

## Features of formation concentration profile in structured materials

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**Abstract.** The paper presents analysis of dependence of the penetration depth of the implanted aluminium ions in structured titanium. Ion implantation was performed repetitively pulsed particle beam ion source "MEVVA-V.RU". In the interpretation of the observed patterns of energy accounted for heterogeneous composition of the beam vacuum-arc source, is represented by three components. Within the simulation found that in samples with relatively fine grains (ultrafine samples) largely contribute to diffusion processes, in particular radiation-induced diffusion in comparison with fine-grained samples.

### 1. Introduction

One of the important directions of modifying the physicochemical properties of structural materials is the method of exposure beams of metallic ions. This method allows the synthesis of ion in the surface layers of metals and alloys and, thus, receive the phase of a transition metal and aluminium, which have high mechanical strength, wear resistance, corrosion resistance [1]. The use of titanium in different structural states is lately increasingly used in various fields of science and technology. To date, a number of studies on the effect of ion irradiation on the structural and phase characteristics and other properties of the metal in a coarse state.

However, implantation nanostructure and fine-grained materials is considerable interest in the prospect of wide application. Microscopic processes that occur in the process of ion implantation of titanium in different structural states, little analyzed and investigated. Therefore, studies of the characteristics of the formation of concentration profiles of implanted ions in titanium with different structural states are relevant.

The starting material of the target for the implantation of aluminium ions selected rod of commercially pure titanium VT1-0. For the formation of nano- and submicrocrystalline (SMS) state titanium billet was subjected to repeated uniaxial pressing with the change to the deformation axis at a rate of 10-2 s<sup>-1</sup> with decreasing temperature in the range of 773-673 between the pressing cycle. After the stage, the deformation of the titanium specimens were deformed by rolling in multiple brook rolls at room temperature, then to increase the plasticity of the titanium billet-Gigue. The average amount received by the elements in the structure of the titanium after such processing, was 0.2 microns – SMS state. Titanium samples with different grain sizes were made of titanium rods SMS by annealing time at various temperatures. Implantation of titanium materials with aluminium ions was carried out on vacuum-arc ion source "MEVVA-V.RU" in frequency pulsed mode [1]. Terms titanium implant specimens are shown in table 1. Obtained by layering Auger electron spectroscopy concentration profiles of aluminum in titanium samples are shown in figure 1 [1].

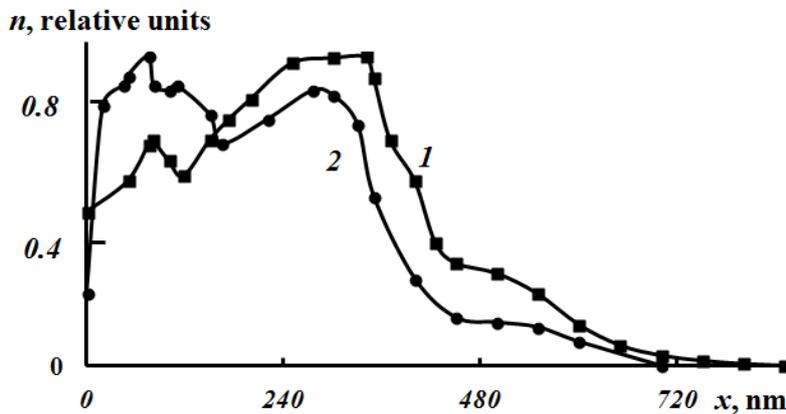


**2. Model and Results**

Ion source "MEVVA-V.RU" maintains the uniformity of the beam and is characterized by a decrease in the flow of ionic contamination.

**Table 1.** Modes of irradiation of titanium with different structural states of aluminium ion source "MEVVA-V.RU"

Modes	Grain size (microns)	Type of structure	The dose of irradiation (ion/cm <sup>2</sup> )	Time implantation (h)	The target temperature (K)	The accelerating voltage (kV)
1	0,3	Ultrafine-grained (UFG)	1·10 <sup>18</sup>	5,25	623	50
2	1,5	Fine-grained (FG)				



**Figure 1.** Experimental concentration profiles of aluminum ions in titanium modes: 1 – mode 1; 2 – mode 2

However, the proportion of the aluminium ions in the beam is 85% (balance nitrogen impurity (9.5%), oxygen (4.5%) and hydrogen (1%)), which affects the mass transfer processes taking place during implantation. When using ion sources of vacuum arc ion beam energy is heterogeneous and contains 38% Al<sup>+</sup>, 51% Al<sup>2+</sup>, Al<sup>3+</sup> + 38% [2]. Consequently, the composition of the energy beam is represented by three components with energies of 50, 100, 150 keV.

To describe the concentration profiles for materials with grain sizes used in any two-stage model. It is assumed that in the first minute implantation (for a small dose of implanted ions and low concentration of generated defects) impurity advantageously distributed statistically (the profile is described using functions Pearson fourth type and sputtering surface of the target). In subsequent times the formation of the profiles contributing to the processes of radiation-stimulated diffusion and heat. The total energy of the inhomogeneous profile for the beam (in this case the three components aluminium) based additive process can be represented as:

$$n(x) = \sum_{i=1}^3 F_i n_p(x, E_i) + F_i n_d(x, E_i) + F_i n_\tau(x, E_i), \tag{1}$$

where  $F_i$  – the dose of implanted ions, corresponding to the energy  $E_i$ ;  $n_p(x, E_i)$  – describes the statistical distribution of the original;  $n_d(x, E_i)$  – takes into account the contribution of radiation-stimulated diffusion;  $n_\tau(x, E_i)$  – is the contribution of thermal diffusion.

