Materials Physics and Mechanics 39 (2018) 75-80 Received: November 1, 2017

EMISSION PROPERTIES OF AN ARRAY OF SILICON NANOCONES

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Abstract. In this paper we investigate the emission properties of an array of silicon nanocones containing cobalt nanoparticles at their vertices. Nanocones are formed on a silicon substrate by deposition a cobalt film, processing it to obtain an array of nanoparticles with a diameter of 20-30 nm and subsequent etching of silicon. Nanocones of silicon are separated from the conductive substrate by a layer of silicon oxynitride with the thickness of 8 nm. The results of modeling the current transfer in Si(Sb)/SiO_xN_y/Co nanocones and an estimation of their emission properties are presented.

Keywords: electron transport, emission, nanocone, oxynitride, silicon

1. Introdiction

At the present time, nanoelectronics expands its capabilities; new directions are developing and traditional areas are improving, such as vacuum electronics. In recent years, vacuum nanoelectronics was developed which is directed to application of nanostructures with vacuum spacing, containing emitters for field emission [1, 2]. The advantages of such nanostructures involve no need to create a vacuum by air pumping, and no need for cathodes heating. In addition, a high speed of electrons in vacuum gaps permits to increase significantly the operating frequency of devices. The technological possibilities of creation of nanoelectronic vacuum devices are determined by silicon technology. On its basis, it is possible to form vacuum silicon nanostructures, functionally analogous to traditional vacuum tubes (triodes, pentodes, etc.). For the implementation of vacuum nanoelectronics devices into industry, some problems remain to be solved, related to increasing the efficiency of field emission of semiconductor (silicon) cathodes, the reproducibility of the formation of nanostructures, and the stability of their functioning, associated mainly with degradation of point cathodes.

In this paper the emission properties of an array of silicon nanocones containing cobalt nanoparticles at their vertices are investigated. Nanocones are formed on a silicon substrate by depositing a cobalt film, its processing to producing of an array of nanoparticles with a diameter of 20-30 nm, and subsequent silicon etching. The silicon nanocones are separated from the conductive substrate by a layer of silicon oxynitride SiO_xN_y with the thickness of 8 nm. The purpose of this work is the simulation of the current transfer in n-Si(Sb)/SiO_xN_y/Co nanocones and the evaluation of their autoemission properties.

2. Model

To model the current transfer in the n-Si(Sb)/SiO_xN_y/Co heterostructure, we assume that the current transfer is monopolar, and the main mechanism of electron transport in SiO_xN_y is the capture on trap centers and subsequent ionization of such centers in a strong electric field. This mechanism is valid for the case of carrier transport in wide-gap semiconductors and dielectrics in strong electric fields at a high concentration of trap centers [3]. SiO_xN_y is

http://dx.doi.org/10.18720/MPM.3912018_12

characterized by a relatively high concentration of traps. To increase it, an electric breakdown can be carried out, which results in a pre-breakdown condition characterized by increasing the trap concentration almost up to 1020cm^{-3} [4]. In this case, the current-transfer equation and Poisson's equation, taking into account trapping and ionization in the stationary case, reduce to the following system of equations [5]:

$$n_t(F) = N_t[1 + (q/J\sigma)P(F)]^{-1}, \tag{1}$$

$$\frac{\partial F(x)}{\partial x} = q\frac{n_t(F)}{\varepsilon\varepsilon_0}, \tag{2}$$

where q is the electron charge, J is the current density, P is the ionization probability of a trap center, F is the electric field intensity, N_t is the concentration of the trap centers, σ is the capture cross section of electron per trap, ε, ε_0 are the relative dielectric constant of SiO_xN_y and the vacuum permittivity respectively. After the transformations, we obtain the system of equations characterizing the electric field intensity and the current density [5]:

$$J = \frac{(q/\sigma)\int_{F_0}^{F_d} P(F)FdF}{(q/\varepsilon\varepsilon_0)N_tU_g+(1/2)\left(F_d^2-F_0^2\right)}, \tag{3}$$

$$\frac{\int_{F_0}^{F_d} P(F)dF}{\int_{F_0}^{F_d} P(F)FdF} = \frac{(q/\varepsilon\varepsilon_0)N_td+(F_d-F_0)}{(q/\varepsilon\varepsilon_0)N_tU_g+(1/2)\left(F_d^2-F_0^2\right)}. \tag{4}$$

Here F_0, F_d are the electric field intensity at the Si/ SiO_xN_y and SiO_xN_y/Co interface, d is the SiO_xN_y thickness, and U_g is the voltage drop at SiO_xN_y.

