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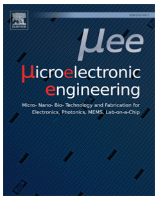

Research paper

Semipolar AlN on Si(100): Technology and properties

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ABSTRACT

Initial stages of the semipolar AlN layer formation by chloride-hydride vapor phase epitaxy on a misoriented Si(100) substrate with a thin intermediate nano-SiC layer grown by atomic substitution method are investigated. It is found that once the growth rate of AlN layer on a nano-SiC/Si(100) substrate is about 0.02 μm/h, the layer is formed in a polar direction. On the other hand, at the growth rate of 1 μm/h the layer is formed in a semipolar direction. We propose the model of the semipolar AlN layer growth based on the formation of the special structure on the SiC layer synthesized by atomic substitution and on the possibility of the matching of the quasi-lattices of Al(20 − 23) and 3C—SiC(100) planes assuming bonding of four atoms from the layer to four atoms of the 3C—SiC quasi-lattice consisting of three lattice unit cells in one of the directions.

Aluminum nitride (AlN) is a prospective material for devices intended for ultraviolet optoelectronics, power, high-frequency electronics and biosensorics. Besides it is an efficient buffer layer material for the formation of epitaxial layer on foreign substrates. However, a strong piezoelectric polarization peculiar for III–N wurzite polar structures promotes formation of the structures with reduced internal fields called as semipolar structures. On the basis of this approach, many attempts were undertaken to synthesize the semipolar aluminum nitride on different substrates, such as r-sapphire [1], r-$LiAlO_2$ [2], α-ZnO [3], and m-SiC [4].

Recently it was found that the semipolar AlN can be grown on Si (100) substrates with a thin intermediate 3C—SiC layer. Application of 3C—SiC as buffer layer enables reduction of the mismatch in lattice constants and thermal expansion coefficients of the silicon substrate and the layer. Once the AlN is grown epitaxially by metal-organic chemical vapor deposition (MOCVD) on the 3C—SiC/Si(100) substrate the layer at first nucleates in the form of AlN cubic crystals, and then transforms to the hexagonal aluminum nitride [5]. In the process of AlN epitaxy on the 3C—SiC/Si(100) quasi-substrate by magnetron sputtering the transition of the orientation of the AlN layer from (002) to (101) was observed when the composition of the N_2/Ar gas mixture was changed [6]. On a Si(100) substrate with the preliminary formed nano-SiC layer the GaN(20–23) layer was grown by HVPE [7], and the light-emitting diode InGaN/GaN(20–23) structures with thin AlN buffer layers were obtained by MOCVD [8]. However, no data on the conditions of nucleation and growth of the semipolar AlN on silicon substrate is available so far.

In this paper we investigate the conditions for nucleation and growth of the semipolar AlN by HVPE on a Si(100) substrate with a thin intermediate SiC layer.

Two kinds of SiC films grown on silicon substrates by topochemical substitution of atoms were used to study the mechanism of the semipolar AlN growth. Boron-doped p-type silicon substrates (KBD) with the specific resistance of 20 Ω·cm were used in the experiments. Silicon substrates were misoriented from the (100) plane by 4° towards ⟨110⟩ direction. The process temperature, time of the SiC film growth and composition of the gas mixture were corresponded with the optimal synthesis conditions proposed in [9]. The synthesis was performed at 1250°C in a CO + SiH_4 gas mixture. The synthesis duration was 20 min. Two different CO partial pressures were used. Sample Nos. 1 and 2 were synthesized with CO partial pressures of 0.6 and 1 Torr, respectively. The reasons for using different CO partial pressures in the synthesis process will be discussed later. The thicknesses of SiC layers in the samples Nos. 1 and 2 were 80 and 50 nm, respectively.

Then on the surfaces of SiC layers the AlN layers were grown by HVPE at $T = 1080$ °C, as in [10,11]. The thickness of the layers was in the range ~0.3–1 μm. The III/V flux ratio in the growth zone was about 500. The AlN layers were grown with the rate of either 0.02 μm/h or 1 μm/h both on the substrate No. 1 and on the substrate No. 2. To this end, each of the substrates Nos. 1 and 2 was cut on several pieces. The

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AlN/SiC/Si(100) structures obtained were studied by x-ray diffraction, scanning electron microscopy (SEM), and transmission electron microscopy (TEM).

