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Modeling of Schottky Barrier Height and Volt-Amper Characteristics for Transition Metal-solid Solution $(SiC)_{1-x}(AlN)_x$

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Proposed nonlinear defect concentration model of metal-semiconductor contact. It is shown that taking into account nonlinear dependence of the Fermi energy EF defect concentration leads to higher barrier Schottky in 15-25 %. Calculated Volt-Amper characteristics of the diodes are consistent with experiment.

Keywords: Schottky barrier, Silicon carbide, Solid solutions, Volt-amper characteristics, Metal-semiconductor transitions.

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The paper considers a simple non-linear contact model defects on the concentration of metal-semiconductor Schottky barrier is formed when superficial defective E_i, States localized at the interface. It is shown that taking into account nonlinear dependence of the Fermi energy EF defect concentration leads to higher barrier Schottky in 15-25 %. The calculated barrier heights are used for analyzing current characteristics of structures $M/(SiC)_{1-x}(AlN)_x$. The calculation results are compared with experimental results.

The potential barrier height Schottky barrier ΦB to contact metal-semiconductor Schottky diodes parameter is the most important, field effect transistors and other elements (Instrumentation) power electronics with the superficial barrier structures. Therefore, the study of Schottky barrier in structures on the basis of new and under-studied semiconducting materials still remains an urgent task of semiconductor physics. In this regard, the undoubted interest structure: metal (M: Ni, Al, Mo, Au)/ solid solution of silicon carbide with aluminum nitride ($(SiC)_{1-x}(AlN)_x$), in particular $Al/n-(SiC)_{1-x}(AlN)_x$ [1, 2].

The potential barrier height calculation ΦB for $Al/n–(SiC)_{1-x}(AlN)_x$ on the generalized theory of Bardeen and Schottky-Motta [2, 3] never gave a credible agreement with experiments in the field of small surface densities of States [1, 2]. However, earlier in the works [4, 5] was offered a fairly simple model contact metal (M) – semiconductor (*n*–4H–SiC) with localized at the surface States of defects Ei (BSLD-model). While Volt-Amper characteristics (VACH) diodes Ni/4H–SiC ($x = 0$) with Schottky barrier (SB) good agreement with experiments [6].

In this paper, we developed a model BSLD [4, 5, 7] and are the results of the simulations and calculations of the barrier height Schottky contact $M/(SiC)_{1-x}(AlN)_x$ with different content *x*. Calculating Volt-Amper characteristics type structure $Al/n–(SiC)_{1-x}(AlN)_x$ as a function of various system parameters (*U* – voltage electric field, *T* – temperature, – bandgap, *x*-dependent concentration AlN in solid solution, Ni – density (concentration) of isolated States defects per unit of surface, E_i – surface localized defect status). The results of the calculations are compared with the experimental results for structures $Al/n–(SiC)_{1-x}(AlN)_x$.

The paper considers a modified surface concentrations Schottky barrier model State. Are results of calculations of Schottky barrier with localized in the area of contact conditions defects (BSLD [4, 5]), but in a higher concentration (non-linear) defects ($Ni = c \times 10^{13}$ sm^{-2} eV; $c = 0$-30). In this model, along with the concentration of defects Ni enter the numbers filling *nx*(*c*), defined as Gamiltone operation (2), which leads to a better agreement with the Schottky barrier value experience when Ni < 10^{13} sm^{-2} eV^{-1}. Then the barrier height is determined by the formula [3, 6]:

$$\Phi_B^x(c) = \Phi_m - \chi + \Delta\Phi_x(c)$$
$$\Delta\Phi_x(c) = 4\pi\left(e^2 / 4\pi\varepsilon_0\varepsilon\right)\lambda N_i n_x(c) \quad (1)$$

Here Φ_m – work function of metal, χ – the electronic affinity, $\Delta\Phi_x(c)$ – potential barrier on contact due to tunneling of electrons between metal and localized kvazi-level, λ – the thickness of the double layer dielectric permeability $\varepsilon_0\varepsilon$, Ni – isolated defect states density, $n_x(c)$ – number of filling a localized level E_i с полушириной $\Gamma = \pi\rho V$ (*V* – hybridization energy of metals and localized states), ρ – continuous, assumption, density State of metal, EF – Fermi energy.

Then the semiconductor located in contact with metal, characterized by superficial defective states |*d*>, energy which E_i lie in the forbidden zone. Interaction level |*d*> with metal that can be described is operator Gamiltone of Anderson [4, 7]:

$$H = \sum_k \varepsilon_k c_k^+ c_k + E_i d_i^+ d_i + V \cdot \sum_k (c_k^+ d_i + h.c.). \quad (2)$$

Here ε_k – the energy of the electrons in the metal; *V* – matrix element hybridization of metal |*k*> and defective |*d*> states; *c* + *k* – operator birth electron in state |*k*>; d_i^+ – operator birth electron in state |*d*>.

