Properties of spectral parameters of multi-cascade nanostructure, being a model of quantum cascade detector

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Motivation for research

To improve purposefully the characteristics of multi-cascade devices, in particular quantum cascade detectors (QCD), it is necessary to develop a realistic theory that would take into account the main features of their operation. In the majority of theoretical papers, a simplified model of a separate active region or a separate QCD cascade was studied. Although this approach allowed to study the energy spectra, intensities of quantum transitions and other quantum-mechanical characteristics of a separate single-cascade element of the nanodevice, but it did not assumed the multi-cascade structure of real QCD.

In this paper we present the developed theory and investigated spectral properties of multi-cascade nanostructures with potential of closed-type and Kronig-Penny potential, being two models for QCD structural element. Choice of the closed model is justified by the fact that it adequately describes multi-cascade structural elements of experimental QCD. Developing the theory of spectral characteristics of nanostructures in closed model it is useful to study the features of the spectrum in the Kronig-Penny model as a limit case of an infinite periodic structure, for the sake of comparison.

Theory of electron states of multi-cascade nanostructure in closed-model and Kronig-Penny model

Nanostructure with a closed (C) potential [1] and with a Kronig-Penny (KP) potential [2] is observed as two models of a multi-cascade structural element of typical experimental QCDs [3, 4]. In both models we use the same multilayered element (Fig. 1), formed by N identical three-well nanostructures - cascades. It is assumed that the considered multilayered structure in C-model is located in the external massive medium-barrier while in the infinite KP-model, it satisfies the conditions of Born-Karman periodicity. Under such conditions, taking into account the insignificant difference between the values of the lattice constants of layers-wells and barriers, the problem is to study the spectral properties of structures in the approximation of effective mass and rectangular potentials. In these models of N-cascade structure the potentials are periodic functions of coordinate (z) with the period equal to the length (d) of separate cascade.

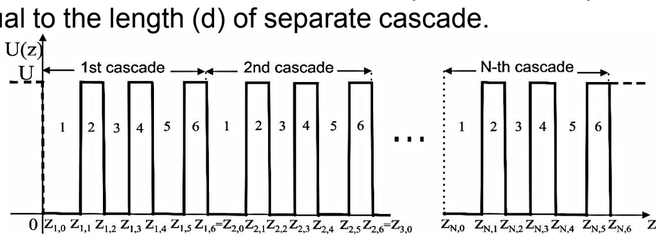

Fig.1. Potential profile of N-cascade nanostructure. Dotted lines indicate the potential of the external semi-infinite medium in the C-model

In C- and KP-models, the corresponding stationary Schrödinger equations are valid for an electron

$$\left(-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m_{C,KP}(z)}\frac{d}{dz}+U_{C,KP}(z)\right)\Psi^{C,KP}(z)=E\Psi^{C,KP}(z),$$

from which the exact expressions are obtained for wave functions Ψ^{KP} and Ψ^{C} [1,2].

At all heterostructure interfaces, in both models, the conditions of continuity of wave functions and probabilities of flux densities, as well as the conditions of wave functions normality, must be satisfied [1, 2]. Requiring the finite wave functions $\Psi^{C}(z)$ at z→±∞ in the C-model and using Born-Karman condition $\Psi^{KP}(z+L)=\Psi^{KP}(z)$ and Bloch's theorem $\Psi^{KP}(z+d)=e^{iKd}\Psi^{KP}(z)$, $(K=\frac{2\pi}{L}g,$ g = 0,1,…, N-1) in KP-model together with the boundary equations, we obtain dispersion equations. From the latter, the energies E_n^C and E_n^{KP} (n =1,2, …) are numerically calculated for the both models.

Properties of electron states of a multi-cascade nanostructure in two models

The studied models are based on a three-well cascade based on GaAs/$Al_{0.33}Ga_{0.67}As$ semiconductors used in experimental QCDs. The geometrical sizes of potential wells (a_1=6.8 nm, a_2=2.4 nm, a_3=3.7 nm) and barriers (b_1=b_2=b_3=3 nm) of a separate cascade were chosen such that the energies of electron states satisfactorily modeled the energy scheme of typical QCD cascades [3] with two operating levels and "phonon ladder" levels.

