MICROSCOPIC STRUCTURE OF THE SEMICONDUCTOR SURFACE IN THE EXTERNAL ELECTRIC FIELD

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Abstract

In this paper a theoretical model for the free semiconductor surface is proposed. The principled capability of the correct calculation of the electrostatic potential of the real semiconductors surface is demonstrated on the example of Silicon surface. The potential relief $V(\vec{r},F)$ of Si(100) surface are investigated theoretically using methods of nonlocal electrostatics. It is shown, that taking into account the microscopic structure of the free semiconductor surface can lead to the local change of the potential barrier height along the surface. $V(\vec{r},F)$ (and its amplitude $\delta\phi(\vec{r})$) is determined by the microscopic structure of the real surface and the bulk (macroscopic) parameters of the semiconductor.

1. Introduction

The progress in up-to-date vacuum microelectronics requires the development of better theoretical models for calculations of the emission characteristics. It is known that emission properties depend on the bulk properties of the field emission cathodes, their geometric shapes and the state of their surfaces. For the theoretical calculation of the current-voltage characteristics and optimization of the field emitter parameters it is necessary to know a precise shape of the potential barrier in the presence of an external electric field F. Recently semiconductor materials (silicon, diamond, diamond-like-carbon ets.) are considered to be promising for vacuum microelectronics devices [1-3].

The theoretical comprehension of an autoelectronic emission from the real semiconductor surfaces is one of the most actual problems of vacuum microelectronics [4]. As against the emission characteristics of metals, which are well explained by available theoretical models, the emission characteristics of the non-metal cathodes in a number of cases have not adequate theoretical interpretation. Mainly it is connected to essential distinction in the bulk properties of metals and semiconductors and as a result in essential distinctions in its emission characteristics. The emission characteristics of the main semiconductors (including Silicon) are very sensitive to the preparation conditions, which can change the state of the free semiconductor surface (for example, in the result of the reconstruction of the surface). For the metals the presence of the fixed charged surface states (CSS) on a free surface (for example, the dangling bonds) leads to the formation of a screening layer of the free electrons in the vacuum region [5,6]. It is known, that in the case of the semiconductors the fixed CSS on the free surface leads to the formation of the space charge region (SCR) in its bulk with the concentration of the free carriers (electrons or holes) which are essentially different from its bulk concentration [7,8]. Surface properties of semiconductors including the emission and adsorption characteristics are considerably influenced by change in the CSS.

In this paper the distribution of the total potential $V(\vec{r},F)$ in the external electric field F from the exact solution of the nonlocal Poisson equation for the semiconductor-vacuum system is determined. It is shown that the correct account of the screening properties of the semiconductor provides the continuity (finiteness) of the potential $V(\vec{r},F)$ at the semiconductor-vacuum interface and the common (vacuum) level of the counting out of the energy [9-11].

The continuity (finiteness) of the potential $V(x,F)$ on the semiconductor surface allows us to enter correctly the lateral distribution of the fixed CSS $\sigma_s(y,z)$ along the surface. In the given work the density of the fixed charge $\sigma_s(y,z)$ on the semiconductor surface connects with the microscopic (atomic) structure of the semiconductor surface, which is determined by experimental investigations or by microscopic (quantum-chemistry) calculations of the specific semiconductor surface. The introducing of the distribution of fixed CSS $\sigma_s(y,z)$ in the model form, which is used in the microscopic calculations [8,12-14], has allowed us to link the macroscopic characteristics of the semiconductor with the microscopic structure of the surface in frameworks of the proposed theory. In this paper the potential relief $V(\vec{r},F)$ of n-Si(100) surface are investigated theoretically using methods of nonlocal electrostatics. It is shown, that the microscopic structure of the free semiconductor surface can lead to the local change of height of a potential barrier along the surface. The total potential $V(\vec{r},F)$ (and its oscillating part $\delta\phi(\vec{r})$) is determined not only by the microscopic structure of the real surface (fixed CSS) but also the macroscopic properties (bulk parameters) of semiconductors.

2. Fundamentals of the theoretical method

In this section we consider the problem of a point charge e interaction with the surface of a semi-infinite semiconductor in an external electric field F taking into account the screening effects in its bulk and the density of fixed charged surface states (CSS) $\sigma_s(y,z)$ on the free semiconductor surface.

