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Quality improvement of III-nitride epilayers and their heterostructures grown on vicinal substrates by rf-MBE

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Abstract

III-nitride films and their heterostructures are grown on vicinal sapphire and 4H-SiC (0 0 0 1) substrates by plasma-assisted molecular beam epitaxy (rf-MBE). Surface morphologies, optical, structural and electrical properties of the films and heterostructures are systematically characterized. Dramatic improvements of the film quality are demonstrated. Furthermore, high electron mobility of the two-dimensional electron gas (2DEG) in the AlGaN/GaN heterostructure exceeding 1500 $cm^2/V s$ at room temperature in all-MBE-grown samples is obtained, which is extremely important for the electronic device applications. The performance of the results clearly shows the potential of the vicinal substrate usage for the III-nitride growth.

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1. Introduction

III-nitride semiconductors are promising owing to their potential applications to both optical and electronic devices [1–4]. Recent researches on III-nitrides have been concentrated on how to improve the material quality for the high performance of device operations. Among them, ultra-flat surface, low dislocation density and high structural quality of nitride films are hot topics of study. Molecular beam epitaxy (MBE), as one of the major epitaxial growth techniques, has attracted great attention because of its distinctive features of excellent abrupt interface controllability, etc. As applications to other III–V semiconductor materials, MBE technique is also expectable for III-nitride semiconductor growth because many works have demonstrated excellent results using MBE technique to grow III-nitrides and their heterostructures on GaN template and bulk GaN substrates [5–9]. However, qualities of all-MBE-grown III-nitride films and their heterostructures, directly on the foreign substrates such as sapphire, SiC, Si, etc., are still not satisfied in comparison with those grown by metalorganic chemical vapor deposition (MOCVD) at present. Therefore, it is imperative to find breakthrough techniques to grow device-quality III-nitrides by MBE such as those by MOCVD.

Recently, we have proposed a technique of using vicinal substrates for the growth of III-nitrides in MBE growth. Using this technique, we successfully realize the ultra-flat stepped surface with high structural qualities by MBE, which are comparable to those grown by MOCVD [10]. Vicinal substrates are well used in the III–V materials and Si, which can enhance the step-flow growth. However, in the growth of III-nitride materials, vicinal substrate has not been widely used until now. There are several reports concerning the growth and characterization of the III-nitride films on the vicinal substrates mainly grown by MOCVD and hydride vapor phase epitaxy (HVPE) [11–17]. In their works, structural, optical and electrical properties of GaN films are described, where the usage of

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vicinal substrates demonstrates the positive effect on the improvements of the film qualities. One of the main problems for growing MBE III-nitrides is the low growth temperature, which makes it difficult to realize the step-flow growth mode, resulting in rough surface morphologies. Vicinal substrate usage can enhance the step-flow growth and solve the above problem to realize ultra-flat surface in the MBE growth of III-nitrides. There are also many other unique phenomena by using vicinal substrates, which are different from the usage of conventional on-axis substrates. Therefore, it is necessary to master an overall image when using vicinal substrate to grow III-nitride films and their heterostructures by MBE.

In this paper, we report the systematical investigating results of the III-nitride films and their heterostructures grown on vicinal substrates by plasma-assisted MBE (rf-MBE). From our experimental results, the dramatic improvements of the quality both in films and heterostructures are demonstrated.

