# Modeling of Morphology of Semiconductor Surfaces with Quantum Nanowires

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**Abstract.** In the present work we present a possibility to model morphology of surfaces of nanostructured semiconductor films containing quantum nanowires by use of our own theory based on the map for fractal evolution of measure and method for reconstruction of dynamical chaos.
**Keywords:** Semiconductor, Fractal, Nanostructure, Quantum Nanowire.

## 1   Introduction

At the present time nanocluster semiconductor films have been attracting considerable attention because they may have different applications in new electronic devices. Modern methods of microscopy (such as atomic-force, scanning tunneling, etc.) demonstrate the nanocluster structure of semiconductor thin films. As usual, such structures are irregular, self-affine, and self-similar. So, we can consider nanoclusters as fractal and multi-fractal objects. Self-similarity means that similarity factors are equal each other for all variables. Self-affinity corresponds to different values of similarity factors for different variables.

Nanostructures can be classified into different types (for example, we can consider nanostructures as quantum dots, quantum wires, and superlattices (quantum wells)). These types of nanostructures are widely used in modern electronics, for example, for creation of lasers, solar cells, detectors, quick-operating devices and so on.

Surfaces of semiconductor thin films containing quantum-sized structures with specified geometrical and topological characteristics have the unique

optical properties. Using of such semiconductor films in electronics can lead to increasing of efficiency of optoelectronic devices, particularly, for increasing of efficiency of solar cells. For example, nanostructured semiconductor films can be used as covering of surfaces of optoelectronic devices for reduction of scattering and reflection of light.

## 2 Map for fractal evolution of measure

For modeling of morphology of surfaces of semiconductor thin films containing quantum-sized structures of different types we must know distribution of electrons, holes and impurities depending on fractal dimension of their sets. For this aim in the present work we use the universal map for fractal evolution of measure [1, 2].

From the criterion of fractal measure it is possible to obtain the universal map describing its alternated evolution. The map describes chaotic oscillations with characteristics corresponding to criteria of self-organization.

Let us to consider evolution on time of $x(t)$ which is the module of a function related with fractal measure (we consider measure as an additive value characterized by a measurable set) as

$$\frac{dx(t)}{dt} = sign\left(\frac{dx(t)}{dt}\right)\frac{|\Delta x|}{|\Delta t|^{1-\gamma_0}},\tag{1}$$

where $\gamma_0$ is a statistical characteristic of the set of $t$. Parameter $\gamma_0$ is used for supporting the Lipshitz–Hölder condition due to limitation of $\frac{dx}{dt}$. Module of increment of function $|\Delta x|$ which is relative dimensionless scale of measurement of $x(t)$) can be replaced according to the condition of the fractal measure $x(t)$ as

$$x = x_0(|\Delta x|)^{-(D-d)}, \ |\Delta x| = \left(\left|\frac{x}{x_0}\right|\right)^{-\frac{1}{\gamma}}, \ \gamma = D - d,\tag{2}$$

where $x_0$ is non-fractal regular measure, $D$ is fractal dimension of the set of $x(t)$, $d$ is topological dimension of measure for a carrier. By the substitution of Eq. (2) to Eq. (1) we can obtain the equation with finite differences.

Let us designate the discrete form of the sign function as $\mu_i$. $\Delta t > 0$, therefore, signum function $sign\left(\dfrac{dx(t)}{dt}\right)$ depends only on value of $\Delta x_i$. We can define its variation on discrete variable $i$ as

$$\mu_{i+1} = \frac{\Delta x_{i+1}}{\Delta x_i}\Big|_{x_i = x_{i+1}} = \frac{dx_{i+1}}{dx_i} \ . \tag{3}$$

As usual, values $\mu_{i+1} = \pm 1$ are used for linear description of evolution of perturbations. Obviously, it is possible to define $\mu_{i+1}$ via $\mu_i$. We don't use any limitations for module of this value.