An exact solution of this problem may be obtained in the framework of non-local electrostatics [9-11]. The Green's function of a longitudinal self-consistent field $D(q;x,x')$ describing the screened Coulomb interaction between the charges at the points x and x' is determined by the Poisson equation [9]

$$\left(\frac{\partial^2}{\partial x^2}-q^2\right)\cdot D(q,x,x')-4\pi e^2\int dx'\Pi(q;x,x')D(q;x',x)=\delta(x-x'), \qquad (1)$$

where $\delta(z)$ is the delta-function; $\Pi(q;x,x')$ is the polarization operator of the inhomogeneous system, $q=\{q_y,q_z\}$ is the two-dimensional component of the wave vector and $k_\perp$ is the component of the wave vector which is normal to the interface:

$$\left.\begin{aligned}&\Pi(q;x,x')=\\&\left[\Pi_1(q,x-x')+\Pi_1(q;x+x')\right]\theta(-x)\theta(-x')+\left[\Pi_2(q;x-x')+\Pi_2(q;x+x')\right]\theta(x)\theta(x'),\\&\Pi_j(q;x\mp x')=\int_{-\infty}^{\infty}\frac{dk_\perp}{2\pi}\cdot\frac{k_\perp^2+q^2}{4\pi e^2}\cdot\left[\varepsilon_j(k_\perp,q)-1\right]\cdot\exp(ik_\perp(x\mp x')).\end{aligned}\right\} \qquad (2)$$

The approximation (2) corresponds to the specular reflection of the longitudinal polarisation waves from the interface (x=0), $\theta(x)$ is the step-function, $j=1$ is used for the semiconductor region $x\le 0$, while $j=2$ for the vacuum region $x\ge 0$.

The solution of the homogeneous Poisson equation (1) for the Fourier coefficients $D_j(q;x,x')$ can be written in the following form

$$\left.\begin{aligned} &D_j(q;x,x') = \\ &-a_j(q;x)\theta(x)\partial D_j(q;0,x') + a_j(q;x)\theta(-x)\partial D_j(q;0,x') + b_{j,j-1}(q;x,x') \end{aligned}\right\}, \quad (3)$$

where the function $\partial D_j(q;0,x') = \left.\dfrac{\partial D_j(q;x,x')}{\partial x}\right|_{x=0}$ is the derivative in the case of $\varepsilon_j(\vec{k}) \to 1$ for $\vec{k} \to \infty$ and $\partial D_j(q;,0,x') = \varepsilon_j \left.\dfrac{\partial D_j(q;x,x')}{\partial x}\right|_{x=0}$ if $\varepsilon_j(\vec{k}) \to \varepsilon_j$ while $\vec{k} \to \infty$. The functions $a_j(q;x)$ are the solutions of the homogeneous Poisson equation (1) in the case when the polarization operator $\Pi(q;x,x')$ has the form (2) and $\sigma_s(q) = 0$, $F(q) = 0$

$$a_j(q;x) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{dk_\perp \exp(ik_\perp x)}{\varepsilon_j(k_\perp,q)\cdot(k_\perp^2+q^2)}, \quad (4)$$

where $\varepsilon_1(k_\perp,q) = \varepsilon(\vec{k})$ is a dielectric permittivity function of semiconductor and $\varepsilon_2(k_\perp,q) = 1$ in vacuum region. The functions $b_{j,j-1}(q;x,x') = b_j(q;x)\,\delta_{j,j-1}$ are the particular solution of the Poisson equation (1) with the zero boundary conditions

$$b_j(q;x,x') = \frac{1}{2}\left[a_j(q;x-x') + a_j(q;x+x')\right], \quad (5)$$

where $\delta_{j,j-1}$ is the Kronecker symbol.

Taking into account a continuous character of potential behavior at the semiconductor-vacuum interface $x = 0$ and the continuity jump of the normal component of the electrostatic induction vector at the surface ($x = 0$) in the external field F the boundary conditions have the following form

$$\left.\begin{aligned} &D_j(q;0,x') - D_{j-1}(q;0,x') = 0 \\ &\partial D_j(q;0,x') - \partial D_{j-1}(q;0,x') = 4\pi\sigma_s(q) \pm F(q) \end{aligned}\right\}, \quad (6)$$

where $\sigma_s(q)$ is the Fourier component of the density of charges on the surface and $F(q)$ is the Fourier component of the external electric field F [10], the sign in (6) depends on the sign of the external electric field F.

