

## The influence of TiB<sub>2</sub>-thin film thickness on metal - GaAs structural characteristics

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The X-ray diffraction and Atomic Force Microscope investigations of TiB<sub>2</sub>/GaAs as-produced and annealed device structures has been carried out. The samples were obtained by magnetron sputtering on previously photon cleaned Czochralski-grown (001) GaAs substrates doped by Te up to concentration  $10^{18} \text{ cm}^{-3}$ . The magnetron sputtering was carried out in the argon atmosphere at pressure in the chamber  $5 \cdot 10^{-3}$  torr. The currents of sputtering were 0.3 and 0.4A, and thickness of TiB<sub>2</sub>-films was from 10 nm up to 50 nm. The samples annealing was carried out in a stream of hydrogen in the furnace at temperatures 400, 600, and 800 °C during 1 minute with heating velocity of 1800°C/min. It was shown that film thickness and magnetron sputtering current determines the film surface and interface structural parameters as well as a features of processes of structural relaxation under short-term thermal annealing.

### 1. Introduction

It has been well known that microelectronics devices based on metal-semiconductor junction operation stability and reliability is determined by the nature of solid-phase interactions between the layers forming the contact. The increasing operating requirement of devices have imposed the necessity of development of new materials and processes for device production.

One of them could be the titanium diboride films and short-term thermal annealing (STA) treatment [1]. The TiB<sub>2</sub> compound has a low expansion coefficient, good adhesion to metals and other materials. It is characterized by high melting points and hardness, as well as has a good electrical conductivity. It makes possible the microelectronic application of TiB<sub>2</sub>. Beside this, the transition metal borides are inert with respect to copper, silver and gold. So, they can be used as the layer, which prevents the diffusion of mobile impurities [2]. The STA could improve the produced device characteristics, but the appropriate conditions must be determined. To clarify the processes which take place in TiB<sub>2</sub>/GaAs device structure under STA treatments the complex of structural investigations has been carried out.

### 2. Experiment

The metal films were obtained by magnetron sputtering on previously photon cleaned Czochralski-grown (001) GaAs substrates doped by Te up to concentration  $10^{18} \text{ cm}^{-3}$  (dislocation density was  $10^7 \text{ cm}^{-2}$ ). The magnetron sputtering was carried out in the argon atmosphere at pressure in the chamber  $5 \cdot 10^{-3}$  torr. The currents of sputtering were 0.3 and 0.4A, the growth velocity was approximately 5 Å/s, and thickness of TiB<sub>2</sub>-films was from 10 nm up to 50 nm. The contacts annealing was carried out in a stream of hydrogen in the furnace at temperatures 400, 600, and 800 °C during 1 minute with heating velocity of 1800°C/min.

X-ray scattering measurements were performed using the x-ray source with Cu K<sub>α</sub> line monochromatized by Ge (220) crystal. Samples surface morphology and features studies were performed

by Atomic Force Microscope (Nanoscope D3000, Digital Instruments). The scan was taken by 100µm scanner using silicon tip (radius of curvature ~50 Å) in tapping mode.

### 3. Results and discussion

The x-ray measurements of substrate atomic planes curvature radius [3] near the contacts indicates that all structures were concave at the metal film side, so the metal film was tensed and substrate was compressed. The deformation in investigated samples was estimated according to

the relation  $e = \frac{t \sin \alpha}{2l}$ , where  $t$  is the thickness of a substrate,  $\alpha$  - angle of Bragg pike displacement under sample translation on the distance  $l$ . As shown on fig.1, deformation is determined by thickness of film and sputtering current. A little bit higher initial deformation in structures obtained at 0.4A sputtering current is explained by more equilibrium conditions of TiB<sub>2</sub> film formation than at 0.3A.