We can rewrite Eq. (1) at $x_0 = 1$ with regard to Eqs. (2) and (3) as

$$\frac{x_{i+1}}{\Delta t} = \frac{x_i}{\Delta t} + \mu_i |x_i|^{-\frac{1}{\gamma}} \Delta t^{\gamma_0 - 1} = \frac{x_i}{\Delta t} + \mu_i |x_i|^{-\frac{1}{\gamma}} \frac{\Delta t^{\gamma_0}}{\Delta t} =$$
$$= \left( x_i \Delta t^{-\gamma_0} + \mu_i |x_i|^{-\frac{1}{\gamma}} \right) \frac{\Delta t^{\gamma_0}}{\Delta t} \ . \tag{4}$$

Let us to eliminate $\gamma_0$ from the Eq. (4) due to choosing of identical moments of time. We use a discrete algorithm and we model the relation $x_i \Delta t^{-\gamma_0}$ via $\gamma_0$ because only this relation (not $x_i \Delta t^{\gamma_0}$) corresponds to transition to chaos.

Meaning of using of $\gamma_0$ corresponds to realization of the following condition:

$$\frac{\Delta x_i}{x_i} \left( \frac{\Delta t}{\tau} \right)^{\gamma_0} = const \equiv C \ . \tag{5}$$

Here $\tau$ is characteristic time.

Mathematical operations reduced to calculation of the Riemannian measure if $\gamma_0 = 0$. In this case $\Delta t = 1$.

At $\gamma_0 \neq 0$ we have a possibility to find the Lebesgue measure with regard to the dependence of $\Delta t^{\gamma_0}$ on increment of function $\Delta x_i(\gamma, x_i)$ as

$$\left( \frac{\Delta t}{\tau} \right)^{-\gamma_0} = \frac{1}{C} \frac{\Delta x_i(\gamma, x_i)}{x_i} = \frac{(|x_i|)^{-1/\gamma}}{C x_i} \tag{6}$$

Meaning of parameter $C$ can be interpreted as an analog of base $B$ (complexity) of a signal used for the description of spectra:

$$B = \tau_k \Delta\omega . \tag{7}$$

Here $\tau_k$ is typical correlation time and $\Delta\omega$ is bandwidth. According to the definition, value of the parameter $C$ characterizes complexity of choosing accuracy for the description of signals with chaotic nature. It is well-known that measure of a fractal object depends on accuracy of observation. So, theoretical results contain the constant parameter $C$ characterizing accuracy of observation. Therefore, this parameter can be equal to $10^{-2}, 10^{-3}$, and so on. If sign of the derivative in Eq. (1) defined by external conditions (for example, by noise-type excitations), so, we must use absolute values of $\Delta x$ and $\Delta t^{\gamma_0}$ in Eq. (5).

Let us take into account that $\Delta t = \tau$. So, we can rewrite Eq. (4) as

$$x_{i+1} = \left(\frac{1}{C} + \mu_i\right)|x_i|^{-\frac{1}{\gamma}} . \tag{8}$$

If we differentiate Eq. (8) we have the following expression:

$$\mu_{i+1} = \left(\frac{\Delta x_{i+1}}{\Delta x_i}\right)_{x_i = x_{i+1}} = -\frac{1}{\gamma}\left(\frac{1}{C} + \mu_i\right)|x_i|^{-\frac{1}{\gamma}-1} . \tag{9}$$

Relations (8) and (9) are the map for the description of fractal evolution of measure.

Distribution of electrons, holes and impurities in a nanostructured semiconductor can be described via the map for alternation of fractal measure by the following way:

$$
\begin{aligned}
X_{k,i+1} &= \left(\frac{1}{C_k} + \sum_{k=1}^{3}\mu_{k,i}\right)\left|\frac{X_{k,i}}{X_{k,0}}\right|^{-\frac{1}{\gamma_k}} \\
\mu_{k,i+1} &= -\frac{1}{\gamma_k}\left(\frac{1}{C_k} + \sum_{k=1}^{3}\mu_{k,i}\right)\left|\frac{X_{k,i}}{X_{k,0}}\right|^{-\frac{1}{\gamma_k}-1}
\end{aligned}
\tag{10}
$$

where $k = (1, 2, 3) \equiv (n, p, a)$; (here $(n, p, a)$ describe distributions of electrons, holes and impurities correspondently), $P_k$ is precision factor of resolution, $\gamma_k$ is difference between fractal and topological dimensions, $X_{k,0}$ is equilibrium

concentrations of current carriers (electrons and holes) and impurities, $\mu$ is sign function.