To perform calculations using system (3, 4), it is necessary to determine the dependence of the ionization probability P on the electric field strength F. It is determined by the ionization mechanism and depends on parameters of the trap center. Three mechanisms of trap ionization are considered, namely: the Poole-Frenkel mechanism, the mechanism of tunnel ionization of charged centers, and the mechanism of multiphonon tunneling ionization of neutral centers [5, 6]. The equations for the ionization probability by means of these mechanisms are given in [5]. By specifying the functions $P(F)$ and the corresponding parameters of the traps, one may calculate the distribution of field intensity in SiO_xN_y and the current density in it, depending on the applied external bias.

According to Refs. [6-8], the multiphonon effects lead the probability of the trap ionization to be dependent on the electric field applied as

$$P(F) = \nu\exp(-w_t/kT)\, exp\left(\sqrt{Zq^3F/\pi\varepsilon\varepsilon_0/kT^*}\right), \tag{5}$$

where w_t is the energy of thermal ionization of a trap, k is the Boltzmann constant, v is the frequency factor, and T is the absolute temperature of the sample. The effective temperature T^* is defined from

$$\frac{1}{kT^*} = \frac{1}{kT} \pm \frac{2\tau_1}{h} = \frac{\tau_2}{h}, \tag{6}$$

where the time constants $\tau_1(_2)$ characterize the tunneling transition of the trap from the ground state to the ionized state, in which an electron occupies the highest energy level in the trap but still has zero kinetic energy [6]. The plus sign corresponds to a weak electron–phonon coupling, while the minus sign stands for a strong one.

Tunneling effects dominate in the fields of $F \sim F_T = (2\text{-}3)10^8$ V/m while the influence of the trap charge leads to increasing the barrier transparency by lowering its height [6]. On the other side, multiphonon ionization in the electric field is also accompanied by tunneling. The probability of multiphonon tunneling ionization as a function of the electric field can be written as [6]

$$P(F) = p(0)exp\left(\frac{q^2F^2\tau_2^3}{3hm_e}\right), \tag{7}$$

where $p(0)$ is the ionization probability at $F = 0$.

In the case of multiphonon transitions with electron tunneling, the probability of ionization, taking into account the Coulomb charge of a trap, can be written as [6]

$$P(F) = p(0)exp\left(\frac{q^2F^2\tau_2^3}{3hm_e}\right)exp\left(\frac{2qm_e}{\varepsilon\varepsilon_0\tau_2hF}\ln\frac{4q^2F^2\tau_2^3}{hm_e}\right). \qquad (8)$$

For neutral traps the multiphonon tunneling ionization occurs in an electric field [7]. In order to model this process the following parameters should be introduced: phonon energy $w_{ph}=\hbar\omega$, thermal w_t and optical w_{opt} energy of the trap ionization. There are several models of this mechanism based on a classical description of oscillations of a trap center [9] and on a quantum mechanical approach according to the theory of Makram-Ebeid and Lannoo [10]. Classical and quantum mechanical approaches, as has been shown in Ref. [11], provide similar results if the electric field is in the range of 3×10^7–1×10^9 V/m and the temperature varies from 300 to 425 K. Sizable difference between these two approaches appears only at lower temperatures, at larger electric field and at larger phonon energy. In the case of the multiphonon tunneling ionization of a neutral trap, the classical model of oscillations of trapping centers has been applied to describe the ionization probability [7]

$$P(F) = \frac{qF}{2\sqrt{2m_ew_{opt}}}\times exp\left[-\frac{4w_{opt}^{3/2}}{3}\frac{\sqrt{2m_e}}{hqF}+\frac{4m_e}{h^2}\frac{w_{ph}w_{opt}(w_{opt}-w_t)}{q^2F^2}coth\frac{w_{ph}}{2kT}\right]. \qquad (9)$$

3. Results and Discussion

Structure parameters: the thickness of SiO_xN_y is 8 nm, the traps concentration in SiO_xN_y, N_t=(2-10)10^{19} cm^{-3}, the flat-band voltage is 0.05-0.15 V, the capture cross section of the electron per trap is 5×10^{-13} cm^2, The energy of the traps w_t= 0.4-1.7 eV, the frequency of traps oscillations is 10^{10} Hz, the effective temperature in the Poole-Frenkel ionization mechanism is 380-420 K. The dielectric constant $\varepsilon = 5$. With the help of a method of measuring of the injection of electrons from silicon to SiO_xN_y by the Fowler-Nordheim mechanism in [12] the barrier for electrons at the Si/SiO_xN_y interface was estimated, being taken as 2.9 eV.

