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The effect of AlN buffer layer morphology on the structural quality of a semipolar GaN layer grown on a Si(001) substrate, according to transmission electron microscopy data

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Structural features of the interface between a semipolar gallium nitride layer and buffer layer of aluminum nitride grown on a SiC/Si(001) template misoriented by an angle of 7° were studied by high-resolution transmission electron microscopy. The effect of interface morphology on the structural quality of the gallium nitride layer was revealed: faceted structure of the buffer layer surface reduces the threading dislocations density.

Keywords: semipolar GaN, transmission electron microscopy, dislocation, Si(001) substrate

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Compounds Al/Ga/In−N (III-nitrides) and their alloys are direct−gap semiconductors with the bandgap of 0.7 eV for InN to 6.2 eV for AlN [1]. In this connection, III-nitrides are promising materials for creating wide−spectral− range optoelectronic devices. Nowadays the GaN substrates for homoepitaxy are very expensive. Therefore, III-nitrides are synthesized by heteroepitaxy on sapphire or silicon−carbide substrates that possess such drawbacks as high price and small diameter. Silicon wafers have at present large sizes; using wafers of the (001) orientation allows integration into the well developed silicon technology. Unfortunately, considerable lattice mismatch and significant difference in the thermal expansion factors of silicon and gallium nitride (35% [2], 50% [3]) negatively affect the active layer quality. To overcome this disadvantage, various buffer layers are used. In addition to defects of active layer crystal structure, a source of a significant decrease in the efficiency of light−emitting devices is the presence in wurzite−type gallium nitrides of considerable internal electrostatic fields induced by piezoelectric and spontaneous polarization [4,5]. Paper [6] showed theoretically that one of the ways to overcome this problem is growing the GaN layer in the semipolar orientation, when the GaN [0001] direction (polar axis c) does not coincide with the film growing direction.

At present most researchers use nanostructured substrates formed by using the high−cost procedure of selective chemical etching [7–9]. Concurrently, attempts are taken to synthesize GaN layers on vicinal Si(001) substrates without selective etching. In this case, a problem arises of how to improve structural quality of epitaxial layers in order to increase the efficiency of device structures constructed on them. Our investigation showed that the most promising in this field is heterostructure GaN/AlN/SiC/Si(001) since the use of the concerted atom displacement method [10] for synthesizing the SiC buffer layer results in that the buffer layer surface contains SiC(111) facets [11]. These facets are deviated from the surface normal by 54.7°, which is close to the angle of $\sim 45°$ that is optimal for reducing the polarization effect [6]. What is important is that the layer should be in the monocrystalline rather than in the polycrystalline state, as, e.g., in [12,13].

Most defects are formed in the area of interface between the epitaxial layer and substrate. The goal of this work is to study by high−resolution transmission electron microscopy (TEM) structural features of the GaN/AlN interface in the GaN/AlN/SiC/Si(001) heterostructure.

A combined SiC/Si substrate was fabricated on a Si(001) wafer 1.5″ in diameter misoriented by 7° in the ⟨110⟩ direction according to the procedure described in [10]. As our earlier investigations showed, such substrates enable formation of semipolar GaN layers. Then the AlN buffer layer (0.8 μm) was synthesized by the chloride−hydride gas−phase epitaxy at the substrate temperature of 1080°C; the main GaN layer (15 μm) was fabricated at 1050°C.

The interface structural state was studied by using transmission electron microscopes Titan 80-300 (with the accelerating voltage of 300 kV) and Philips EM420 (100 kV). The microscopy samples were prepared according to the standard procedure comprising polishing and ion etching.