We can use known values of $\gamma_k$ for self-similar case (coefficients of similarity are equal each other for all variables) and for self-affine set (coefficients of similarity are different for different variables). Normalized values of informational entropy of self-similar and self-affine sets $I_2 = 0.806$ and $I_1 = 0.567$ correspondently [3, 4].

On the base of the map of alternation (10) describing evolution of a system according to the condition of fractality of measure we can model morphology of quantum dots ($\gamma > 2$), quantum wires ($\gamma > 1$) and quantum wells ($\gamma > 0$) located on surfaces of semiconductor thin films (topological dimension $d = 2$). So, type of nanostructures in a nanocluster semiconductor is determined by fractal dimensions of sets of electrons, holes and impurities. Numerical values of fractal dimensions describe steady self-similar and self-affine sets.

We apply the well-known method for reconstruction of dynamic chaos [5] for modeling of relief of semiconductor surfaces containing quantum nanowires. According to the method multi-dimensional images characterizing a chaotic phenomenon can be constructed via a one-dimensional realization by the following way.

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 divisible to $\tau$. Parameter $\tau$ can be interpreted as a fixed delay. So, we can write a set of discrete variables as

$$
\begin{aligned}
& n_1 : n_1(t_1), \ldots\ldots\ldots\ldots\ldots\ldots\ldots n_1(t_N) \\
& n_2 : n_1(t_1 + \tau), \ldots\ldots\ldots\ldots\ldots n_1(t_N + \tau) \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& n_{i-1} : n_1(t_1 + (j-1)\tau), \ldots\ldots\ldots n_1(t_N + (j-1)\tau)
\end{aligned}
\tag{11}
$$

Linear independence of the variables in phase space is necessary. This condition can be achieved by the corresponding choice of numerical value of $\tau$. All these variables can be defined via single data sequence $n_{i+1} = f(n_i)$. So, application of the described approach let us to describe dynamics of a system in multi-dimensional space via a single one-dimensional data sequence. Current values of electron concentration in a nanocluster semiconductor can be defined from the map for alternation of fractal measure (Eq. (10)). In our case the dependence of electron concentration on spatial step can be considered as required one-dimensional dependence.

## 3 Results of numerical analyses

Results of computer simulation of morphology of semiconductor surfaces containing quantum-sized structures according to the described approach are presented below.

(a)
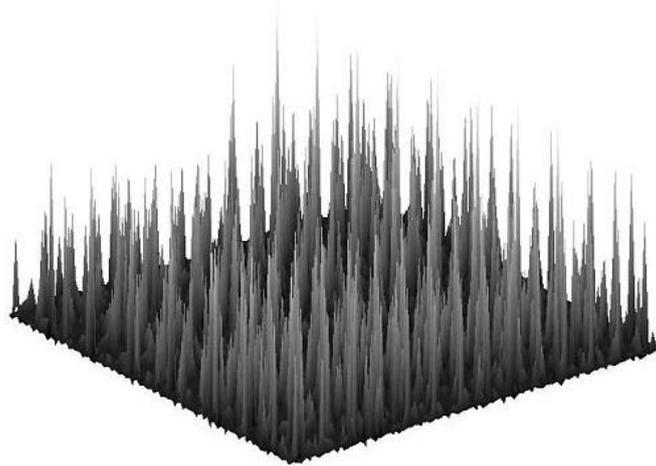


(b)
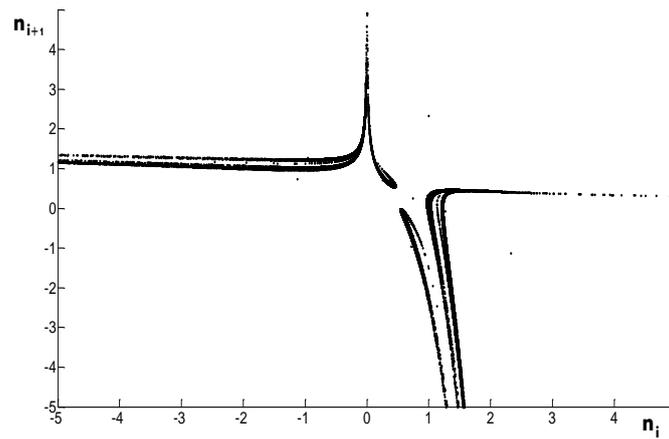


Figure 1. Model of a surface containing vertical quantum nanowires (a) and its phase plane ( $n_i$, $n_{i+1}$ ) (b).