Assuming that the level of localized defective condition |*d*> overlaps with the broader zone of conductivity of metal is determined by the number of its filling $nd = n_x(c)$:

$$n_x(c) = (1/\pi) \cdot arc\cot\left((E_i - E_F)/\Gamma\right) \quad (3)$$

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Consider that the position of EF relative ceiling valence band of the semiconductor bandgap with (= 3.3 eV, a = 0.56, b = 3.86 [2, 8]), determined by the ratio of [4]:

$$E_F = \chi + E_g^x - \Phi_m - \Delta\Phi_x(c). \quad (4)$$

Then for the potential barrier height Schottky $\Phi_x B$ и $n_x(c)$ по (3) и (1) taking into account the non-linear concentration with components, we obtain [7]:

$$\Gamma\delta_x(c) = p - (1-\xi_i)E_g^x + k\eta c(1 - c\nu) \quad (5)$$

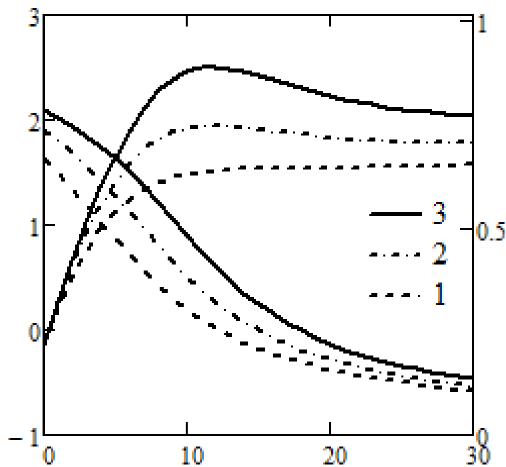
$n_x(c) = (1/\pi)\cdot \mathrm{arc\,cot}\,\delta x(c)$,

$$\Phi_B^x(c) = p + k\eta c 2n_x(c) \quad (6)$$

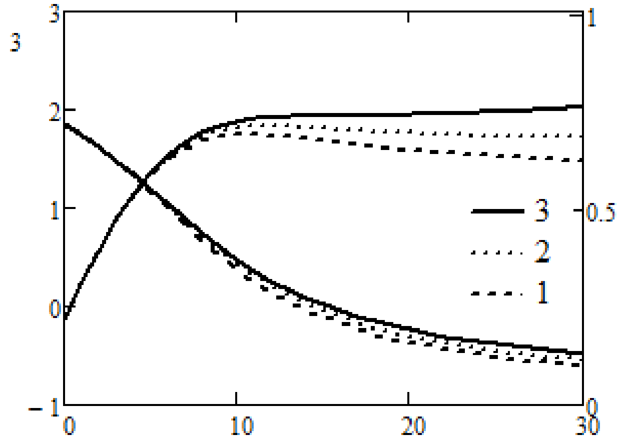
where $\eta = 0.5 \div 2.0$; $k = 0.272$ and for values $EF = E_g/2$, and $\Gamma = 0.5 \div 2.0$ value: $\tau = 2/\pi\Gamma$, $p = \Phi m - \chi$; and for Al in SiC – AlN. The results of calculations on (5)-(6) Schottky barrier height as a function of the parameters of nonlinear models ξ_i, x and c presented in figures 1-4. When $\nu = 0$ formula (5)-(6) give initial results in linear models with (BSLD-model) [4, 5].

2. Schottky barrier height calculation ΦB_x for diodes based on SiC-AlN. Formula (5)-(6) allow you to compare the calculations and conclusions of this work with the results obtained in the framework of generalized theory Badrina and Schottky-Motta [3]. Analysis of the results of this work BSLPS model is generally consistent with the results obtained in the two above mentioned models BSLD (localized defects [4, 5]) and generalized model Bardeen and Schottky-Motta [2, 3]. This is in spite of the different approach to the nature of the Schottky barrier ΦBx type structures M/n-SiC : AlN по BSLD [5, 7] and generalized model [2, 3]. The transition from linear iteration over c to the quadratic in EF and non-linear for ΦB_x and $n_x(c)$ Schottky barrier leads to increased from 15 до 25 %.