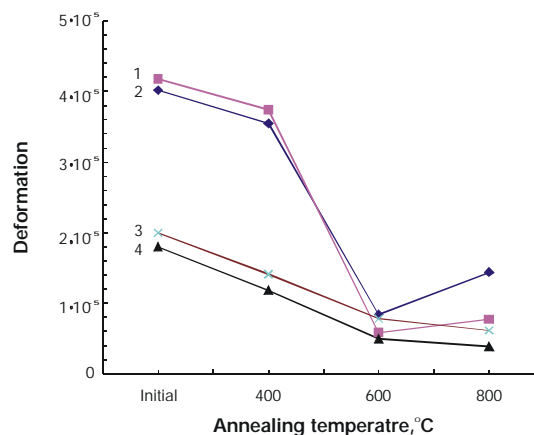


Fig. 1. Deformation  $e$  vs annealing temperature: 1,2 - structures with 50 nm TiB<sub>2</sub> film thickness, obtained at 0.4 A and 0.3A sputtering current, respectively; 3,4 - structures with 10 nm film thickness, obtained at 0.4 A and 0.3A, respectively.

Table 1. The changes of roughness  $R_q$  for  $TiB_2$  film with different thickness under short-term annealing.  $e$  indicates the relative deviation of  $R_q$  in different points of film surface.

	TiB <sub>2</sub> /GaAs 10 nm, 0.4 A		TiB <sub>2</sub> /GaAs 50 nm, 0.4 A	
	$R_q$ , nm	$e$ , %	$R_q$ , nm	$e$ , %
Initial state	0.219	4.70	0.470	27.28
After annealing at 400 °C	0.259	10.04	0.530	24.18
After annealing at 600 °C	1.063	5.30	0.568	22.87
After annealing at 800 °C	1.841	19.35	28.566	12.22

It is confirmed by AFM measurements of roughness  $R_q$ . The roughness of films obtained at 0.3A is higher and more inhomogeneous. The value of roughness  $R_q$  was calculated according to the equation:

$$R_q = \sqrt{\frac{\sum (Z_i - Z_{ave})^2}{N}}$$

where  $Z_{ave}$  is the average of the Z values in the given area,  $Z_i$  is the current Z value,  $N$  is the number of points in the given area. The STA causes to decreasing of deformation in all samples, but residual strains in structures with 50 nm film thickness relax nonmonotonously with increasing annealing temperature and have a minimum after annealing at 600°C. This nonmonotony is determined by higher deformation in initial state.

The residual strains relaxation (deformation decreasing) is accompanied with changes of roughness (table 1) and surface shape transformation (fig.2.).

The roughness of annealed film increases with increasing of annealing temperature. The  $R_q$  changes are significant in samples annealed at 600 °C and for samples with 50 nm  $TiB_2$  films we could observe the sharp roughness increasing after annealing at 800 °C.

Described changes of deformation and surface morphology for investigated structures may be explained by the intensive processes of structural relaxation in  $TiB_2$ -GaAs interface under STA treatment. As it was shown in our previous paper [4], the decay of  $Ga_xTi_{1-x}As$  and  $Ga_xB_{1-x}As$  solid solutions which were formed under magnetron sputtering of titanium diboride films, dislocation generation, point defects redistribution and structure ordering take place in an interface region.

It was found by using of AFM that for samples with thickness 10 nm the surface in initials state is covered by parallel rows of hills (fig.3.a,b). After STA treatment at 800 °C no ordered hills arrangement can be found (fig. 3. c). So, it could be supposed that we observed textures on magnetron sputtered thin films of titanium diboride.

To examine this assumption the x-ray diffraction spectra in grazing incidence geometry were registered. On