$n_0 = p_0 = 0.25$, $a_0 = 1.7$   $C_n = C_p = C_a = 0.999$.  $\gamma_n = \gamma_p = \gamma_a = 2 + I_1$,  $\tau = 10$.

Varying the parameters $C_k$, $\gamma_k$, $X_{k,0}$ and $\mu$ in Eq. (10), it is possible to model morphology of surfaces with different cluster structure.

It is well-known that semiconductor surfaces can contain point, lined, spatial and volumetric structures. Type of nanostructures can be taken into account by assignment of $\gamma_k$.

Influence of substrate can be taken into account by assignment of corresponding values of $X_{k,0}$, which are equilibrium concentrations of electron, holes and impurities.

Resolution of the modeled image can be controlled by parameter $C_k$ which is the is precision factor of resolution ranged from 0 to 1.

We accept $\tau$ equal to 10. Fractional values of initial concentrations correspond to valency of semiconductor substrate and impurity atoms.

Model of morphology of semiconductor with quantum nanowires is shown in Figure 1(a). Its phase plane characterizing distribution of current carriers is shown in Figure 1(b). We can see that phase plane contain steady phase trajectories tending to infinity. This fact confirms that the considered systems can by described by use of theory of dynamical chaos. In this case chaotic processes are close to stochastic behavior.

Varying the values of fractal dimension we can obtain models of surfaces with quantum nanowires with different height and location.

Influence of insignificant variation of concentration of impurities on morphology of semiconductor surfaces containing vertical nanowires is shown in Figure 2. We can see that even insignificant variation of concentration of impurities leads to remarkable changing of morphology of the considered semiconductor film.

Models of surfaces with quantum nanowires presented in Figures 1 and 2 are identical to experimental photos made by use modern methods of microscopy [6-10].

By use of the theory it's possible to model so called horizontal quantum nanowires also. These structures can be considered as lateral ordered arrays of quantum dots. Models of semiconductor surfaces containing quantum dots are shown in Figure 3(a) and Figure 3(b). We can see that increasing of concentration of impurities leads to changing of height of nanoclusters and theirs relative disposition.

Varying parameters in Eqs. (10) and (11), we can model surfaces with arranged arrays of quantum dots. These arrays can be considered and horizontal quantum wires.

Phase plane for such structures contains steady phase trajectories. As indicated above, this fact corresponds to existence of dynamical chaos in the considered systems.

