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DESCRIPTION OF ELECTROPHYSICAL CHARACTERISTICS FOR MIS-STRUCTURES WITH CdHgTe-BASED QUANTUM WELLS UNDER THE 8–300 K [1]

Description of theoretical model for energy-band spectrum calculation for the heteroepitaxial CdHgTe (MCT) structures grown by molecular-beam epitaxy (MBE) method with the single quantum wells (QW) is presented in this work. This computation model allows to calculate different electro-physical properties of this structures and allows to explain features of their C–V and G–V characteristics in the wide temperature range, i.e. from «helium» till room temperatures.

Keywords: *$Cd_xHg_{1-x}Te$ grown by MBE, quantum well, energy-band diagram, metal-insulator-semiconductor (MIS) structure, C–V characteristic, G–V characteristic.*

At present, experimental methodics of low-temperature ($T \sim 8$ K) semiconductor heterostructures research including structures with quantum wells by the impedance spectroscopy method are increasingly available. One of the impedance spectroscopy methods is the method of capacity-voltage characteristics [1, 2].

Results of experimental research of admittance (total conductivity) for metal-insulator-semiconductor structures based on $Cd_xHg_{1-x}Te$ grown by MBE with single quantum wells are presented in [3]. In this scientific work describes results of admittance research for MIS-structures based on MBE MCT with QW under the range temperature from 8 till 300 K. Considered structures include single quantum wells on the basis of material HgTe with the QW width 5,6 and 7,1 nm. Composition of these structures barrier layers with the width 30 nm is 0.65 mole fractions and 0,62 mole fraction respectively. After the comparison results of these investigations with structures without quantum wells authors have made the following conclusion: quantum well may cause the essential influence on complex conductivity structure under the near-«helium» temperatures.

Hence, it is too difficult to interpret the influence of quantum well on the structure electro-physical parameters. The cause of this is absence of theoretical model at present which allows to carry out precise quantitative estimation for influence of dimensional quantization on heteroepitaxial MBE MCT structures properties [4, 5].

There are brief description of basic principles of self-consistent electrostatic potential theoretical model for semiconductor heterostructure in this article. This model are based on joint decision of Poisson and Schrödinger equations for heterostructure comprising a quantum well. Similar theoretical model have been used by us for a infrared photoluminescence spectra calculation for MCT structures comprising potential and quantum wells [6].

At the formulation of the problem we have taken into account the fact that all structures under consideration were grown by the molecular-beam epitaxy method on the «Ob'-M» MBE-equipment in the Institute of semiconductor physics (Novosibirsk). Poisson equation solution is used for electrostatic potential calculation. We use following view of Poisson equation for *n*-type MBE MCT heterostructures:

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}\varphi(z)}{\mathrm{d}z}\right)=\frac{q}{\varepsilon_0}\left[n(z,\varphi)-p(z,\varphi)-N_d^{+\mathrm{int}}(z)-N_d^{+\mathrm{dop}}(z)\right], \quad (1)$$

where φ is electrostatic potential distribution for structure; ε is the relative permittivity of the material; *n*, *p* are concentrations of electrons and holes; $N_d^{+\mathrm{int}}$, $N_d^{+\mathrm{dop}}$ are concentrations of ionized donors and acceptors impurities due to intrinsic defects and dopant respectively. Composition dependence of $N_d^{+\mathrm{int}}$ value was defined earlier by us [6]:

$$N_d^{+\mathrm{int}}(x)=(1{,}26x-0{,}26)\cdot 10^{16}\ [\mathrm{cm}^{-3}]. \quad (2)$$

In structures comprising a quantum wells spatial distribution of electrostatic potential defines also by the concentrations of 2D-electrons and 2D-holes in the dimensional quantization subband in a quantum well. It is necessary to now dimensional quantization levels energies and envelope wave function to de-

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fine values of these concentrations. Dimensional quantization levels energies and envelope wave functions can be obtained by the Schrödinger equation solution:

$$\left[-\frac{\hbar^2}{2m^*(z)}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+U(z)\right]\psi_i(z)=E_i\psi_i(z), \tag{3}$$

where $\psi_i(z)$ are the envelope wave functions for dimensional quantization level with number i; E_i is dimensional quantization energy; $U(z)$ is spatial distribution of potential energy ($E_c(z)$ for electrons, $E_v(z)$ for holes).

Using the explicit form for n and p expressions which describe the distribution of concentrations of charge carriers in nonhomogeneous potential profile structure [6] as well as expressions for 2D-elecrones and 2D-holes in a quantum well [4] we can obtain the common view of Poisson equation for structure under consideration:

$$\frac{\mathrm{d}^2\varphi(z)}{\mathrm{d}z^2}=\frac{1{,}8\cdot10^{-8}}{\varepsilon(z)}\left[\begin{array}{l} n_0\exp\left(\left(q\varphi(z)+\Delta\chi(z)\right)\Big/kT\right)\left(\dfrac{m_c^*(z)}{m_c^*}\right)^{3/2}- \\ -p_0\exp\left(-\left(q\varphi(z)+\Delta\chi(z)+\Delta E_g(z)\right)\Big/kT\right)+ \\ +\sum\limits_{n=1}^{2}\dfrac{m_e^*kT}{\pi\hbar^2}\ln\left(\exp\left[\left(F-E_{en}\right)\Big/kT\right]+1\right)\left|\psi_{en}(z)\right|^2- \\ -\sum\limits_{n=1}^{2}\dfrac{m_{hh}^*kT}{\pi\hbar^2}\ln\left(\exp\left[\left(E_{hhn}-F\right)\Big/kT\right]+1\right)\left|\psi_{hhn}(z)\right|^2- \\ -\sum\limits_{n=1}^{2}\dfrac{m_{hl}^*kT}{\pi\hbar^2}\ln\left(\exp\left[\left(E_{hln}-F\right)\Big/kT\right]+1\right)\left|\psi_{hln}(z)\right|^2- \\ -N_d^{+\mathrm{int}}(z)-N_d^{+\mathrm{dop}}(z) \end{array}\right]. \tag{4}$$