The function $D_j(q;x,x)$ can be written in the following form

$$D_j(q;x,x) = D_j^0(q;x,x) + \Delta D_j(q;x), \quad (7)$$

where $D_j^0(q;x,x)$ determines unambiguously the polarization component $V_j^0(x)$ of the potential, this component being connected to the difference in the bulk properties of adjacent media (so-called potential of image forces in local electrostatics):

$$V_j^0(x) = -e\int q\cdot dq\left[D_j^0(q;x,x) + e/2q\right]. \quad (8)$$

The second term in Eq. (7) $\Delta D_j(q;x)$ is the solution of the homogeneous equation (1) with the boundary conditions (3), which determines $\Delta V(\vec{r},F)$ component of the total potential

$$V(\vec{r},F) = V^0(x) + \Delta V(\vec{r},F). \quad (9$$

$\Delta D_j(q,x)$ is caused by charging condition of the macroscopic sharp semiconductor surface and also depends on the external field F:

$$\Delta V(\vec{r},F) = -e\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dq_y dq_z}{(2\pi)^2}\exp[i(q_y y + q_z z)]\cdot\Delta D(q;\vec{r},F)\,. \qquad (10)$$

For the semiconductor-vacuum system the Green functions $D_j^0(q;x,x)$ have the following form [10,11]

$$D_1^0(q;x,x) = \frac{eqa^2(q;|x|)}{1+qa(q;0)} - \frac{e}{2}\left[a(q;0)+a(q;2|x|)\right], \qquad x\le 0, \qquad (11)$$

$$D_2^0(q;x,x) = \frac{e}{2q}\left[\frac{1-qa(q;0)}{1+qa(q;0)}\exp(-2qx)-1\right], \qquad x\ge 0\,. \qquad (12)$$

The Green functions $\Delta D_j(q;x)$ in the case of the field emission from semiconductors are expressed as follows

$$\Delta D_1(q;x) = \frac{\left[4\pi\sigma_s(q)-F(q)\right]\cdot a(q;|x|)}{1+qa(q;0)}, \quad x\le 0, \qquad (13)$$

$$\Delta D_2(q;x) = \frac{\left[4\pi\sigma_s(q)-F(q)\right]\cdot a(0;x)}{1+qa(q;0)}, \quad x\ge 0\,. \qquad (14)$$

Let us consider the interaction of a point charge e with the surface of the semi-infinite semiconductor taking into account the screening effects induced both by free carriers (electrons or holes) and by bound electrons of ion islands. We determine the dielectric function of the semiconductor in the region $x\le 0$ in the following form [9]

$$\varepsilon(\vec{k}) = 1 + \frac{\varepsilon-1}{1+\left(\vec{k}^2/\lambda^2\right)(\varepsilon-1)} + \frac{\kappa^2}{\vec{k}^2}, \qquad \vec{k}^2 = k_\perp^2 + q^2, \qquad (15)$$

where ε is the dielectric constant of a crystal lattice in a homogeneous field (when $\vec{k}\to 0$), λ^{-1} is the effective screening length by bound electrons equal in the order of magnitude to the ion (atom) radius, $\kappa^2 = \dfrac{4\pi e^2 n}{\varepsilon k_B T}$ in the Debye-Huckel approximation (DHA) in a case of non-degenerate electronic gas, k_B is the Boltzmann constant; n is the concentration of free electrons (or holes) in the bulk of semiconductors (in this work we consider the n- type semiconductor) and $\kappa^2 = 6\pi e^2 n/\varepsilon E_F$ in the Thomas-Fermi approximation (TFA) in a case of degenerate electronic gas, E_F is Fermi energy of free electrons in the semiconductor. The first two terms in Eq. (15) correspond to the interpolation Inkson model [15]. As was shown in Ref. [9], such a combination of the Inkson model with DHA (or TFA), leading to the asymptote $\varepsilon(\vec{k}) \approx 1 + \dfrac{(\lambda^2+\kappa^2)}{\vec{k}^2}$ when $k >> \lambda$, provides the continuity of the full electrostatic potential $V(\vec{r},F)$ (11) at the surface for $x = 0$.

By substituting of Eq. (15) into Eq. (4) we obtain upon integrating over $k_\perp$

$$a_1(q;x) = \frac{1}{\beta_+^2-\beta_-^2}\left[\frac{e^{-|x|\beta_+}}{\beta_+}\left(\beta_+^2 - q^2 - \kappa^2\frac{\Lambda^2}{\varepsilon}\right) - \frac{e^{-|x|\beta_-}}{\beta_-}\left(\beta_-^2 - q^2 - \kappa^2\frac{\Lambda^2}{\varepsilon}\right)\right], \qquad (16)$$

here

$$\beta_\pm^2 = \frac{1}{2}\left[\kappa^2(1+\Lambda^2)+2q^2\right] \pm \frac{\kappa^2}{2}\sqrt{(1+\Lambda^2)^2 - \frac{4\Lambda^2}{\varepsilon}}\,, \quad \Lambda = \frac{\lambda}{\kappa}\sqrt{\frac{\varepsilon}{\varepsilon-1}}\,.$$