(a)
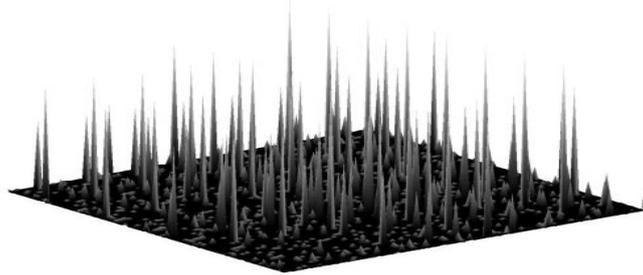


(b)
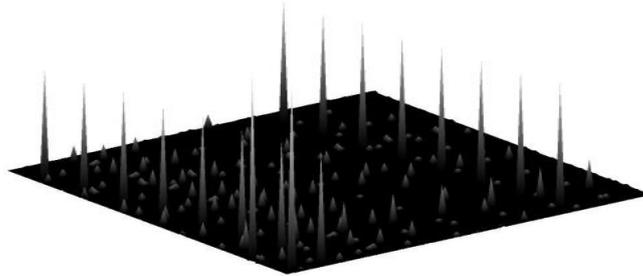


(c)
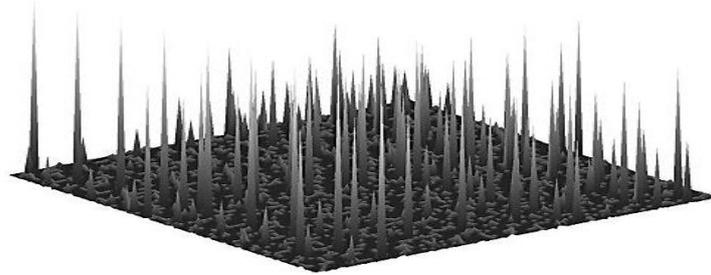


(d)
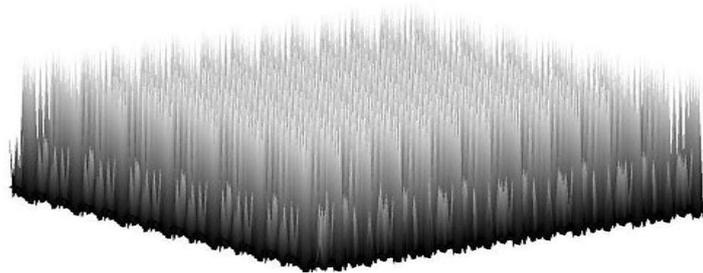


Figure 2. Influence of concentration of impurities on morphology of a surface
of nanostructured semiconductor film.

$$n_0 = p_0 = 0.25, \ C_n = C_p = C_a = 0.996. \ \gamma_n = \gamma_p = \gamma_a = 2 + I_2, \ \tau = 10,$$

$$(a) - a_0 = 1.0, \ (b) - a_0 = 1.2, \ (c) - a_0 = 1.4, \ (d) - a_0 = 1.6.$$

(a)
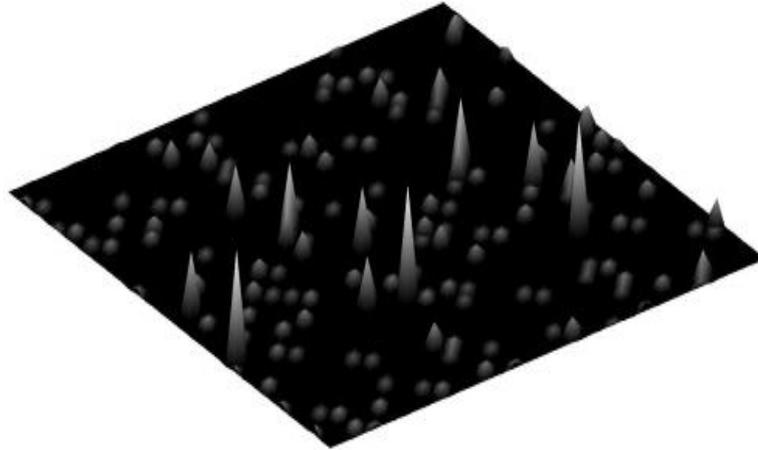


(b)
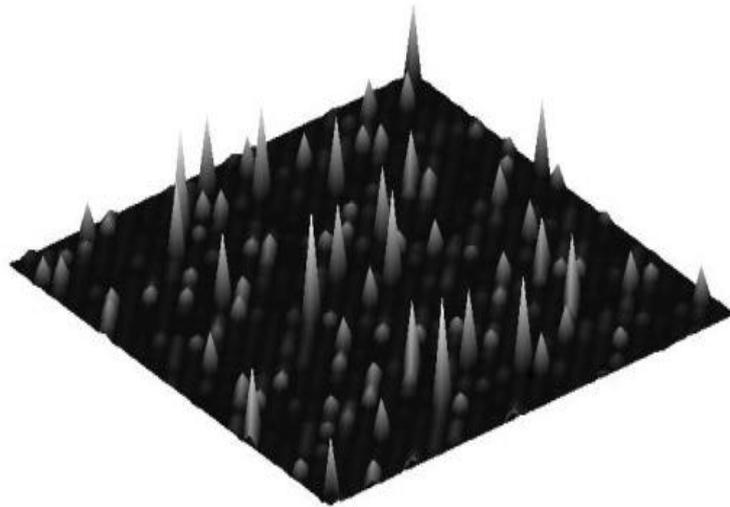


Figure 3. Models of surfaces containing quantum dots.
$n_0 = p_0 = 0.25$, $C_n = C_p = C_a = 0.999$. $\gamma_n = \gamma_p = 3 + I_1$, $\gamma_a = 3 + I_2$, $\tau = 15$,
$(a) - a_0 = 0.95$, $(b) - a_0 = 1.3$.

