Strain Relaxation via Misfit Dislocation in Step-Graded InGaN Heteroepitaxial Layers Grown on Semipolar $(11\bar{2}2)$ and $(1\bar{1}01)$ GaN

Md. Arafat Hossain, Md. Mahbub Hasan, and Md. Rafiqul Islam

***Abstract*—A theoretical existence of misfit dislocation (MD) and strain relaxation has been reported in compositionally step graded $In_xGa_{1-x}N$ grown on the two favored planes of GaN using the total dislocation energy at each interface. The results also compared with uniform layer of $In_{0.17}Ga_{0.83}N$ and $In_{0.14}Ga_{0.86}N$ grown differently on GaN. Due to having residual strain and a step increase in indium (In) composition a lower misfit strain in upper layers and hence larger critical thickness at each interface has been reported. These effects significantly reduced the misfit dislocation from 2.6×10^5 cm^{-1} to 9.5×10^4 cm^{-1} and from 4.0×10^5 cm^{-1} to 1.5×10^5 cm^{-1} in step-graded $In_{0.14}Ga_{0.86}N$(500nm)/$In_{0.09}Ga_{0.91}N$(100nm)/$In_{0.05}Ga_{0.95}N$(100nm) /GaN layers grown on $(11\bar{2}2)$ and $(1\bar{1}01)$ planes respectively instead of an without graded $In_{0.14}Ga_{0.86}N$ (700nm)/GaN layer. A small residual strain of 0.0007 after 700 nm graded layer thickness has been reported with 87.04% strain relaxation.**

***Index Terms*—Critical thickness, burger vector, misfit dislocation, threading dislocation, step-graded layer.**

I. Introduction

Throughout the last decade III-Nitride semiconductors have heen receiving much attention due to their large, direct band gap to create a new generation of electronic and optoelectronic devices. But in heteroepitaxial nitride semiconductors the large lattice mismatch between layers and layer-substrate interface leads to degrade the quality of these promising material systems and hence the performance of their constituent devices. The process of misfit strain relaxation is one of the key factors for improving device performance. The very common mode of strain relaxation is the formation of misfit dislocation by bending of preexisting threading dislocation (TD) on basal plane [1]. The experimental results also proved the strain relaxation mechanism by formation of MD at layer substrate interface in case of InGaN thin film grown on m-GaN [2]. The high density of MD greatly degrades the device performance. So a material system with low MD is highly desirable for future generation electronic and optoelectronic devices fabrication.

The heteroepitaxial layers may be grown on substrate directly or with an intermediate buffer layer which may be grown with compositionally grading. A high density of MD has been reported for uniform composition heteroepitaxial layer on mismatched substrate which degrades the performance of the device significantly [3]. Hence from the very beginning, the heterosructure researchers have been trying to find the way of improving performance of these devices by reducing the MDs. The MD density may be decreased significantly by grading the epitaxial layer with different approach of compositionally grading such as linear grading, nonlinear grading and step grading. Most of the experimental work with graded heteroepitaxial layer has been carried out on linear and nonlinear grading [4]-[5]. Some authors developed reaction model for dislocation reduction in (0001) wurtzite epitaxial GaN thin films [6]. But these models are not sufficient to explain the mechanism of MD formation in wurtzite structure or any approach to reduce the MD at layer-substrate interface. Some experimental works have been carried out on step graded layer grown in different cubic material system such as SiGe/Si, InGaAs/GaAs and reported that this technology may be a promising solution for MD reduction during epitaxial growth [7]-[8]. A very few experimental works has been done on step graded wurtzite materials and they found strong evidence of MD reduction in InGaN epitaxial layer grown on GaN substrate [3], [9]. Though some mathematical model has been developed for cubic structure there is no such work on wurtzite materials for MD reduction via step grading. Thus, a detail theoretical study of MD formation and their reduction in step graded wurtzite structure is greatly needed for high quality material systems for future generation electronic and optoelectronic devices. In this paper we have present a theoretical evidence of low density MD formation during the step increase in In composition with the thickness of InGaN grown on two possible planes of GaN instead of uniform thick single layer of InGaN.

