

Fractality of Nanostructured Semiconductor Films

Z. Zh. Zhanabayev and T. Yu. Grevtseva*

Al-Farabi Kazakh National University, Tole bi Street, 96, Almaty 050012, Kazakhstan

(Received 24 August 2007; Accepted 25 October 2007; Published 9 November 2007)

We present a model of spatial distribution of electrons, holes, clusters of intrinsic and admixtures (defects of different types) in nanostructured semiconductor thin films. We obtain intermittent, heterogeneous distributions of concentration typical for images of surfaces obtained by scanning tunneling microscopy, atomic-force microscopy and electron microscopy by numerical analyses. [DOI: 10.1380/ejsnt.2007.132]

Keywords: Semiconductor; Fractal; Nanocluster; Computer simulation; Nano-scaling imaging; Atomic force microscopy; Scanning electron microscopy; Scanning tunneling microscopy

I. INTRODUCTION

Microscopy demonstrates the nanocluster structure of semiconductor thin films. Such structures are hierarchically self-similar and self-affine, i.e. fractal. For the description of the physical phenomena obtained in thin semiconductor films it is necessary to describe the distribution of current carriers depending on fractal dimension of their set. Determination of fractal dimensions of heterogeneous, anisotropic (affine) objects is a stand-alone scientific problem. However, we can make use of values of fractal dimensions of model fractals and well-known values of fractal dimensions for self-similar (informational) and self-affine (entropy) sets [1, 2]. The aim of this paper is to determine fractal distribution of concentration of current carriers in nanostructured semiconductors and to compare the theoretical results to the experimental microscopy data.

II. EQUATIONS FOR NON-EQUILIBRIUM DISTRIBUTION OF CURRENT CARRIERS

Let us designate concentrations of quasi-particles (electrons, holes and clusters of intrinsic and admixture atoms which are defects of different types) as n, p, a , respectively. We examine variation of concentration on coordinate x near the point $x = x_*$, where x_* is a coordinate of the center of a cluster. Let us assume that centers of clustering are intrinsic atoms and molecules or atoms and molecules of an admixture. In general, clustering is aggregation (formation of friable conglomerations) of atoms, molecules and uniformity neutral defects.

In order to take into account the irregularity of the motion of current carriers in a fractal surroundings it is necessary to adopt the Lipshtz-Hölder condition. The derivative is limited by means of this condition due to fractional power of argument's increment $\alpha < 1$. Let us take this power as $\alpha = 1 - \gamma_0$, where γ_0 is a fractal dimension of decomposition points set of the argument axis. $\gamma_0 = 0$ provides the usual derivative. Thus, the derivative of concentration of electrons $n(x)$ can be written via final

differences as

$$\frac{dn(x)}{dx} = \pm \frac{\delta_n}{|x - x_*|^{1-\gamma_0n}}, \quad (1)$$

where δ_n is scale of measurement of $n(x)$. Coordinate and concentration in Eq. (1) are the dimensionless values which are relative to some characteristic scales. Sign “-” (“+”) corresponds to positive (negative) difference $\delta_n = n(x) - n(x_*)$.

Fractal measure $n(x)$ is given by

$$n(x) = n_0(x)\delta_n^{-(D_n-d)}, \quad (2)$$

where d is the topological dimension of cell with the spatial scale δ_n , D_n is the fractal dimension of set of all various cells and $n_0(x)$ is the equilibrium (non-fractal) concentration of electrons. Excluding δ_n from Eqs. (1) and (2) we obtain

$$\frac{dn(x)}{dx} = \pm |x - x_*|^{\gamma_0n-1} \left| \frac{n(x)}{n_0(x)} \right|^{-\frac{1}{\gamma_n}}, \quad (3)$$

$$\gamma_n = D_n - d, d = 0, 1, 2, 3.$$

Non-equilibrium concentration $n(x_1)$ for the fixed value of x_1 is determined by boundary conditions as $n(x = x_1) = n_1$.

We rewrite Eq. (3) for the description of a set of randomly (due to dynamical, thermal factors) disposed clusters with various structure, i.e. for $x_* = \{x_{*j}(n, p, a)\}, j = 1, 2, \dots$, where x_{*j} are the random numbers in the range of $0 < x_{*j} < x_{\max}$. In that case the alternation of signs “+” and “-” in Eq. (1) will be random. For the description of this alternation we can use $\text{sign}(\xi(x))$, where $\xi(x)$ is delta-correlated random process. Position of electron in the range of $0 < x_{*j} < x_{\max}$ is also defined by a probabilistic approach. This probability we shall define as

$$P_n(x) = |\psi_n(n, a, p, x)|^2 |x - x_*|, \quad (4)$$

where $\psi_n(n, a, p, x)$ is wave function of an electron located in a field of a cluster. This function should be chosen for simple models of interaction of an electron to a cluster.

