

The texture of thin films of aluminum nitride obtained by magnetron sputtering

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The results of studying the texture of thin aluminum nitride films obtained by magnetron sputtering are presented. The dependence of the crystallite size and degree of preferential orientation on the conditions of the thin films formation (pressure, discharge power, composition of the plasma-forming gas) is considered.

Keywords: aluminum nitride films, magnetron sputtering, texture, size of the coherent scattering region.

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Thin films of aluminum nitride (AlN) have recently found wide application in microelectronics due to their excellent acoustic properties [1,2].

In modern science and industry, various methods of fabricating thin films are widely used, e.g. ion-plasma, ion-beam and thermal-vacuum deposition methods [2]. One of the most efficient methods for producing thin films is magnetron sputtering.

However, physical properties of piezoelectric AlN films significantly depend on the deposition parameters and conditions [5,6] which determine the arrangement of aluminum and nitrogen atoms on the substrate and, hence, the resulting film microstructure.

In a broader sense, the thin film internal microstructure refers to the grain size, stress, strain, and texture, that is, the preferential orientation of grains (crystallites) in the films. The film microstructure depends significantly on the substrate on which the film is applied, as well as on the fabrication conditions. The problem of controlling the texture has become an important challenge in thin-film technology. The texturing degree often varies during the thin film growth, and the most pronounced texture gets achieved only after the layer reaches a certain thickness. Thus, to optimize the deposition process, the thin film manufacturers need information on textures for different production-process conditions.

Despite the existence of numerous studies devoted to the formation of thin aluminum nitride films by magnetron sputtering, up-to-date models do not allow predicting the thin film structure resulting when different sputtering parameters are varying [3,7,8]; in addition, the relationship between the deposition parameters and physical properties of the resulting film has not been established for the modes specified in the paper. Since these films are to be used as piezoelectric layers in bulk-acoustic-wave microelectronic resonators, and their properties directly affect functional properties of these devices, establishing the dependence of

the film structure and texture on specific process modes is indeed important and determines the relevance of this study.

Structural and morphological properties fully determine the possibility of using thin aluminum-nitride films in devices of one or another type [9]. Particularly, thin AlN films to be used in devices based on surface acoustic waves should have a smooth surface and predominant orientation (002), since piezoelectric properties are strongly dependent on the film crystallographic orientation. Thus, the goal of this work was to study the texture of AlN thin films obtained by magnetron sputtering, namely, to determine the size and degree of preferential crystallite orientation depending on the conditions of thin film formation (pressure, discharge power, composition of the plasma-forming gas).

The AlN films to be studied were formed on glass-ceramic substrates by magnetron sputtering of an Al target (99.99%) in the Ar/N₂ reactive environment by using a setup for applying multicomponent coatings. Prior to sputtering, the substrates were chemically treated; then they were placed in a vacuum chamber where, in order to additionally clean the target from possible oxides before the film formation, the target was sputtered in argon; in the process, the substrate was closed by a shutter and power fed to the target exceeded that used in the AlN film formation by 10–15%.

Production process modes for the AlN films were the following. Ratios between the Ar/N₂ flows (in standard cubic centimeters per minute, sccm) were varied: 4/5 and 4/10. Power fed to the target was varied from 400 to 900 W, the substrate temperature was 350 °C, and the pressure ranged from 0.07 to 0.1 Pa. The target-to-substrate distance was 100 mm. The pressure was chosen so that the particles' mean free path was comparable to the target-to-substrate distance. It is known that, when the chamber pressure is 0.1 Pa, the mean free path is 10 cm; that at the pressure of 0.07 Pa is ~ 13 cm. The target was mounted at 10–11 cm from the substrate. Thus, the mechanism of