Different force experienced by the grown up TD has been calculated in different slip system in InGaN structure which is based on Matthews-Blakeslee balance force model considering the Peierls force [10]. This result showed that basal plane slip does not experience a shear component of lattice mismatch stress and only the active slip systems $1/3<11\bar{2}3>[11\bar{2}2]$ and $1/3<11\bar{2}3>[1\bar{1}01]$ have finite value of shear stress force hence favorable for strain

Manuscript received December 19, 2011; revised January 18, 2012.

M. A. Hossain is with Department of Electrical and Electronic Engineering of Khulna University of Engineering and Technology (KUET), Khulna-9203, Bangladesh (e-mail: arafat_kuet_eee@ yahoo.com).

M. M. Hasan is with the Department of Advanced Technology Fusion, Saga University, Japan, and on leave from the Khulna University of Engineering and Technology (KUET), Khulna-9203, Bangladesh (e-mail: hasanimahbub@yahoo.com).

M. R. Islam is with Department of Electrical and Electronic Engineering of Khulna University of Engineering and Technology (KUET), Khulna-9203, Bangladesh (e-mail: rafiq043@yahoo.com).

relaxation by producing MD [10]-[11]. The misfit force is responsible for generation of MD which depends upon the degree of mismatch. In this work we have reported that a lower misfit force experienced by the pre-existing TD during the step increase in indium composition leads to lower MD formation. In addition, due to having residual strain a further decrease in the misfit strain results in the upper layers and hence lower MD density has been reported.

II. Theory

In almost all heteroepitaxial growth of interest, the epitaxial layer has a relaxed lattice constant which is different from that of the substrate. As the epitaxial layer thickness increases, so does the strain energy stored in the pseudomorphic layer. At some thickness, called the critical layer thickness (h_c), it becomes energetically favorable for the introduction of MD in the interface that relaxes some of the mismatch strain [1]. The critical layer thickness developed by the Matthews-Blakeslee balance force model is modified to calculate the h_c for each step increase in In composition

$$h_{ci} = \frac{b_i\left(1-\nu_i\cos^2\theta\right)}{8\pi\left(1+\nu_i\right)\left|\varepsilon_{mi}\right|\sin\theta\sin\varphi}\ln\left(\frac{h_{ci}}{r_{0i}}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$\varepsilon_{mi} = \frac{a_{i-1}-a_i}{a_i} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

where the index i in the subscript indicates the step number for increasing In composition in $In_xGa_{1-x}N$, b is the length of burger vector, ν is the Poisson ratio, φ is the angle between the slip plane and normal to the film-substrate interface, θ is the angle between the dislocation line and the burger vector and the outer and inner cut-off radii of the elastic media adjoining the dislocation is $r_0=b/2$. The in plane lattice misfit strain for i^{th} layer can be calculated by Eq. (2). For slip to occur, the slip system should experience resolved share component stress acting on slip plane and slip direction. The primary slip system (basal plane) and the prism plane does not experience the share component of lattice mismatch stress. Thus they are inactive for MD formation.

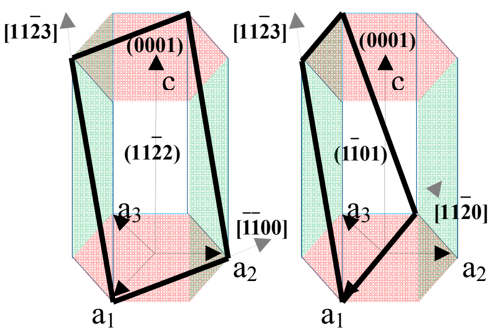


Fig. 1. $1/3<11\bar{2}3>[11\bar{2}2]$ and $1/3<11\bar{2}3>[1\bar{1}01]$ plane orientation in InGaN structure.

Srinivasan et al. estimated theoretically the appropriate slip systems for the misfit dislocations in $In_xGa_{1-x}N$ crystal as $1/3<11\bar{2}3>[11\bar{2}2]$ and $1/3<11\bar{2}3>[1\bar{1}01]$ [10]. Among them the first one shows greater resolve share stress on c-plane and hence most favorable for MD formation. Fig. 1(a) and (b) show the two favored planes for MD formation in InGaN and the parameters used for calculation on both planes are listed in Table I.

