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Rutherford backscattering study on high dose Mg-ion implanted GaN bulk single crystal

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Lattice displacements before and after annealing for the high dose Mg-ion implanted GaN with 5.0 x 10^{15} cm^{-2} and 1.0 x 10^{16} cm^{-2} are evaluated by Rutherford backscattering spectroscopy (RBS) using 1.5-MeV H^+ ions. The Mg-ion implantation into GaN bulk single crystal is performed at room temperature with implantation energy of 150 keV. Annealing is performed at 1230℃ for 1 min in a nitrogen atmosphere. Although the gallium displacement for the dose of 5.0 x 10^{15} cm^{-2} is observed, the surface of GaN for the dose of 1.0 x 10^{16} cm^{-2} shows the polycrystalline-like feature. The high dose Mg-ion implanted GaN such as 1.0 x 10^{16} cm^{-2} remains the lattice displacement in the implanted layer under the present annealing condition. From photoluminescence measurements, the band edge emission for un-implanted GaN is observed at 358 nm (3.46 eV), but this emission is not observed for as-implanted GaN and annealed ones. The disappearance of the band edge emission is considered to be due to the collapse of the crystal structure of the GaN surface due to the Mg-ion implantation.

I. Introduction

GaN exhibits unique electrical, optical and thermal properties, which make it a promising material for optoelectronic and high-power devices. The characterization of p-n junction by Mg-ion implantation into GaN has been reported by several research groups[1, 2], but the formation of p-type by Mg-ion implantation into GaN is very difficult. In this study, lattice displacements before and after annealing for the high dose Mg-ion implanted GaN with 5.0 x 10^{15} cm^{-2} and 1.0 x 10^{16} cm^{-2} are evaluated by Rutherford backscattering spectroscopy (RBS). The evaluation of Mg-implantation induced defects is also performed by photoluminescence (PL) measurements.

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II. Experimental

GaN bulk single crystals with a thickness of 450 ± 30 μm were provided from Hitachi Cable, Ltd. The Mg-ion implantation into GaN bulk single crystal was performed at room temperature with implantation energy of 150 keV and doses were 5.0 x 10^{15} cm^{-2} and 1.0 x 10^{16} cm^{-2}. Since the Mg concentration by a TRIM simulation is maximum at 180 nm in depth, most of the Mg-ions remain near the surface of GaN. Annealing was performed at 1230°C for 1 min in a nitrogen atmosphere. To evaluate the lattice displacement, RBS analysis was performed using the Van de Graaff accelerator of Hosei University. 1.5-MeV H^+ ions were used in the present experiment because the kinematic factor of N atoms for He-ion as a probing beam is very small. The experimental arrangement has already been reported elsewhere[3, 4)]. The samples were mounted on a triple axis goniometer and the backscattered ions were collected by a silicon surface barrier detector placed at a scattering angle of $\theta = 150$ º. The beam spot and the beam divergence were ~1.0 mm in diameter and ~0.03 º, respectively. The sheet resistance was measured by van der Pauw method. PL measurements were performed using a He-Cd laser at 17 K.

III. Result & Discussion

Figure 1 and 2 show the random and aligned spectra of RBS for the dose of 5.0 x 10^{15} cm^{-2} and 1.0 x 10^{16} cm^{-2}, respectively. The minimum yield χ_{min} is calculated by χ_{min} = aligned yield / random yield. The displacement of Ga atoms was estimated by the following equation [5, 6)]

$$N_D = N_{Ga\ or\ N}\ (\chi_{min} - \chi^0_{min}\ )\ /\ 1 - \chi^0_{min}, \qquad (1)$$