Fig. 1 presents the results of Schottky barrier values dependency analysis ΦB_x and n_x the concentration of defects c and from depth levels E_i (Fig. 1a) and from the decomposition ν (Fig. 1 b). This dependence has been received by the equations (5) and (6) for $\Phi_x B$ and $n_x(c)$ from the composition x when x = 0.2; 0.5; 0.7.



a). When $Eg = 3.3$ and $Ei = \xi i E_g$ (ξi = 0.3; 0.5; 0.7), ν = 1/200, for curves 1, 2 and 3 accordingly



b). When $E_i = 0.5\ E_g$ ν = 1/120; ν = 1/200; ν = 1/700 for curves 1, 2 and 3 accordingly

Fig. 1 – Dependence of barrier height Schottky $\Phi_x B$ (a) and numbers fill the defect states $n_x(c)$ the concentration of defects c and the composition of the x (a) and parameter values ν (b) for system n-Al/p-$(SiC)_{1-x}(AlN)_x$

3. Current-voltage characteristics n-Al/p-$(SiC)_{1-x}(AlN)_x$ diodes. Formula (5) and (6) for different values of the system parameters n-Al/p-$(SiC)_{1-x}(AlN)_x$ [T, E_q^x, E_i, Φ_{B_0}, n, c, x] used when calculating the current dependencies $I(V)$ According to the classical theory of emission termo-elektron diode voltage V [1, 10]:

$$I(V) = sAT^2 \cdot \exp(-\frac{\Phi_B^X(c)}{kT}) \cdot [\exp(\frac{qV}{nkT}) - 1] = \\ = I_0 \cdot [\exp(\frac{qV}{nkT}) - 1]. \quad (7)$$

It is known that there are qualitative similarity of characteristics of Schottky Barrier diodes with and ordinary p-n transitions [10]. In particular on the experiences observed the similarity of some characteristics of the diode type 4H-SiC [1], n-SiC/p-$(SiC)_{1-x}(AlN)x$ [8, 9], n-Al/p-$(SiC)_{1-x}(AlN)_x$ [2]. In the classical theory of Schottky barrier height is considered to be unchanged and used its effective value ΦB_0. Fig. 2 shows the current-voltage characteristics for ΦB_0 = 1.1; 1.26; 1.29; 1.4; that meets the the LEDs on the Ni, Al, Mo, Au and for model values ΦB_0 = 1.7: curves 1, 2, 3, 4 and 5 accordingly.

Current values $I\,(U)$ when n = 1 and 2 presented in Fig. 3. There's also a marked data experiences [2, 8]. Observed at high voltages (U > 1V) Figure 3 discrepancy theory with experiment apparently connected with the change in size and shape of the potential barrier at the transition or the inclusion of other mechanism of current transport, for example,

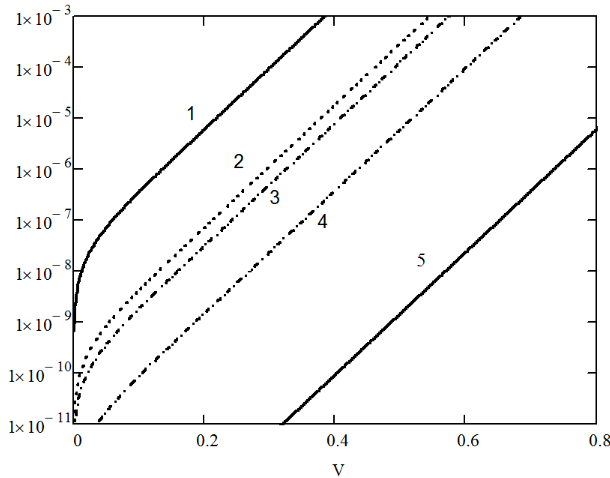


Fig. 2 – Direct Current-voltage characteristics for Ni, Al, Mo, Au (and ΦB_0 = 1.7 eV) for n-M/p-$(SiC)_{1-x}(AlN)_x$ with ΦB_0: 1 – 1.1; 2 – 1.26; 3 – 1.29; 4 – 1.4 and 5 – 1.7 eV accordingly

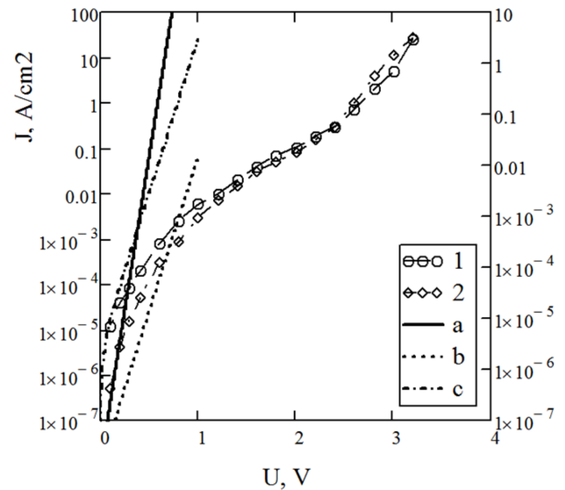


Fig. 3 – Direct Current-voltage characteristics n-Al/p-$(SiC)_{1-x}(AlN)_x$ when T = 293 K: curve 1 – x = 0.10 (n = 1 – curve a, n = 2 – b); curve 2 – x = 0.15 (n = 2 – c); 1 and 2 – experimental data on [2, 8]