TABLE I: Parameters for Favored Slip Systems in Wuzrite Crystal Structure Showing b, φ and θ

Possible Slip	b	φ	θ
$1/3<11\bar{2}3>[11\bar{2}2]$	$\sqrt{a^2(x)+c^2(x)}$	$\arctan\dfrac{a(x)}{c(x)}$	90°
$1/3<11\bar{2}3>[1\bar{1}01]$	$\sqrt{a^2(x)+c^2(x)}$	$\arctan\dfrac{\sqrt{3}a(x)}{2c(x)}$	74.79°

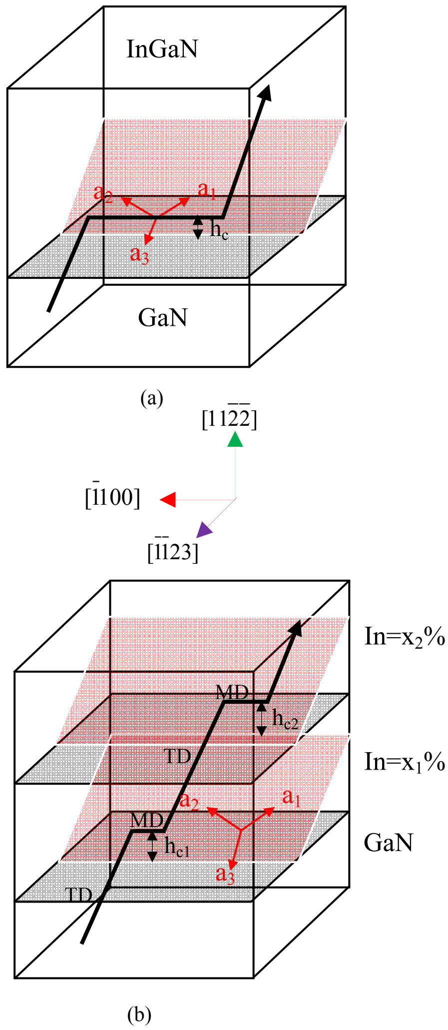


Fig. 2. The grown in dislocation elongates at the interface tocreate a length of misfit dislocation for (a) single uniform layer (b) step-graded layer.

Fig. 2 (a) and (b) presents the effect of compositionally step grading of InGaN grown on GaN in formation of MD. It is clear that each step increase in In composition results in lower MD formation from the pre-existing TD glided from GaN.

In case of material with hexagonal symmetry the only non-zero component of biaxial misfit stress tensor and elastic energy per unit area of the interface takes the form [12]

$$\sigma_{xx} = \sigma_{yy} = \left(c_{11} + c_{12} - \frac{2{c_{13}}^2}{c_{33}} \right) \varepsilon \quad \ldots\ldots\ldots\ldots..(3)$$

$$W = \left(c_{11} + c_{12} - \frac{2{c_{13}}^2}{c_{33}} \right) \varepsilon^2 h \quad \ldots\ldots\ldots\ldots\ldots(4)$$

where c_{ij} are elastic constant and h is the thickness of the epitaxial layer grown on the GaN substrate.

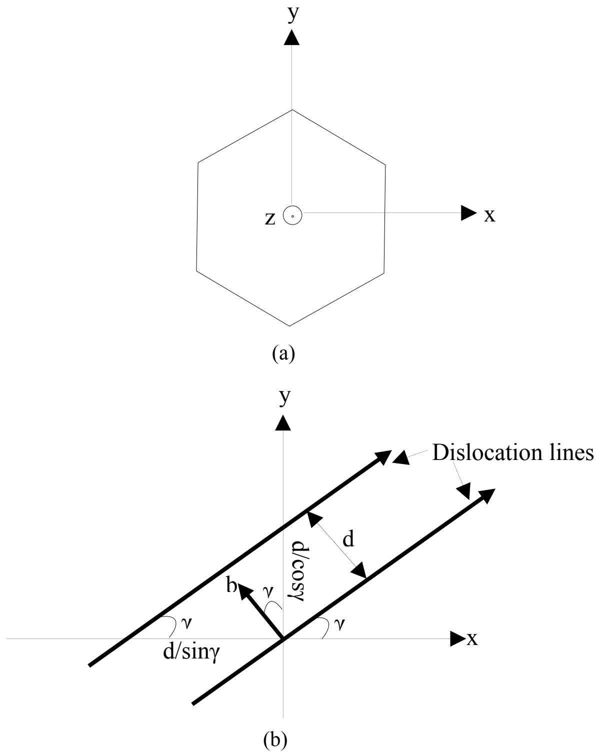


Fig. 3. The three coordinate system for dislocation in wuzrite structure where the z-axis is perpendicular to the c-plane and the dislocation line lies along the y-axis (a) and geometrical represantation of equally distributed dislocation array (b).