where $N_{Ga\ or\ N}$ is the Ga and N density (4.38 x 10^{22} cm^{-3}) of the crystal, χ^0_{min} is the minimum yield for the un-implanted sample and χ_{min} is the observed minimum yield for implanted one. From the aligned spectra along the c-axis of GaN, the displacement of Ga atoms and N atoms was observed near the GaN surface. For the displacement of Ga atoms, the minimum yield χ^0_{min} is 2 % for the un-implanted GaN. The minimum yield χ_{min} for the dose of 5.0 x 10^{15} cm^{-2} is 14 % for the as-implanted GaN and 7 % for the annealed ones. The displaced Ga atom concentrations estimated from the χ_{min} values were 5.8 x 10^{21} cm^{-3} for the as-implanted GaN and 2.7 x 10^{21} cm^{-3} for the annealed ones, whereas χ_{min} for the dose of 1.0 x 10^{16} cm^{-2} is 50 % for the as-implanted GaN and 22 % for the annealed ones. The displaced Ga atoms were 2.2 x 10^{22} cm^{-3} for the as-implanted GaN and 9.3 x 10^{21} cm^{-3} for the annealed ones. For the displacement of N atoms, the minimum yield χ^0_{min} is 22 % for the un-implanted GaN. The minimum yield χ_{min} for the dose of 5.0 x 10^{15} cm^{-2} is 40 % for the as-implanted GaN and 33 % for the annealed ones. The displaced Ga atom concentrations estimated from the χ_{min} values were 1.0 x 10^{22} cm^{-3} for the as-implanted GaN and 6.7 x 10^{21} cm^{-3} for the annealed ones, whereas χ_{min} for the dose of 1.0 x 10^{16} cm^{-2} is 77 % for the as-implanted GaN and 52 % for the annealed ones. The displaced N atoms were 3.1 x 10^{22} cm^{-3} for the as-implanted GaN and 1.7 x 10^{22} cm^{-3} for the annealed ones. These results show that the Ga and N displacement increases with increasing Mg-ion dose and decreases by annealing. Also, Ga vacancy, N vacancy and N interstitial were introduced in Mg-ion implanted GaN.

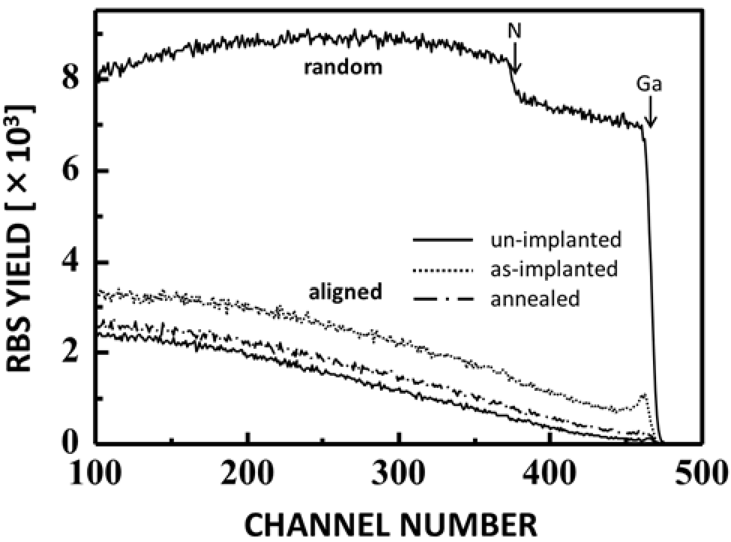

Fig. 1 The random and aligned spectra of RBS for the Mg dose of 5.0×10^{15} cm^{-2}.

