Opto-Electronics Review 26 (2018) 195–200

Contents lists available at ScienceDirect

Opto-Electronics Review

journal homepage: http://www.journals.elsevier.com/opto-electronics review

Full Length Article

Nanostructures with Ge–Si quantum dots for infrared photodetectors

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ARTICLE INFO

Article history:
Received 15 January 2018
Received in revised form 10 April 2018
Accepted 9 June 2018

Keywords:
Molecular beam epitaxy
Heterostructures
Dark current
Noise
Detectivity

ABSTRACT

In this paper questions of optimization of growth conditions in the method of molecular beam epitaxy for creation of high-efficient quantum dot infrared photodetectors are considered. As a model material system for theoretical investigations, heterostructures with germanium-silicon quantum dots on the silicon surface are chosen. For calculations of the dependencies of quantum dots array parameters on synthesis conditions the kinetic model of growth of differently shaped quantum dots based on the general nucleation theory is proposed. The theory is improved by taking into account the change in free energy of nucleation of an island due to the formation of additional edges of islands and due to the dependence of surface energies of facets of quantum dots on the thickness of a 2D wetting layer during the Stranski–Krastanow growth. Calculations of noise and signal characteristics of infrared photodetectors based on heterostructures with quantum dots of germanium on silicon are done. Dark current in such structures caused by thermal emission and barrier tunneling of carriers, as well as detectivity of the photodetector in the approximation of limitation by generation-recombination noises are estimated. Moreover, the presence of dispersion of quantum dots by size is taken into account in the calculations of the generation-recombination noises. Results of calculations of the properties of structures with quantum dots and their dependencies on growth parameters, as well as the characteristics of quantum dot photodetectors are presented. Comparison of the estimated parameters of quantum dots ensembles and the characteristics of quantum dot photodetectors with experimental data is carried out.

1. Introduction

Researchers pay great attention to creation of various electronic devices based on the structures with quantum dots of germanium on silicon since early 1990's, when they were obtained in the experiments [1,2] by the method of molecular beam epitaxy (MBE) for the first time. There are infrared photodetectors, fast-speed transistors and solar cells among these devices [3–5]. Such a high interest to the Ge-Si heterostructures with quantum dots is due to the number of unique properties of these structures caused by the effects of size quantization [6–8]. These new phenomena appearing in the structures with quantum dots make them attractive to device application [9,10].

Infrared photodetectors may be used in the wide range of various applications: for military and civil needs, in energetics, medicine, and industry. Photodetectors are required to have high operating characteristics (such as sensitivity and detectivity), to operate at high temperatures, and to have a reasonably low price. To date, the basic material for creation of infrared photodetectors is mercury-cadmium telluride (MCT). However, there are some technological difficulties connected with the synthesis of MCT epitaxial layers. And now quantum dot infrared photodetectors may become good alternative to traditional MCT detectors [11–13].

Principles of quantum dot infrared photodetectors operation are analogous to those of quantum well infrared photodetectors. The principal difference is only the restriction in all three dimensions of the charge carrier motion in a quantum dot [14]. It is expected that due to this restriction quantum dot photodetectors will provide better characteristics, namely higher operating temperatures, lower dark currents and higher photoelectric gains [13]. Finally, that may result in higher response and detectivity [15].

To date, not all the potential advantages of photodetectors with quantum dots are realized. It may be explained both by low degree of islands homogeneity in the array, and by non-optimal energy structure of such detectors. For example, quantum dots may have additional energy levels located between the ground and excited states, which are responsible for the absorption of the radiation of

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https://doi.org/10.1016/j.opelre.2018.06.002
1230-3402/

the given wavelength. Moreover, the excited energy level may be rather distant from the conduction band and high applied biases are required. These factors increase dark current and decrease absorption coefficient. Finally, they lessen detectivity of quantum dot photodetectors compared with the predicted ultimate characteristics [11].

The most perspective method of quantum dots creation is molecular beam epitaxy. This method is based on the effects of self-organization of semiconductor nanostructures in heteroepitaxial systems. For various applications it is necessary to create heterostructures with quantum dots with different properties. These properties are defined by such parameters of quantum dots as their shape, average size, size distribution function and surface density. So, the important task is to estimate optimum growth conditions for obtaining heterostructures with given properties.

The aim of this paper was the calculation of noise characteristics of quantum dot photodetectors, firstly, taking into account generation-recombination noises, and, secondly, with the respect to the dispersion of quantum dots in array by sizes, for the further optimization of growth conditions in the method of molecular beam epitaxy for creation of photodetectors with improved detectivity.

2. Methods

Dark current of a photodetector is the current caused by various sources other than by incident signal flux (for example, background radiation or thermal generation of carriers). It is well known, that the dark current of a quantum dot photodetector is mainly caused by the processes of the thermal generation of carriers and barrier tunneling in the presence of the electric field. In this case dark current density may be written as [16]:

$$j_d = 2q(2\pi m^* K_B T/h^2)^{3/2}\exp(-E_a/K_B T)\mu F[1+(\mu F/v_s)^2]^{-1/2}, \quad (1)$$

where q is the electron charge, m^* is the effective mass of charge carrier in barrier layer, K_B is the Boltzmann's constant, T is the temperature, h is the Planck's constant, E_a is the activation energy, F is the applied electric field, μ is the mobility and v_s is the maximum carrier speed.