In order to calculate the partially relaxed misfit strain let us consider an array of misfit dislocation be inclined by an angle γ from the x-axis as shown in fig. 3. The c-plane edge component burger vector, $b_c = b\cos\varphi\sin\theta$. Let d is the distance between two neighbor dislocations. In such a system the average strain for a layer with thickness h and total three arrays of misfit dislocations which are simultaneously rotated by 60° can be calculated by Eq. (5), (6) and (7), (8) respectively.

$$\varepsilon_{xx}(\gamma) = \frac{b_c \sin\gamma}{\dfrac{d}{\sin\gamma}} = \frac{b_c}{d}\sin^2\gamma \quad \ldots\ldots\ldots\ldots\ldots(5)$$

$$\varepsilon_{yy}(\gamma) = \frac{b_c \cos\gamma}{\dfrac{d}{\cos\gamma}} = \frac{b_c}{d}\cos^2\gamma \quad \ldots\ldots\ldots\ldots\ldots(6)$$

$$\varepsilon^{\gamma}{}_{xx} = \varepsilon_{xx}(\gamma) + \varepsilon_{xx}\left(\gamma + \pi/3\right) + \varepsilon_{xx}\left(\gamma + 2\pi/3\right) = \frac{3b_c}{2d} \quad \ldots(7)$$

$$\varepsilon^{\gamma}{}_{yy} = \varepsilon_{yy}(\gamma) + \varepsilon_{yy}\left(\gamma + \pi/3\right) + \varepsilon_{yy}\left(\gamma + 2\pi/3\right) = \frac{3b_c}{2d} \quad \ldots(8)$$

Now the strain in the epitaxial layer is partially relaxed by the misfit strain. Therefore the residual strain after a thickness of h is

$$|\varepsilon_i| = \left| |\varepsilon_{mi}| - \left| \frac{3b_{ci}}{2d_i} \right| \right| = \left| |\varepsilon_{mi}| - \left| \frac{3}{2} b_{ci}\rho_{MDi} \right| \right| \quad \ldots(9)$$

where, i = 1, 2, 3 …. residual strain of the first, second, third layer and so on. The total energy stored by the array of misfit dislocation in the i[th] layer with partially relaxed misfit strain

$$E_{ti} = \left(c_{11} + c_{12} - \frac{2{c_{13}}^2}{c_{33}} \right) \left(|\varepsilon_{mi}| - \left| \frac{3}{2} b_{ci}\rho_{MDi} \right| \right)^2 h_i + \frac{3}{d} b_{ci} \left(c_{11} + c_{12} - \frac{2{c_{13}}^2}{c_{33}} \right) \varepsilon_{mi} h_{ci} \frac{\ln \dfrac{h_i}{r_{0i}}}{\ln \dfrac{h_{ci}}{r_{0i}}} \quad \ldots. \quad .(10)$$

The first term of this equation is due to the strain energy and the second term counted for energy per unit length of an array of dislocation per unit area lying in the layer substrate interface. It is assumed that the dislocation spacing d is such that it minimizes the total energy, E_{ti}. So the misfit dislocation density is found by differentiating Eq. (10) and results in Eq. (11). The layer grown upon the partially relaxed layer of thickness h_i, will experience a misfit strain less by the residual strain ε_i of the previous layer and calculated by Eq. (12).