By substituting Eq. (16) into (11), (12) and then into Eq. (8) we obtain the real space distribution of the polarization component $V_j^0(x)$ (so-called potential of image forces in local electrostatics) from the common vacuum level in a semiconductor-vacuum system in the integrated form. We want to notice, that $V_j^0(x)$ is connected only with the difference in the bulk properties of the contacting media and it does not vary depending on the σ_s and external field F. When $|x| \to -\infty$ the function $D_1^0(q;x,x) = -\frac{1}{2}a_1(q;0)$ and the potential of image forces $V_1^0(x)$ is the continuity on the surface for $x = 0$ and at $|x| \to -\infty$ it defines the electronic affinity energy in a bulk of semiconductor. Under the condition $V_1^0(-\infty) = -E_c$, where E_c is the bottom of conduction band of the semiconductor, we can obtain the parameter λ.

In this work we assume, that σ_s is formed by the fixed charges on a free surface of the semiconductor $\sigma_s = \sum_{i=1}^{\nu} \sigma_i = const$ (ν is the number of types of the surface charges, which define the complete charge density σ_s on a free surface of the semiconductor).

After substitution of Eq. (16) into (13), (14) and then into Eq. (8) we obtain a potential $\Delta V_j(x,F)$ for the semiconductor-vacuum system in the case of the macroscopic homogeneous interface $\sigma_s = const$ and $F = const$ ($\sigma_s(q) = (2\pi)^2 \sigma_s \delta(q_y)\delta(q_z)$ and $F(q) = (2\pi)^2 F\delta(q_y)\delta(q_z)$) in the following form

$$\Delta V_1(|x|,F) = -e(4\pi\sigma_s + F)\cdot a_1(0;|x|);\ (x \le 0,\ \text{in the semiconductor region}); \quad (17)$$

$$\Delta V_2(x,F) = -e(4\pi\sigma_s + F)\cdot a_1(0;0) - eFx;\quad (x \ge 0,\ \text{in the vacuum}). \quad (18)$$

It is seen from these formulas that the field penetration effect as well as the polarization part $V_j^0(x)$ (potential of image forces) of the total potential are determined by the screening properties of the semiconductor.

Let us take into account a microscopic structure of the semiconductor surface assuming, that σ_s is formed by the ordered lattices (for the simplicity we assume a square lattices) of the each type i of the fixed CSS or CD on a free surface (for example, the dangling bonds, the impurities ets.) with two-dimensional concentration $N_i = a_i^{-2}$, where a_i is the lattice constant of square lattice of the i-type of the surface charge. This consideration corresponds to a Fourier-component $\sigma_s(q)$ of the charge density at the ordered lattices of the surface charges, which is widely used in the microscopic quantum-chemical calculations)

$$\sigma_s(q) = \sum_{i=1}^{\nu} \sigma_i(q) = (2\pi)^2 \sum_{i=1}^{\nu} e_i^* N_i \left[\delta(q_y)\delta(q_z) + \delta\left(q_y - 2\pi/a_i\right)\delta\left(q_z - 2\pi/a_i\right) \right] \quad (19)$$

where $\sigma_i = e_i^* N_i$ and e_i^* is the effective charge of the i-type of the surface lattice.

From Eqs. (7)-(13) the complete potential $V_j(\vec{r},F)$ of the system, can be obtained taking into account Eqs. (15)-(16) and (19) in the following form

$$V_j(\vec{r},F) = V_j^0(x) + \Delta V_j(x,F) + \Delta w_j(\vec{r}) \quad (20)$$

The modulated part $\Delta w_j(\vec{r})$ can be written from Eqs. (10), (13),(14),(16) and Eq. (19) with taking into account the charge structure of the specific semiconductor surface. As will be shown by our calculations in the next section (on the example of specific Si(100) surface) the amplitude of the oscillation part $\Delta w_j(\vec{r})$ of the full potential $V_j(\vec{r},F)$ is determined by the bulk properties of Silicon and subsides into the semiconductor and into the vacuum region.

3. Results and conclusions

Silicon is one of most suitable material for fabricating field emitter arrays in batch technology. In the present work is considered the n- type Silicon. We take into account a microscopic structure of the fixed charge density $\sigma_s(y,z)$ along Si(100) surface assuming, that it is formed by an ordered lattice (for the simplicity we assume a square lattice) of the surface atoms. Really the Silicon surface is far from ideal and the CSS is formed by defects. The presence of charged defects (CD) on a surface of the semiconductor can reduce not only to the change of a macroscopic potential barrier for the electrons (actually to change of threshold voltage), but also to the local downturn (growth) of height of a potential barrier. According to the proposed model we obtained that taking into account the microscopic structure of the free semiconductor surface allows us to determine the local emission (adsorption) centres.