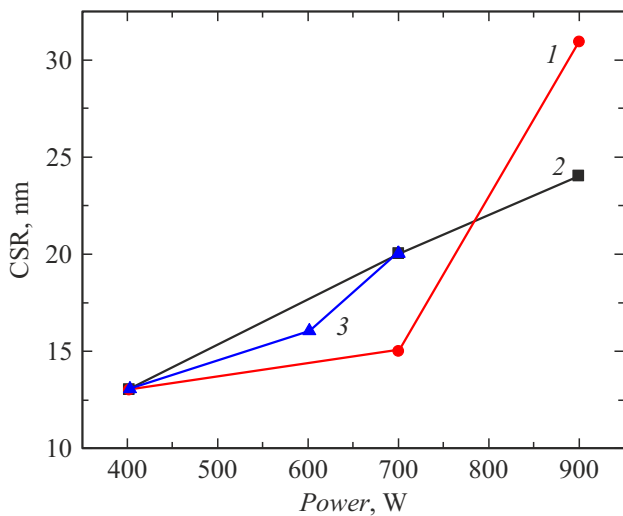


Figure 1. CSR size versus the discharge power. 1 — 10 sccm, 0.1 Pa; 2 — 5 sccm, 0.1 Pa; 3 — 5 sccm, 0.07 Pa.

delivering sputtered aluminum atoms to the substrate is a collisionless process. The AlN deposition temperature was chosen so that, in combination with the pressure calculated via the Thornton model of the structural zones of thin film formation, the thin film formation mode would fall into the T [10] zone, which enabled growing thin films with a close-packed columnar structure; in this case, the crystallites grow perpendicular to the substrate, i.e. along the (002) axis. In our previous studies [11–14], we have found the optimal values of the magnetron discharge power and ratios between the plasma-forming gas flows.

Diffraction analysis of the thin AlN film structural parameters was performed on diffractometer XRD-6000 based on the $\text{CuK}\alpha$ radiation. The subject of examination was phase compositions and structural parameters of the samples. The coherent scattering regions (CSRs) and preferential orientation of the films were analyzed using the

PDF 4+ databases and POWDER CELL 2.4 code for the full-profile analysis.

Fig. 1 presents the CSR size dependence on the magnetron discharge power. It is evident that the CSR size increases with the magnetron discharge power increasing from 400 to 900 W. As the magnetron discharge power increases, the adatoms' energy and surface mobility increases, which leads to the formation of larger crystallites.

Fig. 2 presents the CSR size dependence on the gas pressure. For the films obtained at the nitrogen concentration in the gas mixture of 10 sccm, CSR decreases with increasing pressure (Fig. 2, *a*), while at the nitrogen concentration of 5 sccm an inverse relationship is observed (Fig. 2, *b*). This may be explained by that at a higher concentration of nitrogen atoms in the working gas plasma (10 sccm) the number of high-energy aluminum atoms getting on the substrate decreases. Along with this, an increase in the working gas pressure leads to scattering of sputtered aluminum atoms because of their collision with argon atoms. The joint effect of these two factors is a decrease in the migration capacity of Al atoms deposited on the substrate, which leads to a decrease in the crystallite size. At lower nitrogen concentrations (5 sccm), the crystallite size increases with increasing working gas pressure, which is associated with the acceleration of diffusion of aluminum atoms adsorbed on the substrate surface and capturing small crystallites by larger ones.

Fig. 3 presents the dependence of the preferential orientation (002) degree on the magnetron discharge power. An increase in the magnetron discharge power leads to an increase in the deposition rate. Thin films deposited at a low discharge power have a low degree of orientation along the (002) plane, which may be associated with the fact that atoms sputtered in the direction of the substrate have energy insufficient to form a well-oriented structure. Further increase in power leads to a change in the microstructure and to the formation of a textured film with grains misoriented relative to each other, which is because the increase in the deposition rate promotes a

