UDC 530.1

MODELING OF SEMICONDUCTOR NANOSTRUCTURES BY USE OF METHODS OF DYNAMICAL CHAOS

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We present a possibility to model morphology of nanostructured semiconductor films by use of equation for fractal evolution of measure. Using of the theory let us to describe structure of films containing different quantum-size structures including quantum dots, quantum nanowires and quantum wells. We have investigated influence of different parameters on morphology of nanocluster semiconductor films. Histograms describing distribution of nanostructures on height have been constructed. Results of numeric analysis have been compared with corresponding experimental data.

Keywords: nanocluster, semiconductor, fractal, morphology, dynamical chaos.

Introduction

Nanocluster semiconductor films are perspective materials for modern electronics. Characteristic sizesof nanostructures are comparablewith thedeBrogli wavelength.Itleads to appearance of characteristic quantum-size effects in nanostructures. Even insignificant distinction in structure of nanocluster films can lead to noticeable changesof their electrical and optical properties[1-3].Therefore, study of structure of semiconductor films with different nanostructuresis the problem of interest.

Equation for fractal evolution of measure

It's possible to use methods of dynamical chaos for the description of complex topology of semiconductor surfaces containing nanostructures. We can use this approach because dynamical chaos can be characterized by a statistical characteristic similar to characteristics of stochastic processes. I.e., it is necessary to describe dynamics of chaos with an alternatedand fractal structure close to the structure of nanofilms. For this aim we use the new equation for fractal evolution of measure (additive value) describing chaotic oscillations with characteristics corresponding to criteria of self-organization [2, 3]. Thus, distribution of electrons, holes and impurities in a nanostructured semiconductor can be described by the following system:

$$\begin{cases} n_{i+1} = \left(\frac{1}{C_n} + \mu_i\right)\left|\frac{n_i}{n_0}\right|^{-\frac{1}{\gamma_n}}; \;\; p_{i+1} = \left(\frac{1}{C_p} + \mu_i\right)\left|\frac{p_i}{p_0}\right|^{-\frac{1}{\gamma_p}}; \;\; a_{i+1} = \left(\frac{1}{C_a} + \mu_i\right)\left|\frac{a_i}{a_0}\right|^{-\frac{1}{\gamma_a}}; \\ \mu_{n_{i+1}} = -\frac{1}{\gamma_n}\left(\frac{1}{C_n} + \mu_i\right)\left|\frac{n_i}{n_0}\right|^{-\frac{1}{\gamma_n}-1}; \;\; \mu_{p_{i+1}} = -\frac{1}{\gamma_p}\left(\frac{1}{C_p} + \mu_i\right)\left|\frac{p_i}{p_0}\right|^{-\frac{1}{\gamma_p}-1}; \\ \mu_{a_{i+1}} = -\frac{1}{\gamma_a}\left(\frac{1}{C_a} + \mu_i\right)\left|\frac{a_i}{a_0}\right|^{-\frac{1}{\gamma_a}-1}; \;\; \mu_i = \mu_{n_i} + \mu_{p_i} + \mu_{a_i}. \end{cases} \quad (1)$$

where n, p, a are non-equilibrium (fractal) concentration of electrons, holes and impurities, respectively, C_n, C_p, C_a are constants describing degree of resolution accuracy, $\gamma_n, \gamma_p, \gamma_a$ aredifference between fractal and topological dimensions of sets of electrons, holes and impurities, n_0, p_0, a_0 are equilibrium (non-fractal) concentrations of charge carriers and impurities, μ_n, μ_p, μ_{a_i} are sign functions.

