Diffusion theory and optimization of ohmic contacts to n-layer of bipolar nanoheterostructures

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Abstract. Ohmic contacts to n-layers of gallium arsenide-based heterobipolar nanoheterostructures obtained by layer electron-beam evaporation Ge/Au/Ni/Au are studied. Time and temperature dependencies of diffusion profiles of doping Ge distribution are calculated. The interface of metal-semiconductor is analyzed with SEM, then an RTA installation design and methodology of RTA are suggested based on the results of this study. This allows to obtain ohmic contacts with low resistance and minimum transition layer.

1. Introduction
Ohmic contact to the n-layers nanoheterostructures based on gallium arsenide are widely used in microwave, digital and optical devices. Despite the enormous amount of work on metallization systems based on thin layers of Ag, Ni, Pt, Pd, Ti and other materials, [1-3] Au/Ge based metallization systems are most widely used at the moment [4,5]. To obtain ohmic contact an electron beam vacuum deposition and a special heat treatment - RTA, in which diffusion processes take place, in order to create a heavily doped region with low resistance between the semiconductors and metallization, - are used. This mechanism is still not fully comprehensible. In practice, it turns out that the doping mechanism that occurs at the interface metal/GaAs section is very complicated, and the resistivity of the Ni-Au-Ge/GaAs contact is very sensitive to heat exposure processing procedure. Developed metallization schemes allow to obtain the minimum of contact resistance at the level of 0.1-0.2 Ohms*mm, but literature data indicate that the extent of the transition layer in this case is a few tenths of a micron [6]. We assumed that the thickness of the material forming eutectic alloy determines transition layer thickness. We modeled distribution of impurities in the transition layer. On the basis of the calculation of diffusion profiles, we have optimized the time and temperature of ohmic contacts annealing.

2. Theoretical background
To calculate the diffusion of thin layer of the germanium to gallium arsenide was examined diffusion from a limited supply in to the semi-infinite body at a relatively short time. Since the modeling problem consists in calculating the impurity distribution profile in depth, we consider the one-dimensional case. The calculation of diffusion processes reduces to solving a differential equation with given initial and boundary conditions. For a description of diffusion process, we use the Fick’s second law:

$$\frac{\partial N}{\partial t} = D \frac{\partial^2 N}{\partial x^2}$$  (1)
where $N$ – the concentration of diffused particles, $D$ is the diffusion coefficient, $t$ is the diffusion time and $x$ is the doping depth. This equation is used to describe diffusion processes. The maximum surface concentration of the diffusing impurity corresponds to the limit of its solubility $N_0$ for a given body. During this process, we are creating a highly doped layer in the surface region of the semiconductor. Border conditions:

$$N = N_0, \text{ at } x = 0, \ t > 0.$$  \hspace{1cm} (2)

The concentration tends to zero in the volume of the body. Initial conditions:

$$N = 0, \text{ at } x \gg 0, \ t > 0.$$  \hspace{1cm} (3)

The solution of the diffusion equation has the form:

$$N(x,t) = N_0 \exp\left(-\frac{x^2}{4Dt}\right).$$  \hspace{1cm} (4)

The diffusion coefficient of the impurity depends on the temperature according to the Arrhenius law:

$$D = D_0 \exp\left(\frac{E_a}{kT}\right)$$  \hspace{1cm} (5)

where $E_a$ is the diffusion activation energy, $D_0$ is the diffusion coefficient value at $E_a = 0$, $T$ is the absolute temperature, and $k$ is the Boltzmann constant.

We used the package MATLAB applications. The program builds a dopant distribution profiles in the gallium arsenide. Profile defined by the expression (5). The purpose of the calculations was to form a transitional layer of minimum depth. This is necessary to avoid puncturing the emitter layer of the heterobipolar structure. The greater depth of the transition layer will lead to the penetration of the contact layer, which is less to the contact with a rather high level of resistance. We must learn to obtain a transitional layer of a certain depth with high accuracy. Germanium is an electrically active impurity for gallium arsenide, in order to obtain an ohmic contact, the concentration of the dopant in the near-contact region should be at least $10^{19}$ cm$^{-3}$. The solubility limit of Ge in GaAs is determined by the maximum concentration of Ga vacancies in GaAs. These vacancies are formed during diffusion and are replaced by germanium atoms. In the case of diffusion of pure Ge, the vacancy concentration and, accordingly, the solubility limit are $10^{17}$ cm$^{-3}$ [7]. To increase the degree of doping, the diffusion of germanium is carried out in the presence of gold, since in this case gallium leaves the semiconductor more actively, forming AuGa compounds, the concentration of vacancies reaches $5\times10^{19}$ cm$^{-3}$. In only one of five cases, germanium occupying a vacancy is an electrically active impurity, in the remaining cases the impurity is neutral [7,8]. The donor impurity concentration was calculated, since it determines the parameters of the contact. Accordingly, the solubility limit in this case will be $10^{19}$ cm$^{-3}$. We have received doping profiles (figure 1).

