UDC 537.311.33:622.382.33

O. A. KULINICH, V. A. SMYNTYNA, M. A. GLAUBERMAN, G. G. CHEMERESUK, I. R. YATSUNSKY

Training, Scientific-Investigation and Production Center at Odessa I. I. Mechnikov National University
(4 Marshala Govorova str., Odessa 65063, Ukraine,e-mail: eltech@elaninet.com)

CURRENT FLOW PROCESS SIMULATION IN METAL—SILICON STRUCTURES

The model of current flow process simulation in metal—silicon structures with used modern method of investigation within the limits of thermo-electric, drift-diffusion and tunnel-resonant theories and it bases on barrier properties of structural defects.
Key words: silicon, metal, model, current, dislocation.

1. INTODUCTION

The deviation of experimental current—voltage characteristics (I-V) of structures metal—silicon from theoretically calculated ones defines a subject of the given research. In some cases it is impossible to explain, why in experimental I-V characteristics the value of current is smaller, than theoretically calculated current even if one takes into account the effects which change the parameters of barrier. The presence the large density for structural defects in near-surface layers of silicon can increase current. The presence of located defects or impurity precipitated states in forbidden zone of silicon can explain the raise of conductivity. [1, 2]. However, when the density of structural defects is less than 10^{12} m^{-2}, the experimental current not only doesn't increase, but on the contrary, in most cases, decreases.

The purpose of work is the definition of structural defects and physical properties of silicon layers in metal—silicon interface; the definition for possible influence of impurities (oxygen, etc.) on properties of investigated silicon layers; the definition for influence of these layers on electrophysical characteristics in metal—silicon structures and suggestion of current flow model in view of their real structure.

2. EXPERIMENTAL DETAILS

The structures of nickel—silicon with Schottky-barrier and the ohmic contacts manufactured on p-Si (10(100)) and n-Si (10(100)) silicon wafer by the ordinary planar process (fig. 1) were studied.

Investigation of silicon surface after removal of metal was carried out by scanning electronic microscopy (by electronic scanning microscope «Cam-Scan» with «Link-860» X-Ray microanalyser), by optical methods (by metallographic microscope MMR-2R), by Auger spectrometer LAS-3000 (beam diameter — 5 microns), by X-Ray topography method (Fujiwara method). To detect structural defects, the silicon surface layer-by-layer etching away with selective Sekko (for surface 100) and Sirtl (for surface 111) etchants with preliminary treatment in Karo intermixture and peroxide-ammonia solution was led [3].

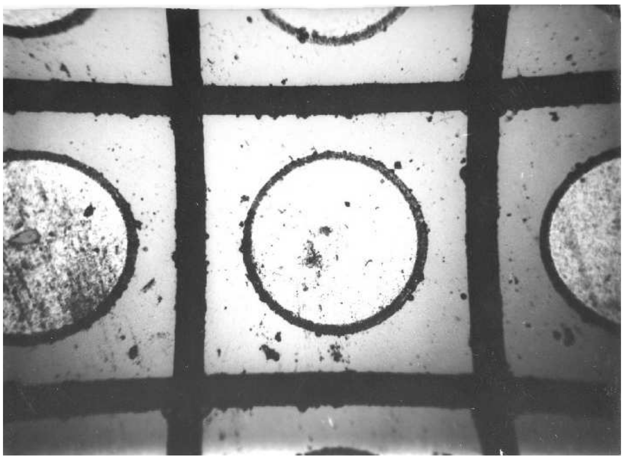

Fig. 1 Electronic image of nickel silicon contacts with Schottky barrier

3. RESULTS AND DISCUSSION

In most cases, not only the deviation of procedure parameters from the given ones and the differences in parameters of metal and silicon, but also defective structure of source silicon are caused for formation of defects in structures metal—silicon. Figure 2 shows the electronic image of dislocation defects obtained at surface p-Si (10 (100)) after etching for 2 minutes (Sekko etchant). The picture is obtained in the mode of conductivity. Dark areas correspond to the increased conductivity, light areas — to the reduced conductivity. In some cases, the dendrites of alkali metals salts (KCl) and twinning lamellas were observed. (fig. 3, 4). The typical image of a silicon surface SHB 10 (100) after removal of a nickel layer and treatment with Sekko etchant is shown in fig. 5 (obtained by microscope MMR-2P).

