BALLISTIC CONDUCTANCE AND IMPEDANCE OF ONE-DIMENSIONAL SYSTEMS

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General expressions for the resistance and impedance of one-dimensional ideal nanoconductors and semiconductors of finite length are obtained and illustrated for models of the systems of parallel regular atomic chains the electronic structure of which was modeled on the basis of the method of null-range potentials.

1. Introduction

If a point defect is located on the surface or in the bulk of a nonmetallic crystal, then energy levels may appear in each forbidden band of its one-electronic spectrum. On the association of defects into a cluster, such a level splits into a multiplet, the number of sublevels of which coincides in general with that of the defects forming a cluster. If such defects form an infinite regular chain or one-dimensional path of parallel chains, then impurity levels merge into waveguide bands inside the forbidden band of a crystal-matrix. Electrons or holes of such bands are located near the chain, but can move freely along it. Depending on the depth of an impurity level E_0, the waveguide band is either entirely located inside the forbidden band or it overlaps partly the adjacent bands. The same waveguide bands are formed along one-dimensional periodic atomic structures such as carbon nanotubes and nanowires formed inside pores produced by MeV-energy heavy ions in different materials.

If the Fermi level crosses several waveguide bands, then the concerned one-dimensional structures are conductors, whose finite conductivity is caused at low temperatures and in the absence of defects only by the scattering of carriers on contacts at their ends. Notice that the resistance R_0 of an ideal conducting one-atomic chain at zero temperature is the universal constant [1]

$$R_0 = \frac{\pi\hbar}{e^2} = 1.293 \times 10^4 \Omega.$$

One-dimensional conductors such as carbon nanotubes [2—4] or metal nanobridges [5, 6] and under certain conditions nanowires in pores produced by the beams of MeV-energy heavy ions [7] can be considered as the connection of n ideal parallel one-atomic chains. Therefore, their electronic spectrum contains n, maybe overlapping, waveguide bands. Electric resistance of such conductors is R_0/n', where $n' \leq n$ is the number of the waveguide bands crossing the Fermi level.

In this paper, these results are generalized on the case where the Fermi level of a system of parallel one-atomic chains gets on the top edge of one or several occupied waveguide bands whereupon it is non-conducting at zero temperature. In addition, a simple expression for the impedance of the investigated structures in a harmonic field is deduced.

The aforementioned statements follow directly from the general concepts of the elementary quantum theory of solids and are true for any model of quantum particle motion in a periodic field. Therefore, without loss of generality, for the specification of the electron dynamics in waveguide bands formed along real periodic chains of defects in crystals or along one-dimensional periodic atomic structures like carbon nanotubes, it is enough to use the elementary model in which the atomic carcass of the one-dimensional structure is considered as a periodic sequence of null-range potentials (NRP) [8, 9]. Despite a rather poor description of the electronic structure of single atoms, a great advantage of such a model is in the accurate account of all peculiar properties of electronic spectra of quantum dots, atomic chains, and crystals resulting from their geometry. The last section of the paper is devoted to the description of one-electronic states of the considered structures in frameworks of the NRP model as a base for the numerical illustrations and estimates for specific one-dimensional periodic compounds.

2. Resistance of One-dimensional Structures

Let's consider now a finite quasi-one-dimensional system of length L such that it is reasonable to speak about a quasi-wave vector k. If a potential difference U is applied to the ends of the system, then an electric current may flow. For the calculation of conductance, we use

the Boltzmann kinetic equation in the approximation of relaxation time. In this approximation, a change of the equilibrium electron distribution Fermi function $\delta n(E(k))$ at a rather small displacement U is determined by the expression

$$\delta n(k) = -e\frac{U}{L}V(k)\tau(E)\frac{\partial n(E)}{\partial E}, \quad (1)$$

where $V(k)$ is the electron speed with quasi-momentum k and energy $E(k)$,

$$V(E(k)) = \frac{1}{\hbar}\frac{\partial E(k)}{\partial k},$$

$\tau(E)$ is the relaxation time of carriers with energy E. Taking into account that the unique mechanism of relaxation in an ideal system is the scattering or absorption of carriers on the contacts, we put

$$\tau(E) = \frac{L}{|V(E)|}. \quad (2)$$

According to (1), the current caused by a displacement U is given by the expression

$$I = \frac{e}{\pi}\sum_{\alpha}\int\limits_{0}^{\pi/a}\delta n(E_\alpha(k))eV(E_\alpha(k))dk, \quad (3)$$

in which the summation is formally performed over all one-dimensional bands $E_\alpha(k)$.

