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A Simulation Analysis of Dislocations Reduction in InxGa1-xN/GaNHeterostructure Using Step-graded Interlayers

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Abstract:- To reduce the misfit dislocation densityis a great challenge for semiconductor devices. Misfit dislocation generation is harmful for device performance. In this paper, we have used different techniques to reduce misfit dislocation. We have studied and calculated the critical layer thickness by varying In composition and we have compared the result between two models i.e. Matthews-Blakeslee and People-Bean model. Matthews-Blakeslee model shows the better performance than People-Bean model. Then we have analyzed the misfit dislocation generation by varying layer thickness and compared the result between two graded layer i.e. uniform graded layer and step graded layer for different three planes such as 1/3<11-23>{11-22},1/3<1-101>{11-22},1/3<11-23>{0001}. Here it is remarkable that we are also able to show the edge, screw as well as mixed dislocation density by varying layer thickness among these planes. Step graded layer displays the lesser misfit dislocation generation than uniform graded layer. Then we have investigated the inter layer effects. If we use more number of interlayer, the dislocation density can be reduced with sharply.

Keywords:- *InGaN;dislocation;critical layer thickness; In composition;step graded layer;inter layer effect.*

I. INTRODUCTION

During the last decade III-Nitride semiconductors have been receiving much concentration due to their large, direct band gap to build 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 essential devices. 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. Many researchers have been analyzed to reduce misfit dislocation generation. Md. Arafat Hossain, Md. Mahbub Hasan, and Md. Rafiqul Islam [1] have calculated the critical layer thickness in each step graded layer using the Matthews-Blakeslee balance force model that critical layer thickness is inversely dependent with In composition. The critical thicknesses are found to be 13.5 nm and 11.5 nm for x1=0.09 and x2=0.17, the MD has been decreased from $2.2\times10^{5}\text{cm}^{-1}$ to $1.6\times10^{5}\text{cm}^{-1}$. Authors [2] reported that the critical thickness have been found to be 12.4, 13.9 and 3.3 nm in (11-22), (1-101) and (0001) slip respectively for 10% In composition. Durjoy Dev, Anisul Islam, Md. Rafiqul Islam, Md. Arafat Hossain and A. Yamamoto [3] have calculated the value of critical layer thickness at x=0.2 is 6.792 nm and the edge MD densities of 3.25×10^{11}, 9.39×10^{10}, 6.7×10^{10}, 4.74×10^{10}, 4.45×10^{10} and 4.24×10^{10} cm^{-2} have been calculated for 0, 1, 2, 3, 4 and 5 interlayer respectively. The present article presents a theoretical analysis of different types of critical layer thickness by using Matthews-Blakeslee and People – Bean force balance model, MDs generation by using uniform graded layer and step graded layer and effects of interlayer number on their reduction. In this work 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 three possible planes of GaN. We have observed that more number of interlayer reduce the dislocation density sharply.

II. THEORY

All mechanical properties of GaN and InN used in the subsequent calculations are summarized in this subsection. Lattice parameters of wurtzite GaN and InN are given in Table 1.1[7]. The lattice parameters for $In_xGa_{1-x}N$ are derived using Vegard's law.In approximately all heteroepitaxial development of interest, the epitaxial layer has a stress-free 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 a few thickness, called the critical layer thickness (hc), it becomes energetically approving for the introduction of MD in the interface that relaxes some of the mismatch strain.The critical layer thickness developed by the Matthews-Blakeslee balance force model is modified to calculate the hc for each step increase in In composition [4].

Table 1.1: Lattice parameters of GaN and InN used in the calculations throughout this work [8].

Materials	a[$\overset{o}{A}$]	$c[\overset{o}{A}]$
GaN	3.189	5.185
InN	3.538	5.702

$$h_c = \frac{b(1-\cos^2\theta)}{8\pi(1+\vartheta)|\epsilon_m|\sin\theta\sin\emptyset}\ln\left(\frac{h_c}{r_0}\right) \qquad (1)$$

The index b is the length of burger vector, v 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 burger vector and r0 is dislocation cut-off parameter.

