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The Influence of Substrate and Buffer Layers on the Structure of GaN Thin Films During Radio-Frequency Sputtering

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Thin GaN films are obtained on sapphire (Al_2O_3) substrates and amorphous quartz (υ-SiO_2) substrates with $MgAl_2O_4$, AlN, and ZnO buffer layers using radio-frequency (RF) ion-plasma spraying in a nitrogen atmosphere. Based on x-ray phase analysis, the phase composition of the obtained films is investigated, and the sizes of the nanocrystallites forming the deposited GaN films, as well as the average stresses in the crystal lattices, are determined. As found, the smallest crystallite sizes and the highest mechanical stresses are characteristic for thin GaN films deposited on quartz substrates with an $MgAl_2O_4$ buffer layer.

Методом високочастотного (ВЧ) йонно-плазмового розпорошення в атмосфері азоту одержано тонкі плівки GaN на сапфірових підкладинках (Al_2O_3) та підкладинках з аморфного кварцу (υ-SiO_2) із буферними підшарами $MgAl_2O_4$, AlN і ZnO. На основі рентґенофазової аналізи досліджено фазовий склад одержаних плівок, визначено розміри нанокристалітів, які формують осаджені плівки GaN, та середні напруження кристалічних ґратниць. Встановлено, що найменші розміри кристалітів і найбільші механічні напруження характерні для тонких плівок GaN, осаджених на кварцові підкладинки з буферним підшаром $MgAl_2O_4$.

Key words: gallium nitride, thin films, buffer layer, RF sputtering.

Ключові слова: нітрид Ґалію, тонкі плівки, буферний підшар, високочастотне напорошення.

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1. INTRODUCTION

Compounds based on gallium nitride (GaN) and gallium oxide (Ga_2O_3) are promising materials for optoelectronic applications. They are used to produce semiconductor lasers and light-emitting diodes, which emit in the blue and ultraviolet regions of the spectrum, and are also used as detectors of ultraviolet radiation [1–8]. Along with this, high-power fast-acting transistors based on GaN have also become widely used. Such devices surpass their silicon counterparts in terms of operating frequencies and power densities [9–13].

An important technical task in the creation of various electronic devices based on thin GaN films is to obtain films of perfect quality with a controlled composition of intrinsic defects. Such atomic defects largely determine the absorption and emission spectra, the type and magnitude of electrical conductivity, and a number of other optical and electrical properties of the material.

To obtain samples of the required quality based on thin GaN films in electronic or optoelectronic device technologies, it is important to find optimal substrates, which match GaN in terms of crystal-lattice parameters and thermal-expansion coefficient. Another approach to solving this problem is to use thin buffer layers, whose characteristics are consistent with the high-temperature growth modes of the main gallium-nitride layer. The properties of the buffer layer used are indirectly determined by the properties of the main thin-film layer deposited on it. At the same time, optimisation of the deposition mode of films of the required quality is only possible, if there is a suitable buffer layer. In general, the procedure for determining the optimal parameters for the deposition of thin GaN films is complex and multifaceted.

Based on this, this work conducts structural studies of thin GaN films obtained by radio-frequency (RF) ion-plasma spraying on various substrates and $MgAl_2O_4$, AlN, and ZnO buffer sublayers. The RF ion-plasma spraying method is considered optimal for obtaining homogeneous semiconductor and dielectric films [14].

2. EXPERIMENTAL TECHNIQUE

Thin GaN films with a thickness of 0.3–1.0 μm were obtained by radio-frequency ion-plasma spraying in a nitrogen atmosphere. The films were deposited on sapphire (Al_2O_3) substrates and amorphous quartz (υ-SiO_2) substrates, on which there are corresponding buffer sublayers of $MgAl_2O_4$ (υ-$SiO_2 + MgAl_2O_4$), AlN (υ-SiO_2 + AlN) and ZnO (υ-SiO_2 + ZnO).

The structure and phase composition of the obtained gallium-nitride films were studied by x-ray diffraction analysis (Shimadzu XDR-600). X-ray structural studies showed the presence of a polycrystalline structure with a predominant orientation in the (002) and (011) planes, depending on the type of substrate. At the same time, all diffraction maxima are identified according to the selection rules for the ideal hexagonal structure of wurtzite.

3. RESULTS AND DISCUSSION

One of the most reliable methods for determining the composition and structure of a substance under investigation is x-ray phase analysis. The diffraction patterns we obtained for thin GaN films on various substrates and buffer layers are shown in Fig.

Analysis of the obtained diffractograms shows that the structure of the deposited films differs slightly depending on the type of substrate or buffer layer. In particular, it has been established that films deposited on sapphire (Al_2O_3) substrates and quartz (υ-SiO_2) substrates with $MgAl_2O_4$ and AlN sublayers have a dominant orientation in the (011) plane. At the same time, films deposited on a quartz substrate with a ZnO sublayer have a dominant orientation in the (002) plane. In addition, we have established that, for thin GaN films deposited on a υ-$SiO_2 + MgAl_2O_4$ substrate, there is a slight shift of the maximum dominant characteristic reflection band from the (011) plane towards smaller 2Θ-angle values up to 36.35°. For gallium-nitride films deposited on pure sapphire (Al_2O_3) sub-