Let's consider a simple regular chain of monovalent atoms which has only one band and therefore is a metal. In this case, formula (3) is reduced to the form

$$I = \frac{e^2U}{\pi\hbar}\int\limits_{E_{\min}}^{E_{\max}}\left(-\frac{\partial n(E)}{\partial E}\right)dE =$$

$$= \frac{e^2}{\pi\hbar}U\left[n(E_{\min}) - n(E_{\max})\right]. \quad (4)$$

Thus, the ballistic resistance of the considered system is

$$R = \frac{\pi\hbar}{e^2[n(E_{\min}) - n(E_{\max})]}. \quad (5)$$

At low temperatures where the relation $[n(E_{\min}) - n(E_{\max})] \approx 1$ holds, the formula becomes the universal constant, the quantum of resistance $R_0 = \frac{\pi\hbar}{e^2}$.

It is easy to generalize the given formula for a case where the system has more than one band and the Fermi level crosses p bands:

$$R = R_0\left(\sum_{\alpha}^{p}\left[n(E^\alpha_{\min}) - n(E^\alpha_{\max})\right]\right)^{-1}.$$

If the edges of bands are far enough from the Fermi level, that is, if the electronic gas of a conductor is degenerate, then

$$R = \frac{R_0}{p}.$$

The given formula shows that the ballistic conductance does not depend on parameters of the system, but depends only on the number of bands crossing the Fermi level.

In semiconductors where the chemical potential level μ lies in an interval between two bands, formula (3) is transformed into the expression

$$I = -\frac{e^2}{\pi\hbar}U\left[-\int\limits_{-\infty}^{E_v}\frac{\partial n_h}{\partial E}dE + \int\limits_{E_c}^{\infty}\frac{\partial n_e}{\partial E}dE\right],$$

where n_e and n_h are the distribution Fermi functions for electrons and holes, respectively, E_v and E_c are the levels corresponding to the top of the valence band and the bottom of the conduction band, respectively and integrals should be spread onto the bands nearest to μ. We have expanded the limits of integration up to $\pm\infty$, which does not result in errors as far as the widths of bands $\ll k_{\rm B}T$.

Taking into account that, for a one-dimensional pure semiconductor,

$$\mu = E_v + \frac{E_g}{2} - \frac{1}{4}kT\ln\left(\frac{m^*_e}{m^*_h}\right),$$

where m^*_e and m^*_h are the effective masses of electrons and holes, respectively, E_g is the width of the forbidden band, we get the following expression for its ballistic electric resistance:

$$R = R_0 e^{\frac{E_g}{2k_{\rm B}T}}\left[\left(\frac{m^*_e}{m^*_h}\right)^{1/4} + \left(\frac{m^*_e}{m^*_h}\right)^{-1/4}\right]^{-1}.$$

Thus, upon a reduction of temperature, R of one-dimensional pure semiconductors grows exponentially. However, in semiconductors with a narrow forbidden band at temperatures $k_{\rm B}T \gg \frac{1}{2}E_g$, the ballistic resistance is at least twice less than R_0.

3. Impedance of One-dimensional Conductor

Let's consider now the case where the applied electric displacement changes by the harmonic law with frequency ω: $U(t) = Ue^{-i\omega t}$. To find the dependence of the ballistic conductance on the frequency, we use, as before, the Boltzmann kinetic equation in the approximation of relaxation time. In this approximation,

$$\delta n(k,t) = -e\frac{U}{L}\frac{V(k)\tau(E)}{1-i\omega\tau(E)}\frac{\partial n(E)}{\partial E}e^{-i\omega t}.$$

Respectively, with the account of (3), we obtain

$$I(t) = -\frac{e^2}{\pi}\sum_{\alpha}\int\limits_{-\pi/a}^{\pi/a}\frac{\partial n(E_\alpha(k))}{\partial E}\frac{V(E_\alpha(k))}{1-i\omega\frac{L}{|V(E_\alpha(k))|}}dk\cdot U(t).$$