Let us discuss the reason why the SiC layers were synthesized at different partial pressures of CO gas. In accordance with available data reviewed in [9], the main feature of the SiC growth on Si is the formation of the set of dilatation dipoles in the near-surface region of the silicon lattice. These dilatation dipoles are the stable complexes consisting of the dilatation centers as interstitial carbon atom and silicon vacancy ("C" – "V_{Si}"). In a crystal with cubic symmetry these two dilatation centers attract each other elastically. This attraction results in the formation of the [111] planes independent of the initial crystallographic plane of Si substrate on which a SiC was synthesized. Formation of these planes on vicinal (100) surfaces misoriented by 4–7 causes formation of the tilted facets [9], which act as new surfaces for the growth of semipolar hexagonal crystals as AlN and GaN [10]. As shown in [9], the morphology, density and sizes of the facets depend in a great extent on the partial pressure of CO being maintained in the process of the topochemical synthesis of SiC. At low CO partial pressures, a thicker and rough SiC films with the developed surface morphology are formed. On the other hand, at high CO partial pressures the films are more thin and flat. At very high CO partial pressures, extremely flat SiC films with the roughness of about 1 nm or even less can be obtained [9]. At low CO partial pressures, mountain-peak-like three-dimensional structures are formed (Fig. 1). Note that these structures should not be confused with the nuclei formed in the process of the standard film growth methods. In accordance with [9], in the course of growth the SiC nuclei are formed inside the Si substrate, while on its surface the SiC islands appear that are pushed from below by gas-phase reaction products. At high CO partial pressure the facets formed at the vicinal (100) surfaces will have different structure. In particular, the initial ⟨011⟩ silicon steps transforms after SiC growth to rather large (111) facets [10,11], whereas the initial silicon (100) terraces are covered with small (111) facets with the size not exceeding 1–2 nm. Moreover, while the initial faces of the (011) steps are covered by the (111) faces oriented in one direction only, since the steps remove initial degeneration on formation of the elastic dipole [9], on the terraces all kinds of facets with (111) planes can be formed. It is known that the angle between these planes can be either zero, or 70 32′. As a result, the terraces will look like saw-tooth structures and large tilted facets will occur on their boundaries. So, the nucleation of the AlN layer on such structures will depend in a great extent on supersaturation, or on the layer growth rate. Once the supersaturation is high (high growth rate), the critical radius of the nuclei is low [12]. In this case, the critical radius will sense and discriminate the structure of small facets on a terrace and the structure of large facets on the steps. As the area of the terraces exceeds the area of the facets on the steps, the terraces will determine the morphology and orientation of the forming AlN layer. Therefore, the morphology and orientation of the AlN layers grown on the substrates No.1 and No. 2 will be essentially different. On the other hand, at slow supersaturation (low growth rate) the morphology of the AlN layers grown on these two substrates will be similar.

X-ray diffraction studies of the AlN layers confirmed our assumptions and show that the formation of the AlN layer by HVPE in polar or semipolar direction is determined by the structure of the SiC layer. In particular, on the sample No. 1 which surface is covered with the pyramidal protrusions the semipolar structure AlN(20–23) on SiC/Si(100) is formed when the growth rate of AlN layer is about 1 μm/h (high supersaturation). At the more flat surface of the sample No. 2 under the same conditions the AlN layer is formed with different inclination and its plane will be tilted from the polar state by only 15°. If the AlN layer growth rate is only about 0.02 μm/h (low supersaturation), then the AlN(0002) layer grows on both SiC/Si(100) substrates Nos. 1 and 2. This result is clearly seen in SEM images (Fig. 1). In particular, the surface is flat if the layer growth rate is 0.02 μm/h (Fig. 2c), while on the surface of the layer grown at the rate of ~1 μm/h the agglomerations of AlN grains are clearly visible (Fig. 1c).

TEM image of the cross-section of the AlN/SiC/Si(100) structure grown with the rate of 1 μm/h (Fig. 1b) indicates that the inclination of the layer from the 3C–SiC(111) surface with three-dimensional

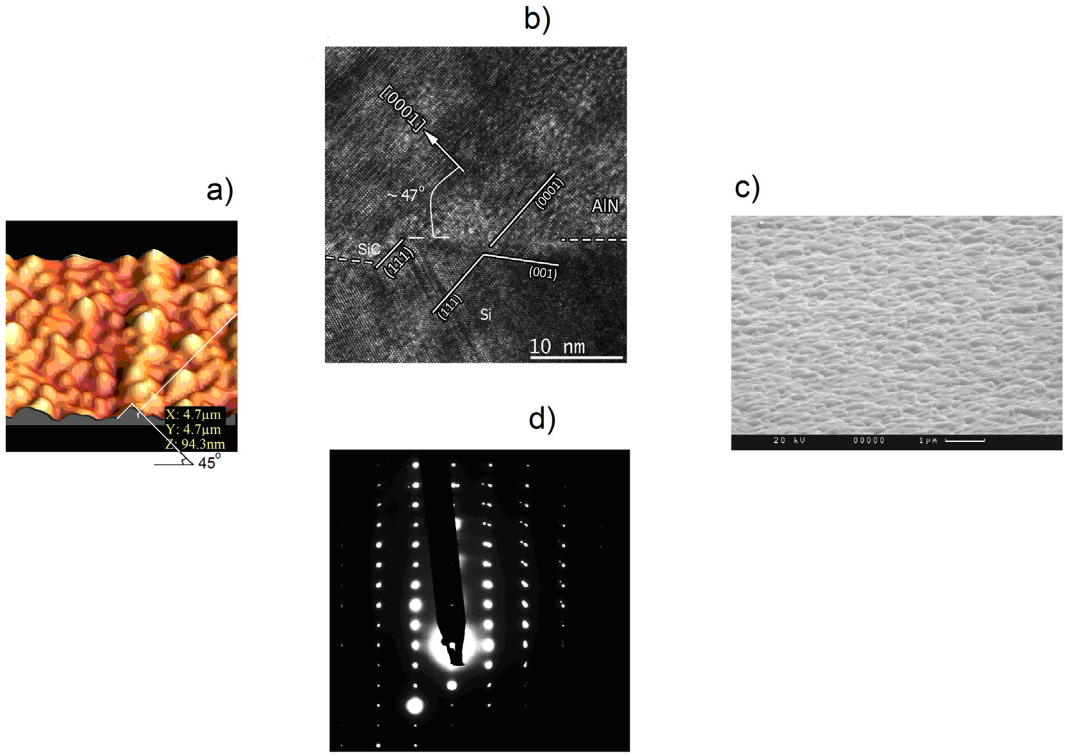

Fig. 1. AFM image of the SiC/Si(100) surface (a), TEM image of the cross-section of the AlN/3C–SiC structure (b), SEM image of the AlN surface (c) and diffraction pattern of the semipolar AlN (d) for the sample No. 1.