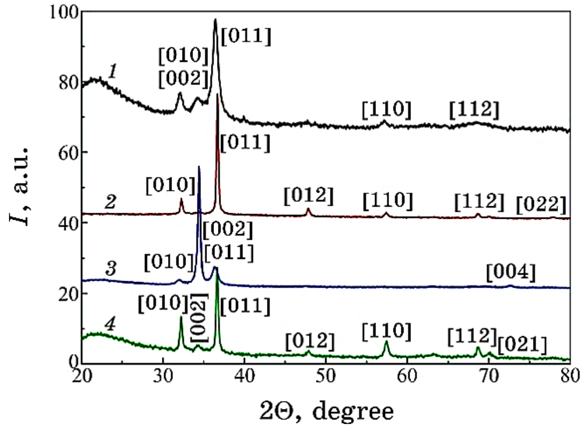

Fig. X-ray diffractograms of thin GaN films deposited on a quartz substrate with an $MgAl_2O_4$ underlayer (*1*), on a pure sapphire substrate (*2*), on a quartz substrate with a ZnO underlayer (*3*), and an AlN underlayer (*4*).

strates and υ-$SiO_2 + AlN$ substrates, the 2Θ-angle values for this reflection band are of 36.68° and 36.65°, respectively. The reason for this shift is most likely a slight increase in the interplanar distances in GaN films on υ-$SiO_2 + MgAl_2O_4$ substrates relative to films on the other two types of substrates. Considering that the value of the detected shift exceeds the instrumental error of the experiment ($\Delta 2\Theta > 0.07°$), it can be stated that the packing density of GaN films on υ-$SiO_2 + MgAl_2O_4$ substrates is lower than on the Al_2O_3 and υ-$SiO_2 + AlN$ substrates. This situation is consistent with previous studies, which have shown that the packing density of thin films is determined by technological parameters and the type of substrate and is lower than the packing density of single-crystal samples [15].

It is known that the widths of diffraction bands are determined by the sizes of nanocrystals (areas of coherent scattering) and the presence of defects and mechanical stresses in the sample [16]. This allows the obtained results to be used to determine the size of the particles, which form the obtained thin films, and to analyse the mechanical stresses in the samples.

According to Debye and Scherrer, the relationship between the half-width of the diffraction band and the size of the crystallites d is given by the expression

$$d = \frac{0.94\lambda}{\beta \cos\Theta}, \tag{1}$$

where λ is the wavelength of the diffracting wave, which is of 0.15418 nm (CuK_α radiation) in our case, β is the half-width of the diffraction band (width at half height), and Θ is the diffraction angle.

Another reason for the broadening of diffraction bands is imperfections in the structure of crystallites and defects, which cause stress in crystallites. Stress-related broadening is described by the expression

$$\varepsilon = \frac{\beta}{4\mathrm{tg}\Theta}, \tag{2}$$

where ε is the average value of the crystal-lattice stresses.

If the broadening of the bands is caused by the presence of very small particles in the sample, then, the characteristic bands will have values close to $\beta\cos\Theta$. Otherwise, in the presence of stresses, the diffraction bands will have values close to the ratio $\beta/(4\mathrm{tg}\Theta)$.

The results of calculations of the crystallite sizes d and the average values of the crystal-lattice stresses ε in gallium-nitride films depending on the substrate type are given in Table.

Analysis of the results presented in Table indicates that the sizes

TABLE. Analysis of diffraction-band broadening in thin GaN films depending on the substrate type and buffer layer.

Substrates	Characteristic band	Angle 2Θ, degree	β	*d*, nm	ε
Al_2O_3	(011)	36.68	0.0040	38.2	0.0031
υ-SiO_2 + $MgAl_2O_4$	(011)	36.35	0.0116	13.2	0.0088
υ-SiO_2 + AlN	(011)	36.65	0.0052	29.4	0.0039
υ-SiO_2 + ZnO	(002)	34.42	0.0059	25.7	0.0047

of nanocrystals forming thin GaN films are determined by the type of substrate and buffer layer, on which these films are deposited. At the same time, the smallest size of nanocrystals and the highest stresses in them are observed for thin GaN films deposited on quartz substrates with an $MgAl_2O_4$ buffer layer. Other types of substrates and buffer layers are characterised by larger sizes of nanocrystals, which form GaN films and lower stresses. The ε values we obtained indicate that thin GaN films obtained by RF sputtering in a nitrogen atmosphere are characterised by rather low average crystal-lattice stresses. For example, in thin films based on Y_2O_3 obtained by RF sputtering in different atmospheres, the ε values vary from 0.0125 to 0.0148 [17].

4. CONCLUSIONS

Based on x-ray phase analysis data, it was established that thin GaN films obtained by RF sputtering in a nitrogen atmosphere form a hexagonal wurtzite structure on sapphire (Al_2O_3) substrates and quartz (υ-SiO_2) substrates with $MgAl_2O_4$, AlN and ZnO. Analysis of the width of the diffraction bands showed that the sizes of nanocrystals forming gallium-nitride films on these substrates vary from 13.2 to 38.2 nm, depending on the type of substrate. It was found that low average crystal-lattice stresses are observed in the deposited GaN films for all types of substrates. At the same time, the smallest crystal sizes and the highest mechanical stresses are characteristic of thin GaN films deposited on a quartz substrate with an $MgAl_2O_4$ buffer layer.

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