It's well seen, that the typical etch pits characteristic for dislocations and stacking faults

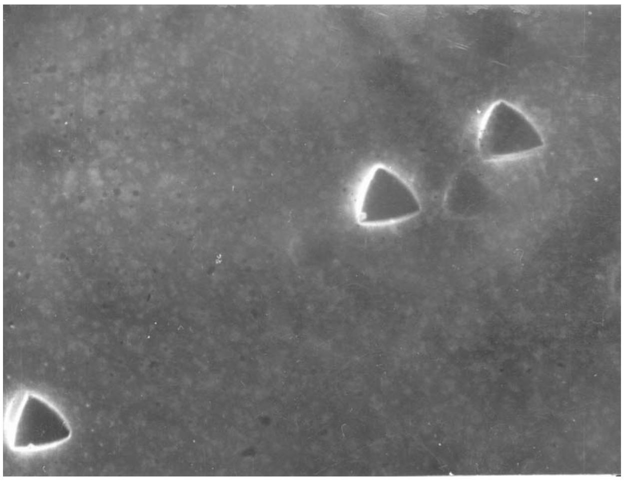

Fig. 2 Electronic image of dislocations on silicon surface (the method of conductivity)

Fig. 3 Electronic image of dendrite on a surface of silicon SHB-10 (100)

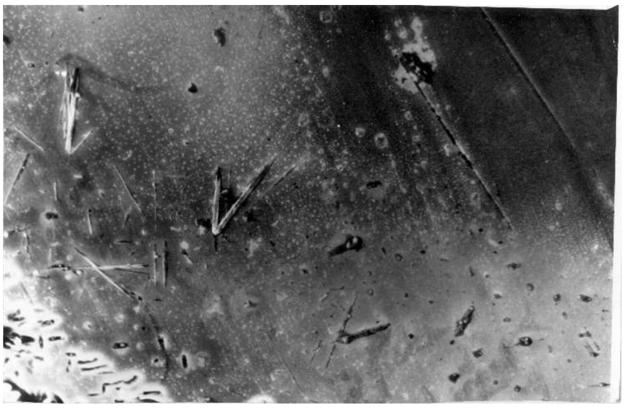

Fig. 4 Electronic image of twinning lamellas

are absent. The presence of such pits on silicon surface is connected with etched metal and they appear at the accelerated thermodiffusion of metal along structural defects of silicon. The attempts to obtain the image of Si surface by electron microscope «Cam — Scan«turned out to be unsuccessful. The irradiated silicon surface

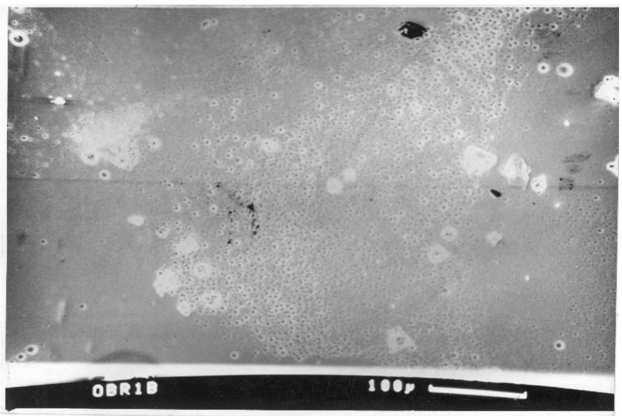

Fig. 5 Optical image of silicon surface after removal of nickel and etching during 5 minutes (microscope MMR-2P)

