Improving Si Doping Efficiency in GaAsN Epilayers by Using (211)B and (311)B GaAs Substrates

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1. Introduction

III-V nitrides Ga (In) AsN are promising semiconductors for the fabrication of high-efficiency multijunction solar cells owing to a proper ~1.0 eV bandgap for the key subcell and lattice matching to GaAs/Ge [1]. A nice bipolar electrical conduction is essential to achieve a high conversion efficiency in photovoltaic applications. Silicon is an important dopant in many III-V compound semiconductors. However, Si doping efficiency decreases dramatically in traditional (100) orientated Ga (In) AsN layer with the increase of N composition, which leads to poor optical and electrical properties [2, 3]. This work aims to show that a quite high Si doping efficiency can be realized at relatively high N fraction by engineering the growth orientation of GaAsN.

Despite a thorough knowledge on its doping physics in GaAs during the last decades, the incorporation behavior of Si is more complicated in GaAsN due to its interaction with N. Mutual passivation is suggested to occur between Si and N with the form of Si-N complexes [4]. The true construction of the complex is still in debate. Both SiGa-NAs pairs and (Si-N)As split interstitials have been predicted theoretically [5, 6]. On the other hand, most research efforts restricted to the limited crystallographic orientations: typically (100). We have found that N incorporation in undoped GaAsN can be significantly enhanced on (311)B GaAs substrate while keeping impressive carrier lifetime as compared with (100) GaAsN layers [7]. It is thus important to understand how the crystallographic orientation influences dopant incorporations, and the related interaction between Si and N. In this work, Si doping behavior was studied in GaAsN epilayers with (211)B, (311)B and (100) growth orientations. A model based on the atomic bonding geometries between Si/N adatoms and adsorption sites was discussed to explain the observed phenomena.

2. Experiments

For parallel comparison, (211)B, (311)B and (100) GaAs substrates were loaded on a single holder to grow ~1μm GaAsN layers by using the chemical beam epitaxy (CBE) system. The surface structure of (n11) substrate can be considered to be composed of (100) and (111) components. As illustrated in Figure 1, the corresponding atom ratio of <111> and <100> direction components on the growth surfaces is 2:1 and 1:1 for (211) and (311) substrates. Triethylgallium (TEGa), trisdimethylaminoarsenic (TDMAAs) and monomethylhydrazine (MMHy) were used as Ga, As and N sources, respectively. Si doping was achieved via a constant supply of 0.7 sccm SiH$_4$ gas during the growth. Flow rates of TEGa and TDMAAs were fixed to 0.1 and 1.0sccm, while MMHy flow rate was varied from 0 to 9 sccm to examine the effect of N composition on the Si incorporation. The growth temperature is 460°C. For Hall measurement, evaporated In was annealed at 350°C in N$_2$ for 5 minutes to form the Van der Pauw configuration. High resolution X-ray diffraction (HRXRD) was measured via Philips X’pert Pro diffractometer. 2θ/ω scan of (422), (311) and (400) reflections were performed on samples grown on (211), (311) and (100) substrates, respectively. N composition was determined from Bragg angles of the GaAs and GaAsN reflections.

3. Results and Discussion

Figure 2(a) shows the variation of electron density as a function of N composition in GaAsN layers on different GaAs substrates. As compared with Si doped GaAs, Si doping efficiency decreases remarkably for all three substrates at low N incorporation, which implies that even a small amount of N introduction will lead to the formation of N-related charge trapping centers. Although a constant supply of SiH$_4$ gas was applied during the epitaxial growth,
Hall measurement results showed that an increasing free carrier concentration accompanies the increasing N composition in (211)B and (311)B GaAsN layers. The electron density tends to saturate as N flow rate continues increasing. Furthermore, such a saturation occurs at higher N content in (211)B as compared with (311)B sample. On the contrary, free electron density decreases gradually with the rise of N content for (100) samples. It implies that increasing N incorporation enhances compensation and/or passivation to Si donors (SiGa) as growth follows (100) orientation. The mobilities for three growth orientation in Figure 2(b) exhibit similar decreasing behaviors which are mainly limited by N-related scatters. Saturated values of ~200 and 250 cm²/Vs were recorded for (211)/(311)B and (100) GaAsN layers, respectively.

(a)

![Graph](image1)

(b)

![Graph](image2)

Fig. 2 (a) Electron density and (2) mobility as a function of N composition in GaAsN layers grown on (100), (211)B and (311)B substrates.

The different doping behavior of Si in response to the increasing N incorporation might be explained by different bonding status on three substrate surfaces. Taking the (100) component as terraces and (111) component as step edges, a high density of three-bond sites can be formed with the aid of two atoms on terraces and one adatom bonded to step edges. Such three-dangling-bond sites on (211)B and (311)B substrates are V sites in nature, which act as energetically favorable sites for N adatom owing to its larger electronegativity than As [7]. With the increase of N flow rate, enhanced N incorporation into these three-dangling bond V sites will suppress its occupation by Si. Thus, the compensation effect from SiAs reduces significantly. Since the density of three-dangling bond V sites for (211)B substrate is higher than that for (311)B substrate, the saturation of Si doping occurs at relatively high N composition. For (100) substrate, the competition between N and As occurs on two-dangling bond sites. The formation of N-Si complex is enhanced with the increasing supply of N sources; and Si dopant is deactivated in (100) GaAsN samples.

3. Conclusions

The compensation and/or passivation of Si doping in GaAsN epilayer can be suppressed by using (211)B and (311)B substrates, and efficient Si doping was achieved at relatively high N incorporation. The atomic bonding geometries on the growing surface are suggested to account for the phenomena.

Acknowledgements

Part of this work is supported by the New Energy Development Organization (NEDO) under the ministry of Economy, Trade and Industry, Japan.

References