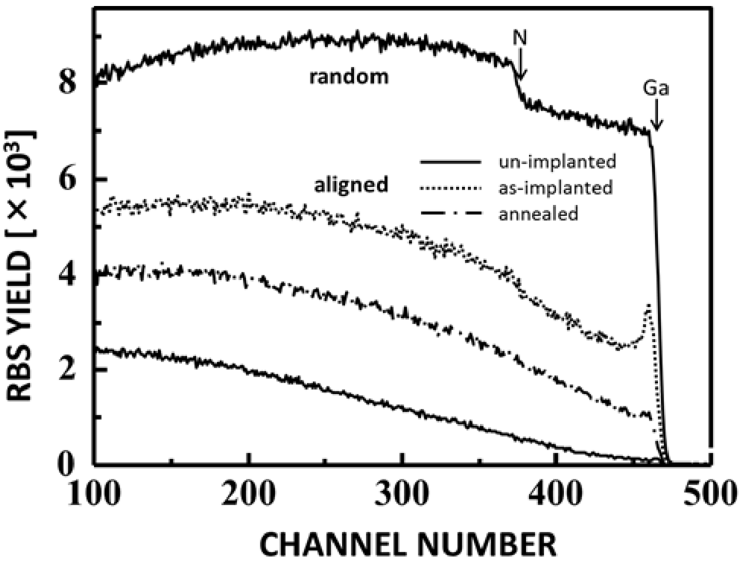

Fig. 2 The random and aligned spectra of RBS for the Mg dose of 1.0×10^{16} cm^{-2}.

Figure 3 and 4 show the channeling dip of RBS for each Mg dose. The lattice displacement r_x of Ga atoms from the c-axis row was estimated using the following equation [7)]

$$\frac{\varphi_i}{\varphi_c} = \frac{\ln[(Ca/r_x)^2+1]}{\ln[(Ca/\rho)^2+1]}, \quad (2)$$

where φ_i is the half angular width of channeling dip for the implanted samples, φ_c that for the un-implanted samples, C the constant (C$\sim\sqrt{3}$), a the Thomas-Fermi screening radius (a=0.013 Å), and ρ the thermal vibration amplitude[8)] calculated using the Debye temperature (600 K for GaN [9)]) at 300 K (ρ=0.039 Å). Form the axial half-angle $\varphi_{1/2}$ of the angular yield profile along the c-axis, the average displacement of Ga atoms from the c-axis for the dose of 5.0 x 10^{15} cm^{-2} was 0.041 Å for the as-implanted GaN and 0.040 Å for the annealed ones. On the other hand, the $\varphi_{1/2}$ value for the dose of 1.0 x 10^{16} cm^{-2} without annealing was broadened, showing the polycrystalline-like feature near the surface. This is similar to the channeling in Si overlaid with Al film [10)].

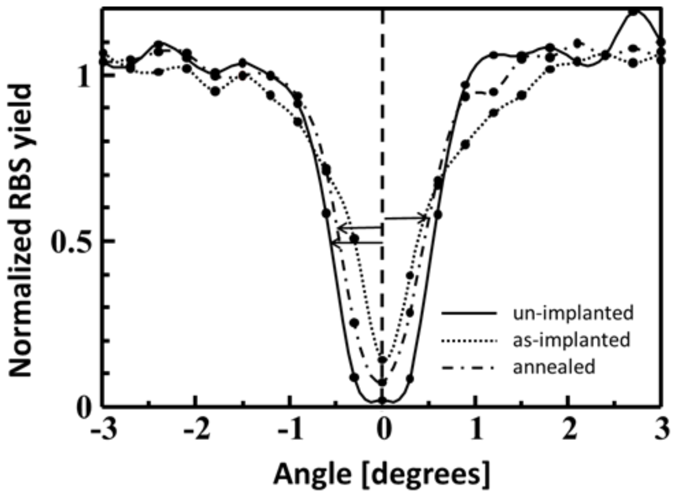

Fig. 3 The channeling dip of RBS for the Mg dose of 5.0 x 10^{15} cm^{-2}. The axial half-angle $\varphi_{1/2}$ is 0.56 ° for un-implanted GaN, 0.46 ° for as-implanted GaN and 0.50 ° for annealed GaN, resistivity.