was strongly charged by electron beam and there was no opportunity to obtain the electron image of surface. All the abovementioned indicates that the investigated layers are of mosaic block formation and show some dielectric properties. The investigation in properties of these small-block structures by X-ray topographic Fujiwara method determined, that the neighbor blocks are disoriented at the angles of 0,0510° up to 0.0620°. The Auger-analysis has confirmed the presence of metal and oxygen impurities in the investigated layers. At the further etching of silicon surface (up to 3 minutes) dislocation structure (dislocation density make up to 10^{10} m^{-2}), included 60°- and partial dislocations and decorated with oxygen (fig. 6) were revealed. The appeared typical structural defects testify to occurrence of normal crystal structure Si. After etching during 5 minutes the separate disloca-

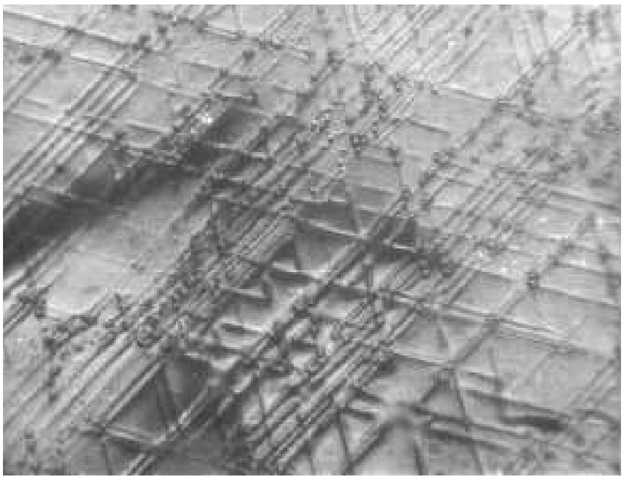

Fig. 6 The electronic image of dislocation structures (1×2300)

tions and glide lines appeared instead of dislocation structures (fig. 7). We have established, that thickness of transition layers, consisted of disorder silicon and dislocation structure areas, is proportional to the thicknesses of applied metal that is clear if one recollects, that the increase in metal thickness results in the in-

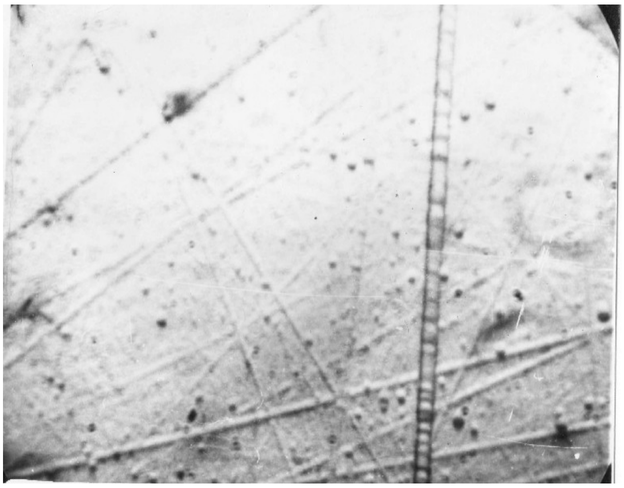

Fig. 7 The electronic image of dislocations at etching during 5 minutes

crease in mechanical strain of the interface which value strongly exceeds the limit of silicon plastic flow. Structural defects of source silicon also influence on the transition layer thickness. The raise of structural defects density leads to increase in number of accelerated diffusion channels during metal application that result in increase in mechanical strain at interface.