For a conductor, the real part of the conductance which determines the energy dissipation is

$$\mathrm{Re}G(\omega) = \frac{e^2}{\pi\hbar}\int\limits_{E_{\min}}^{E_{\max}}\frac{V^2}{V^2+\omega^2L^2}\left(-\frac{\partial n(E)}{\partial E}\right)dE. \qquad (6)$$

As the expression $\left(-\frac{\partial n(E)}{\partial E}\right)$ behaves similarly to the delta function centered at the Fermi level, the main contribution to (6) has form

$$\mathrm{Re}G(\omega) = \frac{e^2}{\pi\hbar}\frac{V_{\mathrm{F}}^2}{V_F^2+\omega^2L^2}.$$

Notice that, in contrast to static conductivity, this expression includes such parameters of the system as its length L and the electron speed V_{F} at the Fermi level. If the Fermi level crosses some bands, then

$$\mathrm{Re}G(\omega) = \frac{e^2}{\pi\hbar}\sum_{\alpha}^{p}\frac{V_{\mathrm{F}_\alpha}^2}{V_{F_\alpha}^2+\omega^2L^2}.$$

For a semiconductor, formula (6) looks as

$$\mathrm{Re}G(\omega) = \frac{e^2}{\pi\hbar}\left[-\int\limits_{-\infty}^{E_v}\frac{V^2}{V^2+\omega^2L^2}\left(-\frac{\partial n_h}{\partial E}\right)dE+\right.$$

$$\left.+\int\limits_{E_c}^{\infty}\frac{V^2}{V^2+\omega^2L^2}\left(-\frac{\partial n_e}{\partial E}\right)dE\right].$$

The derivatives in the integrands fall down exponentially by moving away from the edges of bands, and the basic contributions to integrals are given by the vicinities of the edges. Hence, for the calculation of $\mathrm{Re}G(\omega)$, we can use the effective mass approximation and, assuming that the semiconductor is non-degenerate, change the Fermi distribution by the Boltzmann one.

As a result, we get

$$\mathrm{Re}G(\omega) = \frac{e^2}{\pi\hbar}e^{-\frac{Eg}{2k_{\mathrm{B}}T}}\times$$

$$\times\left\{\left(\frac{m_e^*}{m_h^*}\right)^{\frac{1}{4}}\left(1-\frac{\omega^2}{\omega_h^2}e^{\frac{\omega^2}{\omega_h^2}}\,\mathrm{Ei}\left(\frac{\omega^2}{\omega_h^2}\right)\right)+\right.$$

$$\left.+\left(\frac{m_h^*}{m_e^*}\right)^{\frac{1}{4}}\left(1-\frac{\omega^2}{\omega_e^2}e^{\frac{\omega^2}{\omega_e^2}}\,\mathrm{Ei}\left(\frac{\omega^2}{\omega_e^2}\right)\right)\right\},$$

where $\omega_h^2 = \frac{2k_{\mathrm{B}}T}{m_h^*L^2}$, $\omega_e^2 = \frac{2k_{\mathrm{B}}T}{m_e^*L^2}$, $\mathrm{Ei}(x) = \int\limits_x^{+\infty}\frac{e^{-t}}{t}dt$.

For $x \to 0$, the asymptotic expression

$$xe^x\int\limits_x^{+\infty}\frac{e^{-t}}{t}dt \approx (-C-\ln(x))x$$

is valid, where $C = 0.5772$ is the Euler constant. Then, for $\omega < \omega_e$ and $\omega < \omega_h$, we obtain

$$\mathrm{Re}G(\omega) = \frac{e^2}{\pi\hbar}e^{-\frac{Eg}{2k_{\mathrm{B}}T}}\times$$

$$\times\left\{\left(\frac{m_e^*}{m_h^*}\right)^{\frac{1}{4}}\left(1+C\frac{\omega^2}{\omega_h^2}+\frac{\omega^2}{\omega_h^2}\ln\left(\frac{\omega^2}{\omega_h^2}\right)\right)+\right.$$

$$\left.+\left(\frac{m_h^*}{m_e^*}\right)^{\frac{1}{4}}\left(1+C\frac{\omega^2}{\omega_e^2}+\frac{\omega^2}{\omega_e^2}\ln\left(\frac{\omega^2}{\omega_e^2}\right)\right)\right\}.$$