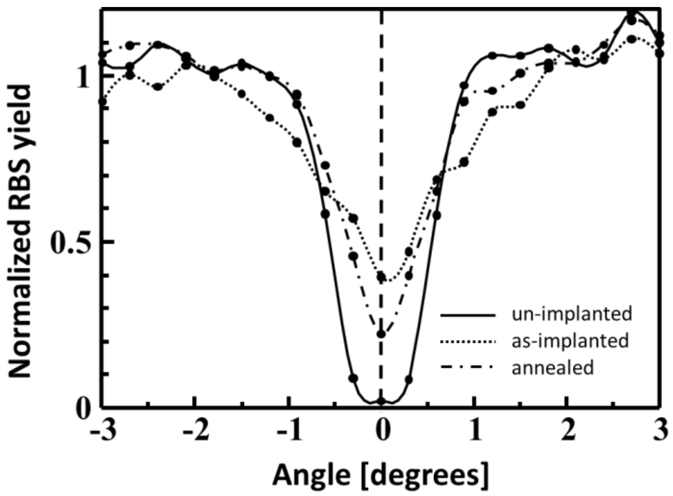

Fig. 4 The channeling dip of RBS for the Mg dose of 1.0 x 10^{16} cm^{-2}.

From van der Pauw measurements, the sheet resistance was 2.5 x 10^2 Ω/sq. for un-implanted GaN. The sheet resistance for the dose of 5.0 x 10^{15} cm^{-2} was 1.9 x 10^8 Ω/sq. for as-implanted GaN and 8.9 x 10^3 Ω/sq. for annealed ones. The sheet resistance for the dose of 1.0 x 10^{16} cm^{-2} was 3.2 x 10^9 Ω/sq. for as-implanted GaN and 4.4 x 10^5 Ω/sq. for annealed ones. These results show that the resistance after the Mg ion implantation is higher than before the implantation and the resistance decreases after annealing. However, the sheet resistance of the annealed GaN is higher than the un-implanted ones. Increase in resistance would be mainly attributed to the carrier compensation effect due to the acceptor level of Ga vacancy and the deep donor level of N interstitial.

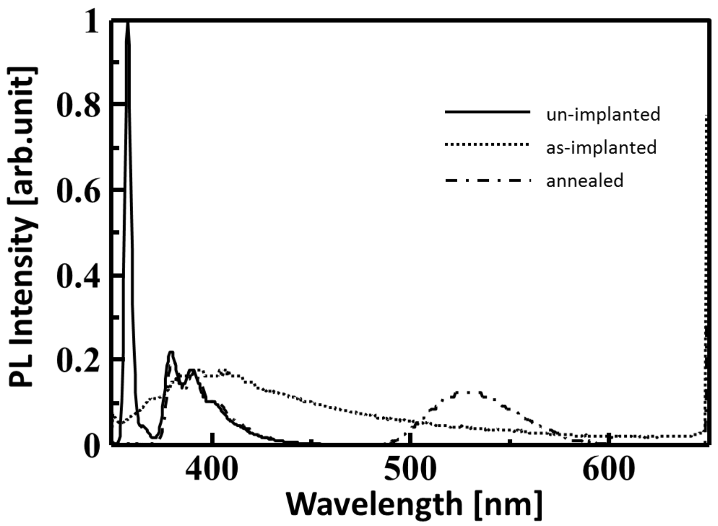

Fig. 5 PL spectra for un-implanted, as-implanted and annealed GaN for the Mg dose of 5.0 x 10^{15} cm^{-2}.