$$\rho_{MDi} = \frac{1}{d_i} = \frac{2|\varepsilon_{mi}|}{3b_i \sin\theta\cos\varphi} \left(1 - \frac{h_{ci} \ln \dfrac{h_i}{r_{0i}}}{h \ln \dfrac{h_{ci}}{r_{0i}}} \right) \quad \ldots\ldots..(11)$$

$$|\varepsilon_{m(i+1)}| = \left| \frac{a_{li} - a_{l(i+1)}}{a_{l(i+1)}} \right| - |\varepsilon_i| \quad \ldots\ldots\ldots\ldots\ldots(12)$$

The misfit dislocation density $\rho_{MD(i+1)}$ for the *(i+1)* layer will be updated using the Eq. (11) and (12) and corresponding residual strain ε_{i+1} from Eq. (9) and the results takes the form as Eq. (13) and (14). The parameters used for different possible slip system have used from the TABLE I.

$$\rho_{MD(i+1)} = \frac{2|\varepsilon_{m(i+1)}|}{3b_{(i+1)} \sin\theta\cos\varphi} \left(1 - \frac{h_{c(i+1)} \ln \dfrac{h_{(i+1)}}{r_{0(i+1)}}}{h \ln \dfrac{h_{c(i+1)}}{r_{0(i+1)}}} \right) \quad \ldots\ldots(13)$$

$$|\varepsilon_{i+1}| = \left\| \varepsilon_{m(i+1)} \right| - \left| \frac{3}{2} b_{c(i+1)} \rho_{MD\ (i+1)} \right\| \quad ......(14)$$

III. Result and Discussion

The Matthews-Blakeslee balance force model has been used to calculate the critical layer thickness in each step graded layer. Fig.4. shows that critical layer thickness is inversely dependent with In composition and so the misfit strain. Hence a step increase in In composition leads to larger critical thickness at each interface. In two step-increased In composition layer, the critical thicknesses are found to be 13.5 nm and 11.5 nm for x_1=0.09 and x_2=0.17. For three step-increased layer the critical thicknesses are found to be 29.1nm, 38.6nm and 29.1nm for x_1=0.05, x_2=0.09 and x_3=0. 14 respectively. In case of step-graded layer the critical thickness at each layer has been calculated by considering the relative misfit stress in any layer with respect to its previous layer. Therefore, at each step increase composition a large critical thickness also ceases to rapid increase in MD which has been shown in Fig. 5(a) and 6(a). The same value of critical thickness has been considered during the growth on both $1/3 < 11\bar{2}3 > [11\bar{2}2]$ and $1/3 < 11\bar{2}3 > [1\bar{1}01]$ slip systems.

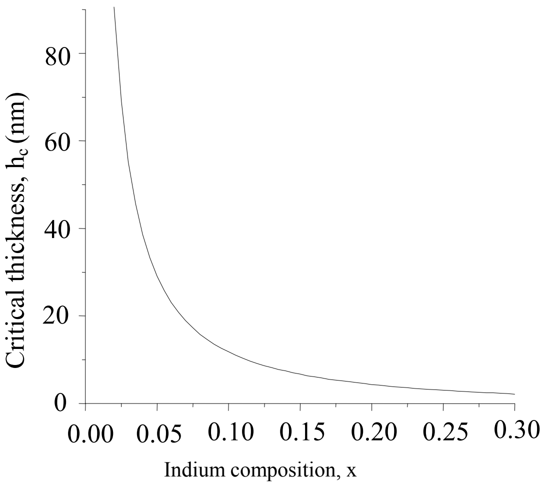
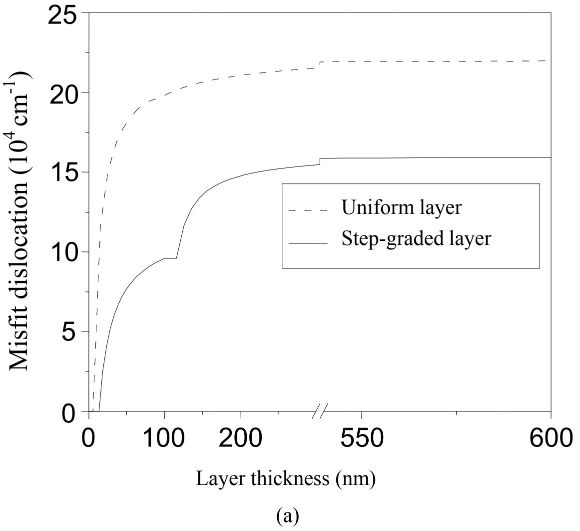
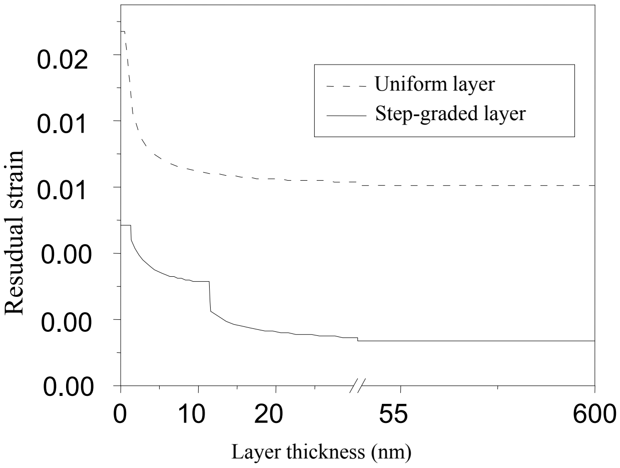