4. Numerical Modeling

The basic features of the electronic structure of the considered systems are manifested already for periodic chains with two atoms in an elementary cell. We assume that cells of such chains (Fig. 1) are located along the axis x and their position is defined by radius vectors $\vec{n} = n\vec{a}$, and the relative displacement of atoms inside a cell is defined by the radius vector $\vec{c}$. According to the method of NRP, the interaction of an electron (or a hole if the chain is formed by a donor impurity in

nonmetallic crystals) with atoms of a chain is modeled not by a periodic potential but by a periodic sequence of boundary conditions imposed on the wave function of an electron $\Psi(\vec{r})$ at the points where there are atoms [8], [9]:

$$\lim_{\rho_{n,s}\to 0}\left[\frac{\partial}{\partial\rho_{n,s}}(\rho_{n,s}\Psi)-b\rho_{n,s}\Psi\right]=0, \tag{7}$$

$$\rho_{n,s}=|\vec{r}-n\vec{a}-s\vec{c}|\,, \qquad n=0,\pm1,...,\qquad s=0,1.$$

Here, the unique parameter of interaction b is chosen so that the energy E_0 of ionization of an isolated atom or impurity equals $\frac{\hbar^2b^2}{2m}$, where m is the mass or effective mass of a carrier. Thus, it is assumed that the wave function $\Psi(\vec{r},E)$ for the state of a carrier with energy $E(<0)$ in the waveguide band satisfies the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\Psi=E\Psi \tag{8}$$

everywhere except for points (7). Setting

$$\gamma=\sqrt{-\frac{2m}{\hbar^2}E}$$

let's present wave function of the carrier as:

$$\Psi(\vec{r},E)=\sum_{n=-\infty}^{+\infty}A_n\frac{e^{-\gamma|\vec{r}-n\vec{a}|}}{|\vec{r}-n\vec{a}|}+\sum_{n=-\infty}^{+\infty}B_n\frac{e^{-\gamma|\vec{r}-(\vec{c}+n\vec{a})|}}{|\vec{r}-(\vec{c}+n\vec{a})|}. \tag{9}$$

Note that, for any choice of coefficients A_n, B_n providing the convergence of the corresponding series, function (9) satisfies Eq. (8) everywhere except for the points $n\vec{a}, \vec{c}+n\vec{a}$. Boundary conditions (7) result in the following homogeneous system of equations for A_n, B_n:

$$\begin{cases}\sum\limits_{n=-\infty}^{+\infty}\alpha_{n'n}A_n+\sum\limits_{n=-\infty}^{+\infty}\beta_{n'n}B_n=0,\\ \sum\limits_{n=-\infty}^{+\infty}\tilde{\beta}_{n'n}A_n+\sum\limits_{n=-\infty}^{+\infty}\alpha_{n'n}B_n=0,\end{cases} \tag{10}$$

$n'=0,\pm1,\pm2...$

Here,

$$\alpha_{n'n}=(-\gamma-b)\delta_{n'n}+\frac{e^{-\gamma|n'-n|a}}{|n'-n|\,a}\,(1-\delta_{n'n})\,,$$

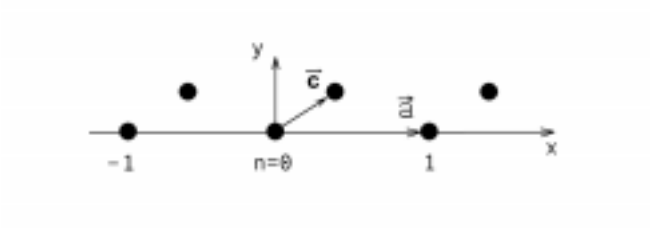

Fig. 1

$$\beta_{n'n}=\frac{e^{-\gamma|(n'-n)\vec{a}-\vec{c}|}}{|(n'-n)\vec{a}-\vec{c}|},\quad \tilde{\beta}_{n'n}=\frac{e^{-\gamma|(n'-n)\vec{a}+\vec{c}|}}{|(n'-n)\vec{a}+\vec{c}|}. \tag{11}$$

