



Full Length Article

Peculiarities of the AlN crystalline phase formation in a result of the electron-stimulated reconstruction transition ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ – (1 × 1)

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ABSTRACT

In the present work, it was found for the first time that an electron beam used in reflection high-energy electron diffraction technique stimulates a reconstruction transition from a sapphire ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ superstructure which is chemically inert under an ammonia flux to an unreconstructed (1 × 1) structure with subsequent surface nitridation. The electron beam initiates electron-stimulated oxygen desorption from the sapphire surface followed by formation of oxygen vacancies, which are potential energetically accessible centers for the primary nuclei formation of the AlN crystalline phase.

1. Introduction

After Isamu Akasaki [1], Hiroshi Amano [2], and Shuji Nakamura [3] success in obtaining on a sapphire substrate a first bright blue LED based on III-nitride semiconductor compounds, these semiconductors are considered as a very promising materials for opto- and electronic applications. Despite the fact that, today native AlN and GaN substrates are gradually beginning to be used for growing III-nitride structures, foreign substrates are still widely applied in industrial technology. One of the most common substrates is a sapphire (Al₂O₃) substrate. Sapphire is transparent in the visible and UV wavelength ranges, has a rather high thermal conductivity (40 W/m·K at 300 K), is thermally stable, has high crystalline perfection and much cheaper than SiC or native nitride substrates.

On the Al₂O₃ surface, after being placed in the loading chamber, adsorbed carbon and hydroxyl groups are retained [4–6], and the surface may consist of mixed cationic/anionic areas [7]. Since the Al₂O₃ substrate for epitaxial growth is initially “epi-ready” prepared, it is preliminary annealed before loading to the growth chamber without additional chemical treatment. Annealing leads to the surface cleaning from residual impurity gases and improving the structural properties of the substrate surface, increasing the terraces size between steps [8–10], and decreasing the roughness [9]. When the samples are heated to high temperatures (over 1150 °C), a reconstruction transition (1 × 1) → ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ on the sapphire surface occurs [11,12]. The sapphire

($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ surface reconstruction was investigated in the classical work of French and Somorjai (1970) by the low energy electron diffraction technique (LEED) [11]. The reconstruction model is shown in Fig. 1a. It was found that the ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ superstructure is formed upon high-temperature annealing, and the reverse reconstruction transition ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ → (1 × 1) is possible when the sapphire surface is exposed to oxygen (at high temperatures about of 1000–1200 °C). It was also indicated that the ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ superstructure can be obtained by direct Al deposition on a clean unreconstructed sapphire surface and further annealing of the surface at a temperatures of about 800 °C. The surface reconstructed ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ layer has been described as an oxygen-depleted layer or, in other words, as partially reduced aluminum oxide (i.e., containing suboxides AlO, Al₂O). A model of a surface reconstructed monolayer (ML) as an suboxide with a rectangular lattice 4.40 × 4.57 Å² (Fig. 1c) rotated by 9° relative to the sapphire lattice (Fig. 1b) was proposed. Later, the ($\sqrt{31} \times \sqrt{31}$)R $\pm 9^\circ$ reconstruction was investigated using X-ray diffraction in [12–15]. Based on the obtained diffraction data, the authors of these works rejected the Somorjai model, proposing a model in the form of a hexagonal structure consisting of two metallic Al crystal planes (111) with certain structural distortions and partial disordering in comparison with the ideal hexagonal structure of the bulk aluminum crystal (111) planes (Fig. 1d).

It is expected that such an aluminum-enriched surface is more suitable for nitridation - an integral part of the III-nitrides growth

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