Thus, by consideration of current flow process in such structures the presence of structural defects and their possibility to influence on conductivity in metal-silicon structures with Schottky-barrier is necessary to take into account. It is well-known, that the presence of structural defects in semiconductor influences both on the lifetime and for the mean free path of charge carriers. For example, in silicon the dislocation 60° forms potential barrier, which height, basically, depends on concentration of dopant impurity and distance between charges in dislocation core. Mobility μ_{qd} with the account of dislocation barriers scattering (N — density of dislocations) can be calculated as [4]

$$\mu_{qd} = \frac{3q}{8RNVm^*}, \quad (1)$$

where q — elementary charge, m^* — effective mass of charge carriers, N — dislocation density, R — radius of dislocations space charge, V — velocity of electron scattering. If one does not take into account «interference» of dispersion processes, the resulting mobility can be written as

$$\frac{1}{\mu} = \frac{1}{\mu_{qf}} + \frac{1}{\mu_{qd}} + \frac{1}{\mu_{qs}} + \frac{1}{\mu_{qi}}, \quad (2)$$

where μ — the resulting mobility, μ_{qs} — mobility for the intersurface scattering mechanisms, μ_{qi} — mobility for the ionized impurity scattering mechanisms, μ_{qf} — mobility for the phonon scattering mechanisms.

Thus, current flow process occurs at the presence of structural defects of dislocation type generated in space of structure, and at the presence of disorder silicon areas. Experimental investigations show, that thickness of disordered silicon area is much less than the area of dislocation structures, and resistance at current flow is much less in the area of dislocations. Therefore, in design for models of current flow through metal—silicon structure it is necessary to take into account the part of current which flows in the area of dislocation structures, and the thermionic, drift-diffusion and tunnel-resonant theories should be used.

Let's consider, current flow processes through metal—silicon structure with Schottky barrier. There are L dislocation structures and M dislocations in one. The distance between dislocations, at their maximum density, is less than the doubled radius of space-charge zone of dislocations. The energetic circuit of metal — silicon structure Schottky-barrier at presence of dislocation structures is submitted in fig. 8.

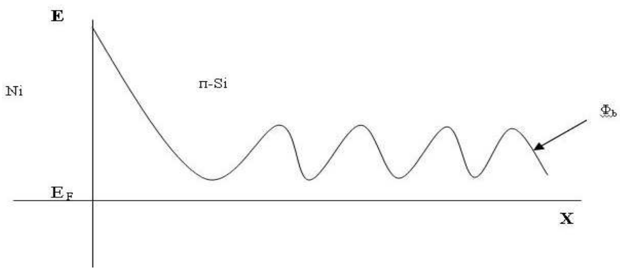

Fig. 8 The power circuit of metal—silicon structure at presence of dislocation structures: E — energy, E_F — Fermi level, X — distance from interface, Φ_b — height of dislocation barrier

We shall consider, firstly, current flow process in approach of the thermionic theory. Within the frames of this theory current flow through area of dislocation barriers can be written as [5].

$$I = A^{**}T^2S\left[\exp\left(\frac{qV}{kT}\right) - \exp\left(\frac{-qV}{kT}\right)\right]\exp\left(\frac{-\Phi_b}{kT}\right), \quad (3)$$

where A^{**} — the modified Richardson constant, T — temperature, V — voltage drop in the space-charge region of Schottky barrier. As considered, all barriers have the identical height, such current will pass through all parallel dislocation structures, S — area of metal—silicon contact.

Current which flows through Schottky barrier of metal—silicon contact will be defined as [5]

$$I_1 = A^{**}T^2S\left[\exp\left(\frac{qV}{kT}\right) - 1\right]\exp\left(\frac{-\Phi_a}{kT}\right), \quad (4)$$

where Φ_a — height of Schottky barrier.

