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Formation mechanism of V defects in the InGaN/GaN multiple quantum wells grown on GaN layers with low threading dislocation density

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V-defect formation of the $In_xGa_{1-x}N$/GaN multiple quantum wells (MQWs) grown on GaN layers with different threading dislocation (TD) densities was investigated. From cross-sectional transmission electron microscopy, we found that *all* V defects are *not* always connected with TDs at their bottom. By increasing the indium composition in the $In_xGa_{1-x}N$ well layer or decreasing the TD density of the thick GaN layer, many V defects are generated from the stacking mismatch boundaries induced by stacking faults which are formed within the MQW due to the strain relaxation. Also, TD density in the thick GaN layer affects not only the origin of V-defect formation but also the critical indium composition of the $In_xGa_{1-x}N$ well on the formation of V defects. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1384906]

Nitride alloys (GaN, AlGaN, and InGaN) are of particular interest due to their ability to cover a wide spectral range and high-temperature stability that is not possible with other III–V semiconductors.[1] The growth of these alloys is primarily done on sapphire substrates using metalorganic chemical vapor deposition (MOCVD)[2] and molecular beam epitaxy (MBE).[3] However, because of a large lattice mismatch and a thermal expansion coefficient difference between GaN and sapphire, a GaN layer contains several defects such as threading dislocations (TDs), stacking faults, and inversion domain boundaries (IDBs).[4,5] It is usually accepted that the high defect density results in poor optical property and shorter device lifetime.[6] Also, these defects affect the structural and optical quality of the active layer composed of the InGaN/GaN multiple quantum well (MQW) structure.[7] Especially, it has been reported that TDs disrupt the InGaN/GaN MQW and initiate the V defect using transmission electron microscopy (TEM) and atomic force microscopy (AFM).[7–12]

These V defects have an open hexagonal, inverted pyramid with $\{10\bar{1}1\}$ side walls.[8] Several research groups have reported that there is always a TD connected with the bottom of V defect[7–11] and the cause of V-defect formation is the increased strain energy[10] and the reduced Ga incorporation on the $\{10\bar{1}1\}$ pyramid planes in comparison with the (0001) surface.[7,8] Recently, a large improvement has been achieved in the growth of high quality GaN layers with low TD density ($<5\times10^8$ cm^{-2}).[13] Different luminescence properties from the $In_xGa_{1-x}N$/GaN MQWs of the high indium (In) composition were also proposed to be closely related to the In cluster regions.[14,15] However, the previous results of the origin of V defects have mainly been obtained from the InGaN/GaN MQWs of the low In composition (<20%) grown on thick GaN layers with a relatively high dislocation density ($>10^9$ cm^{-2}) and there have been very few studies on the MQWs of the high In composition (⩾30%) grown on high quality GaN layers with a low dislocation density.

In this study, we have examined the effect of the TD density in thick GaN layers on the origin of V-defect formation in the InGaN/GaN MQW structure. We report here that in the highly strained InGaN/GaN MQWs of high In composition grown on high quality GaN, V defects are formed not only at the TDs from the thick GaN layer, but also at the stacking mismatch boundaries (SMBs) related with stacking faults generated due to the strain relaxation.

All samples were grown on *c*-plane sapphire substrates with a nominal 25 nm thick GaN buffer layer by a horizontal MOCVD reactor operating at low pressure. Trimethylgallium (TMGa), trimethylindium (TMIn), and ammonia (NH_3) were used as the source precursors for Ga, In, and N, respectively. In order to analyze the effect of the TD density and the strain on the formation mechanism of V defects, the MQWs composed of six periods of InGaN/GaN were grown on the high TD density GaN (sample A) and the low TD density GaN (samples B and C) GaN layers of ~2 μm thickness. The TD densities of the high TD density and low TD density GaN layer are 10×10^8 and 2×10^8 cm^{-2}, respectively (Table I). To obtain the GaN layers with different TD density, the TMGa flow rate of GaN nucleation layers was

TABLE I. Threading dislocation density in the thick GaN layer, In composition in the $In_{1-x}Ga_xN$ well, V-defect density, and the ratio of the SMB related V-defect density on the total V-defect density of samples.

Sample No.	ρ_{th} (cm^{-2}) in thick GaN	In composition in well (%)	V defect density (cm^{-2})	V_{SF}/V_{tot}
A	10×10^8	30	15×10^8	~0.5
B	2×10^8	24	no	no
C	2×10^8	30	15×10^8	>0.9

