Numerical simulation of parameters of ZnCdHgTe films and ZnCdHgTe-based heterostructures.

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Abstract

Two simple calculation techniques are proposed for numerical modeling and estimation of main parameters determining the operation reliability of active elements based on A^2B^6 materials. In particular, room-temperature processes of charge carriers transport accounting inhomogeneities of epitaxial films surfaces and work function of the heterostructures based on narrow-gap semiconductor solid solution ZnCdHgTe are reported. The calculation algorithm is also presented.

.Introduction

Determination of model parameters and material properties through simulation is seemed to be helpful tool for effective design of different microelectronic devices. In particular, the problem of charge carriers transport is appeared to be of special importance in semiconductor physics and technology using different materials (especially bulk monocrystals and epitaxial films and layers of different thickness).

2. Experiment

The first section of the paper deals with the numerical simulation and consequential determination of low-bias (no more than 150 mV) parameters of carriers leaking on the inhomogeneous surface of the new narrow-gap semiconductor ZnCdHgTe (E_g=360 meV) prepared by the modified liquid-phase epitaxy (LPE) on different A^2B^6 single crystals substrates and proposed as material alternative to the worldwide known semiconductor compound HgCdTe. The technological peculiarities of the growth of large-area ZnCdHgTe epitaxial films required by the modern photonics were caused sufficiently inhomogeneous two-dimensional epilayer surface as aggregates of clusters with typical size of about 2 mm^2 (the typical size of the elemental cluster was estimated to be about 10^{-2}μm).

3. Calculation procedure

Peculiarities of the experimental current-voltage characteristics measured at T = 290 K under the applied bias $V_a = (0.1 \div 0.5)E_g$ were shown a dominant tunneling current leaking in area extent the epilayer surface. Numerical simulation performed according to the experimental data has demonstrated the significant influence of the randomized relief of the epilayer :

$$I = \left(\frac{R}{r}\right) I_s \exp(-\alpha\phi(r)) \exp\left[-e(E_g - V_a)/kT\right], \quad (1)$$

where $\alpha = (4/3\hbar)(m_e^* \varepsilon\varepsilon_0 / \delta N)^{1/2}$, I_s stands for the saturation current (a complete function strongly depending on the main parameters of the material), the cluster size R was estimated to be R = 0.125 mm, δN is the concentration of carriers immediately taking part in process of the charge transport evaluated by the experimental capacitance-voltage measurements. The randomized potential $\phi(r)$ was estimated according to the expression given below:

$$\phi(r) = a(r_0^2)\left[1 - (r_0/r)(1 + R/r_0)\exp(-R/r_0)sh(r/r_0)\right], \quad (2)$$

where $a = e\delta N/\varepsilon\varepsilon_0$, $(r_0)^{-2} = n_i e^2/\varepsilon\varepsilon_0 k_B T$; both parameters are determined by the properties of ZnCdHgTe epifilm, n_i stands for intrinsic carriers concentration of ZnCdHgTe calculated in assumption of the parabolicity of this material band structure. The sections of the theoretical and experimental curves (Fig. 1) are well matched up to applied voltage 0 ÷ 0.15 V. The percolation theory shows the dramatic increase of the calculated values of the current as the applied voltage increases. Such a phenomenon can be explained by formation of the conductive channels localized along the clusters boundaries. Nevertheless, the "p-n-island" conductivity theory gives no similar results due to the protection influence of the native oxide film coating the as-grown epilayers immediately after their growth finishing.

Thus, the described numerical simulation allowed to determine the following factors: (i) some important technological parameters of the modified LPE technique in order to avoid undesirable surface relief of the as-grown film; (ii) results of the calculations gave a possibility to determine the quasi-two-dimensional distribution of the charge carriers and the film surface mobility modulation.