We use the following parameters of Si [16]: dielectric constant is $\varepsilon = 11.9$; effective masses are $m_{\perp} = 0.98$ (transverse) and $m_{l} = 0.19$ (parallel); electron affinity in the bulk is $\chi = -E_c = 4.05\,eV$; temperature is $T = 300°K$; bulk density of the free electrons is $n = 10^{18} cm^{-3}$.

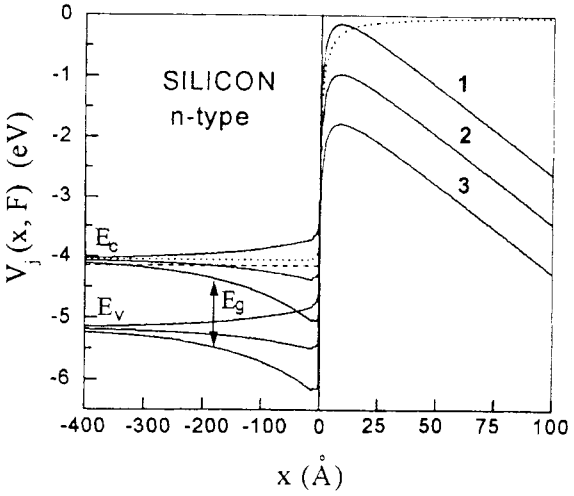

Fig. 1. The distribution of the potential barrier $V_j(x;F)$ in the external electric field $F = 3 \cdot 10^6 V/cm$ for different macroscopic densities of charge on the surface $\sigma_s = -3.4 \cdot 10^{12}\ e/cm^2$ (curve 1), $\sigma_s = 0$ (curve 2) and $\sigma_s = 3.4 \cdot 10^{12}\ e/cm^2$ (curve 3). The dash line is the Fermi energy and the dot line is the potential of image forces.

As was shown before, the macroscopic density of the fixed charge σ_s on the surface determines the Space Charge Region (SCR) in the semiconductor. Since the Silicon surface can exhibit donor or acceptor character [8,12-14], the formation of the potential barrier $V(x,F)$ in the external electric field $F = 3 \cdot 10^6 V/cm$ for different macroscopic densities of charge on the surface $\sigma_s = -3.4 \cdot 10^{12}\ e/cm^2$ (curve 1), $\sigma_s = 0$ (curve 2) and $\sigma_s = 3.4 \cdot 10^{12}\ e/cm^2$ (curve 3) is shown in Fig. 1.

The distribution of the potential $V_j(x,F)$ in Fig.1, which is the direct calculation according to the Eq. (20) with the account (15), demonstrates also the formation of the SCR in the subsurface region of Silicon. Note, that the SCR, which is connected with the redistribution of the free carriers in the semiconductor, ensures the quasielectroneutrality condition in the vacuum region for $x \to \infty$.

As can see from Fig. 1, the correct consideration of the spatial dispersion effects in the semiconductor allows us to obtain not only continuous course of the image forces potential

$V_1^0(x)$ (the dot curves in Fig.1) in the Silicon-vacuum system, but also the common (vacuum) level of the counting of the potential energy [9-11]. The continuous course of the image forces potential $V_j^0(x)$ (and also the full potential $V_j(\vec{r},F)$) at the sharp semiconductor- vacuum interface allows us the correct consideration of microscopic structure of the Silicon surface.

Let's take into account the microscopic structure of the charge density $\sigma(y,z)$ on the surface. Let's assume that $\sigma(y,z)$ is formed by an ordered lattice (for the simplicity we assume a square lattice) of the surfaces atoms with two-dimensional concentration $N_s = 6.8\cdot 10^{14} cm^{-2}$, which is corresponded to Si(100) surface, where $a = \left(N_s\right)^{-2}$ is the size of square lattice. Because the CSS on the free Silicon surface exhibit donor or acceptor character [8] we can introduce the effective charge on the surface atom e_s^* as a parameter, for example $e_1^* = 0.02$. In the case of one type of the CSS on Si(100), when $\nu = 1$ in Eq.(19), the potential relief $V(\vec{r},F)$ is calculated. The amplitude $\delta\phi(\vec{r})$ of the oscillation part of the total potential $V(\vec{r},F)$ is determined by e_1^* and the bulk parameters of semiconductor n,T,ε and for used parameters is $\delta\phi(0,y,z) = 0.016eV$. For the reconstructed Si(100) surface , when the microstructure of the surface is determined by the superlattice (7x7) (with the size of the square lattice is $a_2 \approx 27\,\mathring{A}$), we should enter two types of the CSS ($\nu = 2$ in Eq. (19)) , for example with effective charge on the defects $e_2^* = 0.5$ (in this case the total value of the density of charge is $\sigma_1 = -6.384\cdot 10^{12}\ {}^{e}/_{cm^2}$). Results of the direct calculation $\delta\phi(\vec{r})$ are shown by solid curve in Fig. 2.