The critical layer thickness, hc(x), at which strain relief is expected to occur, can be estimated as a function ofx using the model proposed by People and Bean. The equation for hc(x) as a func-tion of the lattice mismatch and the film structural properties is given by [6]

$$h_c(x) = \left(\frac{1-v(x)}{1+v(x)}\right)\left(\frac{1}{16\pi\sqrt{2}}\right)\left(\frac{b^2}{a(x)}\right)\left[\left(\frac{1}{f^2(x)}\right) ln\left(\frac{h_c(x)}{b}\right)\right] \qquad (2)$$

Where n(x) is Poisson's ratio, a(x) is the bulk lattice constant of the film, b is the slip distance, and f(x)is the lattice mismatch. The value used for b was a_{GaN}, and Vegard's law was assumed to obtain a(x) and n(x).

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 [5]

$$\sigma_{xx} = \sigma_{yy} = \left(C_{11} + C_{12} - \frac{2C_{13}^2}{C_{33}}\right)\epsilon \qquad (3)$$

$$W = \left(C_{11} + C_{12} - \frac{2C_{13}^2}{C_{33}}\right)\epsilon^2 h \qquad (4)$$

where cij are elastic constant and h is the thickness of the epitaxial layer grown on the GaN substrate.Therefore the strain energy per unit area of the interface in the material with hexagonal symmetry is [3]

$$\frac{dW}{dA} = \left(C_{11} + C_{12} - \frac{2C_{13}^2}{C_{33}}\right)\left(|\epsilon_{mi}| - \left|\frac{3}{2}b_{ci}p_i\right|\right)^2 h \qquad (5)$$

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

$$|\epsilon_i| = \left||\epsilon_{mi}| - |\frac{3}{2}b_{ci}p_i|\right| \qquad (6)$$

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 ith layer with partially relaxed misfit strain

$$\in_{total} = \left(C_{11} + C_{12} - \frac{2C_{13}^2}{C_{33}}\right)(\in_{mi} - \left|\frac{3b_{ci}}{2l_i}\right|)^2 h_i + \frac{3b_{ci}}{2l_i}\left(C_{11} + C_{12} - \frac{2C_{13}^2}{C_{33}}\right) \in_m h_c \frac{ln\frac{h_i}{r_o}}{ln\frac{h_c}{r_o}} \tag{7}$$

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 l is such that it minimizes the total energy ε_{total} so the misfit dislocation density is found by differentiating above equation which results in Eq. (8). 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. (8).

$$p_i = \frac{1}{l_i} = \frac{3}{2}\frac{\in_{mi}}{b_i sin\theta cos\ \emptyset}\left(1 - \frac{h_c ln\frac{h_i}{r_o}}{h ln\frac{h_c}{r_o}}\right) \tag{8}$$

$$|\in_{m(1+i)}| = \left|\frac{a_{li} - a_{l(i+1)}}{a_{l(i+1)}}\right| - |\in_i| \tag{9}$$

The misfit dislocation density $\rho_{(i+1)}$ for the (i+1) layer will be updated using the Eq. (8) and (9) corresponding residual strain.

In this paper, the most creative work is to analyze the interlayer effect on edge, screw and mixed dislocation. By using the equation 8, we have observed the effect of one and two interlayer on misfit dislocation .The value of misfit dislocation for edge ,screw, and mixed in one interlayer is comparatively large than two interlayer which is the main point.

III. RESULT AND DISCUSSION

The Matthews-Blakeslee balance force model and People-Bean model has been used to calculate the critical layer thickness in each step graded layer which is shown in figure 1 & 2. The figures show the inverse relationship between critical layer thickness and indium composition. Here step increase in indium composition leads to lower value of critical layer thickness.

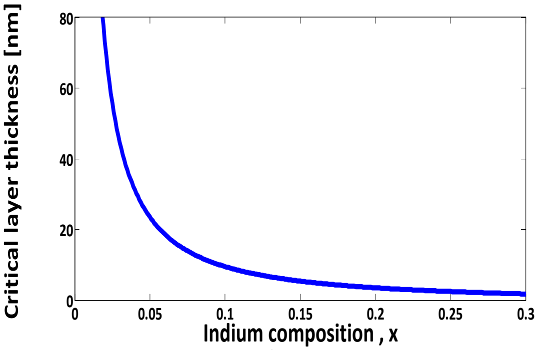

Figure 1: Critical thickness for the In$_x$Ga$_{1-x}$N /GaN system predicted by Matthews and Blakeslee model.