Following the same arguments for a description of concentration of holes $p(x)$ and impurities (clusters) $a(x)$ we

*Corresponding author: kenvp@kazsu.kz

obtain the following system of equations:

$$\frac{dn(x)}{dx} = \text{sign}(\xi(x)) |\psi_n(n, a, p, x)|^2 |x - x_*|^{\gamma_{0n}} \left| \frac{n(x)}{n_0(x)} \right|^{-\frac{1}{\gamma_n}}, \quad (5)$$

$$\frac{dp(x)}{dx} = \text{sign}(\xi(x)) |\psi_p(n, a, p, x)|^2 |x - x_*|^{\gamma_{0p}} \left| \frac{p(x)}{p_0(x)} \right|^{-\frac{1}{\gamma_p}}, \quad (6)$$

$$\frac{da(x)}{dx} = \text{sign}(\xi(x)) |\psi_a(n, a, p, x)|^2 |x - x_*|^{\gamma_{0a}} \left| \frac{a(x)}{a_0(x)} \right|^{-\frac{1}{\gamma_a}}, \quad (7)$$

$$\text{sign}(\xi(x)) = \begin{cases} +1, & \xi(x) > 0 \\ -1, & \xi(x) < 0 \end{cases}.$$

In order to account the specific character of crystal or amorphous structure of semiconductors we can choose the wave functions as Bloch waves, so, we allow for dependence of concentration on the coordinate. Equations (5)–(7) cannot be investigated even for a simplest expression for the wave function due to the stochastic character of these equations. Therefore we examine discrete form of the equations.

III. NON-LINEAR MAP FOR CONCENTRATION OF CURRENT CARRIERS

For simplicity, we rewrite Eq. (1) with the sign “+” via series of discrete numbers n as

$$\frac{n_{i+1}}{\Delta x} = \left(\frac{n_i}{\Delta x} \right)_{\gamma_0} + \frac{\delta_{n,i}}{|\Delta x|^{1-\gamma_{0n}}}, \quad i = 1, 2, 3, \dots, \quad (8)$$

where γ_0 is used for normalization of the given value within the range of the scale of measurement $\delta_{n,i}$ by setting the fractional power γ_0 . From Eq. (1) we have

$$\left(\frac{n_i}{\Delta x} \right)_{\gamma_0} = \frac{n_i \delta_{n,i}}{|\Delta x|^{1-\gamma_{0n}}}. \quad (9)$$

We can use discrete values of n_i taken with the constant step $\Delta x = 1$. Thus, Eqs. (5)–(7) can be written as

$$n_{i+1} = \{n_i + \text{sign}(\xi_i) |\psi_n(a, p_i, i)|^2\} \left| \frac{n_i}{n_0} \right|^{-\frac{1}{\gamma_n}}, \quad (10)$$

$$p_{i+1} = \{p_i + \text{sign}(\xi_i) |\psi_p(a, n_i, i)|^2\} \left| \frac{p_i}{p_0} \right|^{-\frac{1}{\gamma_p}}, \quad (11)$$

$$a_{i+1} = \{a_i + \text{sign}(\xi_i) |\psi_a(n_i, p_i, i)|^2\} \left| \frac{a_i}{a_0} \right|^{-\frac{1}{\gamma_a}}, \quad (12)$$

We shall make use of values of fractal dimensions corresponding to steady self-similar and self-affinity sets for the definition of values $\gamma_n, \gamma_p, \gamma_a$. It is known that specific informational entropy of self-similar set is equal to fractal dimension of a cell of this set. Fixed points of probability

function $P(I)$ and informational entropy $S(I)$ can be used as criteria of similarity as

$$P(I) = e^{-I}, P(I) = \int_I^\infty f(I) dI, \quad (13)$$

$$f(I) = P(I) = e^{-I}, \int_0^\infty f(I) dI = 1,$$

$$S(I) = \int_I^\infty f(I) dI = (I+1)e^{-I}, \quad (14)$$

where I is quantity of information (defining variable), $f(I)$ is density of probability distribution function of information [1, 2]. Their fixed points are determined by formulas

$$P(I_1) = I_1, e^{-I_1} = I_1, I_1 = 0.567, \quad (15)$$

$$S(I_2) = I_2, (I_2+1)e^{-I_2} = I_2, I_2 = 0.806. \quad (16)$$

Different approaches for the determination of wave functions of quasi-particles are possible. Separating the electrons into cluster electrons and free (valence) electrons, we write the Hamiltonian for the examined problem as [3]