The following expressions for the  $n_p(x, E)$  and  $n_d(x, E_i)$ , used in the simulation are shown in [3]. In modeling the values of the moments of distributions of ions for each energy components were taken

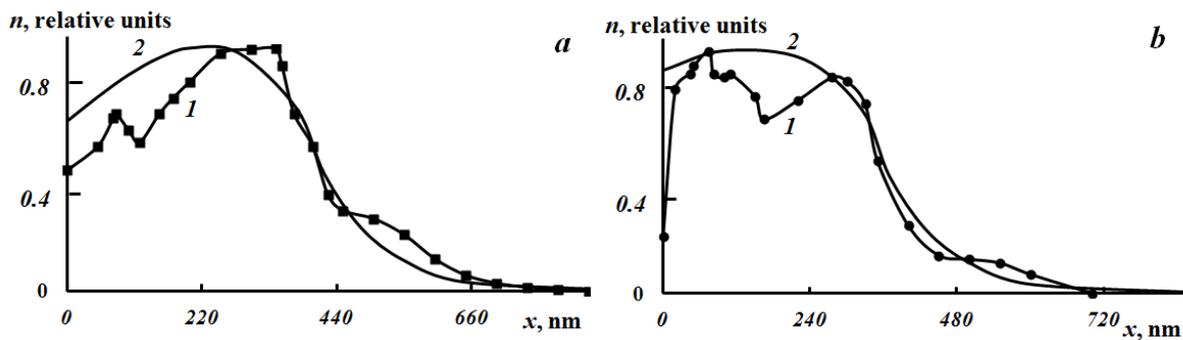
from the program SRIM-2013. The contribution of thermal diffusion was estimated based on their expression:

$$n_{\tau}(x, t) = \int_0^{\infty} n_p(\xi)G(x, \xi, t)d\xi + \int_{t_0}^t \int_0^{\infty} f(\xi, t)G(x, \xi, t - \tau)d\tau d\xi, \quad (2)$$

where  $n_p(x)$  profile formed at time  $t_0$ ;  $t$  – the total time of implantation, the function  $G(x, \xi, t)$  for the Green's function of the boundary value problem [3]. The contribution of diffusion processes is taken into account in the framework of radiation-stimulated diffusion [3] for polyenergetic beam. The share of deposits of statistical and diffusion processes was determined by modeling on the basis of a better agreement between theory and experiment is shown in table 2. The resulting concentration profiles taking into account the contributions of all the mechanisms are shown in figure 2, together with the experimental. Model parameters are given in table 3.

**Table 2.** Mechanisms of formation of concentration profiles in the implantation of titanium ions aluminum

Modes	Mechanisms of formation profiles, share	
	statistical	diffusion
1	0,33	0,67
2	0,40	0,60



**Figure 2.** Experimental (curve 1) and theoretical (curve 2) profiles of aluminum ions in titanium modes: a – mode 1, b – mode 2

**Table 3.** Model parameters to describe the concentration profile of aluminum in titanium

Parameters	Energy (keV)		
	50	100	150
The asymmetry factor $S_k$	0,15	-0,10	-0,26
The sputtering coefficient $S$ (at./ion)	1,3	1,8	2,0
Gain diffusion due to vacancies $d$	40	42	44
The diffusion coefficient defects $D_d$ (cm <sup>2</sup> /s)	$1,8 \cdot 10^{-14}$	$2,0 \cdot 10^{-14}$	$2,1 \cdot 10^{-14}$
The effective diffusion coefficient of the grain boundary $D_{eff}$ (cm <sup>2</sup> /s)	$2,2 \cdot 10^{-13}$	$2,3 \cdot 10^{-13}$	$2,5 \cdot 10^{-13}$
The diffusion length of defects $L_d$ (cm <sup>2</sup> /s)	$3,0 \cdot 10^{-6}$	$3,1 \cdot 10^{-6}$	$3,2 \cdot 10^{-6}$

The modeling found that the share of deposits of diffusion (including thermal diffusion) processes in the formation of the profiles in the UFG titanium slightly higher (about 7-10%) than in the FG titanium, which is associated with an increase in the grain boundary and the corresponding diffusion processes.

### 3. Conclusion

The regularities of mass transfer for the UMP and the Ministry of Health of titanium implant on the vacuum-arc ion source "MEVVA-V.RU". In the interpretation of the observed regularities taken into account heterogeneous composition of the beam, represented by three components. Studies have shown that the formation of concentration profiles in titanium occurs mainly by two mechanisms: an impurity originally distributed statistically, but with increasing doses of implanted particles, the concentration of the ion beam generated by structural defects and spraying the surface, begin to affect a variety of diffusion processes.

It is found that in samples with relatively fine grains (UFG titanium) in the formation of the depth profiles of the target to a greater extent contribute to diffusion processes, in particular radiation-induced diffusion, as compared with the FG samples. The proposed two-stage model allows to obtain qualitative agreement between theory and experiment and identify advantageous mechanisms of profiles at various stages of implantation.

### References

- [1] Kurshina I A, Popova N A, Kalashnikov M P et al. 2011 *News of higher educational institutions. Physics*. 118.
- [2] Nikolaev A G, Oks E M, Yushkov G Y 1998 *Technical Physics* **68** 43.
- [3] Vahnii T V, Vershinin G A, Sharkeev Y P et al. 2010 *Surface. X-ray, neutron and synchrotron the Exploration*. **4** 99.