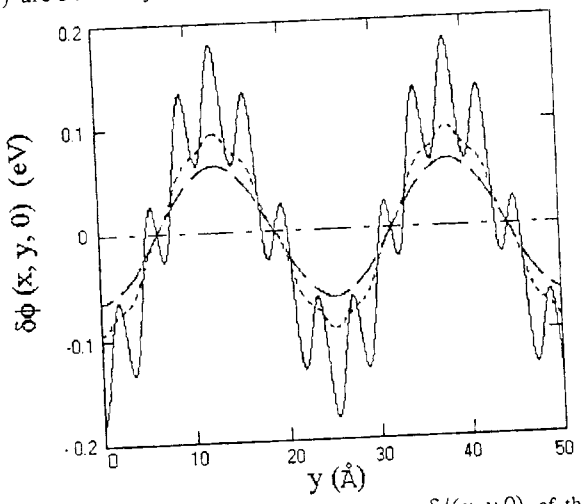

Fig. 2. Lateral distribution of the oscillation part $\delta\phi(x,y,0)$ of the total potential $V(\vec{r},F)$ along Si(100) surface ($\nu = 2$) for $e_1^* = 0.02$, $e_2^* = 0.5$ at x=0 (solid curve), x=1 Å (dot curve) and x=2 Å (dash curve) in the vacuum region for $F = 0$.

The oscillation part $\Delta\phi_2(\vec{r})$ of the full potential barrier $V_j(\vec{r},F)$ is decreasing in the vacuum region (the dot curve for $x = 1\,\mathring{A}$ and the dash curve for $x = 2\,\mathring{A}$ in Fig. 2).

As we can see from Fig. 2 the presence of the superlattice of superficial atoms, which arises for example in result of reconstruction of a surface - in a case $Si(100)-(7\times 7)$, when $e_2^* \neq e_1^*$, results in essential change potential relief of a surface and occurrence of areas of downturn (growth) of a value of the macroscopic potential barrier $V(\vec{r},0)$ (20). Existence of areas of local downturn (growth) of height of a potential barrier along a surface of the semiconductor we link to the microscopic structure of its surface. Our direct calculations according to the proposed model showed that the local downturn

(growth) of a potential barrier can determine the emission (adsorption) centres not only in the place of an arrangement of the defect.

The charged defects (CD) on a surface of the semiconductor (adsorbed atoms or impurities inside the semiconductor) with two-dimensional concentration N_3 can reduce not only to the change of the macroscopic potential barrier for the charged particles (electrons or ions), but also to a local modification of the potential barrier height along the surface and formation of the new adsorption (emission) centres. So the introducing into the structure of the reconstructed surface $n-Si(100)$, which is presented in Fig. 2, the charged impurities with an effective charge $e_3^* = -1$ and two-dimensional concentration N_3, which forms an incommensurable square lattice with the lattice constant $a_3 = 46.17\,\mathring{A}$, results in a modification of a macroscopic (mean) density of charge on a surface $\sigma_3 = 1.557 \cdot 10^{13}\, e/cm^2$ and significant modification of a potential relief of the surface. The lateral distribution of the oscillation part $\delta\phi(\bar{r})$ of the full potential (20) on the reconstructed $n-Si(100)-(7\times 7)$ surface $x = 0$ (solid curve) and its changing into the vacuum for $x = 2\,\mathring{A}$ (dot curve) and for $x = 5\,\mathring{A}$ (dash curve) are shown in Fig. 3.

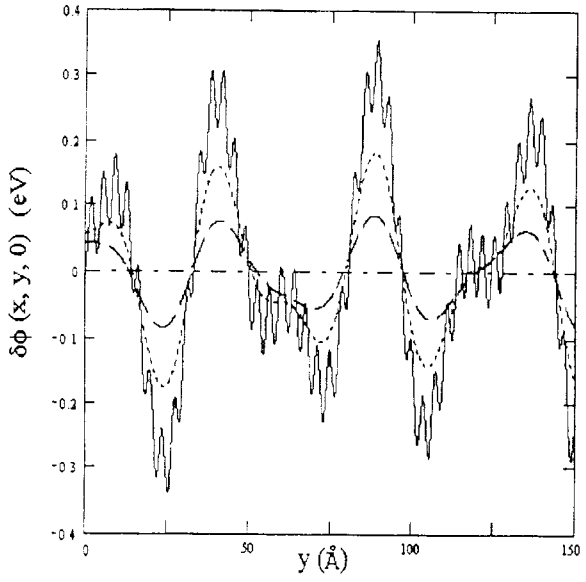

Fig. 3. The lateral distribution of the oscillation part $\delta\phi(x,y,0)$ along Si(100) surface in the vacuum region at $x = 0$ (solid curve), $x = \mathring{A}$ (dot curve) and $x = 5\,\mathring{A}$ (dash curve) for $e_1^* = 0.02$, $e_2^* = 0.5$ and $e_3^* = -1$.

