$th terminal wire unit to the corresponding electrode surface and the adjacent inner wire unit; l is the distance between the neighboring units of a regular part of the wire, $L = l_a + l_1 + (N-1)l + l_N + l_b$ is the total wire length. A form of the rate constants characterizing the elementary hops in a transfer system "electrode a—molecular wire—electrode b" depends strongly on a specific structure of wire units as well as on the coupling of electronic states to vibrational modes (see examples in [6, 7, 9—11]). It is possible, however, to determine the dependence of the current on the number of wire units employing the only relations between the forward and backward rate constants. For the intersite rate constants, these relations read

$$\alpha_0 = \beta_0\, \exp\left[-(E_1 - E_0)/k_{\rm B}T\right],$$

$$\beta_N = \alpha_N\, \exp\left[-(E_N - E_{N+1})/k_{\rm B}T\right],$$

$$\beta = \alpha\, \exp\left[-(E_n - E_{n+1})/k_{\rm B}T\right], \quad (n = 1, ..., N-1)\,, \qquad (13)$$

while the relation between the rate constants characterizing the transitions between the electrodes and the adjacent terminal wire units appears as [7]

$$\chi_a = \chi_{-a}\, \exp\left[-(E_0 - E_{\rm F})/k_{\rm B}T\right],$$

$$\chi_b = \chi_{-b}\,\exp\left[-(E_{N+1} - E_{\rm F} + eV)/k_{\rm B}T\right]. \quad (14)$$

Besides, we have

$$k_2 = k_1\,\exp\left[-(E_0 - E_{N+1})/k_{\rm B}T\right]. \quad (15)$$

[In Eqs. (13) — (15) $k_{\rm B}$ and T are the Boltzmann constant and the absolute temperature, respectively.] It follows from relations (13) — (15) and Eq. (12) that

$$\chi_{-a}\chi_b\beta_0\beta_N\beta^{N-1} = \chi_{-b}\chi_a\alpha_0\alpha_N\,\exp\left(-eV/k_{\rm B}T\right),$$

$$\chi_b\chi_{-a}k_2 = \chi_{-b}\chi_a k_1\,\exp\left(-eV/k_{\rm B}T\right). \quad (16)$$

Therefore, we can reduce expression (9) to a more compact form

$$I = e\Big[1 - \exp\left(-eV/k_{\rm B}T\right)\Big]\,\frac{\chi_a}{\chi_{-a}}\,\frac{F_1}{F_2}, \quad (17)$$

where

$$F_1 = k_1\Big(\frac{1-\gamma^{N-1}}{1-\gamma} + \frac{\alpha}{\beta_0} + \frac{\alpha}{\alpha_N}\gamma^{N-1}\Big) + \frac{\alpha_0}{\beta_0}\alpha \quad (18)$$

and

$$F_2 = \Big(1 + \frac{k_1}{\chi_{-a}} + \frac{k_2}{\chi_{-b}}\Big)\Big(\frac{1-\gamma^{N-1}}{1-\gamma} + \frac{\alpha}{\beta_0} +$$

$$+\frac{\alpha}{\alpha_N}\gamma^{N-1}\Big) + \frac{\alpha\alpha_0}{\beta_0\chi_{-a}} + \frac{\alpha\beta_N}{\chi_{-b}\alpha_N}\gamma^{N-1}. \quad (19)$$