$$H = \sum_i \frac{\mathbf{p}_i^2}{2M_l} + \sum_{l,m} U(\mathbf{R}_l - \mathbf{R}_m) + \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i,l} V(\mathbf{r}_i - \mathbf{R}_l) + \sum_{i,j} \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|}, \quad (17)$$

where l and m are numbers of clusters, indexes i and j are numbers of electrons, \mathbf{P} and M are impulse and mass of cluster, \mathbf{p} and m are impulse and mass of electron, $U(\mathbf{R}_l - \mathbf{R}_m)$ is potential of clusters interaction, $V(\mathbf{r}_i - \mathbf{R}_l)$ is potential of interaction of free electrons to clusters. Each electron interacts to the cluster independently of other electrons. Thus, we write Shrödinger equation as

$$\left\{ \frac{\mathbf{p}_i^2}{2m} + \sum_l V(\mathbf{r}_i - \mathbf{R}_l) \right\} \psi_i(\mathbf{r}_i, \mathbf{R}) = E_i \psi_i(\mathbf{r}_i, \mathbf{R}), \quad (18)$$

where E_i is the energy of electron, $\psi_i(\mathbf{r}_i, \mathbf{R})$ is the wave function of electron. The form of eigenfunction of an electron we choose as the Bloch wave:

$$\psi_{\mathbf{k}}(\mathbf{r}) = U_{\mathbf{k}}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}), U_{\mathbf{R}}(\mathbf{r} + \mathbf{R}) = U_{\mathbf{k}}(\mathbf{r}), \quad (19)$$

where \mathbf{k} is the wave vector. From Eq. (19), it follows that

$$\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{\mathbf{r}} \exp(i\mathbf{k} \cdot \mathbf{R}), \quad (20)$$

It is possible to work with wave functions centered on the centers of clusters \mathbf{R} , i.e. to use the analogues of Vanyi functions $\varphi(\mathbf{r} - \mathbf{R})$ as

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} \varphi(\mathbf{r} - \mathbf{R}) \exp(i\mathbf{k} \cdot \mathbf{R}), \quad (21)$$

It is possible to approximate Vanyi functions by atomic orbitals via approximation of closely coupled interface of electrons to clusters ($\varphi(\mathbf{r} - \mathbf{R}) = \varphi_n(\mathbf{r} - \mathbf{R})$),

$$\varphi_{n,l}(r) = \frac{2}{n^{l+2}(2l+1)!} \sqrt{\frac{(n+l)!}{(n-l-1)!}} (2r)^l e^{-\frac{r}{a}} F\left(-n+l+1, 2l+2, \frac{2r}{a}\right), \quad (22)$$

where n is the index of a energy band, l is orbital quantum number, F is singular hypergeometric function. Equation (21) gives us the dynamics of a hole in center of mass system of an electron-hole pair. At the another extreme case of loosely coupled interface of electron to cluster we can use the plane waves as

$$\psi_n(x) = \psi_p(x) = \psi_a(x) = \cos(k_n x) \cos(k_p x) \cos(k_a x). \quad (23)$$

IV. RESULTS OF THE NUMERICAL ANALYSIS

The results of computer simulation made according to Eqs. (10), (11), (12), (21) and (23) are shown in FIGs. 1–5. Because $\xi(x)$ is random, we do not obtain identical curves, but the curves in different directions are randomly displaced according to their phases. Configuration of a surface of a semiconductor thin film depends on its fractal dimension. Varying the parameters $\gamma_n, \gamma_p, \gamma_a, n_0, p_0$ and a_0 , it is possible to obtain the pictures similar to experimental photos of surfaces of thin semiconductor films [4–8].

Scanning tunneling microscopy image of 5 monolayers Ag deposited on a Si(001) 2×1 substrate at 65 K [4] is shown in FIG. 1. The film was annealed at room temperature at a tunnel current 0.2 nA and a tip voltage of 5 V. Image taken after deposition of 4 monolayers of In on an Si(111)- $\sqrt{3} \times \sqrt{3}$ -Ga (1 monolayer) surface at room temperature [5] is shown in FIG. 2. Topology of surfaces of GaAs(100) [6] shown in FIG. 3 has been investigated before and after short processing in selenium vapour. Surface growing by gas-core epitaxy on p^+ -type substrate obtained in experimental work [7] is shown in FIG. 4. This image has been obtained by atomic-force microscopy at room temperature and atmospheric conditions. The photo of surface of p -CdTe is shown in FIG. 5. Formation of nanosize structures on the surface of the p -CdTe crystals at laser irradiation has been investigated in the experimental work [8]. The photo of the surface has been obtained by atomic-force microscopy.