Taking into account that matrices (11) depend on the difference of indices, we search for a solution of the system (10) in the form

$$A_n=A_0e^{-ikna},\quad B_n=B_0e^{-ikna}. \tag{12}$$

This reduces (10) to the linear homogeneous system

$$\begin{cases}A_0D(\gamma,k)+B_0G(\gamma,k)=0,\\ A_0\overline{G}(\gamma,k)+B_0D(\gamma,k)=0,\end{cases} \tag{13}$$

where

$$D(\gamma,k)=-h-\gamma+\sum_{n=-\infty}^{+\infty}\frac{e^{-\gamma|n|a}}{|n|\,a}e^{ikna},$$

$$G(\gamma,k)=\sum_{n=-\infty}^{+\infty}\frac{e^{-\gamma|n\vec{a}-\vec{c}|}}{|n\vec{a}-\vec{c}|}e^{ikna}. \tag{14}$$

The condition of solvability of (13) yields the dispersion equation

$$D^2(\gamma,k)-|G(\gamma,k)|^2=0$$

connecting the energy and quasi-momentum of an electron in the waveguide band. The ideal chain with two atoms in an elementary cell has two waveguide bands with the energies defined by the equations

$$D(\gamma,k)\pm|G(\gamma,k)|=0. \tag{15}$$

In contrast to a simple one-atomic chain of monovalence atoms which is always a metal, the two-atomic periodic chain, even within the framework of the considered model, can be either a one-dimensional metal or a one-dimensional insulator depending on whether waveguide bands overlap or not. If atoms of one chain

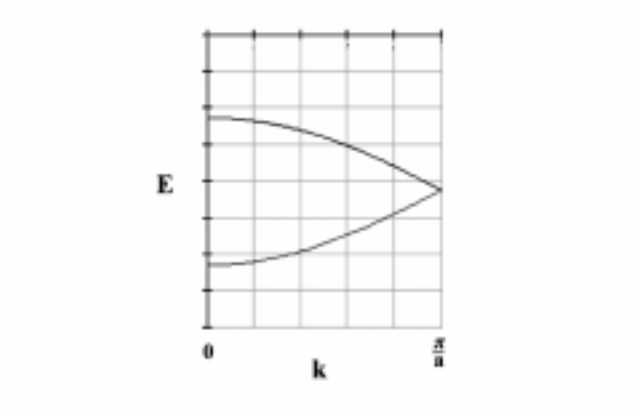

Fig. 2

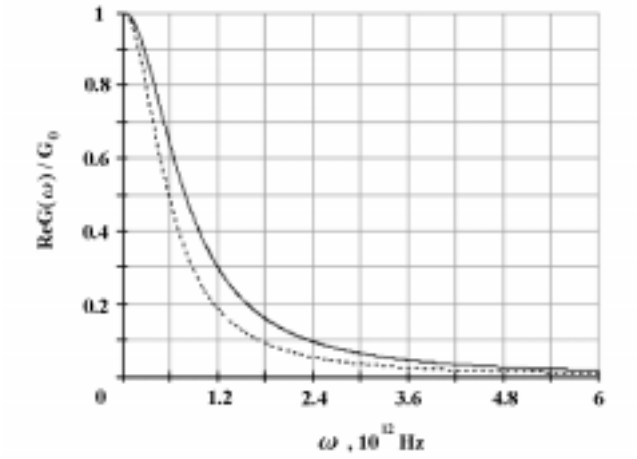

Fig. 4

are exactly in the middle between atoms of another chain (Fig. 2), then one band can be considered as a continuation of other band. That is, the edge of the Brillouin zone $k = \frac{\pi}{a}$ actually is not the edge of bands and is a point of the Peierls instability since a small displacement of one chain along the x-axis results in the appearance of a gap (Fig. 5) at this place. At such a displacement, a metal becomes a semiconductor or an insulator. If the chains of atoms are moved away from each other, then the bottom edge of the top band appears, at a certain moment, below the top edge of the bottom band, and such a system again becomes a metal. A further increase in the distance between the chains, the bands draw together and deform until just the complete merging for large distances.