with tunneling of holes through the barrier in a Valence zone [8, 9]. Fig. 4 direct line Current-voltage characteristics lists as a function of composition x for values of concentration of defects $c = 4$ and 5; $E_i = 0.5\,E_g$ and with voltages $U = 0.10$; 0.15; 0.18; 0.20 V accordingly. According to $I(U)$ from the composition x when x order 0.075 curves of direct current $I(U, x)$ reach the maximum, obviously related to the behavior of the bandgap of the whole. In general data calculations on figures 1-4 are consistent with those experiments [2, 8, 9] and other authors calculations [2, 4, 5]. Dependence of direct current from a concentration of surface States with different values of the depth of the localized level Ei is presented in Fig. 5. Minimum curve 2 in from about 12 is associated with a corresponding maximum Schottky barrier height as a function of the concentration of defects. (Fig. 1a).

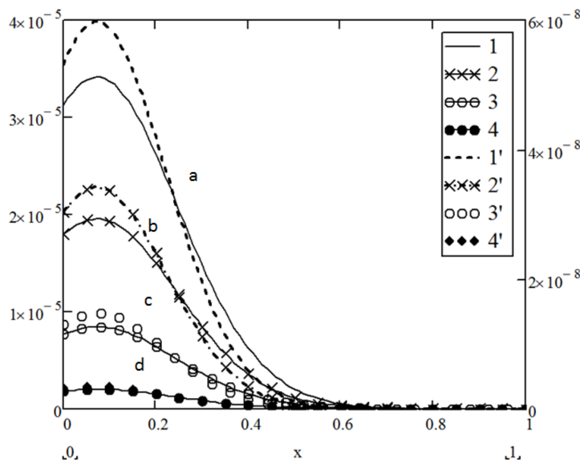


Fig. 4 – Direct current-voltage characteristics as a function of composition for the concentration of defects c: 1,2,3,4 c = 4; and 1´,2´,3´,4´ c = 5 and voltages U: a – 0.10; b – 0.15; c – 0.18;d – 0.20 V

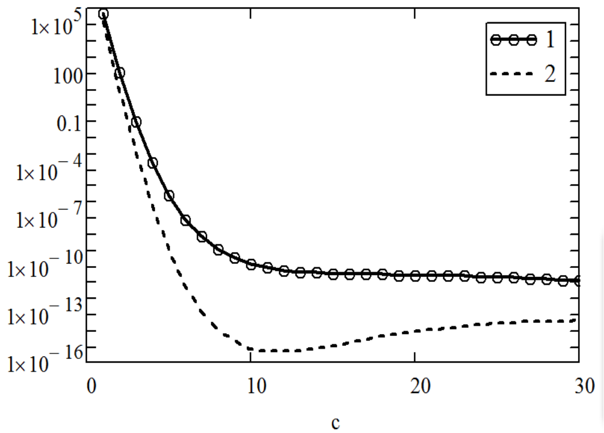


Fig. 5 – Dependence of direct current $I(U)$ the concentration of surface defects c with different values E_i: 1 – $E_i = 0.3Eg$, 2 – $E_i = 0.5E_g$

In the work the model of Schottky barrier with localized at the surface with a non-linear conditions on concentration of defects of the Fermi energy EF. Schottky barrier height calculated under the proposed model for structures Al/n-$(SiC)_{1-x}(AlN)_x$ consistent with the experimental results [1, 3, 6]. The proposed model analyzes the behavior of the Schottky barrier height and current-voltage characteristics of the structures Al/n-$(SiC)_{1-x}(AlN)x$ from the system settings: applied voltage electric field (U), – temperature (T), bandgap solid solution $(SiQ)_{1-x}(AlN)_x$ from the composition of the solid solution (x), the concentration of isolated States defects (Ni) and energy values of surface localized state (Ei).

Using the calculated on BSLPS- models values are built current-voltage characteristics structures Al/n-$(SiC)_{1-x}(AlN)x$ according to the classical theory of termo-elektronics diode issue. Theoretical current-voltage characteristics in the field of small currents and voltages are in good agreement with experimental current-voltage characteristics for such structures. A

method of induction heating modes control algorithm for growing high-voltage heterostructures, layers based on silicon carbide [11]. Received samples used for manufacturing systems with contacts of metal solid solution of silicon carbide Schottky barrier.

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