(a)
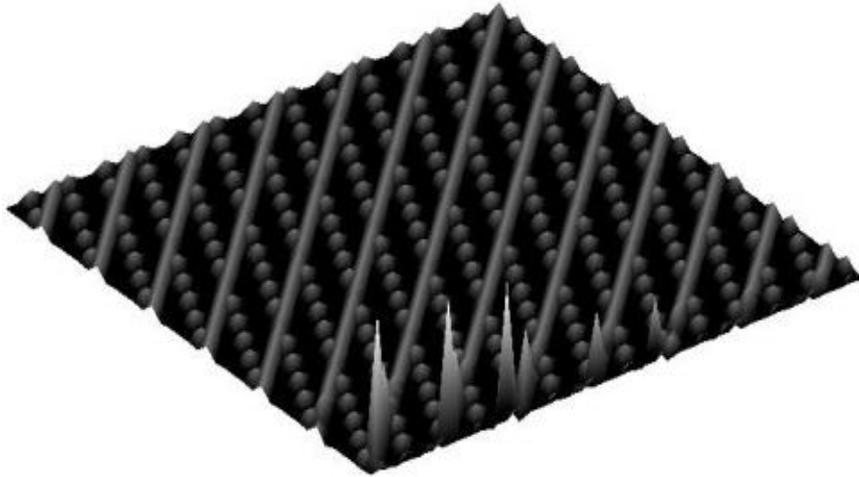


(b)
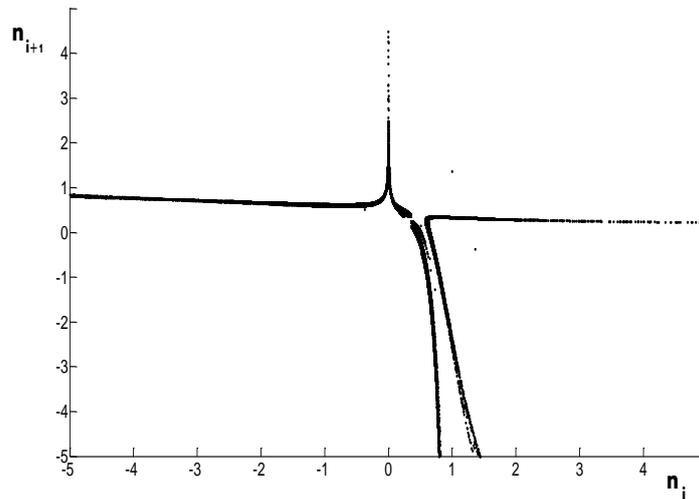


Figure 4. Model of a surface containing horizontal quantum nanowires (a) and its phase plane ( $n_i$, $n_{i+1}$ ) (b).

$n_0 = p_0 = 0.25$ , $a_0 = 1.8$, $C_n = C_p = C_a = 0.999$ . $\gamma_n = \gamma_p = \gamma_a = 2 + I_1$, $\tau = 10$.

Models of surfaces shown in Figures 3 and 4 are in a good agreement with corresponding experimental data [11-18].

## Conclusions

By use of the suggested map for the description fractal evolution of measure we can model different types of nanostructures. For this aim we use quantitative criteria of self-similarity and self-affinity of sets established in our works.

Variation of parameters in Eq. (10) let us model morphology of semiconductor thin films containing vertical nanowires with different height and relative location. Even insignificant variation of concentration of impurities leads to remarkable changing of morphology of surfaces containing quantum-sized structures.

Using of the suggested theory give us a possibility to model quantum dots and lateral arranged arrays of quantum dots which are horizontal quantum nanowires.

Results of presentation of distribution of current carriers in phase plane confirmed that considered systems can be described by use of the theory of dynamical chaos.

Our theoretical results qualitatively conform to the corresponding experimental data.

Theoretical results described in the work can be used for the description of electrical and optical properties of nanostructured semiconductors.

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