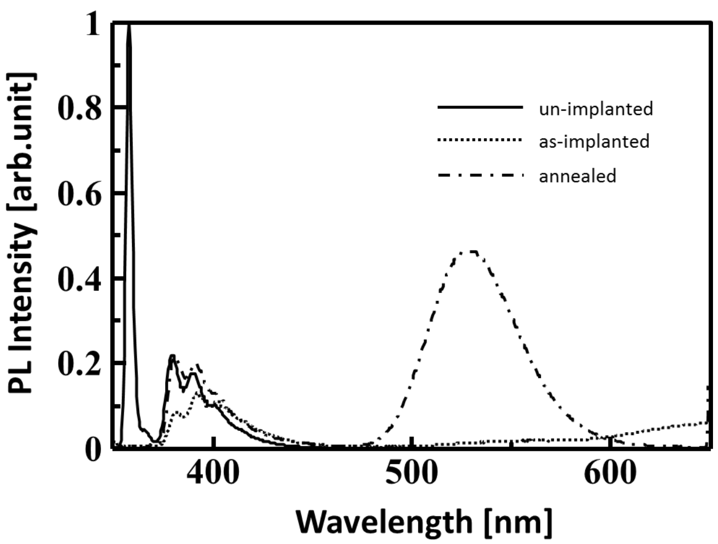

Fig. 6 PL spectra for un-implanted, as-implanted and annealed GaN for the Mg dose of 1.0 x 10^{16} cm^{-2}.

Figure 5 and 6 show PL spectra for un-implanted, as-implanted and annealed GaN for the doses of 5.0×10^{15} cm^{-2} and 1.0×10^{16} cm^{-2}, respectively. The band edge emission for un-implanted GaN was observed at 358 nm (3.46 eV), but this emission was not observed for as-implanted GaN and annealed ones. The disappearance of the band edge emission is considered to be due to the collapse of the crystal structure of the GaN surface due to the Mg-ion implantation. Furthermore, the emissions around 390 nm (3.18 eV) and the strong yellow luminescence at 528 nm (2.35 eV) appeared in the annealed GaN. The strong yellow luminescence suggests the increase in Ga vacancy. The broad emission was observed at around 400 nm after Mg implantation is related to N vacancy donor and some acceptor pairs. This result correlates to the Ga and N displacement evaluated by the random and aligned spectra of RBS. Figure 7 shows the YL model estimated from the photoluminescence at 17 K. Since the usual YL has been proposed as a transition from a shallow donor to V_{Ga} located at about 1.1 eV above the valence band [11].

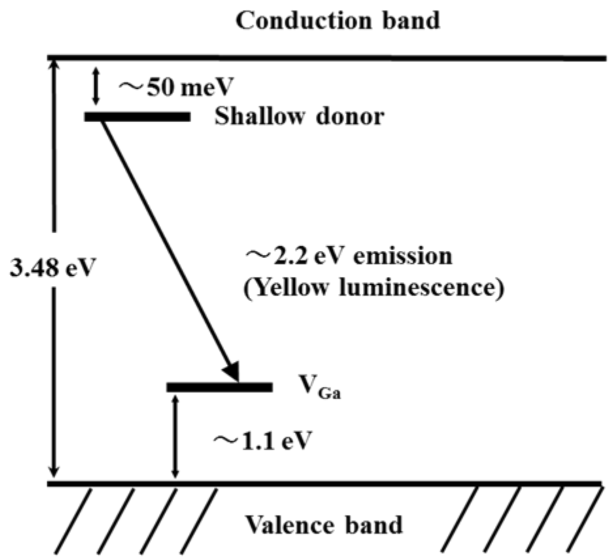

Fig. 7 The YL model evaluated from the photoluminescence at 17 K.

IV. Conclusion

The gallium displacement in Mg-ion implanted GaN bulk single crystals was observed by the Rutherford backscattering method. The surface of GaN for the dose of 1.0×10^{16} cm^{-2} showed polycrystalline-like feature. The high dose Mg-ion implanted GaN such as 1.0×10^{16} cm^{-2} remains the lattice displacement in the implanted layer under the present annealing condition. From the PL measurements, the band edge emission was not observed near the surface of the GaN bulk single crystal. The increase in YL intensity suggests that Ga vacancies in GaN bulk single crystal increased by Mg-ion implantation.

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