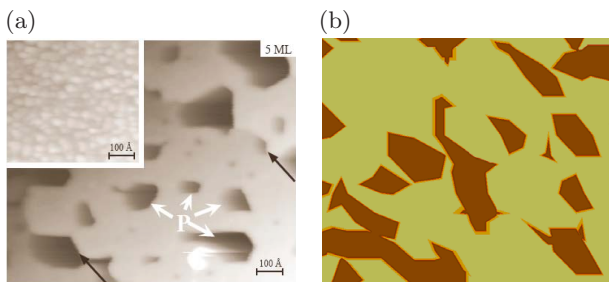


FIG. 1: Microscopy image for the Ag adsorption on a Si surface: (a) experimental data [4], (b) theoretical results: $\gamma_n = \gamma_p = \gamma_a = I_2, n_0 = p_0 = a_0 = 5, n_1 = p_1 = 1, a_1 = 100$.

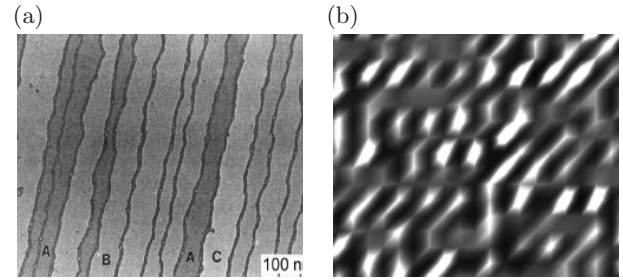


FIG. 2: Image taken after deposition of 4 monolayers of In on a Si surface: (a) experimental data [5], (b) theoretical results: $\gamma_n = I_1, \gamma_p = 2 + I_2, \gamma_a = 3 + I_2, n_0 = p_0 = a_0 = 2.6, n_1 = p_1 = 1, a_1 = 100$.

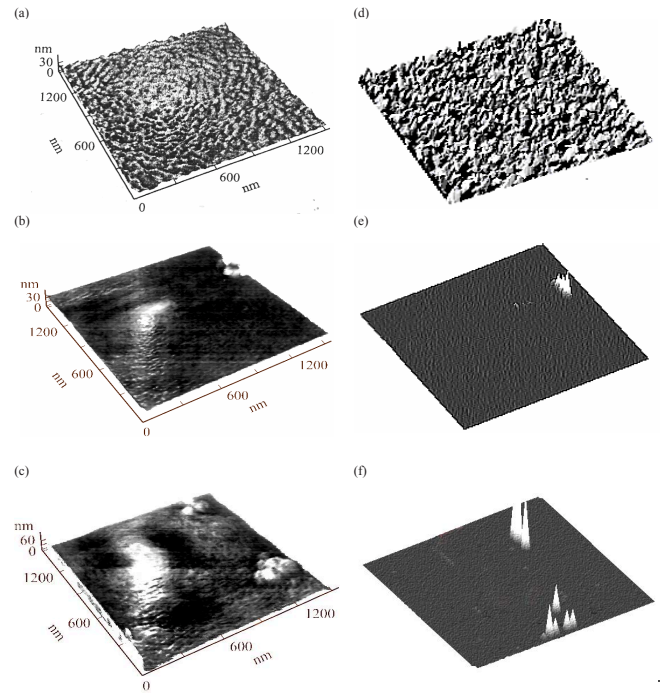


FIG. 3: Image of a surface of GaAs(100). Experimental data [6]: (a) photo of initial surface, (b) photo of surface processed in vapor of Se during 3 minutes, and (c) same during 5 minutes. Theoretical results: (d) $\gamma_n = \gamma_p = \gamma_a = 1 + I_2, n_0 = p_0 = a_0 = 20, n_1 = p_1 = a_1 = 1$, (e) $\gamma_n = \gamma_p = \gamma_a = I_2, n_0 = p_0 = a_0 = 2, n_1 = p_1 = 1, a_1 = 20$, (f) $\gamma_n = \gamma_p = \gamma_a = I_1, n_0 = p_0 = a_0 = 2, n_1 = p_1 = 1, a_1 = 20$.