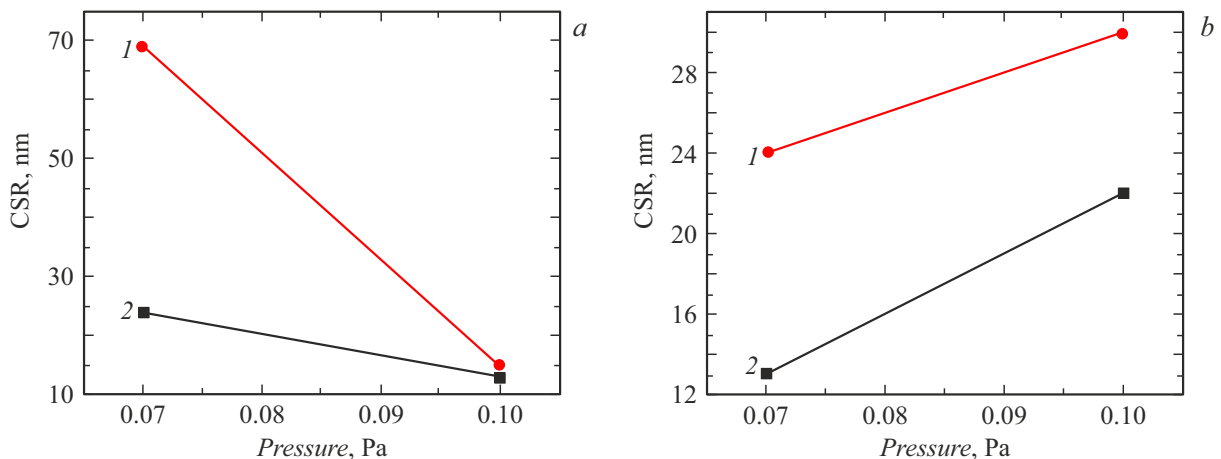


Figure 2. CSR size versus the gas pressure at different nitrogen concentrations: *a* — 10 sccm (1 — 700 W, 2 — 400 W); *b* — 5 sccm (1 — 900 W, 2 — 400 W).

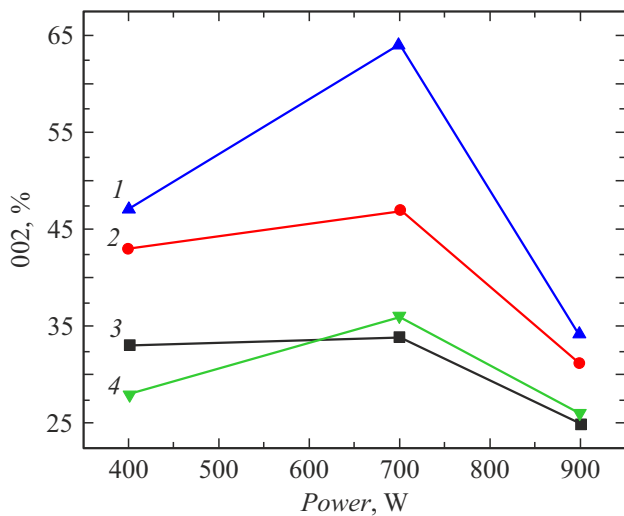


Figure 3. The degree of preferential orientation (002) versus the discharge power. 1 — 10 sccm, 0.07 Pa; 2 — 5 sccm, 0.1 Pa; 3 — 5 sccm, 0.07 Pa; 4 — 10 sccm, 0.1 Pa.

reduction of the surface diffusion. Analysis of experimental data shows that the optimal magnetron discharge power at which crystallites are formed with the highest degree of preferential orientation is 700 W.

