Unidirectional expansion of lattice parameters in GaN induced by ion implantation*

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This paper reports that the 150-keV Mn ions are implanted into GaN thin film grown on Al_2O_3 by metal–organic chemical vapour deposition. The X-ray diffraction reciprocal spacing mapping is applied to study the lattice parameter variation upon implantation and post-annealing. After implantation, a significant expansion is observed in the perpendicular direction. The lattice strain in perpendicular direction strongly depends on ion fluence and implantation geometry and can be partially relaxed by post-annealing. While in the parallel direction, the lattice parameter approximately keeps the same as the unimplanted GaN, which is independent of ion fluence, implantation geometry and post-annealing temperature.

Keywords: GaN, ion implantation, unidirectional strain, X-ray reciprocal space mapping

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1. Introduction

Ion implantation allows the introduction of a precisely controlled amount of impurity into the crystal independent of the solubility of the impurity and has been extensively applied in Si and GaAs based device fabrications. Recently the ion beam process on GaN thin film is heavily investigated by various techniques.[1−5] At the same time, GaN implanted with Mn and other transition metal is demonstrated to be magnetic semiconductor with the Curie temperature up to room temperature.[6−8] Compared with Si and GaAs, some different behaviours in GaN upon implantation have been well established, e.g. a much higher amorphisation threshold,[9−11] on the other hand an extreme difficulty to remove implantation induced damage by thermal annealing.[12] Another common phenomenon in implanted Si or GaAs crystal is the unidirectional strain in the implanted region.The perpendicular strain is positive and increases with ion fluence, while the parallel strain is no more than 0.02%.[13−15] The lattice strain is defined as $\delta d/d_0 = (d_{\rm imp} - d_0)/d_0$, where $d_{\rm imp}$ and d_0 are the lattice parameters for the implanted region and virgin specimen, respectively. A same so-called perpendicular strain has been observed in implanted GaN. Several groups[16−18] find that a new peak appears at lower angles in X-ray diffraction spectra. The main (0002) peak of the virgin GaN film decreases and the new peak gradually shifts to lower angles with increasing implantation fluence. This new peak is due to an expansion of the GaN hexagonal lattice driven by the introduced impurities and disorders of host atoms and not a phase transition in the GaN. However, the investigation on the lattice variation in the parallel direction is rather limited.[19]

Particular implantation results in a kind of 'heterostructure': implanted part and virgin part of the substrate with an unknown lattice mismatch. The implanted part can be fully or partially strained onto the substrate. Lattice strain of an epitaxial semiconductor film has a strong influence on its bandstructure, which is directly related with its magnetic, electronic and optical properties. In this case, in order to detect the in-plane lattice deformation, it arises an ambiguity to rely on a single X-ray diffraction $2\theta/\omega$ scan.[20] Recently, reciprocal-space X-ray mapping (RSM) has been introduced to enhance precision and to expand the area of application of high-resolution X-ray diffraction.[21] The RSM is based on two-dimensional diffraction measurements in the scat-

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tering plane: in the parallel direction (i.e. ω scan) and in the perpendicular direction along the diffraction vector (i.e. $2\theta/\omega$ scan). Correspondingly, a map taken from asymmetric reflection allows one to deduce both the in-plane and the out-of-plane lattice parameters. The RSM technique has been used for strain and composition evaluation in cubic crystals (i.e. SiGe[22]) and hexagonal crystals (i.e. InGaN/GaN heterostructure[20] and quantum well[23]). In this paper, the X-ray reciprocal space mapping is used to measure the lattice variations both in perpendicular and in parallel directions after Mn ion implantation. A strong unidirectional lattice expansion is observed.

2. Experiments

The samples used in this work were hexagonal GaN grown on $Al_2O_3(0001)$ by a metal-organic chemical vapour deposition method. Mn ions with the energy of 150 keV were implanted at room temperature. The fluence was from 1×10^{14} to $1\times10^{16}/\text{cm}^2$. The samples were maintained to be perpendicular to the ion beam (channeled implantation) or tilted by 10° off the ion beam (random implantation) during implantation. With the knowledge of the suppression of implantation-induced damage in GaN by channeled implantation,[18] in this work GaN films were mainly implanted with Mn ions with a channeling geometry and additionally one sample was implanted at a random condition for comparison. High resolution X-ray diffraction was carried out on a Bruker D8 diffractometer system, using four Ge(220) crystals as the monochromator and two 200 μm-slits before the detector. A collimated 1.57-MeV He^+ beam produced by a 5SDH-2 Pelletron was used for Rutherford backscattering/channeling (RBS/C) measurements to determine disorder degree after implantation.