2. Experimental procedure

III-nitride films (AlN and GaN) and AlGaN/GaN heterostructures are grown on vicinal sapphire and 4H-SiC (0 0 0 1) substrates by rf-MBE. The vicinal angles of vicinal substrates change from 0.5° to 2.0°, and the on-axis (just) substrates are also used for comparison. In case of the growth on sapphire (0 0 0 1) substrates, following a 2-h low-temperature (300 °C) nitridation of the substrates [18], ~700-nm-thick AlN and ~2000-nm-thick GaN films (with 200-nm-thick AlN buffer layer) are directly grown at ~700 °C. Detailed growth conditions can be found in our previous publications [10,19]. In case of the growth on 4H-SiC (0 0 0 1) substrates, a 200-nm-thick AlN buffer layer is grown after a galliation treatment of the substrate at first, and then a 1500 nm-thick GaN film is grown on it at ~800 °C. In case of the AlGaN/GaN heterostructure fabrications, ~20-nm-thick AlGaN layers with Al composition varying from 0.2 to 0.4 are grown on the GaN layers with the same structure as described above. Film qualities including surface morphology, optical. structural properties and dislocation behaviors in the films are characterized by atomic force microscopy (AFM), high-resolution photoluminescence (PL), X-ray diffraction (HRXRD) and transmission electron microscopy (TEM). Furthermore, Hall-measurements are applied to characterize the electrical properties of two-dimensional electron gas (2DEG) in AlGaN/GaN heterostructures. Based on the above characterizations, we try to get an overall image of the vicinal substrate usage in III-nitride growth by MBE.

3. Results and discussions

3.1. Surface morphologies of AlN and GaN films

During the AlN and GaN growth, the RHEED shows streak patterns with 1×1 reconstruction, which indicates that the growth of AlN and GaN films is under two-dimensional mode. Fig. 1 illustrates the AFM images of the AlN surface morphology grown on the vicinal sapphire (0 0 0 1) substrates with the inclination direction toward m-axis. It is found that the surface morphologies of AlN films strongly depend on the vicinal angle of the substrate [10]. When the vicinal angle is 0.5° (Fig. 1(a)), well-ordered monolayer (0.23–0.28 nm in height) steps with almost no spiral growth are uniformly formed on the surface. Further increase of the vicinal angle to 1.0° results in a step-bunched surface with macro-steps, and the height of macro-steps is approximately 4–7 monolayers (Fig. 1(b)). As a comparison, AlN grown on a conventional just sapphire (0 0 0 1) substrate shows two-dimensional nucleation growth with many two-dimensional nuclei on the surface as shown in Fig. 1(c). Obviously, the stepped surfaces of AlN indicate that the step-flow growth is enhanced by using vicinal substrates. GaN films grown on the vicinal sapphire and 4H–SiC (0 0 0 1) substrates illustrate surface morphologies similar to those of AlN in Fig. 1. These results suggest that the surface morphologies (not shown here) of III-nitride films can be precisely controlled by the vicinal angle of the substrate.

We also investigate the dependence of the step features on the inclination direction of the substrate because this study is not only for obtaining ultra-flat GaN surfaces, but also for deep understanding of the growth mechanism. Two kinds of the vicinal sapphire (0 0 0 1) substrate are used, which are inclined toward *m*-axis and *a*-axis of the sapphire (0 0 0 1) substrates. Fig. 2 shows the AFM images of the GaN surfaces grown on 0.5° vicinal substrates with different inclination directions. It is clear that the straight step can be obtained when the inclination direction is toward *a*-axis of the substrate (Fig. 2(a)), whereas the step shape is zigzag when the inclination direction is toward *m*-axis of the substrate (Fig. 2(b)). In case of the substrate being inclined toward the *a*-axis, the straight step edges are simply normal to the inclination direction. On the other hand, AFM results clearly show that there are two kinds of edges of the zigzag steps grown on the *m*-axis inclined substrates. The directions of each step-edge (shown in Fig. 2(b) by dotted lines) are normal to $[0 1 \bar{1} 0]_{GaN}$ and $[1 0 \bar{1} 0]_{GaN}$, respectively, which indicate that these two directions are stable for the step-flow growth of the GaN. The above results clearly indicate that the step morphologies of the GaN surface react sensitively to the inclination direction of the substrate.

In order to explain the anisotropic step morphologies described above, it is necessary to consider step structures of the GaN surface in atomic scale. Fig. 3 schematically illustrates the atomic configurations of the GaN surface step with different inclination directions. When the sapphire substrate is inclined toward the *a*-axis, only one kind of atom (Ga or N) uniformly sits at the step-edge with one free bond pointing out as shown in Fig. 3(a). During the step-flow growth, the incorporating rate into the step for the adatom is unique, which results in the uniform