Concentrations of charge carriers and impurities can be considered as a non-linear fractal measures. So,for taking into account existence of hierarchically self-similar small-scale structures in the film we can use second generation of the system (1) written as

$$\begin{cases} n_{i+1} = \left(\frac{1}{C_n} + \mu_i\right)\left(\left(\frac{1}{C_n} + \mu_i\right)\left|\frac{n_i}{n_0}\right|^{-\frac{1}{\gamma_n}}\right)^{-\frac{1}{\gamma_n}}; \; p_{i+1} = \left(\frac{1}{C_p} + \mu_i\right)\left(\left(\frac{1}{C_p} + \mu_i\right)\left|\frac{p_i}{p_0}\right|^{-\frac{1}{\gamma_p}}\right)^{-\frac{1}{\gamma_p}}; \\ a_{i+1} = \left(\frac{1}{C_a} + \mu_i\right)\left(\left(\frac{1}{C_a} + \mu_i\right)\left|\frac{a_i}{a_0}\right|^{-\frac{1}{\gamma_a}}\right)^{-\frac{1}{\gamma_a}}; \; \mu_{n_{i+1}} = -\frac{1}{\gamma_n}\left(\frac{1}{C_n} + \mu_i\right)\left|\frac{n_i}{n_0}\right|^{-\frac{1}{\gamma_n}-1}; \\ \mu_{p_{i+1}} = -\frac{1}{\gamma_p}\left(\frac{1}{C_p} + \mu_i\right)\left|\frac{p_i}{p_0}\right|^{-\frac{1}{\gamma_p}-1}; \; \mu_{a_{i+1}} = -\frac{1}{\gamma_a}\left(\frac{1}{C_a} + \mu_i\right)\left|\frac{a_i}{a_0}\right|^{-\frac{1}{\gamma_a}-1}; \mu_i = \mu_{n_i} + \mu_{p_i} + \mu_{a_i}. \end{cases} \quad (2)$$

Fractal dimensions of sets of electrons, holes and impurities can be defined via criteria of self-organization of complex systems [1-3]. To obtain three-dimensional images of semiconductor surfaceswe usedthe algorithm for reconstruction of dynamical chaos via one-dimensional data sequence [4]. We applied this algorithm for the dependence of electron concentration on spatial step defined by the formulas (1) and (2). For this aim it is necessary to transform the initial sequence of data $n_{i+1} = f(n_i)$ to an array of sets with sequentially increased shifts. The shifts are values multiple of a fixed delay τ. So, we can write a set of discrete variables as

$$\begin{aligned} &n_1 : n_1(t_1), \ldots\ldots\ldots\ldots n_1(t_N) \\ &n_2 : n_1(t_1 + \tau), \ldots\ldots\ldots\ldots n_1(t_N + \tau) \\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ &n_{j-1} : n_1(t_1 + (j-1)\tau), \ldots\ldots\ldots n_1(t_N + (j-1)\tau) \end{aligned} \quad (3)$$

Linear independence of the variables in phase space is necessary. This condition can be achieved by the corresponding choice of numerical value of τ. All these variables can be defined via a single data sequence $n_{i+1} = f(n_i)$. So, application of the described approach let us describe dynamics of a system in multi-dimensional data sequence.

Results of numerical analysis

Using of the described approach let us to describe morphology of surfaces of nanostructured semiconductor films identical to experimental photos made by use of modern methods of microscopy (atomic force, scanning tunneling, etc.). Using of the system of equations (2) unlike the system (1) we can obtain models of surface with smoother surface morphology.

By use of the described approach we can model a variety of quantum-dimensional structures including quantum dots, quantum nanowires and quantum wells. Thus, Figures 1-3 presents computer models of morphology of nanocluster semiconductor films. Nanowires have topological dimension $d=1$, dimension of the fractal volume is $D>3$, therefore, for a wire-likemorphology we have $\gamma = D-d>1$. Similarly, topological dimension of quantum wells is $d=2$. So, difference between fractal and topological dimensions is equal to $\gamma = D-d>1$. Surface models of semiconductor quantum-dimensional structures shown in figures 1-3have been observed in experimental works [5-9].