4. Numerical algorithm

A simple numerical technique has been worked out for calculations of the main parameters of multi-component semiconductor heterostructures. Especially, the procedure deals with numerical treatment of room - temperature capacitance - voltage measurements having for an object the determination of some properties of the semi-

conductor free surface. The examined heterostructure (Fig. 2) was prepared by the modified liquid-phase epitaxy of the new narrow-gap semiconductor solid solution ZnCdHgTe (ZCMT, E_g = 320 meV at 300 K) on (111) CdTe single crystal substrates. The as-grown film surface roughness affects the optical element's scatter, damage threshold and, to some degree, absorption [2].

Thus, this part of the paper presents first results of calculation performed for determination not only the electron affinity but the work function of the sufficiently inhomogeneous surface of ZnCdHgTe epitaxial layer.

The proposed numerical model was refined by means of electron affinity calculation and consequent work function definition because these parameters are seemed to be important for construction of the band diagram of the tested semiconductor heterostructure as a base for further microelectronics active elements design.

Capacitance - voltage ($C = f(V_a)$) measurements were carried out at T = 290 K. Results of the study allowed to estimate the energy spectrum of charge surface states E_{ss} localized at the interface *ZnCdHgTe - CdTe- substrate* (the numerical procedure was described previously [3]) and to define a unique electrostatic potential (V_c). Thus, the experiment gives sufficient information to solve the basic equation (1) numerically [4]:

$$V_c = V_a - \phi_{bp} - \chi_s + \chi_{layer} - E_{gs} + E_{ss}$$

$$+ \frac{k_B T}{2e} \ln\left(\frac{N_{clayer}}{N_{vlayer}} \exp\left(-\frac{E_{cd}}{k_B T} \right) \right), (3)$$

where ϕ_{bp} is the flat-band voltage, χ_s and χ_{layer} are the substrate and ZnCdhgTe epilayer electron affinities, respectively, E_{gs} is band-gap of the substrate, N_c and N_v are the effective states densities in the conductance and valence bands of the epilayer.

The computing scheme is presented below.

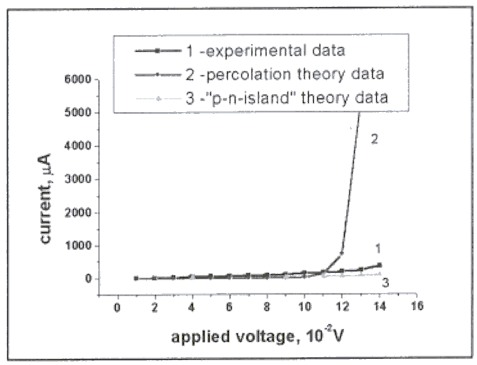


Figure 1. Experimental (curve 1) and simulated (curves 2 and 3, respectively) current-voltage characteristics of the investigated material. As numerical simulation tools the percolation theory and "p-n-island" conductivity models were used. The second theory produces more reliable data giving no sharp increase of the current.

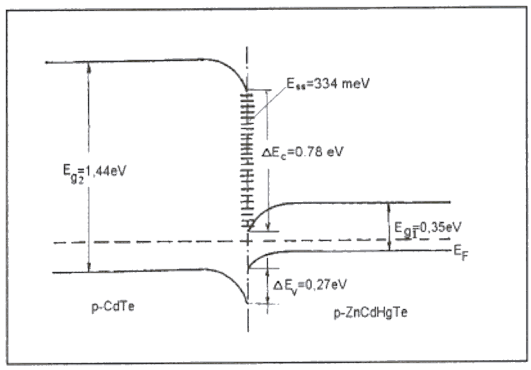
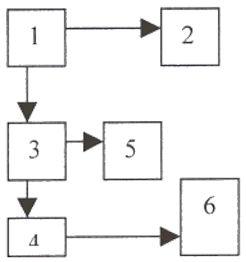


Figure 2. Energy band diagram of the p-p-heterostructure based on new semiconductor ZnCdHgTe calculated according to the method developed in [3].

Computational algorithm:

1. INPUT (experimental values C, V_a);.
2. E_{ss} calculation;
3. Building function $C^{-2}=f(V_a)$;
4. Building function $\chi=f(V_a)$;
5. V_c calculation;
6. OUTPUT: E_{ss} (eV), V_a (V), $\chi(V_a)$, (eV).



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