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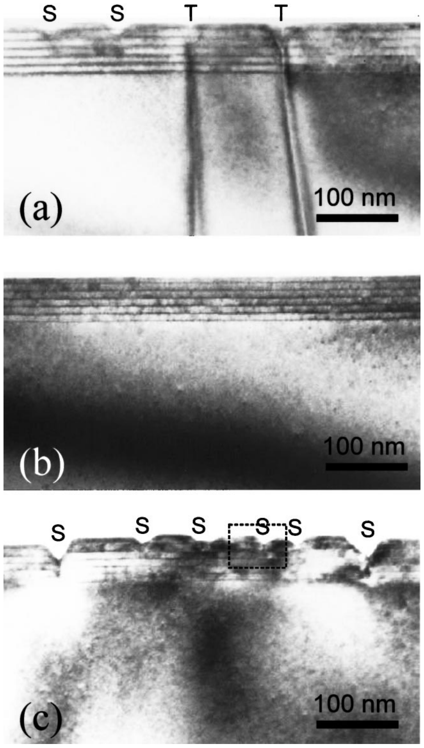

FIG. 1. Cross-sectional bright-field TEM images from (a) the highly strained $In_{0.3}Ga_{0.7}N$/GaN MQW of sample A grown on high TD density GaN, (b) the $In_{0.24}Ga_{0.76}N$/GaN MQW of sample B grown on low TD density GaN, and (c) the highly strained $In_{0.3}Ga_{0.7}N$/GaN MQW of sample C grown on low TD density GaN.

changed. The detail growth conditions of these high TD density and low TD density GaN layers were reported elsewhere.[13] The obtained In compositions of the $In_xGa_{1-x}N$ wells of the samples were 30% (samples A and C) and 24% (sample B) from the (0002) high resolution x-ray diffraction (HRXRD) results, assuming that the films are pseudomorphic. The thicknesses of wells and barriers are 15 and 85 Å, respectively, and no cap layer was grown on the top of InGaN/GaN MQWs.

The formation of V defects in the MQWs was investigated using TEM. TEM specimens were prepared in cross section along [1120] zone axis using a Tripod mechanical polishing followed by low temperature Ar ion milling at 5 kV in a Gatan DuoMill 660 DIF with sector speed control. The ion energy was gradually reduced during the final stages of thinning to minimize the surface damage of MQWs without capping layers. Bright-field (BF) images and high-resolution TEM (HRTEM) images were recorded at 200 kV on a JEOL JEM 2000 EX microscope.

The BF TEM micrographs from the MQW structure of each sample are shown in Fig. 1. It has been reported that a V defect is always connected with a TD from the thick GaN layer at the bottom.[7–11] In addition, because of the low In composition (low strain) in the InGaN well and the high TD density in the GaN thick layer, only a small fraction of the TDs cause the formation of the V defects in the MQWs. However, in sample A with the highly strained $In_{0.3}Ga_{0.7}N$/GaN MQW grown on the high TD density GaN layer as shown in Fig. 1(a), V defects originate from not only TDs (marked with "T") but also other sites (marked with "S"). In addition, the V-defect density in the MQW has a

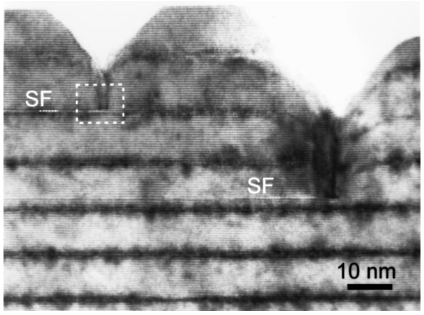

FIG. 2. HRTEM image obtained from the dashed rectangle in Fig. 1(c). The observed V defects have stacking faults on (0001) planes in the their lower position.