(a) (b)

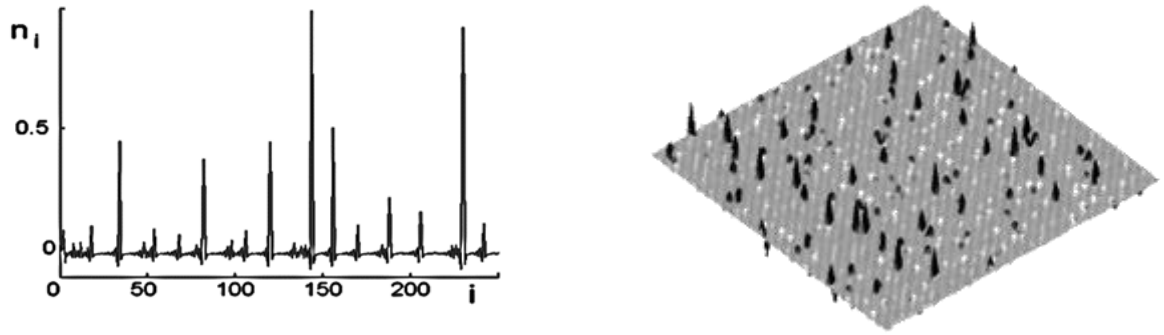

Fig.1. Realization (a) and morphology (b) of quantum dots.
$C_n = C_p = C_a = 0.9$; $\gamma_n = \gamma_p = \gamma_a = 3.806$; $n_0 = p_0 = 1/4$, $a_0 = 1$; $\mu = -1$, $\tau = 15$.

(a) (b)

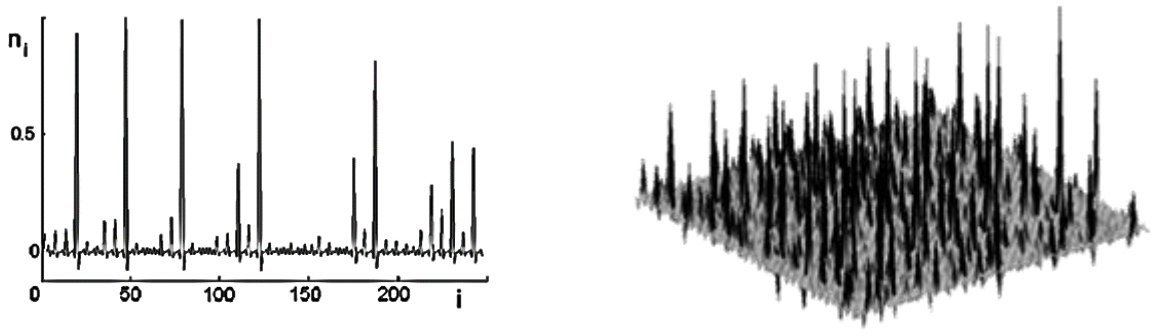

Fig.2. Realization (a) and morphology (b) of quantum nanowires.
$C_n = C_p = C_a = 0.9$; $\gamma_n = \gamma_p = \gamma_a = 2.806$; $n_0 = p_0 = a_0 = 1$; $\mu = -1$, $\tau = 15$.

(a) (b)

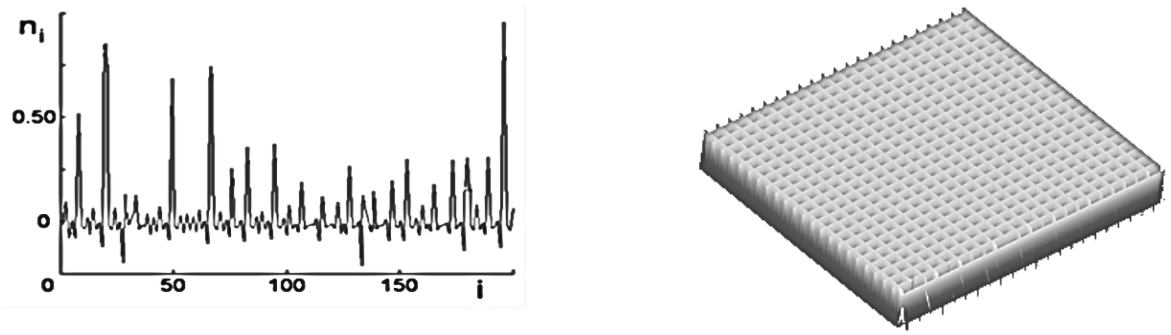

Fig.3. Realization (a) and morphology and (b) of the surface containing quantum well.

$C_n = C_p = C_a = 0.9$; $\gamma_n = 1.806$, $\gamma_p = 1.567$, $\gamma_a = 1.433$; $n_0 = p_0 = 1/4$, $a_0 = 1$; $\mu = -1$, $\tau = 15$.