Currents I and I_1 are identical because dislocation barriers and Schottky barrier connected in series. We shall raise expression (3) in the LM power and multiply by expression (4). We obtained expression for current flow process through metal—silicon contact of Schottky barrier at the presence of dislocation structures

$$I_d = A^{**}T^2 S \exp\left[\frac{-(\Phi_a + LM\Phi_b)}{(LM+1)kT}\right]\times$$

$$\left[\exp\left(\frac{qV}{kT}\right) - \exp\left(\frac{-qV}{kT}\right)\right]^{\frac{LM}{LM+1}} \times$$

$$\times\left[\exp\left(\frac{qV}{kT}\right) - 1\right]^{\frac{1}{LM+1}}. \quad (5)$$

Expression (5) can be used to calculate the influence of one dislocation on current flow process through metal—silicon contact with Schottky barrier. In this case, the expression at $M = L = 1$ can be written as

$$I_d = A^{**}T^2 S \exp\left[\frac{-(\Phi_a + \Phi_b)}{2kT}\right]\times$$

$$\times\left[\exp\left(\frac{qV}{kT}\right) - \exp\left(\frac{-qV}{kT}\right)\right]^{1/2} \times$$

$$\times\left[\exp\left(\frac{qV}{kT}\right) - 1\right]^{1/2}. \quad (6)$$

In case of lack of dislocations, expression (5) coincides with expression (4). Expressions (3)—(6) are obtained at the assumption, that the modified Richardson constant is identical to dislocation barriers and Schottky barrier of metal—silicon contact. Calculation of these constants for dislocation barriers has given the result which differs less than on 1%.

When the dislocation density is such that free path (l) is less than length of space-charge zone (W), one of the thermionic theory position is not carried out. In this case, to describe current flow process through metal—silicon contact in account of dislocations it is necessary to use drift-diffusion theory, and the ratio of forward currents in account of dislocations I_d and without them I can be written as [5]

$$\frac{I_d}{I} = \left[\frac{\mu_{qd}}{\mu_{qd} + \mu_0}\right]\exp\left(\frac{-qV}{kT}\right), \quad (7)$$

where μ_{dq} — mobility of charge carriers at dislocation scattering (described by expression (1)), м $_0$ — mobility of charge carrier without taking into account dislocation scattering. Calculations for space-charge length of nickel—silicon contact with Schottky barrier and free path for n-Si (111) show, that at dislocation density (10^{12} m^{-2}) their values are identical. It means that at the given density of dislocations (10^{10} m^{-2}) the free path is much more than length of space-charge zone and the approximation of the thermionic theory (expression (5)) with participation of dislocations should be used.

Let's consider what place occupies tunnel-resonant current flow process in account of dislocation levels in general current flow through metal—silicon contact (fig. 8). Let's label Γ for spread of dislocations energy state, and W for matrix element of transition, the transparence of barrier D_d in account of dislocation level E_0 can be written as

$$D_d = \frac{(W\Gamma)^2}{(E - E_0)^2 + (\Gamma/2)^2}, \quad (8)$$

where E — electron energy.

The general transparence of barrier is equal to

$$D = D_0 + D_d, \quad (9)$$

where D_0 — quasi-classic transparence of barrier without taking into account dislocations, which depend on the shape of potential barrier and the other parameters. Expression for surface density of current has the ordinary view

$$j = -2q\int_p vDf_p(2\pi\hbar)^{-3}\,\mathrm{d}p. \quad (10)$$

For nondegenerate electronic gas and for parabolic potential barrier f_p should depend on Maxwell—Boltsman statistics and expression for current density (10) should look like

$$j = 4\pi qkTm^*(2\pi\hbar)^{-3}\exp\left(\frac{\mu}{kT}\right)\int_{E_c'}^{\infty} D\exp\left(\frac{-E}{kT}\right)\mathrm{d}E, \quad (11)$$

where $E_c' = E_c + qV_0$, m^* — effective mass of electron, V_0 — the external electrical voltage, E_c — energy of conduction band bottom. Integrating (10) at different voltages, we gain the expression for current density as

$$j = A^{**}T^2\exp\left(\frac{-E_0}{kT}\right)\exp\left[\frac{q(V_0 - V_2)}{kT}\right],$$
$$\text{at } E_0 - \Gamma/2 > qV_0, \quad (12)$$

where V_2 — value for drop of electrical voltage in space-charge zone.