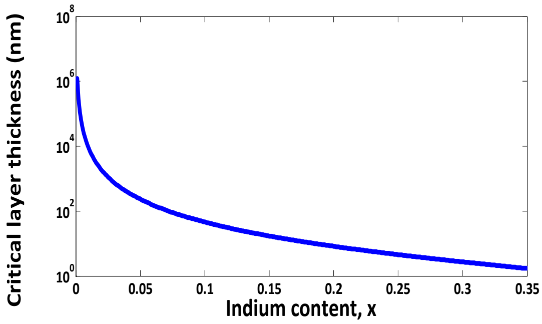

Figure 2: Critical thickness for the In$_x$Ga$_{1-x}$N /GaN system predicted by People and Bean Model

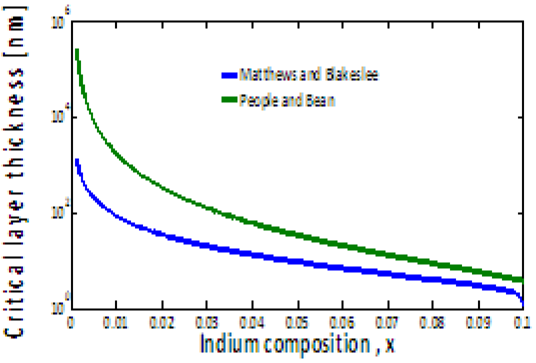

Figure 4: Comparison of critical thickness for the $In_xGa_{1-x}N$ /GaN predicted by Matthews and Blakeslee and People and Bean for screw type dislocation of1/3<11-23>{11-22}.

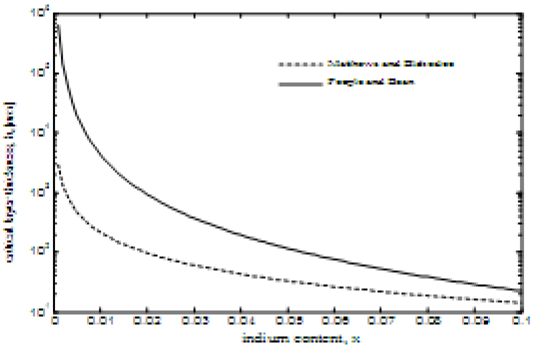

Figure 5: Comparison of critical thickness for the $In_xGa_{1-x}N$ /GaN predicted by Matthews and Blakeslee and People and Bean for mixed type dislocation of 1/3<11-23>{11-22}.

The figure 3, 4, 5 show the comparison relationship between Matthews-Blakeslee and People - Bean force balance model for critical layer thickness to In composition for 1/3<11-23>{11-22} plane . Edge type dislocation from fig.3 shows the different value of critical layer thickness with the step increase in In composition. And for the same value of In composition 0.15 the critical layer thickness for Matthews-Blakeslee model is 9.82nm and 17.3nm for People- Bean method.

In Screw type dislocation from fig.4 for the same value of In composition 0.1 the critical layer thickness for Matthews-Blakeslee model is 2.768nm and 8.279nm for People-Bean method. In Mixed type dislocation from fig.5 for the same value of In composition 0.05 the critical layer thickness for Matthews-Blakeslee model is 33.01nm and 116.3nm for People-Bean method.

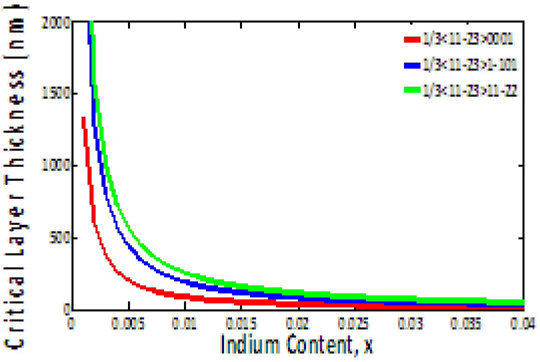

Figure 6: Comparison of critical thickness for the $In_xGa_{1-x}N$ /GaN system predicted by Matthews and Blakeslee at different plane.