Dimensional quantization levels energies E_{en}, E_{hhn} and E_{hln} as well as corresponding envelope wave function ψ_{en}, ψ_{hhn} and ψ_{hln} can be calculated in terms of numerical solution of stationary one-dimensional Schrödinger equation (3). Values $\Delta\chi$ and ΔE_g are the differences between electron affinity and band-gap energy in the coordinate z and their values in the homogeneous layer of structure, e.g. in the barrier layer with the homogeneous potential profile. Composition and temperature dependences for MCT electron affinity, band-gap energy and effective masses used in (4) are described in [6]. Poisson equation solution have been obtained by finite difference method with the use of quasi-linearization [7].

Schrödinger equation have been transformed in terms of in the approximation of the asymmetric rectangular potential well with a barrier of finite height [5]. As a result, we obtain equations for the energy of states:

$$\mathrm{tg}\left[k_1\left(z-\frac{a}{2}\right)\right]=\frac{m_1^*}{m_2^*}\frac{k_2}{k_1}\ -\text{for even states;} \tag{5}$$

$$\mathrm{ctg}\left[k_1\left(z-\frac{a}{2}\right)\right]=-\frac{m_1^*}{m_2^*}\frac{k_2}{k_1}\ -\text{for odd states,} \tag{6}$$

where k_1, k_2 are wave vectors for charge carriers in both quantum well and barrier; m_1^*, m_2^* are effective masses in a well and barrier respectively.

Figure 1 provides an example of using presented method to calculate the energy structure of the QW of the MCT with the composition in a well 0,27 and 0,36 mole fractions and a 10 nm thick.

The capacity-voltage characteristics of the MIS-structure based on MCT QW can be calculated from the voltage balance equation for the structure:

$$V_{\text{MIS}} = -\frac{\varepsilon\varepsilon_0 E_s S_k}{C_i} + \varphi_0 , \tag{7}$$

where V_{MIS} is voltage drop across the MIS-structure, E_s is the electric field at the semiconductor-insulator boundary determined on the basis of self-consistent potential of quantum well structure, S_k is a contact area, C_i is a insulator capacity, φ_0 is value of the surface potential (at the semiconductor-insulator boundary), depending on the applied voltage.

Capacity of MIS-structure can be defined as

$$C = \frac{C_i C_{\text{SCR}}}{C_i + C_{\text{SCR}}}, \tag{8}$$

and capacity the space-charge region (SCR) C_{SCR} was defined as

$$C_{\text{SCR}} = \frac{\Delta Q_{\text{SCR}}}{\Delta\varphi_0}, \; Q_{\text{SCR}} = \varepsilon\varepsilon_0 S_k E_s \tag{9}$$

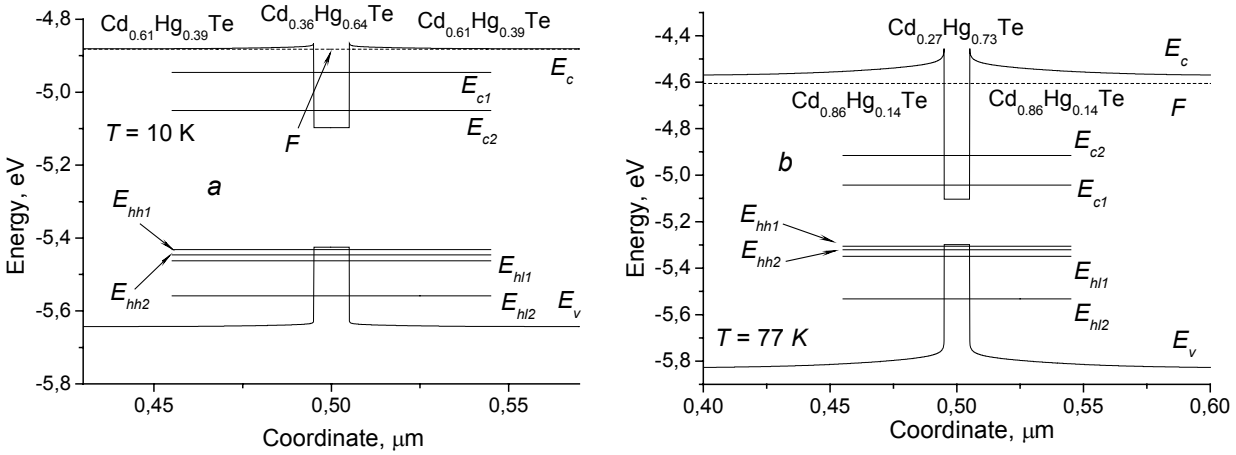

Fig. 1. Energy-band diagram profile for structures with QW $Cd_{0,61}Hg_{0,39}Te/Cd_{0,36}Hg_{0,64}$ (*a*) and $Cd_{0,86}Hg_{0,14}Te/Cd_{0,27}Hg_{0,73}Te$ (*b*) with the QW width 10 nm under the temperature10 K (*a*) and 77 K (*b*).

Thus, this study is devoted to building of physical and mathematical model to carry out numerical calculations of the electrical parameters of the MBE MCT structures, including quantum wells. The model account for the presence of the dimensional quantization levels of the electrons, light and heavy holes in the quantum well.

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