Survey TEM images of the GaN/AlN interface area (Fig. 1, a) were obtained in the Z-contrast mode using a large−angle darkfield circular detector. This mode allows the highest−contrast recording of images of the sample areas of different chemical compositions. One can see that the interface profile has a saw−like shape formed from the aluminum nitride facets. The ratio between the "tooth" short and long sides ranges from 0.2 to 1. As shown by the analysis of images obtained in the high−resolution scanning TEM mode (Fig. 2) and of microdiffraction patterns, the AlN layer surface was formed mainly by facets $(1\bar{1}01)$ and $(\bar{1}101)$. The facet sizes are of about tens of nanometers. Thus, the next GaN layer originates in the areas not larger

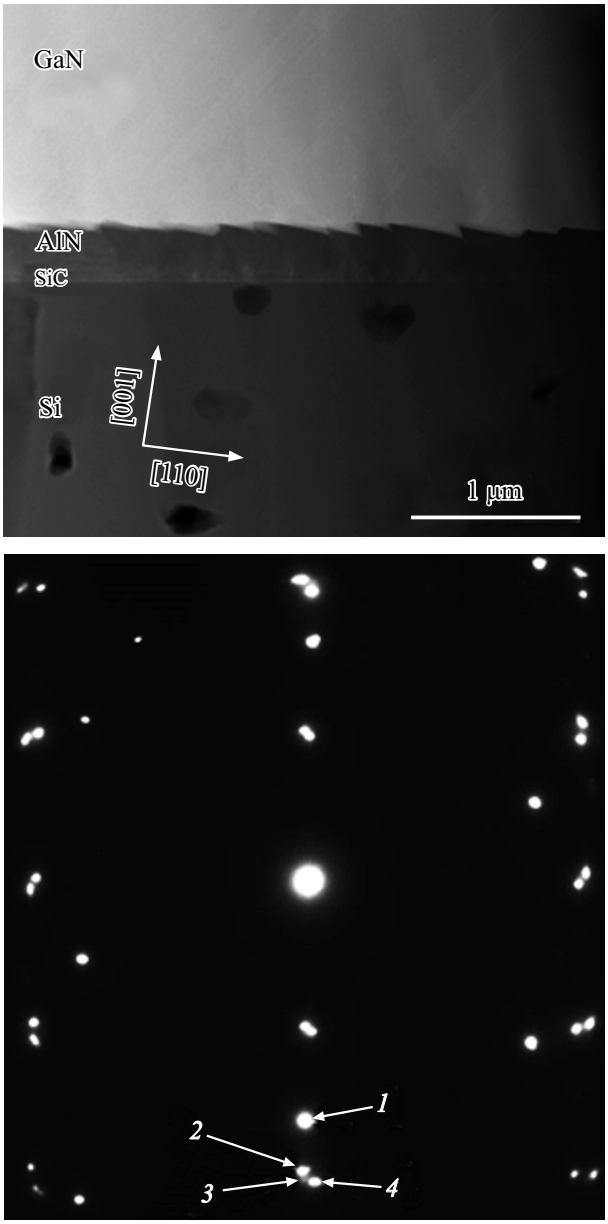

Figure 1. Large−angle darkfield TEM image of the heterostructure cross−section (*a*) and microdiffraction pattern recorded in the area of interfaces (*b*). *1* — reflex $\overline{1}11$ Si, *2* – 0002 GaN, *3* — $\overline{1}11$ SiC, *4* — 0002 AlN.

than the facets represented in the scheme (Fig. 3) by straight line segments *AB* and *AD*. It is known that the absence of dislocations in axial heterostructures formed in nanowhiskers (NWs) is connected with lateral relaxation of elastic stresses. The relaxation is possible because of a small cross section and free lateral surface of the nanowhiskers. In addition, in the case of an axial heterostructure, the substrate (the preceding part of NWs) also reduces the elastic energy by deformation. If the cross section is sufficiently small, the energy of the next NW section with dislocations exceeds the elastic energy of the pseudomorphic layer [14], and axial heterostructures become free of mismatch dislocations. The last is very important: according to the commonly accepted model, only a certain mismatch dislocation segment is located in the interface area, the rest part of the dislocation line spreads up to the interface area, namely, forms a threading dislocation that is a structural defect responsible for the reduction in efficiency of heterostructure−based devices.