The figure 6 shows the Comparison of critical thickness for the $In_xGa_{1-x}N$ /GaN predicted by Matthews and Blakeslee at different plane. For the 1/3<11-23>{11-22} plane the critical layer thickness for 0.2 indium content is 16.99 nm, 11.89 nm for 1/3<11-23>{1-101} plane and 6.802 nm for 1/3<11-23>{0001} plane.

Observing the above figure from 1 to 6 we conclude that the Matthews and Blakeslee model suits more than other model to theoretical and practical works which were performed in the past. So, Matthews and Blakeslee model for critical layer thickness is favorable.

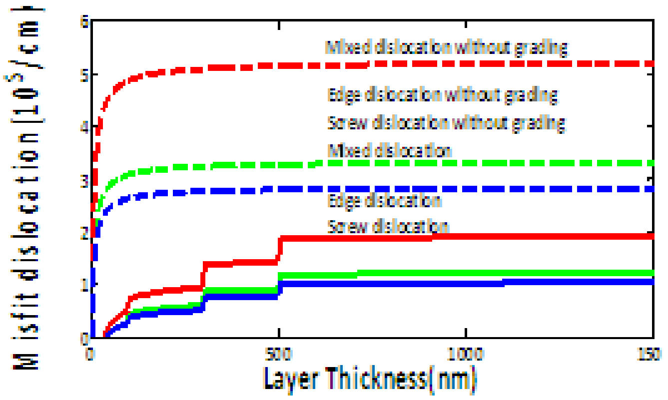

Figure 7: comparison between uniform and step graded layer for the edge, screw and mixed type dislocation with layer thickness for 1/3<11-23>{11-22} plane.

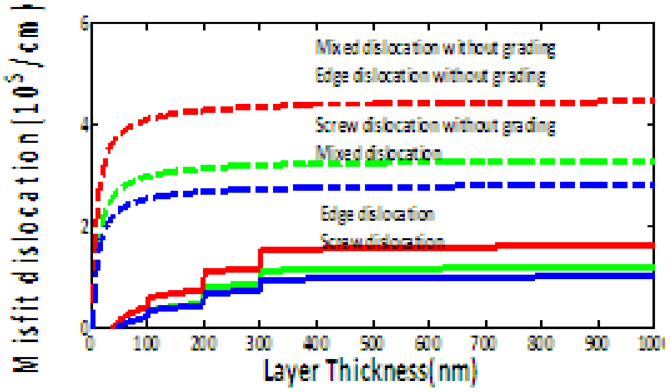

Figure 8: comparison between uniform and step graded layer for the edge, screw and mixed type dislocation with layer thickness for 1/3<11-23>{1-101} plane.

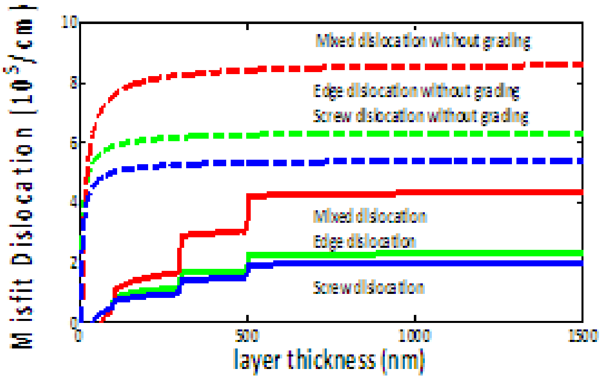

Figure 9: comparison between uniform and step graded layer for the edge, screw and mixed type dislocation with layer thickness for 1/3<11-23>{0001} plane.

The figures 7, 8, 9 shows the comparison between uniform and step graded layer for the edge, screw and mixed type dislocation with layer thickness for different plane. Figure 7 for 1/3<11-23>{11-22} plane states that for uniform layer the edge, screw and mixed type dislocation is much more than step graded layer. For the same point of layer thickness the screw dislocation is 2.826×10^{5} cm^{-1} for uniform layer and 1.034×10^{5} cm^{-1} for step graded layer. On the other hand the edge dislocation for uniform layer is $3.331\times 10^{5}\,cm^{-1}$ and $1.21\times 10^{5}\,cm^{-1}$ for step graded layer and for mixed type dislocation for uniform layer is $5.191\times 10^{5}\,cm^{-1}$ and $1.9\times 10^{5}\,cm^{-1}$ for step graded layer. So, among three types of dislocation, dislocation density is the lowest in screw type. From Fig. 8, for 1/3<11-23>{1-101} plane, screw dislocation is 2.817×10^{5} cm^{-1} for uniform layer and 1.028×10^{5} cm^{-1} for step graded layer. From Fig. 9, for 1/3<11-23>{0001} plane, the screw dislocation is 5.37×10^{5} cm^{-1} for uniform layer and 1.969×10^{5} cm^{-1} for step graded layer. In every plane, the screw type shows the lowest dislocation density with layer thickness and the performance of 1/3<11-23>{11-01} plane is best.
By the above figure 7, 8, 9, we conclude that step graded layer technique is much better than uniform layer to reduce misfit dislocation.