3. Results and discussion

Figure 1 shows the RSMs for the (10$\underline{1}$5) reflections of the Mn implanted GaN samples with different fluences, different implantation geometries and after annealing. Any pair of coordinates (q_x, q_z) in the map correspond to a pair of lattice constants (a, c) of the hexagonal crystal following the equations given below:[24]

$$q_x = \sqrt{\frac{4}{3a^2}(h^2+hk+k^2)},$$
$$q_z = \frac{l}{c}.$$

Implantation results in a kind of heterostructure: implanted part (from the surface to the depth at which ions stop) and virgin part of a thin film with an unknown lattice mismatch. Given the lattice expansion in perpendicular direction in an ion-implanted GaN film,[16−18] the dominant peak with a higher q_z value (i.e. smaller c) is from the unimplanted and hence undamaged GaN and the shoulder peak in lower q_z axis (i.e. larger c) is from the implanted part. The dashed lines in Fig. 1 are asymmetric $2\theta/\omega$ scans of GaN(10$\underline{1}$5). Any point on those lines corresponds to a pair of (a, c) with the same ratio of c/a as a GaN crystal, on the other hand, any point on the left of those lines gives a larger value of c/a (i.e. different symmetry from GaN). Therefore Fig. 1 makes two conclusions

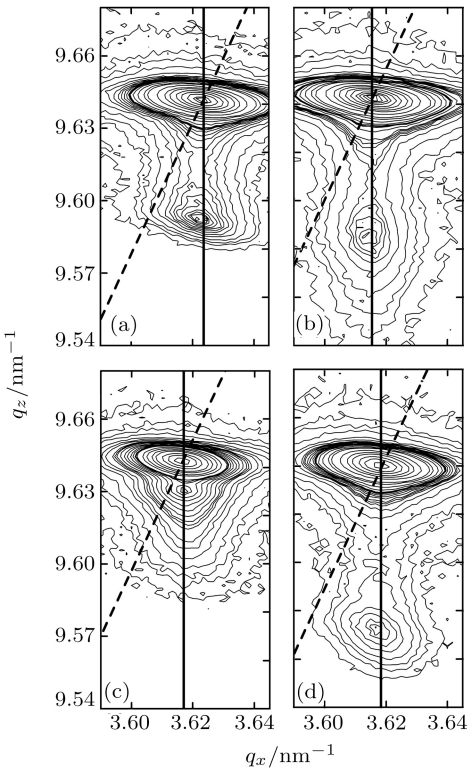


Fig. 1. Reciprocal space maps for the (10$\underline{1}$5) reflections of the Mn implanted GaN samples with different fluences, different implantation geometries and after annealing: (a) $1\times10^{15}/\text{cm}^2$ channeling implantation; (b) $1\times10^{16}/\text{cm}^2$ channeling implantation; (c) $1\times10^{14}/\text{cm}^2$ channeling implantation; (d) $1\times10^{14}/\text{cm}^2$ random implantation. The main peak is from the unimplanted GaN and the shoulder peak in lower q_z axis is from the implanted layer. The solid and dashed lines represent the fully strained and fully relaxed status, respectively.

clear: 1) an asymmetric $2\theta/\omega$ scan can not give reliable information on the implanted GaN (note that the $2\theta/\omega$ scan does not go through the shoulder peak in RSM), while RSM can simultaneously give an accurate measure on both lattice parameters; 2) the implanted

layer has a larger perpendicular lattice parameter and a higher fluence (Fig. 1(b)) or a random implantation (Fig. 1(d)) induces a larger expansion, however, it approximately keeps parallel lattice parameter the same as GaN.

Generally the lattice distortion can be induced by the incorporation of dopants into interstitial sites, the displacement of the Ga or N atom from its mean position, or by the substitution of larger atom into the Ga or N vacancies.[13−16] All of the abovementioned disorders induced by implantation are depth dependent and can be qualitatively measured by RBS/C technique. The energy spectrum of the backscattered channeled ions gives a direct qualitative measure of the profile of displaced atoms as a function of depth. Figure 2 shows the RBS/C spectra of GaN samples implanted with different fluences. The peaks at the higher energy part measure the degree of disorder in GaN films, which is increased with the fluence and is depth dependent. As a direct result, the lattice expansion induced by implantation is depth dependent, which explains the gradual swelling in q_z direction of the peak in RSM from the implanted region. The smallest q_z value corresponds to the maximum strain in perpendicular direction, which is actually the perpendicular strain mentioned in the text. The swelling in q_x direction is generated by the diffuse scattering from the point defects and their aggregation and is the same pronounced in the unimplanted region. Therefore in the q_x direction, the central position of the peak is taken to calculate the parallel lattice parameter.