Calculations. The calculation results are shown in Fig. 1 and 2. As can be seen from the results obtained, the electric field intensity in SiO_xN_y is 10^8 -10^9 V/m. The current density varies in the range of 10^2-10^5 A/m^2 with increasing voltage drop and depends on the trap parameters and trap concentration. The calculations of tunnel ionization of charged centers and multiphonon tunneling ionization of neutral centers are presented in Figs. 3-5. Figure 3 illustrates the current density dependence in the case of tunneling ionization, equation (7) for the ionization probability. A significant current increase starts when the external displacement is greater than 1.5 V. For the tunneling ionization with account of multiphon transitions, equation (8) for the ionization probability, the calculations have shown that the instabilities arise in the distribution of the electric field in silicon oxynitride (Fig. 4a). In this case the solution of equation (4) gives three roots in the region of external biases of 0.2-0.6 V. The stable state is observed at the external bias greater than 0.6 V, while the current density decreases with increasing of external bias (Fig. 4b).

This is caused by the nonlinear change in the ionization probability $P(F)$ with increasing field strength: the probability $P(F)$ rises for F less than 6×10^7 V/m and then decreases.

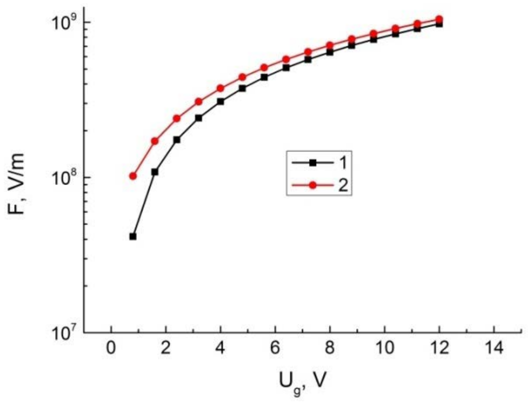

Fig. 1. Dependence of the electric field intensity on the SiO_xN_y interface on the external bias: F_0 – (curve 1), F_d - (curve 2)

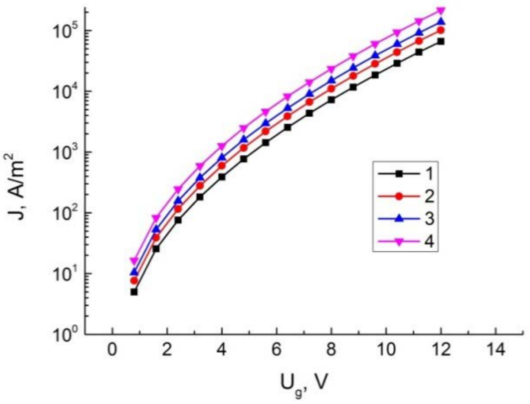

Fig. 2. Current density through silicon oxynitride as a function of external bias at different concentrations of trap centers N_t at the energy w_t = 0.5 eV: N_t (cm^{-3}) = 5×10^{19} (1), 3×10^{19} (2), 2×10^{19} (3), 1×10^{19} (4)

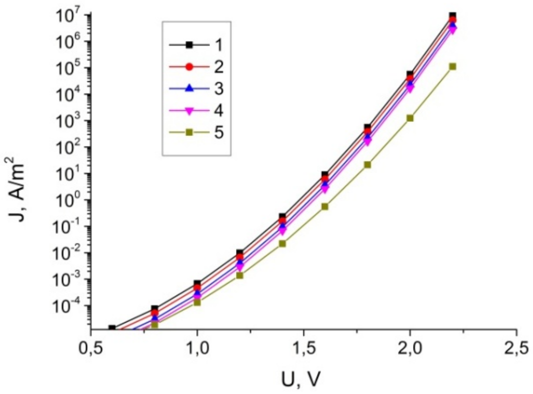

Fig. 3. Current density through silicon oxynitride as a function of external bias at different concentrations of trap centers N_t at the energy w_t = 0.7 eV and N_t (cm^{-3})=2×10^{25} m^{-3} (1); 3×10^{25} m^{-3} (2); 5×10^{25} m^{-3} (3); 7×10^{25} m^{-3} (4,5); ε =7.5 (1-4), ε =10 (5)