From Fig. 3 we can see that the introducing of the doping impurities in a plane of a surface essentially changes (augments) amplitude $\delta\phi(\bar{r})$, so the charged particle in vacuum "feels" the places of the greatest downturn or growth of a potential barrier (minima or maxima of the potential depending on the sign of an interacting charged particles) on the spacing intervals considerably exceeding the direct quantum-chemical interaction.

The direct calculation of the 3D distribution of $\delta\phi(\bar{r})$ on the reconstructed $n-Si(100)-(7\times 7)$ surface $(x = 0)$ in the case of the three types of the CSS and CD ($\nu = 3$ and $e_1^* = 0.02$, $e_2^* = 0.5$ and $e_3^* = -1$) for the two-dimensional concentration $N_3 = 4.69 \cdot 10^{12} cm^{-2}$ is shown in Fig. 4 (corresponds to solid curve in Fig. 3).

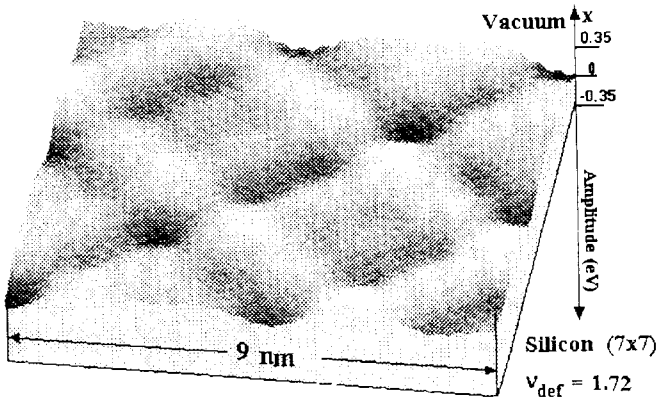

Fig. 4. 3D distribution of $\delta\phi(x,y,0)$ on the Si(100) surface ($x=0$) for the three type of the CSS and charged defects ($\nu=3$) at $e_1^*=0.02$, $e_2^*=0.5$, $e_3^*=-1$ and $N_3=4.691\cdot10^{12}\ cm^{-2}$.

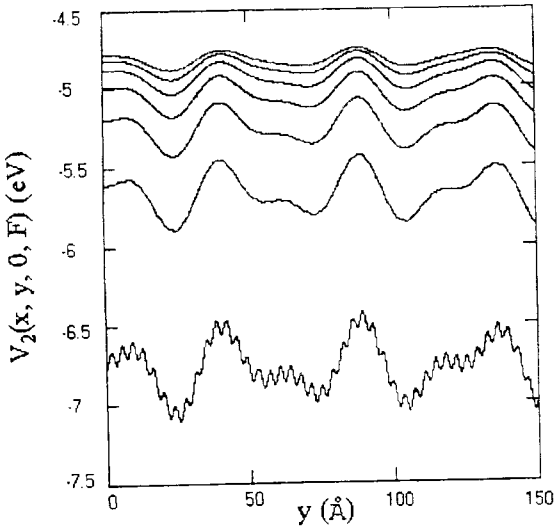

Fig. 5. The change of the potential relief $V(x,y,0,F)$ of Si(100) surface with structure presented in Fig. 4 and solid line in Fig. 3 in the vacuum region at $x = 0;\ 1;\ 2;\ 3;\ 4;\ 5;\ 6\ \mathring{A}$ (from the bottom) for $F=3\cdot10^6\,V/cm$.

Let's note specially, that for the charged particles, which are in the vacuum on spacing intervals $x\to\infty$, the surface of the semiconductor is quasineutral at the expense of redistribution of free carriers (for a semiconductor of a n - type - electrons) - formation of the SCR.

Fig. 5 shows the direct calculations according to Eq. (20) the changings of a full potential barrier $V_s(\bar{r},F)$ of the $n-Si(100)-(7\times7)$ surface (with three types of surface charges $\nu=3$ and with the parameters, which are determined for Figs. 3, 4) in the external electric field $F=3\cdot10^6\,V/cm$ (see in Fig. 1) at the moving from the surface into vacuum at $x=0,1,\ldots,6\,\mathring{A}$ (the bottom-up curves).