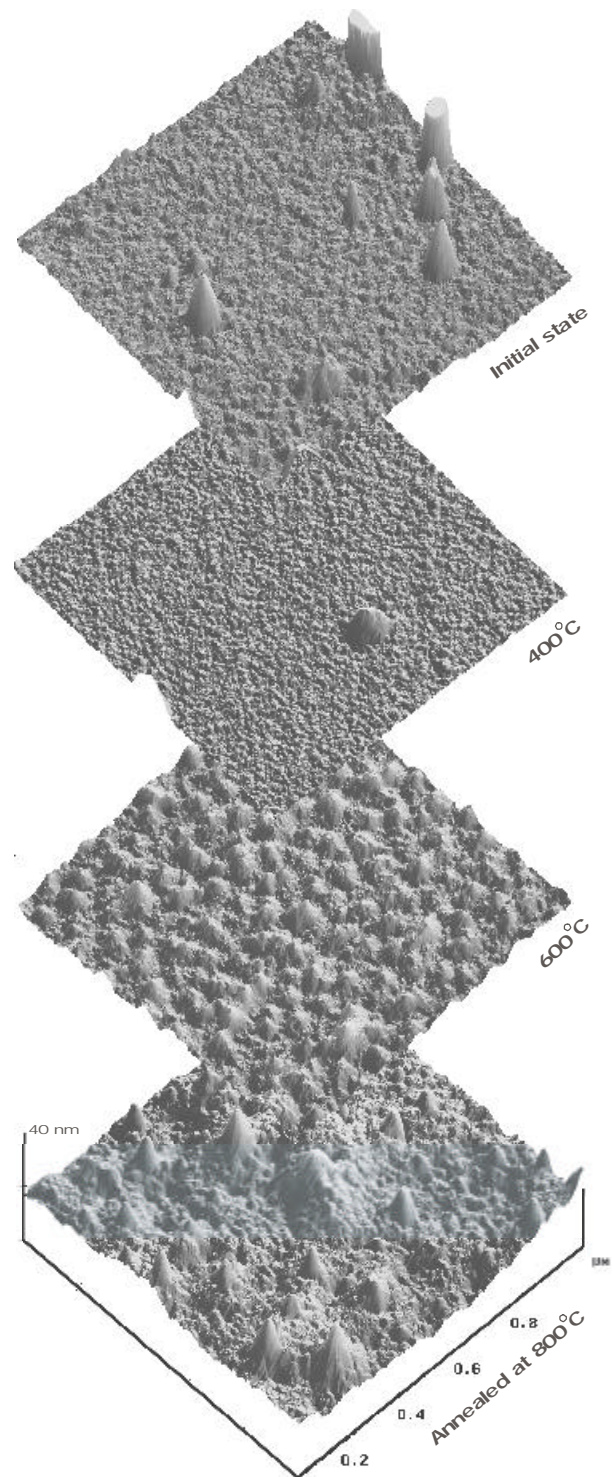


Fig. 2. The transformation of the  $TiB_2$ /GaAs (film thickness 10 nm, sputtering current 0.3 A).surface morphology under short-term thermal annealing.

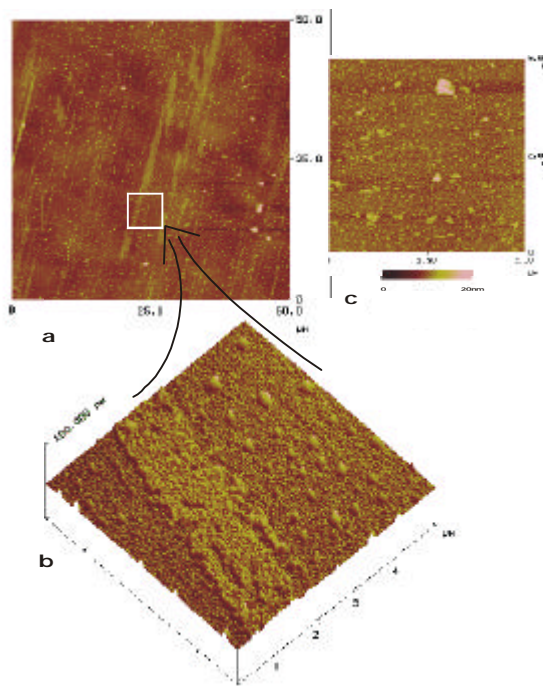


Fig. 3. The AFM images of textured surface of  $\text{TiB}_2/\text{GaAs}$  (10 nm, 0.4A) sample (a - planar image with  $50 \mu\text{m}$  scan, b - 3D image of selected area,  $5 \mu\text{m}$  scan) in initial state and surface after annealing at  $800 \text{ }^\circ\text{C}$  (c - planar image with  $5 \mu\text{m}$  scan).