The figures 10 and 11 show the interlayer effect for the edge, screw and mixed type dislocation with layer thickness for 1/3<11-23>{11-22} plane. In figure 10, we use only one inter layer and which results the dislocation density for screw 2.319×10^{5}cm^{-1}, for edge 2.715 ×10^{5}cm^{-1} and for mixed 4.271 ×10^{5}cm^{-1}. In figure 11, we have used two inter layer and which results the dislocation density for screw 1.809×10^{5}cm^{-1}, for edge 2.118×10^{5} cm^{-1} and for mixed $3.328\times 10^{5}\,cm^{-1}$.

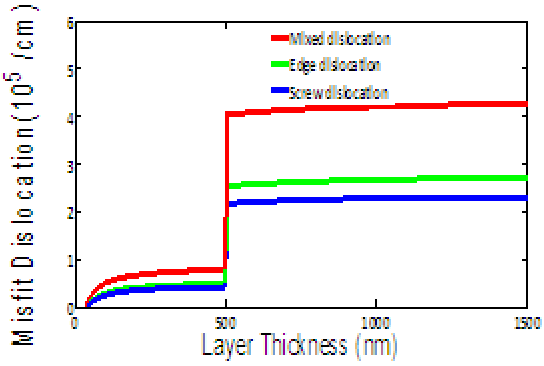

Figure 10: The interlayer effect for the edge, screw and mixed type dislocation with layer thickness for 1/3<11-23>{11-22} plane using one interlayer.

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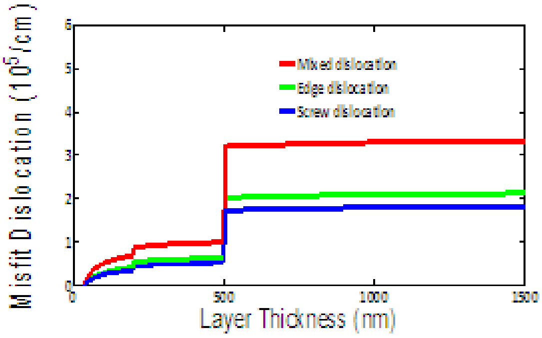

Figure 11: The interlayer effect for the edge, screw and mixed type dislocation with layer thickness for 1/3<11-23>{11-22} plane using two interlayer.

So, the above figure 10 and 11 state that if we use more interlayer the dislocation density can be reduced with sharply. So, interlayer effect is very important to reduce the misfit dislocation as well as for good performance of the fabricated device. But it is important to notify that increasing interlayer also increases the experimental complexity as well as initiates interfacial dislocations in every layer

IV. CONCLUSION

Misfit dislocations, the mechanism of their generation and their properties are a crucial problem in any hetero-epitaxy. The quickly evolving area of applications based on III-nitrides enforced a revision of various models. To fulfil this aim a literature survey was carried out that resulted in identifying several most frequently used critical thickness models. Original results on the misfit dislocation for InGaN/GaN step graded layer systems were presented. A step wise change of lattice mismatch in step-graded interlayer introduces a reduced amount of misfit force and subsequently lesser misfit dislocation generation with thickness. The increase of interlayer enhances this decline up to a definite limit. Therefore, the lower MDs and TDs density in the upper layers as compared to the without graded layer make the step-graded interlayer a better technique for high performance semiconductor device fabrication. However, more attention will be given to obtain reliable experimental data and faithful comparison between theory and experiment in the future work. We will extend the work on misfit dislocation for multiple quantum wells in future.

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