Fig. 4. Critical layer thickness over indium composition in InGaN/Gan structure.

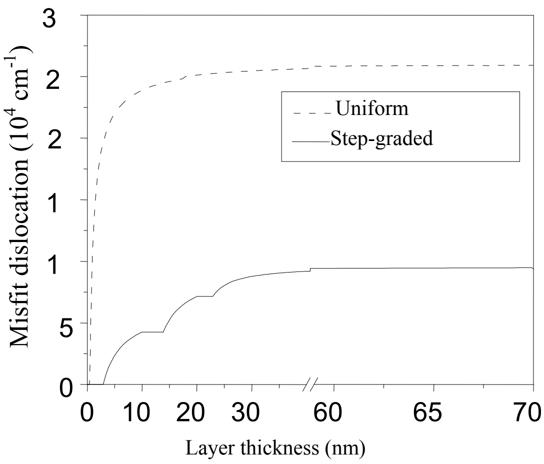


(a)

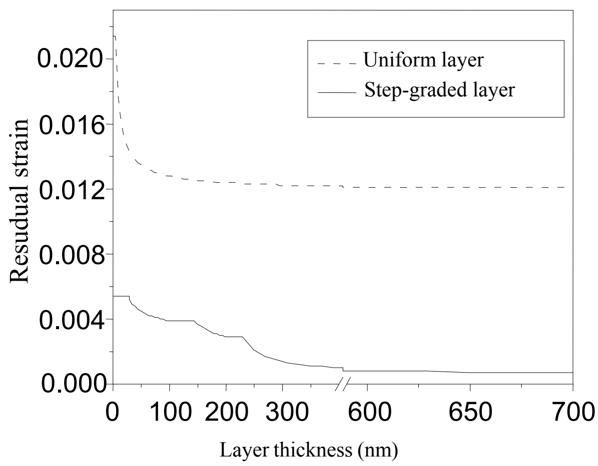


(b)

Fig. 5. Misfit dislocation (a) and strain relaxation (b) profile of $In_{0.17}Ga_{0.83}N$/GaN heterostructure with uniform and two step-graded InGaN layers on $(11\bar{2}2)$ GaN.



(a)



(b)

Fig. 6. Misfit dislocation (a) and strain relaxation (b) profile of $In_{0.14}Ga_{0.86}N$/GaN heterostructure with uniform and three step-graded InGaN layers on $(11\bar{2}2)$ GaN.

The dependence of MD and residual strain on step graded epitaxial layer is shown in Fig. 5, where we calculated the total MD in $In_{0.17}Ga_{0.83}N$ layer grown on $(11\bar{2}2)$ GaN. A single layer of 600 nm $In_{0.17}Ga_{0.83}N$ is compared with two step graded layer having 100 nm $In_{0.09}Ga_{0.91}N$ and 500 nm $In_{0.17}Ga_{0.83}N$ epilayer. The compasrison has been made with a three step-increased In composition layers of 100 nm $In_{0.05}Ga_{0.95}N$, 100 nm $In_{0.09}Ga_{0.91}N$ and 500 nm $In_{0.14}Ga_{0.86}N$ epilayer on $(11\bar{2}2)$ GaN are shown in Fig. 6. A significant MD reduction is observed in the results. The MD has been decreased from 2.2×10^5 cm^{-1} to 1.6×10^5 cm^{-1} and from 2.59×10^5 cm^{-1} to 9.5×10^4 cm^{-1} for two and and three step-graded structure respectively on $(11\bar{2}2)$ GaN.