In this paper we demonstrate the principled capability for the correct calculation of the real surface of semiconductors on the basis of the Green's functions method [9-11] which takes into account the spatial dispersion effects in the semiconductor. The proposed method of theoretical calculation of a potential relief of the real surface of semiconductors and its change in the external electric fields has allowed us within the framework of one model correctly to unify the macroscopic properties of the semiconductor with the microscopic structure of the real specific surface. We want to note, that in the framework of the proposed model we can take into account the microscopic

structure of the surface using the strict quantum-chemical calculations of the specific semiconductor surfaces (not only in the form (19), which is used in this consideration).

The obtained calculations have shown that the distribution of the potential $V_j(\vec{r},F)$ (and in a considerable extent the amplitude of its oscillating part $\delta\phi(\vec{r})$) is determined by macroscopic (volumetric) properties of semiconductors (the level of bulk doping n, the dielectric constant ε, the lattice constant of a semiconductor λ^{-1}) and also the external conditions (the temperature T and the presence of the external electric fields F).

References

1. Physical properties of thin-solid field emission cathodes with molybdenum / C.A.Spindt, I.Brodie, L.Humphrey and E.R.Westerberg // J.Appl. Phys. - 1976. - V. 47, N 12. - P. 5248-5263.
2. Derivation of the image interaction for non-planar pointed emitter geometries: application to field emission I-V characteristics / Jun He, P.H. Cutler, N.M. Miskovsky, T.E. Feuchtwang, T.E. Sullivan, Moon Chung // Surf. Sci. - 1991. - V. 246. - P. 348-364.
3. Field emission cathode array with self-aligned gate electrode fabricated by silicon micromachining / W. Barth, T. Debsky, F. Shi, P. Hudec, I. Kostic, I.W. Rangelow, S. Biehl, T. Iwert, P. Grabiec, K. Studzinska, S. Mitura, I.I. Bekh, A.E. Lushkin, L.G. Il'chenko, V.V. Il'chenko and G. Haindl // J.Vac. Sci. Technol. B. - 2000. -V. 18, N 6. - P. 3544-3548.
4. Modinos A. Field, Thermionic, and Secondary Electron Emission Spectroscopy.- Plenum, New York, 1984.-p. 328.
5. Lang N.D. and Williams A.R. Theory of vacuum chemisorption on simple metals // Phys. Rev. B. - 1978. - V. 18, N 2. - P. 616-636.
6. Lang N.D. The density - functional formalism and the electronic structure of metal surfaces // Sol. St. Fhys. - 1973. - V. 28. - P. 225-300.
7. Sze S.M. Physics of Semiconductor Devices. - J.Wiley & Sons, New York, 1981. - 320.
8. Monch W. Semiconductor Surfaces and Interfaces. Springer-Verlag Berlin Heidelberg, 1995. - p. 442.
9. Il'chenko L.G., Pashitskii E.A., and Romanov Yu.A. Charge interaction in layered systems with spatial dispersion // Surf. Sci.- 1982.- V. 121. - P. 375-395.
10. Il'chenko L.G., Kryuchenko Yu.V. External field penetration effect on current-field characteristics of metal emitters// J.Vac.Sci.Technol. B - 1995. - V. 13, N 2.- P. 566-570.
11. Electrostatic energy and screened charge interaction near the surface of metal with different Fermi surface shape / A.M. Gabovich, L.G. Il'chenko, E.A. Pashitskii and Yu.A. Romanov // Surf. Sci. - 1980. - V. 94. - P. 179-203.
12. Scanning Tunneling Microscopy and Spectroscopy: theory, techniques and applications / Editor Dawn A. Bonnell // - New York, 1993.- p. 436.
13. Scanning Tunneling Microscopy I: General Principles and Applications to Clean and Adsorbate-Covered Surfaces / Eds. H.-J. Guntherodt, R. Wiesendanger // Springer-Verlag Berlin, 1992.- p. 245.
14. Sergei N. Magonov, Myung-Hwan Whangbo. Surface Analysis with STM and AFM: Experimental and Theoretical Aspects of Image Analysis Weinheim. New York; Basel; Cambridge; Tokio: VCH, 1996.
15. Bennet M., Inkson J.C. Exchange and correlation potential in silicon // J. Phys. C. -1977.- V. 10, N 5.-P. 987-999.
16. Jensen K.L. Improved Fowler-Nordheim equation for field emission from semiconductors // J.Vac. Sci. Technol. B. - 1995. - V. 13, N 2. - P. 516-521.