From system (13), we can find a quotient of B_0 and A_0 and, with regard for (12) and (9), get the explicit expression for the Bloch wave functions for the both

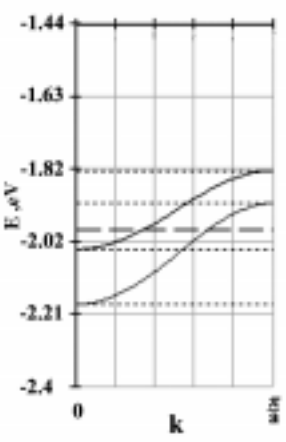

Fig. 3

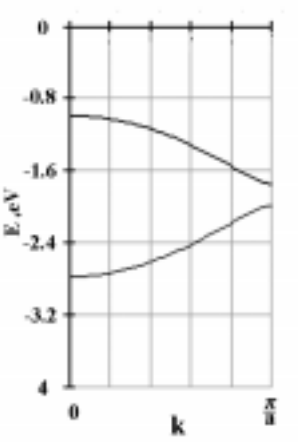

Fig. 5

waveguide bands

$$\psi_{\pm}(\vec{r},k) = A_0 \left(\sum_{n=-\infty}^{+\infty} \frac{e^{-\gamma|r-n\vec{a}|}}{|\vec{r}-n\vec{a}|} e^{-ikna} \pm \right.$$

$$\left. \pm \frac{G(\gamma,k)}{|G(\gamma,k)|} \sum_{n=-\infty}^{+\infty} \frac{e^{-\gamma|\vec{r}-(\vec{c}+n\vec{a})|}}{|\vec{r}-(\vec{c}+n\vec{a})|} e^{-ikna} \right).$$

Example 1

As an example, we consider the system of two parallel identical chains of atoms with an ionization potential of 2 eV and with the period $a = 4.245$ Å. The band scheme of such a system is shown in Fig. 3. The Fermi level is depicted by a dashed line. It crosses both bands, therefore the conductivity will be the sum of two terms. Contributions from different bands are different in view of the distinction of speeds at the Fermi level. For the top band, $V_{\mathrm{F}_c} = 5.68 \times 10^4$ m/s. For the bottom band, $V_{\mathrm{F}_v} = 7.78 \times 10^4$ m/s. The dependence of the conductivity of each channel $\frac{\mathrm{Re}G(\omega)}{G_0}$, where $G_0 = \frac{e^2}{\pi\hbar}$, on the frequency ω is shown in Fig. 4.

Example 2

As another example, we consider the system of two parallel identical chains of atoms with an ionization potential of 2 eV and with the period $a = 4.245$ Å and the displacement vector $\vec{c} = (2$ Å, 1 Å). The band scheme of such a system is shown in Fig. 5. The gap

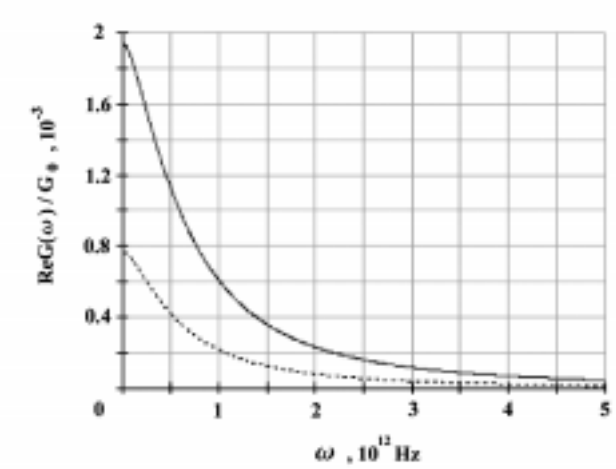

Fig. 6

between bands $Eg = 0.24$ eV. The dependence of conductivity $\frac{\mathrm{Re}G(\omega)}{G_0}$ on the frequency ω at 300 K (solid line) and 250 K (dashed line) is shown in Fig. 6. The numerical examples show that changes of the resistance of the considered one-dimensional conductors and semiconductors with temperature and frequency are great enough to be registered in nanosystems by using the available experimental techniques.

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БАЛІСТИЧНА ПРОВІДНІСТЬ ТА ІМПЕДАНС ОДНОВИМІРНИХ СИСТЕМ

С.В. Тищенко

Р е з ю м е

Отримано вирази для опору та імпедансу одновимірних ідеальних нанопровідників та напівпровідників скінченної довжини. Отримані результати проілюстровано для моделей у вигляді систем паралельних регулярних атомних ланцюжків, електронна структура яких моделювалась на основі методу потенціалів нульового радіуса.