Calculations show that in a separate three-well nanostructure (N=1) in both models (C, KP) there are four electron states with the energies E_1^C=53.2 meV, E_2^C=106.2 meV, E_3^C=159.8 meV, E_4^C=212.0 meV And E_1^{KP}=52.8 meV,E_2^{KP}=107.1 meV, E_3^{KP}=157.8 meV, E_4^{KP}=218.9 meV, respectively. The wave functions of the states n=1 and n=4 in C- and KP-models are localized in the first potential well and strongly overlap. Since, an intensive quantum transition with absorption of electromagnetic radiation in the IR range is possible between these states. In the states n=3 and n=2, the electron is localized in the second and third potential wells so that their energies ($E_{n=3}^{C,KP}$, $E_{n=2}^{C,KP}$) form the "phonon ladder", within which, according to the main idea of experimental papers [3], the electron with phonon-assisted processes tunnels between the active regions of multi-cascade structure.

Let us analyze the evolution of electron energy spectrum as a function of the number (N) of nanostructure cascades. The increase of number N leads to the formation of groups of levels (subbands) in the small vicinity of energies ($E_n^{C,KP}$) of single-cascade (N=1) in C- and KP-structure. Fig. 2 shows the energies as functions of N only in four energy intervals, which contain all levels of the respective subbands. Also, for the convenience of further analysis in this and the following figures, double energy indexation is introduced $E_{ns}^{C,KP}$, where n is a number of the subzone and s is the number of energy level in the n-th subband.

From Fig. 2 it is clear that if N increases, the number of levels ($p_n^{C,KP}$) in the subbands increases too. In C-structure, in each n-th subband the number of levels is equal to the number of cascades $p_n^C=N$ and in the KP-structure it depends on the parity of N and is equal to $p_n^{KP}=(N+1)/2$ for the odd N and $p_n^{KP}=N/2$ for the even. In the limit case N→∞, according to physical considerations, continuous energy subbands are formed in the both structure models. The widths of the subbands in the KP-structure (Γ_n^{KP}) for an even number of cascades is independent of N while for the odd number they increase rapidly coinciding with Γ_n^{KP}. In C-structure, the widths (Γ_n^C) of all subbands increase asymptotically approaching Γ_n^{KP} for bigger N. In both models, at fixed N, the widths of the subbands increase if number n becomes bigger.

Also Fig. 2 shows that in the closed structure at N>1 in the high-energy vicinity of the first subband (n=1) and low-energy vicinity of the fourth subband (n=4), there are one separate energy level $E_{1p_1^C}^C$ and E_{41}^C. To identify the physical causes of their existence ($E_{1p_1^C}^C$, E_{41}^C) in the C-model and their absence in KP-model, we have calculated the probability density distributions ($|\Psi_{ns}^{KP,C}(z)|^2$) and probabilities $W_{ns}^{KP,C}(i)=\int_{z_{i,0}}^{z_{i,6}}|\Psi_{ns}^{KP,C}(z)|^2dz$ of the electron location in the cascades (i).

From Fig. 3a it is seen that in KP-model, for all states (s=1, 2, 3) of the n-th subband the functions $|\Psi_{ns}^{KP}(z)|^2$ are the same in all cascades. Therefore, the probabilities of electron location in different cascades (i=1,..,N) of KP-structures are the same for all states and are equal to $W_{ns}^{KP}(i)=1/N$.

The properties of $|\Psi_{ns}^{C}(z)|^2$ functions are different in C-model. In particular, Fig. 3b shows that electron in the states with energies $E_{n=1\,s=5}^C$ and $E_{n=4\,s=1}^C$ is localized only in the first cascade ($W_{n=1\,s=5}^C(1)=0.99$, $W_{n=4\,s=1}^C(1)=0.66$), and in other states of the first (n=1) and fourth (n=4) subbands - with different probabilities in all further cascades. The states of the second (n=2) and third (n=3) subzones are unevenly distributed over all cascades of the structure.