![Figure 1. The germanium diffusion profiles in gallium arsenide. A) RTA time 30 seconds, B) RTA time of 60 seconds, C) RTA time 120 seconds.](image-url)
The calculation shows a significant change in the depth of the impurity from the RTA time and the RTA temperature. There is a strong diffusion of impurities at higher temperatures and times. This allows for smooth transition layers, if you can create a rapid heating and cooling mode.

3. Experimental data
An experiment was conducted to verify the calculations. During the experiment contacts were made to the n-layers of bipolar nanoheterostructures based on gallium arsenide. The wafer was cut into pieces and subjected to heat treatment. A feature of this type of structure is that the depth of the transition layer should not exceed the thickness of the contact layer (not more than 50 nm). After the formation of metallization and mesa, the plate was cut into pieces measuring 1*1 sm² and annealed, the time and temperature of the process were set in accordance with the results of the calculations. In our furnace the cooling rate is comparable to the heating rate [9], which allows us to fix or "freeze" the diffusion front defined by time and heating temperature. Measurement of the contact resistance was made by the method of the transmission line measurement (TLM) with a width of the rectangular metallized regions 100 um [10].

4. Results
Figure 2 shows the dependence of the contact resistance on the temperature and time of RTA. It is a typical shaping of contact resistance process to gallium arsenide [11]. There is a minimum contact resistance. Also, the contact resistance increases with the level of RTA time. This dependence is reduced at high temperatures. Figure 2 shows that at an incineration temperature of 398 °C, the contact resistance is practically independent of the RTA time. This makes it possible to fabricate ohmic contacts with a minimum transition layer. Most likely, the rapid heating and cooling allows you to fix or “freeze” the diffusion front, set the time and temperature of heating.

![Graph showing the dependence of contact resistance on RTA time and RTA temperature](image)

Figure 2. The dependence of contact resistance on RTA time and RTA temperature this case simply justify the caption so that it is as the same width as the graphic.
To determine the depth of doping, a SEM microscopy was used. Figure 3 shows a SEM image of the metal-semiconductor boundaries for different parameters of heat treatment. The cross-sections show the correspondence to the calculated profiles. The transition layer of the contact obtained by annealing for 60 seconds at 398 °C has a depth of about 50 nm (figure 3A), which agrees well with the theory. It can be seen from figure 3B that an increase in the RTA time leads to a blurring of the transition layer, pulling it down into droplets, and also to an increase in its depth. The latter is very critical for heterobipolar structures.

Figure 3. Cross-section SEM image of test sample interfaces at different heat treatment parameters: A) RTA time 60 seconds, temperature 398 °C, transition layer 50 nm. B) RTA time 480 seconds, temperature 398 °C, transition layer 80 nm.

Figure 4. SEM image of heterobipolar transistor.
Figure 4 shows an image of the surface of a heterostructural bipolar transistor (HBT). Ignition time was 60 seconds, RTA temperature 398 °C, contact resistance 0.1 Ω*mm. As a result, ohmic contacts have a smooth surface morphology and smooth edges.

5. Conclusion
We spent RTA process optimization of ohmic contacts to n-layers GaAs-based bipolar nanoheterostructures, based on results of our calculations. Optimization of the heat treatment of ohmic contacts made it possible to reduce the transition layer thickness of up to several hundreds of angstroms, while maintaining the level of contact resistance 0.1 Ohm*mm to n-layers of GaAs. The research on the impact of changes in the contact resistance to nanoheterostructures under the brazing temperature and time revealed the existence of the optimal parameters of the process in which the level of the contact resistance is minimal and depends weakly on variations of the parameters.

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