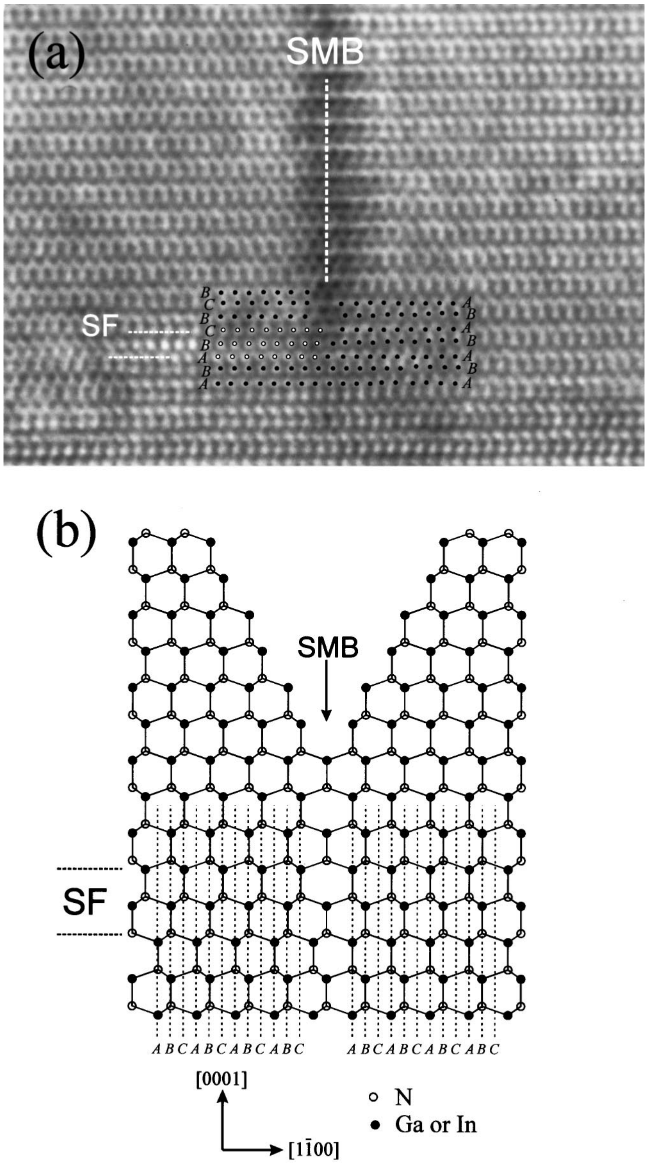

FIG. 3. (a) Magnified HRTEM image from the dashed rectangle in Fig. 2. The stacking order of *ABABABAB* in the left-hand side is transformed into $AB\underline{ABC}BCB$, which indicates stacking fault. Stacking fault generates the stacking mismatch boundaries (SMBs) in the following growth. (b) The geometrical atomic model that shows how the SMB and V defect are generated when the faulted area of the left-hand side meets the corrected stacked area on the right-hand side.

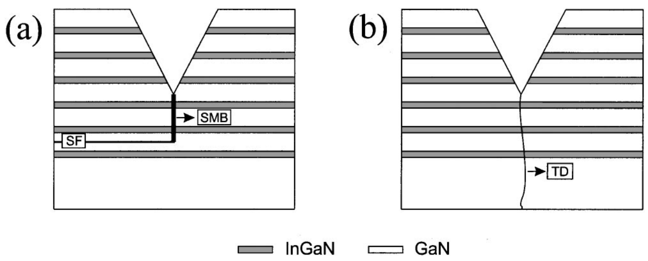

FIG. 4. Schematic models for V-defect formation connected with (a) a threading dislocation (TD) and (b) a SMB induced by stacking faults.

larger value than the TD density in the GaN thick layer as shown in Table I. Therefore, we found that for the MQW grown on the high TD density GaN, V defects are preferentially generated from TDs and by increasing In composition in the $In_xGa_{1-x}N$ well the new formation mechanism, which will be explained below by HRTEM, is induced.

As reported previously, V defects are normally produced in the MQWs with In composition of above ~20% in order to relax the strain. For sample B ($x_{In}=24\%$) grown on the low TD density GaN layer, however, V defects were rarely observed as shown in Fig. 1(b). This result indicates that the TD density in the thick GaN layer affects not only the origin of V-defect formation but also the critical In composition of the $In_xGa_{1-x}N$ well in the formation of V defects. It can be observed in Fig. 1(c) that when the In composition in the MQWs grown on low TD density GaN increased from 24% to 30%, the V-defect density increased and most of the V defects were generated from the site without TD (marked with "S"). Therefore, we found from Fig. 1 that *all* V defects are *not* always connected with TDs at the their bottom.

To illuminate the origin of the V defects with no relation with TDs (marked with "S" in Fig. 1), HRTEM image obtained from the MQW of sample C grown on low TD density GaN [the part indicated as the dashed rectangle in Fig. 1(c)] was investigated. As shown in Fig. 2, the observed V defects have stacking faults on (0001) planes in the their lower position. That is, the stacking order of $ABABABAB$ along the c axis is transformed into that of $AB\underline{ABC}BCB$ in the faulted area [Fig. 3(a)]. Also these stacking faults generate the SMBs in the following growth of the MQW as shown in Figs. 2 and 3(a). SMBs are closely related with stacking faults and finally form the V defects. Figure 3(b) is the geometrical atomic model that shows how the SMB is generated when the faulted area ($AB\underline{ABC}BCB$) of the left-hand side meets the corrected stacked area ($ABABABAB$) of the right-hand side and how the V defect is formed at the SMB. It has been reported that in the InGaN/GaN heterostructure, stacking faults are easily formed in the GaN layer due to the shear in the less compliant GaN layer and low formation energy of stacking faults of only ~20 meV.[16] Therefore, we found that the V defects observed in the highly strained MQW grown on low TD density GaN are mainly connected with the SMBs induced by stacking faults, which is formed due to the relaxation of the large strain in the InGaN/GaN MQWs of high In composition. The ratio of the SMB related V-defect density on the total V-defect density is >90% (Table I).

In conclusion, we have investigated the formation of the V defect in InGaN/GaN MQW structures grown on the thick GaN layers with different TD densities using TEM. We found that unlike other reported results, the different origin of the V defects is observed in the MQWs of the high In composition grown on low TD density GaN. Therefore, we can classify the origin of V defects into two models as shown in Fig. 4. For MQWs with low In composition grown on the high TD density GaN layer, V defects are mainly observed at the vertex of TDs [Fig. 4(a)].[11] However, for MQWs grown with increased In composition or on the low TD density GaN layer, V defects are generated from the SMBs induced by SFs [Fig. 4(b)].

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