Eqs. (17)—(19) define the final form of an inelastic current in the case of a tunnel regime. One can see a mixture between the superexchange contribution characterized by the rate constants k_1 and k_2, and the sequential contribution characterized by the rest rate constants and parameter

$$\gamma \equiv \beta/\alpha = \exp\left(-eVl/Lk_{\rm B}T\right). \quad (20)$$

The mixture of both sequential and superexchange pathways of ET exhibits a rather complicated dependence of the current on the number of regular wire units N. If, however, the inequalities

$$k_1, \alpha_0 \ll \chi_{-a}\,, \quad k_2, \beta_N \ll \chi_{-b} \quad (21)$$

are satisfied during the ET, current (17) is reduced to the sum of two separate contributions,

$$I = \Big[1 - \exp\left(-eV/k_{\rm B}T\right)\Big]\,\Big[I_{\rm sup}(N) + I_{\rm seq}(N)\Big] \quad (22)$$

where

$$I_{\rm sup}(N) = I_{\rm sup}(1)e^{-\lambda(N-1)} \quad (23)$$

and

$$I_{\rm seq}(N) = I_{\rm seq}(1)\Big[1 + \xi\frac{1-\gamma^{N-1}}{1-\gamma}\Big]^{-1} \quad (24)$$

are the superexchange component and the sequential component of an interelectrode current, respectively. Analytic dependence of each component is concentrated in specific factors which contain the decreas parameters

$$\lambda = -2\ln\left[|V_B|/\sqrt{\Delta E_0\Delta E_{N+1}}\right] \quad (25)$$

and

$$\xi = \frac{1 - (\alpha/\alpha_N)(1-\gamma)}{(\alpha/\beta_0) + (\alpha/\alpha_N)}, \quad (26)$$

while quantities

$$I_{\rm sup}(1) = e(\chi_a/\chi_{-a})k_1(1) \quad (27)$$

and

$$I_{\rm seq}(1) = e\frac{\chi_a}{\chi_{-a}}\,\frac{\alpha_0\alpha_N}{\beta_0 + \alpha_N} \quad (28)$$

characterize the current through a single bridging unit. Note that the sequential decrease parameter ξ is defined through elementary rate constants and thus the drop of the sequential part of the current is defined by pure kinetic processes in the transfer system. As to the superexchange decrease parameter λ, it reflects the dynamic properties of the wire. To derive λ, we have utilized the fact that $I_{\rm sup} = e(\chi_a/\chi_{-a})k_1$.The form of the rate constant k_1 is well known in the theory of bridge-assisted donor-acceptor nonadiabatic ET [12—14] so that $k_1 = k_1(1)\exp\left[-\lambda(N-1)\right]$, where $k_1(1)$ is the rate constant for the bridge of a single unit. The parameter λ depends strongly on electron coupling V_B between the neighboring inner wire units as well as on energy gaps $\Delta E_n^{(0)} = E_n - E_0$ and $\Delta E_n^{(N+1)} = E_n - E_{N+1}$, $(n = 1, 2, ..., N)$ between the inner LUMO-levels and the LUMO-levels belonging the terminal groups 0 and $N+1$. Eq. (25) manifests the simplest form of the parameter λ valid at a deep tunnelling when $\Delta E_n^{(0)} \approx \Delta E_0 \equiv E_0 - E_0^{(0)}$, $\Delta E_n^{(N+1)} \approx \Delta E_{N+1} \equiv E_0 - E_{N+1}^{(0)}$, and, additionally, $|V_B| \ll \Delta E_0$, ΔE_{N+1}.

3. Discussion of Results

The derivation of analytic expressions (23) and (24) is the main result of the present work. These expressions allows us to analyze the dependence of the current on the number of wire units and thus to specify the mechanisms of formation of an interelectrode current through a molecular wire. One can see that the superexchange component of the current manifests an exponential drop with N while the sequential component has a smooth decrease. Actually, the N-dependence of the $I_{\rm seq}$ is confined in the factor $(1-\gamma^{N-1})/(1-\gamma)$ which has two limiting values, $N-1$ (at $\gamma \approx 1$) and 1 (at $\gamma \ll 1$). Therefore, we have two limiting cases for the sequential contribution,

$$I_{\rm seq}(N) = \frac{I_{\rm seq}(1)}{1+\xi(N-1)}\,,$$

$$\xi = \frac{1}{(\alpha/\beta_0)+(\alpha/\alpha_N)}\,, \quad (\beta \approx \alpha)\,, \tag{29}$$

and

$$I_{\rm seq}(N) = \frac{I_{\rm seq}(1)}{1+\xi}\,,$$

$$\xi = \frac{1-(\alpha/\alpha_N)}{(\alpha/\beta_0)+(\alpha/\alpha_N)}\,, \quad (\beta \ll \alpha)\,. \tag{30}$$