Fig. 4 presents the dependence of the preferential orientation (002) degree on the gas pressure. In the case of films obtained at the nitrogen concentration of 10 sccm, the (002) orientation degree decreases with increasing pressure (Fig. 4, *a*), while, when the nitrogen concentration is 5 sccm, an increase in the (002) orientation degree with increasing pressure is observed (Fig. 4, *b*). This is explained by the fact that argon ions have a higher atomic mass and, hence, if they dominate in the gas mixture during the target bombardment, a greater number of higher-kinetic-energy aluminum atoms will be knocked out; being deposited on

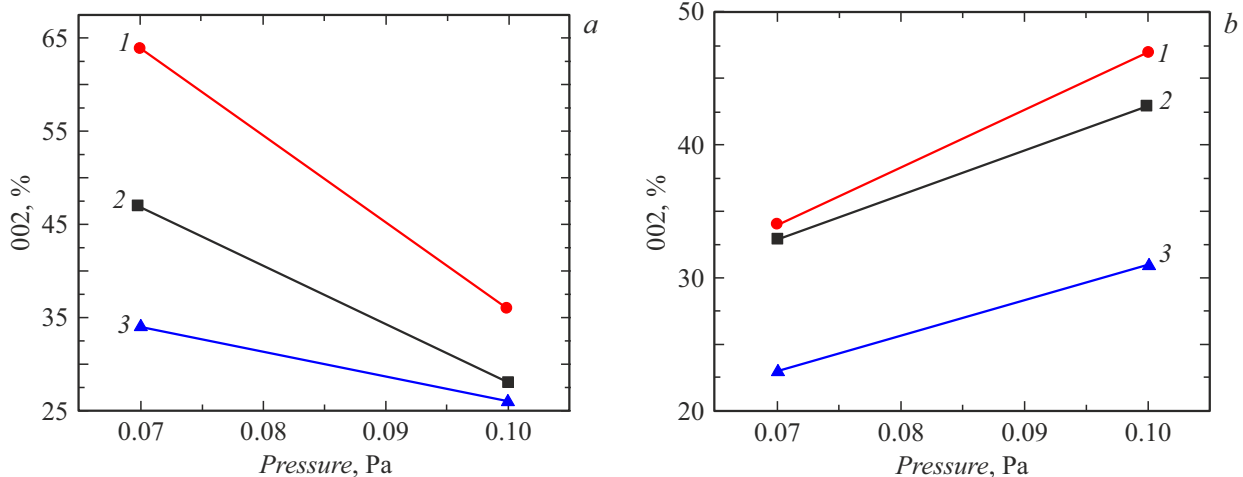


Figure 4. The degree of preferential orientation (002) versus the gas pressure at the nitrogen concentrations of 10 (*a*) and 5 sccm (*b*). 1 — 700 W, 2 — 400 W, 3 — 900 W.

the substrate, those atoms will form the (002) plane. The formation energy of the AlN close-packed (002) plane is higher than that for planes with other orientations, so the high energy of sputtered aluminum atoms will promote the growth of the (002) plane. As the nitrogen concentration increases, the number of collisions between the sputtered aluminum atoms and nitrogen atoms also increases, which leads to a loss of energy and a decrease in the number of high-energy aluminum atoms getting on the substrate and participating in creating the close-packed (002) plane.

Thus, the paper presents the results of studying the texture of thin aluminum nitride films in dependence on the conditions of their formation. Dependence of the CSR size and degree of preferential orientation (002) on the pressure, power and composition of the plasma-forming gas was investigated.

It was found that, when the ratio of gas flows (in sccm) is $\text{Ar}/\text{N}_2 = 4/5$, the fraction of the AlN phase with preferential orientation (002), as well as the crystallite size, increases with increasing pressure, while at the gas flow ratio of $\text{Ar}/\text{N}_2 = 4/10$ an inverse relationship is observed. The CSR sizes and degree of preferential orientation increase with the growth of the magnetron discharge power; however, the crystallites fraction with preferential orientation (002) begins decreasing after the power reaches a certain value. Results of the experimental data analysis have shown that the optimal magnetron discharge power at which crystallites are formed with the maximum degree of preferential orientation (002) is 700 W.

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Conflict of interests

The authors declare that they have no conflict of interests.

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