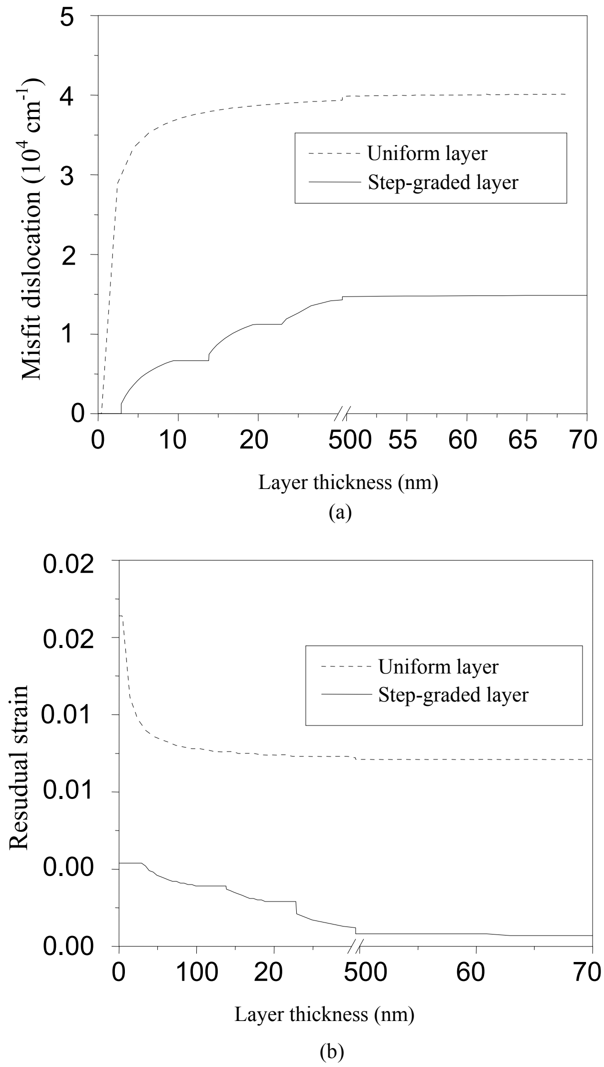


Fig. 7. Misfit dislocation (a) and strain relaxation (b) profile of $In_{0.14}Ga_{0.86}N$/GaN heterostructure with uniform and three step-graded InGaN layers on $(1\bar{1}01)$ GaN.

The result of MD generation and strain relaxation for $In_{0.14}Ga_{0.86}N$ grown on $(1\bar{1}01)$ GaN with three step graded layer and uniform layer is shown in Fig. 7. For the second possible plane of MD generation the MD has been decreased from 4.0×10^5 cm^{-1} to 1.5×10^5 cm^{-1}. The physics behind this phenomenon in during step increase in In composition the grown in TDs experience a relatively lower misfit stress than that of single uniform composition layer. The residual strain profile shown in Fig. 6(b) and 7(b) confirms the evidence of strain relaxation by MD formation. A misfit strains of 0.0093 and 0.0047 have been relaxed by first and second structure of step graded layers.

IV. Conclusion

A lower misfit force experienced by the pre-existing TD during the step increase in In composition leads to lower MD formation in InGaN grown on semipolar $(11\bar{2}2)$ and $(1\bar{1}01)$ GaN. In addition, due to having residual strain a further decrease in the misfit strain is found in the upper layers and hence lower MD density is obtained. The lower MD density and residual strain in the upper layers as compared to the uniform layer make the step graded layer a superior technique for high performance semiconductor device fabrication.