There is the open question on simulation of interaction by precipitated impurity on parameters of dislocations. It is possible to say, that oxygen, revealed with the help of the Auger and X-ray method, is located near dislocation cores, in places of the lowered values for deformation potential and can interact with «unsaturated» or «free» bonds of dislocations with occurrence of the new energy levels in forbidden band of silicon, thus changing electric activity of dislocations.

Thus, at simulation of current flow process through metal—silicon contact at the presence of dislocations with edge boundary one should know not only the parameters of potential barrier and the parameters of silicon, but also principal parameters of dislocations — type and density of dislocations, heights of potential barriers, location of energy levels for dislocations in forbidden zone of silicon (to calculate the occupation degree of dislocation levels, radius of dislocation cylinders and heights of dislocations potential barriers).

References

1. *V. A. Smyntyna*, *O. A. Kulinich*, *M. A. Glauberman*, *G. G. Chemeresuk*, *I. R. Yatsunsky*. Influence of structural defects on electric current in the channel of MOS-transistor // 2005 15th Int. Crimean Conference «Microwave & Telecommunication Technology» (CriMiCo'2005). — IEEE, Moscow, Weber Co. — p. 640—642. (2005).
2. *K. Ravy*. Defects and impurity in semiconductor silicon. M.: Mir. — p. 471 (2001).
3. *O. A. Kulinich*, *M. A. Glauberman*. Influence of defects on an amplification constant of a photoelectric and quantum efficiency of silicon photodetectors. Surface. X-ray, synchrotron and neutron investigations // № 5. — p. 101—106. (2005).
4. *G. Matare*. Electronics of defects in semiconductors. M.: Mir. — 229 p. (2000).
5. *S. Zi*. Physics of semiconductor devices. P. 1. M.: Mir. — 132 p. (2000).

УДК 537.311.33:622.382.33

О. А. Кулініч, *В. А Сминтина*, *М. А. Глауберман*, *Г. Г. Чемересюк*, *І. Р. Яцунський*

МОДЕЛЮВАННЯ ПРОЦЕСУ СТРУМОПЕРЕНОСУ В СТРУКТУРАХ МЕТАЛ—КРЕМНІЙ

В роботі на основі проведених досліджень за допомогою сучасних методів запропонована фізико-математична модель струмопереносу в структурах метал—кремній в межах термоелектронної, дрейфово-дифузіоної та тунельно-резонансних теорій і основана на бар'єрних властивостях структурних дефектів.

Ключові слова: кремній, метал, моделювання, струмоперенос.

UDC 537.311.33:622.382.33

O. A. Kulinich, *V. A. Smyntyna*, *M. A. Glauberman*, *G. G. Chemeresuk*, *I. R. Yatsunsky*

CURRENT FLOW PROCESS SIMULATION IN METAL—SILICON STRUCTURES

The model of current flow process simulation in metal—silicon structures with used modern method of investigation within the limits of thermo-electric, drift-diffusion and tunnel-resonant theories and it bases on barrier properties of structural defects.

Key words: silicon, metal, model, current, dislocation.

УДК 537.311.33:622.382.33

О. А. Кулинич, *В. А Смынтына*, *М. А. Глауберман*, *Г. Г. Чемересюк*, *И. Р. Яцунский*

МОДЕЛИРОВАНИЕ ПРОЦЕССА ТОКОПЕРЕНОСА В СТРУКТУРАХ МЕТАЛЛ—КРЕМНИЙ

В данной роботе на основе исследований, проведенных с помощью современных методов, предложена физико-математическая модель токопереноса в структурах металл—кремний в рамках термоэлектронной, дрейфово-дифузионой и туннельно-резонансных теорий и она основана на барьерных свойствах структурных дефектов.

Ключевые слова: кремний, металл, моделирование, токоперенос.