As a result, the presence of semi-infinite external barriers in C-model causes the emergence of

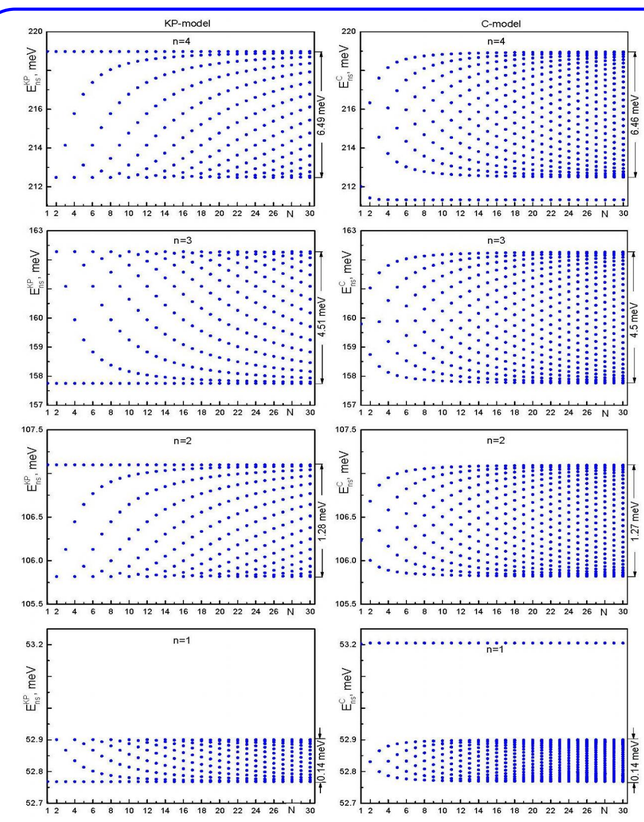

Fig. 2. Electron energy spectrum ($E_{ns}^{C,KP}$) as function of the number of cascades (N) in the nanostructure in the KP- and C-model

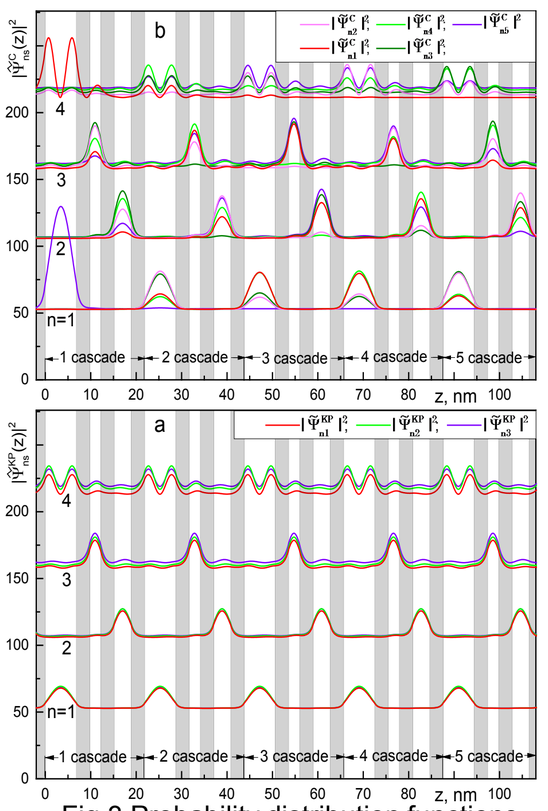

Fig.3 Probability distribution functions ($|\tilde{\Psi}_{ns}^{KP}|^2$,$|\tilde{\Psi}_{ns}^{C}|^2$), normalized with respect to the energies (E_{ns}^{KP},E_{ns}^{C}) in the five-cascade nanostructure in KP- (a) and C-model (b).

strongly localized states ($E_{1p_1^C}^C$ and E_{41}^C) in the near-surface layers, which cannot exist in the infinite Kronig-Penny model. It is obvious that these "near-surface" states can be manifested in real structures of finite sizes.

To study the effect of cascade geometric configurations on the spectral parameters of the electron in the realistic C-model, the energy spectrum (E_{ns}^C) and widths (Γ_n^C) of subbands were calculated depending on the size of potential wells (a_1, a_2, a_3) and potential barriers (b_1, b_2, b_3) of cascade at N = 10. The results are presented in Fig. 4. The figure proves that the dependences of the energy spectrum (E_{ns}^C) of multi-cascade structure on the width of one of the potential well of the cascade (at fixed sizes of the other two) have a nonlinear decreasing character with anti-crossing effect. In the vicinity of the anti-crossings of the two subbands (n and n+1), their widths (Γ_n^C and Γ_{n+1}^C) increase and in other intervals they only decrease.