In the first limiting case, Eq. (29), the $I_{\rm seq}(N)$ demonstrates a hyperbolic decreasing with N. Such a behavior of the current reflects a hopping process at which the forward and backward inner rate constants are equal to each other. Physically, this case corresponds to a small intersite voltage bias so that $\exp(-eVl/Lk_{\rm B}T) \approx 1$. The second limiting case, Eq. (30), is realized at a large intersite voltage bias when $\exp(-eVl/Lk_{\rm B}T) \ll 1$. In the second limiting case, the ET along a regular part of the wire is exclusively defined by the forward rate constant α. It corresponds to a directed ET in the wire such that an interelectrode current does not depend on the number of wire units. Both limiting cases clearly indicate that, at the large number of wire units, the sequential mechanism can become more preferable than the superexchange one. A given conclusion follows from an additive form of the current, Eq. (22). In turn, the additive form appears if and only if inequalities (21) are satisfied during the ET process. The inspection of Eq. (4) shows that all site populations (4) become small in this case.

The proposed model of formation of an inelastic tunnel current supposes a thermal activation of the ET process via a deliver of the transferred electron from the electrode to the adjacent terminal group (the corresponding rates are χ_a and χ_b). After such a deliver, the transferred electron either moves along the wire units (sequential pathway) or performs a distant tunnel hopping between the terminal groups (superexchange pathway). Analytic expressions (22), (23) and (24) allow us to analyze a length-dependence of the current at the fixed voltage and the fixed temperature. Further detalization of the theory depends on experimental results on conductivity of regular molecular wires. Until now such experiments are absent. But, there exists a large perspective to measure microcurrents in a system involving gold islands and organic stearon molecules [15, 16].

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ЗАЛЕЖНІСТЬ ТЕМПЕРАТУРНО АКТИВОВАНОГО НЕПРУЖНОГО І ПРУЖНОГО ТУНЕЛЬНИХ СТРУМІВ КРІЗЬ МОЛЕКУЛЯРНИЙ ПРОВІД ВІД ЙОГО ДОВЖИНИ

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Р е з ю м е

Запропоновано теоретичну модель формування комбінованого пружного і непружного міжелектродних струмів для випадку, коли кінцеві центри проводу відіграють роль донорного і акцепторного центрів. Показано, що струм формується за допомогою двох альтернативних механізмів — суперобмінного та стрибкового. Однак така адитивність допускається лише у тому випадку, якщо виконується певне співвідношення між елементарними константами швидкостей, що характеризують явище переносу у межах загальної системи "електрод—молекулярний провід—електрод". Одержано аналітичну залежність струму від кількості центрів проводу.

ЗАВИСИМОСТЬ ТЕМПЕРАТУРНО АКТИВИРОВАННОГО НЕУПРУГОГО И УПРУГОГО ТУННЕЛЬНЫХ ТОКОВ ЧЕРЕЗ МОЛЕКУЛЯРНЫЙ ПРОВОД ОТ ЕГО ДЛИНЫ

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Р е з ю м е

Предложена теоретическая модель формирования комбинированного упругого и неупругого межэлектродных токов для случая, когда крайние центры провода играют роль донорного и акцепторного центров. Показано, что ток формируется с помощью двух альтернативных механизмов — суперобменного и прыжкового. Однако такая аддитивность допускается только в том случае, когда выполняется определенное соотношение между элементарными константами скоростей, характеризующих переносы в пределах общей системы "электрод—молекулярный провод—электрод". Получена аналитическая зависимость тока от количества звеньев провода.