Let us consider influence of impurities on morphology of surfaces of nanostructured semiconductor films. Figures 4(a-c) show models of surfaces with different concentrations of impurities, and figures 4(d-f) shows corresponding histograms of distribution of quantum-size structures on their height. The figures show that even minor change of concentration of impurities significantly affects to topography of film surfaces (Fig. 4(a, b)). Increasing of concentration of impurities can lead to thickening of films (Fig. 4(c)), and film surfaces become fine-grained. Standard deviation calculated for the surfaces shown in Figures 4(a-c) are equal to 0.018, 0.012 and 0.469, respectively.

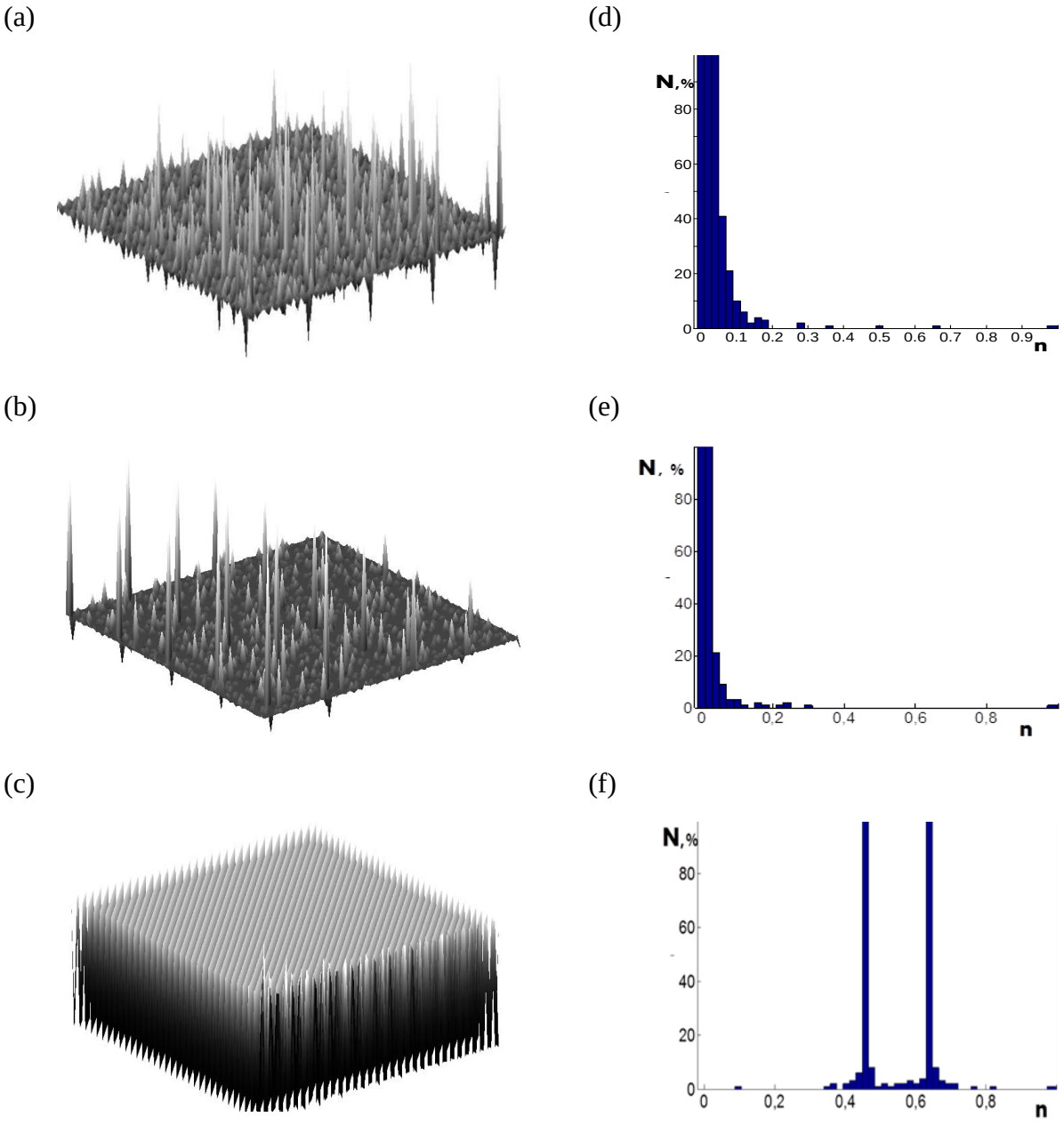

Fig. 4.Influence of impurities on morphology of surface of nanocluster films.