the fig.4 the diffraction spectra for samples with 10 and 50 nm  $\text{TiB}_2$  film thickness are shown. In addition the simulated diffraction pattern for titanium diboride is marked below. The sharp intensive pike for reflection 002 is present in the spectrum of sample with 10 nm  $\text{TiB}_2$  film in initial state (curve 3). There is very small pike for reflection 002 in the spectrum for this sample after annealing at  $800 \text{ }^\circ\text{C}$  (curve 4). So, the 10 nm  $\text{TiB}_2$  films in initial state have a [001] texture and after annealing some recrystallization of film grains takes place. In the case of the 50 nm  $\text{TiB}_2$  films in initial state we can see small wide pike at the position for reflection 002, which slightly increased after annealing at  $800 \text{ }^\circ\text{C}$  (curves 1, 2). In this case we don't speak about texture, but present of tendency to enlargement of polycrystal grains. Furthermore in all spectra the pikes connected with quasiamorphous phase are present. The transformations of these pikes under STA treatment prove the enlargement of nanocrystal grains in this phase. The most quantity of quasiamorphous phase is present in  $\text{TiB}_2$  films with thickness 50 nm obtained at 0.3A sputtering current.

#### 4. Conclusions

X-ray and Atomic Force Microscope investigations of  $\text{TiB}_2/\text{GaAs}$  device structures have shown that the  $\text{TiB}_2$  film thickness and film sputtering current define structural characteristics of the film surface and system as whole as well

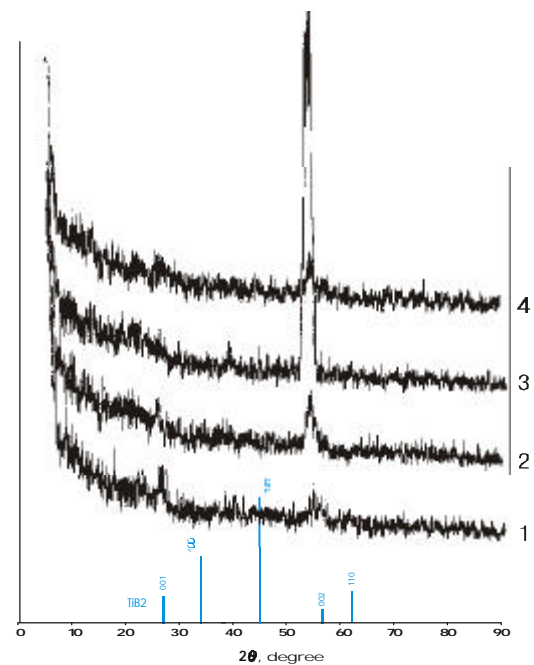


Fig. 4. X-ray diffraction spectra of  $\text{TiB}_2/\text{GaAs}$  surface (grazing angle  $2^\circ$ ): 1,2 - structures with 50 nm  $\text{TiB}_2$  film thickness, obtained at 0.4 A sputtering current, initial state and annealed at  $800 \text{ }^\circ\text{C}$ , respectively; 3,4 - structures with 10 nm film thickness, obtained at 0.4 A, initial state and annealed at  $800 \text{ }^\circ\text{C}$  respectively.

as peculiarities of relaxation processes under short-term thermal treatment. The residual strains increase with raise of sputtering current and film thickness. At sputtering current 0.4A some process of film texturing takes place. The structural relaxation is exhibited in decreasing of mechanical strains in substrate as well as film recrystallization and transformation of surface morphology. The dependence of these processes on annealing temperature has not monotonous character and differs for various structures.

#### Acknowledgements

The help of Dr. I.V. Prokopenko and Dr. R.V. Konakova in results discussion is gratefully acknowledged.

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