Models of nano-scaling images of surfaces plotted according to Eqs. (10), (11), (12) (FIGs. 1(b), 2(b), 3(d),(e), (f), and 4(b)) are placed on the right side of experimental photos. Figures 5(b) and (c) has been plot by using Eq. (10). Figure 5(b) corresponds to the assumption that the function $\varphi_{n,l}(r)$ is equal to radial function of electron at the state $1s$ in an atom of hydrogen. For the other figures this function is defined by Eq. (23). Results of the numeral analyses made by using Eq. (23) correspond to experimental data at relatively little values of fractal

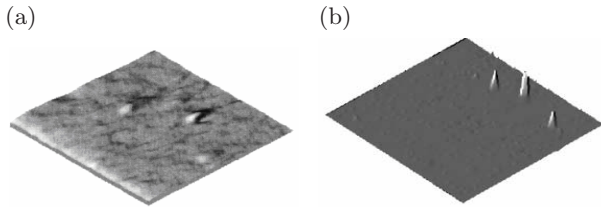


FIG. 4: Morphology of a surface of p -GaAs(100): (a) experimental data [7], (b) theoretical results: $\gamma_n = I_2$, $\gamma_p = \gamma_a = 1 + I_1$, $n_0 = p_0 = a_0 = 1.5$, $n_1 = p_1 = 1$, $a_1 = 15$.

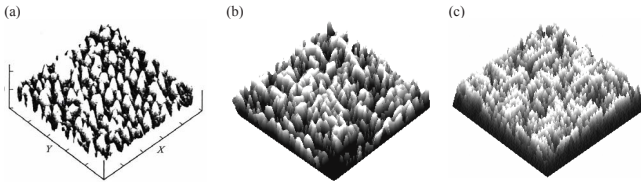


FIG. 5: Image of a surface of p -CdTe. (a) Experimental data [8]; (b) and (c) theoretical results: $\gamma_n = 3 + I_2$, $n_0 = 3$, $n_1 = p_1 = 1$, $a_1 = 10$.

dimension. At great values of fractal dimension application of Bloch-Vanyi functions is preferable. It confirmed by comparison of experimental image in FIG. 5(a) to the models of surfaces shown in FIG. 5(b) and FIG. 5(c).

With the help of the theory we can outline the fol-

lowing properties of fractal surfaces of semiconductors. Quasi-regular linear and flat structures are described by small values of fractal dimension ($\gamma \leq I_1$). Small-scale random formations correspond to relatively large values of $\gamma \geq I_2 + d$, $d = 0, 1, 2, 3$. Stabilizing effect of a substrate on the formation of structures is taken into account by the values of equilibrium concentration of particles ($n_0 > 1, p_0 > 1, a_0 > 1$). Numbers of free and valence electrons in the cluster is taken into account via the choice of Bloch-Vanyi function or of a type of radial function used for its approximation.

V. CONCLUSION

The constructed stochastic and fractal models provide qualitative agreement to different types of microscope images of the surfaces of thin films. Fractal dimension of clusters, sets of electrons and holes, their stochastic distribution, relative concentration of equilibrium components, and type of wave function of electron interacting to cluster are taken into account by the theory. Thus, the method can be future developed to obtain a quantitative description of the morphology of films. Results of the present work can be used for analysis of electrical and optical properties of nanostructured semiconductors.

-
- [1] Z. Zh. Zhanabaev, *Dimensions of self-affine fractals. Fractals and applied sinergetics* edited by F.S. Ivanova (MSPU, Moscow, 2003) pp.198-201.
 - [2] Z. Zh. Zhanabaev and T. Yu. Grevtseva, *Physica B: Condens. Matter* **391**, 12 (2007).
 - [3] B. K. Ridley, *Quantum processes in semiconductors*, University of Essex Clarendon Press, Oxford, 1982.
 - [4] I. Matsuda, T. Tanikawa, S. Hasegawa, H. W. Yeom, K. Tono, and T. Ohta, *e-J. Surf. Sci. Nanotech.* **2**, 169 (2004).
 - [5] T. Yamanaka, *e-J. Surf. Sci. Nanotech.* **1**, 91 (2003).
 - [6] N. N. Bezryadin, G. I. Kotov, I. N. Arsentyev, and A. A. Starodubtsev, *Fizika i Tekhnica Poluprovodnikov* **39**, 1025 (2005).
 - [7] A. V. Panin, A. R. Shugurov, and V. M. Kalygina, *Fizika i Tekhnica Poluprovodnikov* **35**, 78 (2001).
 - [8] A. Baidullaeva, A. B. Vlasenko, L. F. Cuzan, O. S. Litvin, and P. E. Mozol, *Fizika i Tekhnica Poluprovodnikov* **39**, 1064 (2005).