$\gamma_n = \gamma_p = \gamma_a = 2.806$, $n_0 = p_0 = 0.25$, $C_n = C_p = C_a = 0.999$, $\tau = 15$.

(a) - $a_0 = 1.00$; (b) - $a_0 = 1.4$; (c) - $a_0 = 1.8$.

Fig. 5(a-c) showinfluence of scaling factor on topology of the considered films. We consider the scaling factor as difference between fractal and topological dimensions of sets of charge carriers and impurities. Corresponding histograms describing distribution of nanostructures on their height are shown in Fig.5(d-f). For small values of the scaling factorwe observe separated and relatively large nanostructures (Fig.5(a)). Increasing of scaling factor leads to formingof nanostructures with different heights. Standard deviation corresponding to the surfaces shown in Fig.5(a-c) is 0.080, 0.030, and 0.041, respectively.

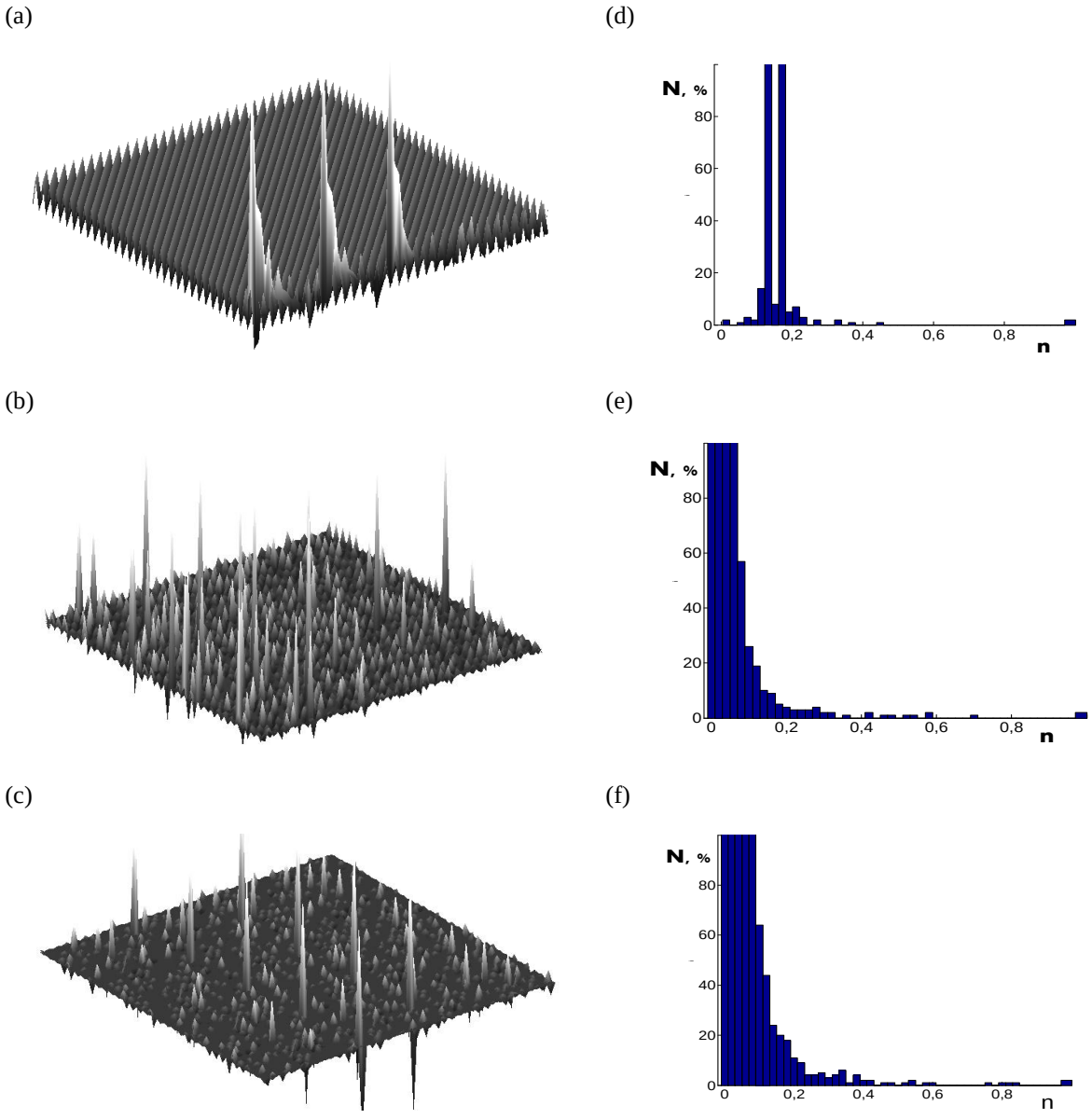

Fig. 5.Influence of scaling factor on relief of semiconductor surfaces.
$\gamma_n = 2.806$, $n_0 = p_0 = 0.25$, $a_0 = 1.00$, $C_n = C_p = C_a = 0.999$, $\tau = 15$, (a) - $\gamma_n = \gamma_p = \gamma_a = 1.5$;
(b) - $\gamma_n = \gamma_p = \gamma_a = 2.5$; (c) - $\gamma_n = \gamma_p = \gamma_a = 3.5$.