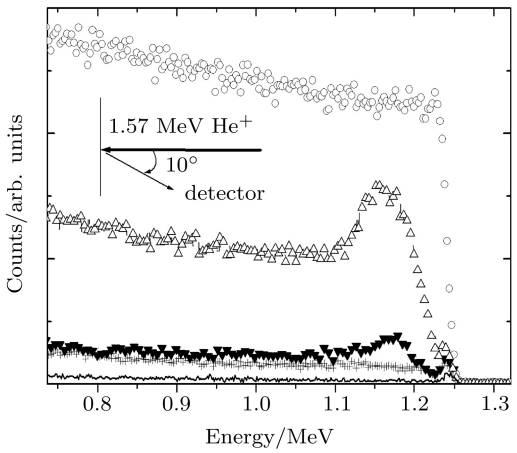


Fig. 2. The RBS spectra of Mn channeled implanted GaN: <0001> aligned spectra for virgin sample (—), 1×10^{14}/cm^2 implanted (+), 1×10^{15}/cm^2 implanted (▼), 1×10^{16}/cm^2 implanted (△) and random spectrum (○).

Figure 3 shows the fluence dependence of perpendicular and parallel strains in Mn-implanted GaN. The perpendicular strain increases gradually with increasing implantation fluence and goes to as high as 1.08% for the highest fluence, while the parallel strains are as minor as below 0.08% for all fluence levels. As fluence rises above 10^{15}/cm^2, the perpendicular strain arrives at a saturation level. The nonlinear behaviour is also observed in implanted Si and GaAs.[13−15] Figure 4 shows the annealing dependence of perpendicular and parallel strains in one sample with channeled implantation in a fluence of 5×10^{14}/cm^2. At an annealing temperature of 200, 400 and 600 °C, only the perpendicular strain is measured by $2\theta/\omega$ scan (not shown). All annealings are performed in nitrogen ambience for a period of 30 min, with sample face to face geometry. Increasing the annealing temperature results in the drastic decrease of the perpendicular strain, but neglectable variation of parallel strain. In RBS/C measurement (not shown), the degree of disorder is decreased with annealing temperature, but not completely restored after 800 °C annealing, which is consistent with RSM measurements.

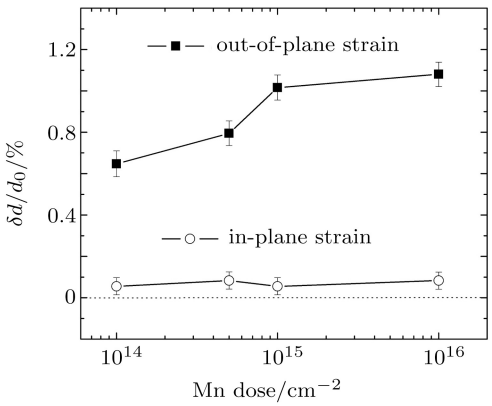


Fig. 3. The fluence dependence of perpendicular and parallel strains in Mn-implanted GaN. The implantation is performed at room temperature with a channeling geometry.

This unidirectional expansion in lattice parameter upon implantation is not a unique observation in Mn-implanted GaN. The same phenomenon has been observed in ion-implanted Si,[13,15] GaAs,[14] and Mg implanted GaN.[19] When ions are implanted into a solid matrix, the incident ions will stop on an interstitial or substitutional lattice site. In the former case, the host lattice will expand. In the latter case, the lattice may expand or shrink, depending on the relative size of host atoms and incident atoms. Implantation of 150-keV Mn^+ ions can only result in a damaged thickness of around 150 nm in GaN, which is much smaller in comparison with the whole GaN layer of 2 μm–3 μm. Therefore the damaged layer is fully compliant

to the unimplanted GaN layer, which serves the same as a substrate.

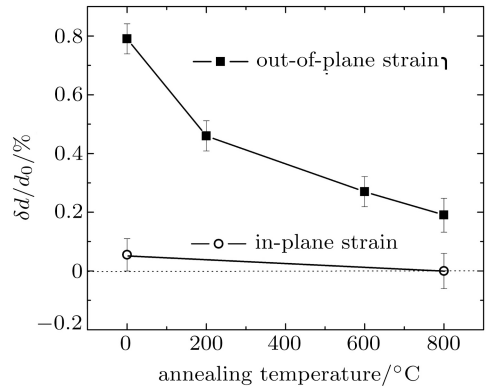


Fig. 4. The isochronal annealing dependence of perpendicular and parallel strains in Mn-implanted GaN (5×10^{14}/cm^2 and channeled implantation). All annealings are performed in nitrogen ambience for a period of 30 min, with sample face to face geometry.

4. Conclusion

In conclusion, Mn-implantation introduced a tensile unidirectional strain in GaN *c*-axis. The perpendicular strain gradually increases with increasing implantation fluence and arrives at a saturation when the fluence is above 10^{15}/cm^2. With the post-annealing, the order in crystal is partially recovered and consequently the perpendicular strain is gradually and partially decreased with increasing annealing temperature. In the parallel direction, the lattice parameter remains approximately the same as that of the unimplanted GaN, which is independent of ion fluence, implantation geometry, and post-annealing temperature. The very pronounced unidirectional strain could significantly alter the band structure in the implanted region, consequently introduce specific stress on the Mn-diluted GaN matrix.

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