References

[1] J. W. Matthews and A. E. Blakeslee, "Defects in Epitaxial Multilayers," *Journal of Crystal Growth* 27, 118-125 (1974)

[2] Takashi Hanada, Taka-aki Shimada, Shi-Yang Ji, Kenji Hobo, Yuhuai Liu, and Takashi Matsuoka, "Strain relaxation mechanism of InGaN thin film grown on *m*-GaN," *Phys. Status Solidi* C 8, No. 2, 444–446 (2011).

[3] M Haeberlen, D Zhu, C McAleese, MJ Kappers and CJ Humphreys, "Dislocation reduction in MOVPE grown GaN layers on (111)Si using SiNx and AlGaN layers," Journal of Physics: Conference Series 209 (2010)

[4] B. Bertoli, D. Sidoti, S. Xhurxhi, T. Kujofsa, S. Cheruku, J. P. Correa, P. B. Rago, E. N. Suarez, F. C. Jain, and J. E. Ayers, "Equilibrium strain and dislocation density in exponentially graded Si1-xGe_x/Si (001)," *Journal of Applied Physics* 108, 113525 (2010)

[5] D. Sidoti, S. Xhurxhi, T. Kujofsa, S. Cheruku, J.Reed, B. Bertoli, P.B. Rago, E.N. Suarez, F.C. Jain, and J.E. Ayers, "Critical Layer Thickness in Exponentially Graded Heteroepitaxial Layers," *Journal of Electronic Materials*, Vol. 39, No. 8, 1140-1145 (2010)

[6] S.K.Mathis, A. E. Romanov, L. F. Chen, G. E. Beltz, W. Pompe, and J. S. Speck, "Modeling of Threading Dislocation Reduction in Growing GaN Layers," *Phys. Stat. sol*. (a) 179, 125 (2000)

[7] P. M. Mooney, J. L. Jordan-Sweet, J. O. Chu, and F. K. LeGoues, "Evolution of strain relaxation in step-graded SiGe/Si structures," *Appl. Phys. Lett*. **66**, 3642 (1995)

[8] V. Krishnamoorthy, Y. W. Lin, and R. M. Park, "Application of 'critical compositional difference concept to growth of low dislocation density($<10^4/cm^2$) $In_xGa_{1-x}As$ ($x\leq0.5$) on GaAs," *Journal of Applied Physics,* 72, 1752, (1992)

[9] G. Macpherson, R. Beanland, and J. P. Goodhew,"A novel design method for the suppression of edge dislocation formation in step-graded InGaAs/GaAs layers," *Philosophical Magazine A*, Vol. 73, No 05, 1439-1450 (1996)

[10] S. Srinivasan, L. Geng, R. Liu, and F. A. Ponce, Y. Narukawa and S. Tanaka, "Slip systems and misfit dislocations in InGaN epilayers," *Applied Physics Letters*, 83, 5187 (2003)

[11] Erin C. Young, Feng Wu, Alexey E. Romanov, Anurag Tyagi, Chad S. Gallinat,Steven P. DenBaars, Shuji Nakamura, and James S. Speck, "Lattice Tilt and Misfit Dislocations in (11_22) Semipolar GaN Heteroepitaxy," *Applied Physics Express* 3, 011004 (2010).

[12] D. Holec, P.M.F.J. Costa, M.J. Kappers, C.J. Humphreys, "Critical thickness calculations for InGaN/GaN," *Journal of Crystal Growth* 303 314–317 (2007)

Md. Arafat Hossain was born in Kushtia, Bangladesh on 02 Sep. 1987. He received Bachelor of Science in Electrical and Electronic Engineering (EEE) from Khulna University of Engineering and Technology (KUET) in March 2009. Currently he is a lecturer and MSc Student of EEE department of KUET. He has some others publications on Indium Nitride (InN) based heterostructure devices. He has also attended many internationally reputed conferences in home and abroad. His specific research interests are on Dislocation Reduction in Semiconductor Growth and InN based Heterostructure Devices.

Md. Mahbub Hasan was born in Jessore, Bangladesh on 21 June 1982. He received B.Sc. and M.Sc. degrees in Electrical and Electronic Engineering (EEE) from Khulna University of Engineering and Technology (KUET) in 2006 and 2010, respectively. Currently he is an Assistant professor (on Leave) of EEE department of KUET and PhD Student of Advanced Technology Fusion department of Saga University, Japan.