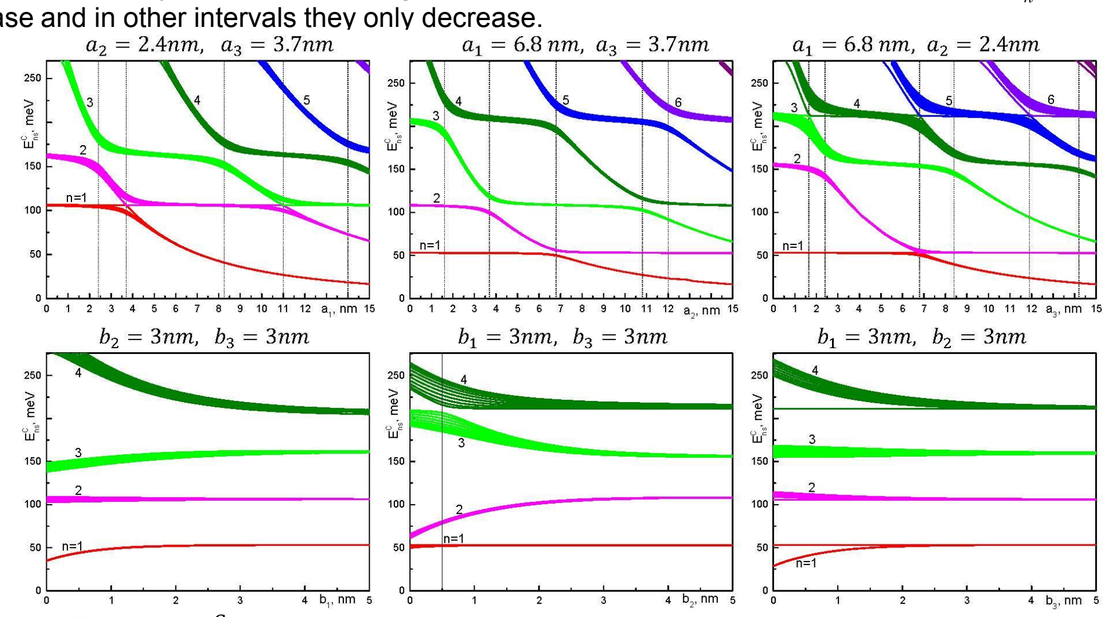

Fig. 4. Energies (E_{ns}^C) of subbands (n) as functions of widths (a_1, a_2, a_3) of potential wells and thicknesses (b_1, b_2, b_3) of potential barriers in ten-cascade (N=10) C-structure

Increasing thickness of one of the barriers at the fixed thicknesses of the other two leads to a decreasing widths (Γ_n^C) of the subbands and to low-energy or high-energy energy shifts depending on the subband number. Herein, the main change of energies occurs in the intervals of small barrier thicknesses (0< b_l<3nm, l=1, 2, 3) while in the region of strong barriers (b_l>3nm) the subbands only narrow almost without varying energy. In the limit case of an infinitely wide potential barrier (b_l→∞), according to the physical considerations and as can be seen from Fig. 4, energy bands are transformed into discrete levels (E_n^C, n=1, 2, 3, 4) of a separate cascade.

Conclusions

The theory is developed and a comparative analysis of the energy spectra of multi-cascade nanostructures with closed-type potential and Kronig-Penny potential, being two models of QCD structural element is performed.

It is shown that in both models the increasing number of cascades (N) leads to the formation of subbands in vicinity of the energies of single-cascade structures. The number of levels in C-model is equal to the number of cascades while in KP-model it is equal to (N+1)/2 for odd N and N/2 for even. The widths of the subbands in C-structure increase at increasing N and asymptotically coincide with the widths of the subbands in KP-structure. For the typical number of cascades in experimental QCD (N=30), the difference between the widths of the subbands in both models does not exceed 1%.

It is shown that the dependences of the subband energies on geometric sizes of potential wells and barriers of multi-cascade structure are similar to the dependences of discrete levels in single-cascade structure. If the energy of the subband increases, the anti-crossing effect is observed. When the thicknesses of the barriers increase, the energies either decreases or increases, depending on the subband number, and quickly reach saturation. The widths of the subbands in vicinity of anti-crossings increase while in all other intervals of the size of the wells and barriers they only decrease.

It is established that in the realistic C-model of multi-cascade nanostructure, the strong localization of the electron in near-surface layers leads to the emergence of separate states, the energies of which almost do not depend on the number of cascades. It should be expected that such "near-surface" states can be manifested in the spectra of real multi-cascade structures by selecting of the appropriate geometric parameters of the cascades.

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