Fig. 6 shows the result of comparing of experimental data [10] devoted to study of morphology of a surface with silicon nanowires, and theoretical model of this surface obtained by use of the described above method. Comparison of Fig. 6(a) and 6(b) shows that results of simulation are qualitatively correspond to the experimental image of the film containing silicon quantum nanowires.

(a) (b)

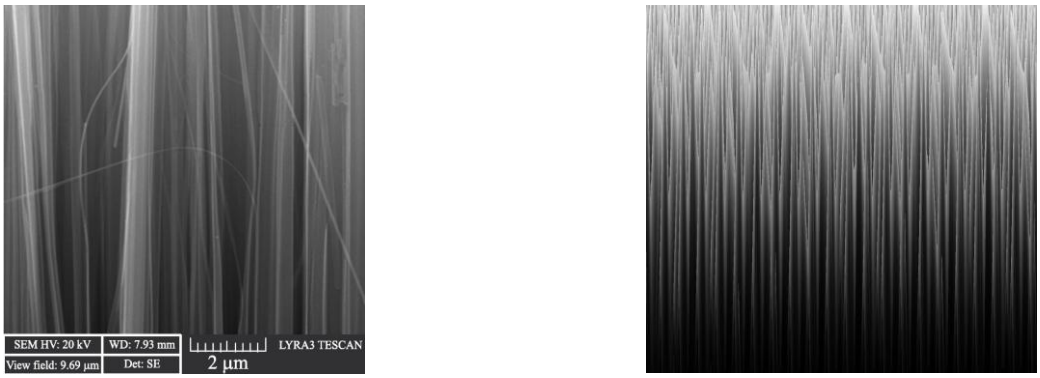

Fig. 6. Silicon quantum nanowires. a) experiment, b) simulation result:
C_n=C_p=C_a=0.99; μ=-1; $n_0 = 0.7$, p_0=0.51; a_0=1.01;γ_n =2.806; γ_p =2.618; γ_a =2.655, τ=15.

Conclusion

Using the equation for fractal evolution of measure let us model different types of nanostructures. Varying parameters in the systems of Equations (1) and (2), we can obtain models of semiconductorsurfaces containing quantum wells, quantum dots, and quantum nanowires with different height and relative arrangement. We built histograms describing distribution of nanostructures on height. These histograms let us characterize size of nanostructures in nanocluster semiconductor films. The obtained theoretical results are in qualitative agreement with the corresponding experimental data.

Theoretical results obtained in the present work can be used for the description of electrical and optical properties of nanostructured semiconductor films.

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