The fact that in the studied structure there occurs a deformation−induced stress relaxation, as in the case of the NW−based heterostructure, is confirmed by the twist of the main layer crystal lattice with respect to the buffer layer lattice toward the substrate, which phenomenon is caused by the saw−like interface shape and the difference

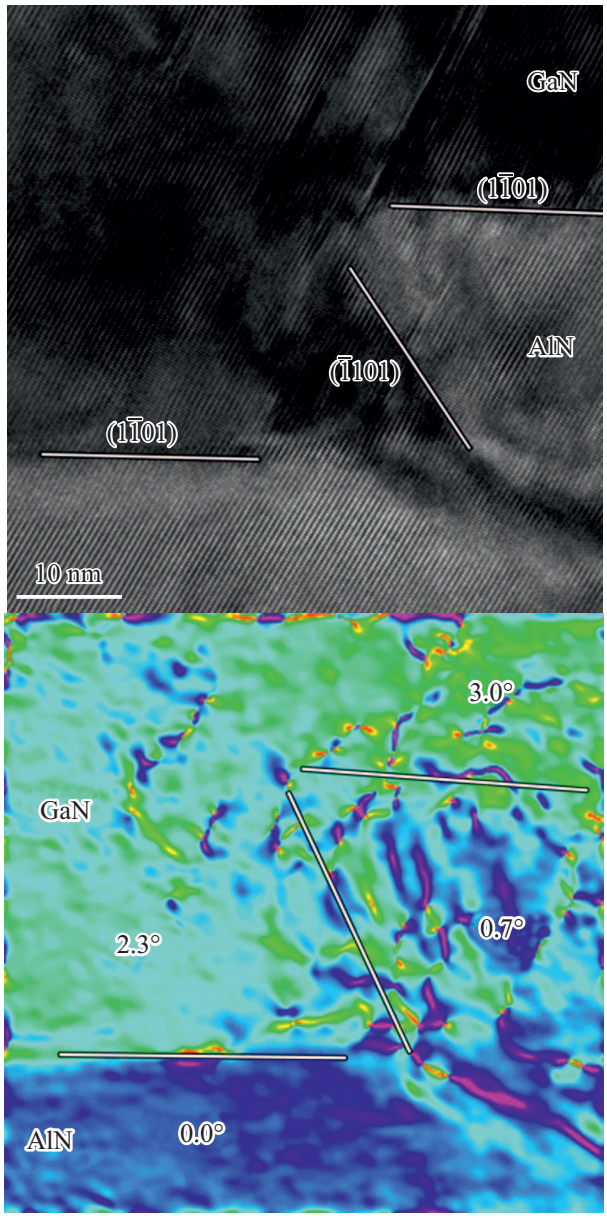

Figure 2. High−resolution TEM image of the GaN/AlN interface area and the corresponding twist map of the (0001) planes. Different colors relate to different twist angles (the colored picture is given in the electronic version of the paper).

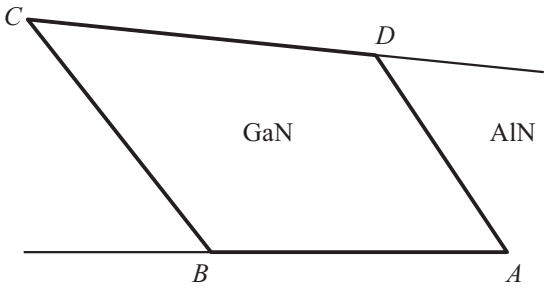

Figure 3. Schematic illustration of the GaN layer formation.

The model dependence of the twist angle of the GaN layer crystal lattice relative to the AlN lattice on the ratio between dimensions of the buffer layer facets $(\bar{1}101)$ and $(1\bar{1}01)$

Dimensions ratio	Twist angle, °
0.25	10
0.5	4.0
0.75	2.2
1	1.2
1.75	0

in the lattices parameters of epitaxial layers [15,16]. In the electron microdiffraction pattern recorded in the interface area (Fig. 1, *b*), reflexes generated by reflections from the GaN(0002) planes do not lie in the same line as reflexes generated by the AlN(0002) planes but are deviated by an angle of about 1° and slightly blurred. A more detailed pattern (Fig. 2) of the GaN crystal lattice twist was obtained by computer processing of the high−resolution TEM image. The figure presents the twist map of the (0001) planes in the interface area in the form of a color palette (the colored version of the figure is given in the electronic version of the paper). Apparently, twists of different segments of the main layer are different; some segments of the buffer layer also get somewhat twisted under the action of elastic stresses, which also reduces the elastic energy.