Activation energy may be written as the sum of two contributions from two different mechanisms of generation of carriers [17]:

$$E_a = E_{0,m}\exp(-F/F_0) + E_{0,n} - \alpha F, \quad (2)$$

where $E_{0,m}$ and $E_{0,n}$ are the activation energies at zero bias for two different mechanisms of carrier transport – microscopic and nanoscale [18]. The activation energy $E_{0,m}$ is defined as the difference between the Fermi level and the lowest energy level in conduction band of barrier layer. This value corresponds to the processes of the thermal emission. The activation energy $E_{0,n}$ is equal to ionization energy of a quantum dot. This energy describes barrier tunneling of carriers. F_0 and α are the fitting parameters characterizing the rate of energy change with applied bias [13].

Due to the inevitable existence of size inhomogeneity between quantum dots in the ensemble, activation energy of tunneling processes changes from one dot to another and it may be described by the Gaussian distribution with the dispersion σ_E^2. The value of σ_E determines the spread in activation energies $E_{0,n}$ caused by size inhomogeneity of the islands. Taking into account this distribution an average dark current density of the photodetector can be written as [13]:

$$j_d = q\mu F[1+(\mu F/v_s)^2]^{-1/2}(2\pi m^* K_B T/h^2)^{3/2} \exp(-(E_{0,m}\exp(-F/F_0) + E_{0,n} - \alpha F - \sigma_E^2/2K_B T)/K_B T)\mathrm{erfc}(-(E_{0,n} - \sigma_E^2/2K_B T)/\sigma_E(2)^{1/2}). \quad (3)$$

For the calculation of quantum dot array parameters, such as the average size L_{av}, the size dispersion δL and the surface density of quantum dots N, the kinetic model of growth of Ge quantum dots on Si [19–22] was used. This model is based on a generalization of the classical nucleation theory and allows one to define the dependencies of quantum dots surface density and size distribution function on growth temperature and deposition rates. For the modelling of quantum dots growth, first of all, such thermodynamic parameters of the Ge/Si system as change in free energy during transition from 2D to 3D growth and equilibrium thickness of the wetting layer were defined [23–25]. Free energy change due to elastic strain relaxation, formation of the additional edges, increase in the surface of the facets and decrease of atoms attraction to the substrate were considered. Moreover, surface energy dependence on the thickness of the deposited material was taken into account. The change in the free energy $\Delta F(i)$ during the transition of i atoms from the wetting layer to an island may be written as a sum of three summands [25]:

$$\Delta F(i) = Ai^{2/3} - B\zeta i + Ci^{1/3}, \quad (4)$$

where $\zeta = h / h_{eq} - 1$ is the wetting layer superstress, h is the Ge wetting layer thickness, h_{eq} is the equilibrium thickness of the wetting layer at which the transition of atoms from the wetting layer to an island becomes energetically favourable. According to the Muller–Kern criterion [26], for the wetting layer thicknesses $h < h_{eq}$ layer-by-layer growth takes place. If $h < h_{eq}$, the 2D to a 3D transition is observed which results in the reduction of free energy [20]. A, B, and C are the parameters depending on the growth temperature and the thermodynamic properties of the materials and characterizing surface energy increase, elastic strain relaxation, and change in the free energy due to the formation of the additional edges, correspondingly.

The equilibrium thickness of the wetting layer h_{eq} may be found by solving the following equation [27]:

$$[1-Z(\varphi)]\lambda\varepsilon_0^2 - 1/d_0\{\gamma_s - [\gamma(0,0) - \gamma(0,\infty)] \exp(-B_0 h_{eq}/d_0) - \gamma(0,\infty)\}\exp(-h_{eq}/k_0 d_0) = 0, \quad (5)$$

where $Z(\varphi)$ is the coefficient of elastic strain relaxation [28–30], φ is the contact angle of quantum dot, λ is the material's modulus of elasticity, ε_0 is the lattices' mismatch, d_0 is the height of one monolayer (ML), γ_s is the specific surface energy of the substrate, k_0 is the relaxation coefficient. $\gamma(\varphi, 0)$ and $\gamma(\varphi, \infty)$ are the specific surface energies of a facet with the contact angle φ on the surface of pure silicon (without the wetting layer) and on the surface of pure strained germanium (infinite wetting layer thickness) respectively [20,26,31–33], B_0 is the dimensionless parameter characterizing the rate of specific surface energy change with the deposited material thickness [34–38].

Then, islands nucleation rate, surface density of quantum dots, rate of atoms arrival to an island, the critical thickness of the wetting layer h_c and quantum dots size distribution function are calculated [21–25].

When considering the contribution of the edges to the free energy of the atoms in an island, to determine the critical thickness h_c of the transition from two-dimensional to three-dimensional growth, it is necessary to solve the following equation for the critical superstress $\zeta_c = (h_c/h_{eq} - 1)$ [25]:

$$4h_{eq}\zeta_c/(6(\pi)^{1/2}d_0 a(\zeta_c+1)F(\zeta_c))[2F(\zeta_c)\tau_{inc} /\zeta_c^2 t_{eq}]^{5/2}\exp[F(\zeta_c)] = 1, \quad (6)$$

where $t_{eq} = h_{eq} / V$ is the growth time for the wetting layer of the equilibrium thickness, V is the growth rate, $\zeta_c = (h_c/h_{eq} - 1)$ is the critical superstress, i_c is the critical number of atoms in an island, at which the function of the free energy $\Delta F(i)$ reaches its maxi-