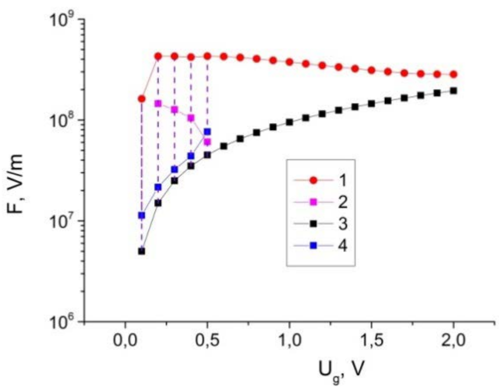

Fig. 4a. Dependence of the electric field intensity on the SiO_xN_y interface on the external bias at N_t=2×10^{25} m^{-3}: F_0 – (curve 3), F_d - (curve 1, 2, 4)

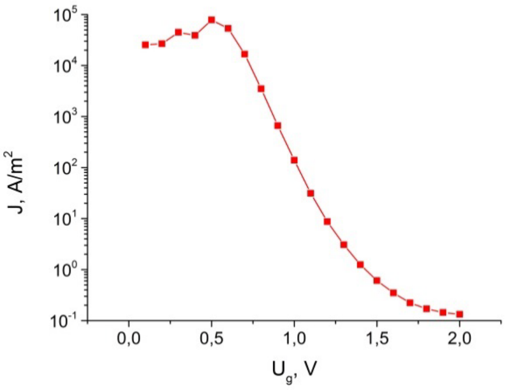

Fig. 4b. Current density through silicon oxynitride as a function of external bias at N_t=2×10^{25} m^{-3}, w_t = 1.7 eV

Similar results were obtained for the ionization of neutral traps; equation (9), Fig. 5. Here, the instability is also observed because of the nonlinear dependence of the ionization probability on the electric field intensity.

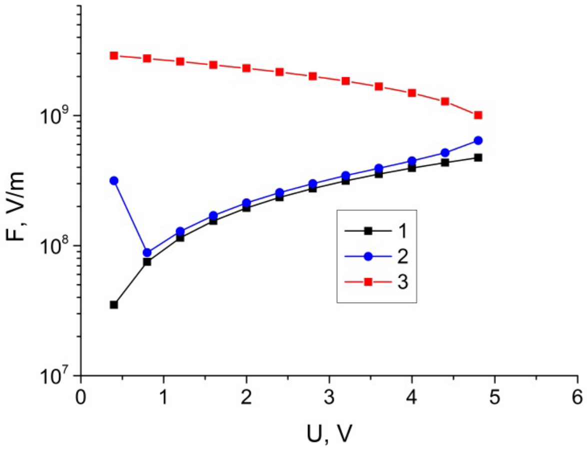

Fig. 5. Dependence of the electric field intensity on the SiO_xN_y interface on an external bias at N_t=5×10^{25} m^{-3}, w_{opt} = 0.6 eV, w_t = 0.48 eV, w_{ph} =0.045 eV: F_0 – (curve 1), F_d - (curve 2, 3)

Estimation of emission characteristics. To obtain the current density of the field emission of 100 A/m^2, taking into account the value of the SiO_xN_y/cobalt surface barrier and the cobalt work function (4.4 eV), the current density in SiO_xN_y should be above 10^4A/m^2. To obtain an emission current density of 100 A/m^2 at field intensity between cobalt and vacuum of about (2-5)10^7V/m, the current density of 2×10^7 - 1.1×10^4A/м^2 in SiO_xN_y is required. As preliminary estimates have shown, this can be achieved by the trap concentration of (2-5)10^{19}cm^{-3} and their energy of 0.4-0.5 eV over conduction band bottom of SiO_xN_y.

4. Conclusions

Simulation of current transfer in the array of silicon nanocones, presenting the n-Si(Sb)/SiO_xN_y/Co nanostructure, is performed. It is found that at the trap concentrations in SiO_xN_y of the order of (2-5)10^{19} cm^{-2} and their energy of 0.5 eV, is possible to reach a current density up to 10^5 A/m^2 that allows obtain the emission current density of 100 A/m^2.

A stable state of current transfer through silicon oxynitride with trap states is observed for the Poole-Frenkel mechanism of multiphonon ionization and the ionization tunneling mechanism. In the case of multiphonon transitions with electron tunneling and neutral traps, the instabilities in the distribution of the electric field intensity as well as the current transfer occur, that can be used for creating emission cathodes in the microwave region.

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