Variability of the crystal lattice twist angle may be explained via a simple geometric model. Consider the gallium nitride nanocrystal *ABCD* generated on the buffer layer (Fig. 3). As the growth surfaces, pyramidal planes $(\bar{1}101)$ and $(1\bar{1}01)$ were chosen because they are most stable in the process of growth; these planes are represented in the scheme with straight line segments *BC* and *CD*. The model is based on the assumptions that the GaN lattice along line segments *BC* and *CD* is fully relaxed and parameters of the GaN lattice along *AB* and *AD* coincide with those for the AlN layer. Lengths of the straight line segments enclosing rectangle *ABCD* were chosen so that the ratio between the lengths of opposite sides were the same as between corresponding interplane distances of the main and buffer layers. For clarity, the line segment lengths ratio shown in the scheme is overstated. Thus, in the framework of the proposed model the ratios between the buffer layer facet sizes may be varied by varying the line segment lengths ratio AD/AB. This model is more complex than that presented in [15] since it takes into consideration the difference in lattice parameters on both facets. There was calculated the difference between angles $180° - \angle CBA$ and $\angle DAB$ which was assumed to be the measure of the main layer lattice twist. The facet sizes were determined from measurements made on the interface area microphotographs. The calculations presented in the table demonstrate a strong dependence of the crystal lattice inclination angle on the ratio between sizes of facets $(\bar{1}101)$ and $(1\bar{1}01)$; just this dependence explains variability of the crystal lattice twist angle. The absence of twisting is possible only at the facet sizes ratio of 1.75; however, geometrically it is impossible to obtain a constant−thickness buffer layer at such a ratio. Evidently, it is possible to reduce the mutual twist of individual main layer segments by decreasing the variation in the ratio between the buffer layer facet sizes. The reduction of the mutual twist results in a decrease in the density of dislocations emerging on the inter−grain boundaries.

The calculated angles are, of cause, significantly overvalued due to the made simplifications. Local measurements of the twist angles (Fig. 2) gave values 2.3 and 3°. Relaxation of the elastic stress induced by the mutual twisting of different GaN layer regions is caused by the bend deformation and edge dislocations in the vicinity of small−angle boundaries. Lines of those dislocations are parallel to the interface within the grain generated on the facet. After leaving the intergrain boundary, the dislocation will spread over the basic plane up to the growth surface, which will negatively affect the device structure that can be potentially formed on the GaN layer. As our estimates showed, in the case of total stress relaxation due to plastic deformation, the mismatch dislocation density is at least half an order of magnitude lower than the dislocation density at small−angle boundaries.

Thus, the faceted structure of the GaN/AlN interface promotes reduction of the mismatch dislocation density due to lateral relaxation of elastic stresses. This manifests itself in relatively low density of threading dislocations ($4 \cdot 10^9\,\mathrm{cm}^{-2}$ at $2\,\mu$m from the interface and $3 \cdot 10^8\,\mathrm{cm}^{-2}$ at the GaN layer surface [17]). By using the significantly more expensive method of substrate masking, the density of $5 \cdot 10^7\,\mathrm{cm}^{-2}$ was reached [18]. Notice that in this case not Si(001) but sapphire was selected as a substrate, which allows easy integration of this method into the silicon technology.

Significant improvement of the GaN structural quality may be reached by reducing the variation in the ratio between sizes of the buffer layer facets. Thus, the method for growing semipolar gallium nitride layers on silicon substrates without preliminary selective etching may be regarded as promising.

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Conflict of interests

The authors declare that they have no conflict of interests.

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