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# Zone Centre Phonon Mode Behavior of Wurtzite Phase of Ternary Nitrides

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***Abstract: The group-III nitrides have been acknowledged as noteworthy materials for researchers in recent times for their extra ordinary properties and applications. The vital property of these materials is their wide and direct band gap, which can also be customized by doping. A common feature of these device structures is the applicability of ternary alloys. Despite of the wide range of the ternary alloys of group-III nitrides only few have been discussed. So in this study we have studied zone centre phonon mode behavior of the ternary alloys $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ for wurtzite phase using de Launey Angular force constant model. The optical phonon modes at zone centre have been found for $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$. The content of Al and In in alloy is in the range 0<x<1. The one mode behavior has been observed for both the alloys and it is found that for wurtzite phase of $In_xGa_{1-x}N$ continuous decreases in magnitude of phonon frequency with the increase in the content of In and for wurtzite phase of $Al_xGa_{1-x}N$ increase in magnitude of phonon frequency is reported with incresae in content of Al, which is due to the fact that frequency varies inversely proportional to the mass, as content of In increases mass of alloy while content of Al decreases the mass of alloy.***

## I. INTRODUCTION

Group-III nitrides are the fundamental building blocks of laser diodes (LDs), light emitting diodes (LEDs), emitter and receiver of optoelectronic devices. An extraordinary property of group-III nitride semiconductors is the utilization of their ternary alloys. The direct band gap of group-III nitride alloys can be continuously extended from infrared (IR) region to ultraviolet (UV) region with suitable concentration of doping. The energy gaps of $In_xGa_{1-x}N$ alloy provides an outstanding match to the full solar band which unlock an chance for high efficiency multifunction solar cells with flexibility of selection of gaps (Wu et al., 2003). $Al_xGa_{1-x}N$ can also be used for water purification. These alloys can meet the requirement of next generation electronic equipment, high frequency, microwave power appliances of high power, smaller dimensions and work under ambient conditions. In recent studies the optical modes of $In_xGa_{1-x}N$ in cubic phase by molecular beam epitaxy were experimentally studied by using Raman spectroscopy and it is observed that the optical modes show a one-mode behavior and their frequency vary linearly with alloy composition (Teles et al., 2004, Santos et al., 2002). The infrared transmission study of both the phases i.e. cubic and wurtzite phase of $Al_xGa_{1-x}N$ has been studied by (Ibanez et al., 2008) in composition range 0<x<0.3 and reported one mode behavior for $Al_xGa_{1-x}N$. To improve the performance of the devices the understanding of the light emission mechanism is essential. Even these materials have such outstanding properties but ternary alloys of cubic and wurtzite phase have been studied much less efficiently. The knowledge of basic properties of these materials is lacking. Therefore, in the present study the zone centre phonon mode behavior of various optical modes of ternary alloys $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$ for wurtzite phase have been investigated by using de Launey angular force constant model to understand the miscibility of one in another with varying composition 0<x<1. The zone centre phonon frequency of these alloys is calculated and results are found to be in admirable agreement with existing experimental and theoretical results with large range of composition.

## II. THEORY

The creation of mixed crystal with special proportion of two undoped crystals results in a fresh set of crystal with physical properties which are in-between pure end members depending upon the composition of pure crystals. The properties may change in different manner with variation of composition. In some mixed crystals properties changes monotonically linearly as a function of composition while in some cases the properties may vary non-linearly (may be slightly non linearly or highly non-linear manner). In some cases, properties are different from the properties of parent crystals at all and these properties are unique to mixed crystals only.

In this study by using de Launey Angular force constant model we have obtained the frequency at zone centre of the In and Al doped GaN with composition varying from 0 to 1. Here two parts of the Interatomic interactions are considered: Central interaction (ion-ion radial interaction), which act along the line joining the centres of two neighbors and angular force which depends upon the angle which the line joining the moving atoms makes with the line joining their equilibrium position. These forces are considered for first and second nearest neighbors. We shall let $\alpha_1$ and $\alpha'_1$ denote the force constant associated with central force and angular force of the nearest neighbor, while $\alpha_2$ and $\alpha'_2$ denote the force constant associated with central and angular force next nearest neighbours. In DAF model by using the coordinates and direction cosines of the neighbors, in the equation of motion given below

$$\vec{F} = -\alpha'(\vec{S}_0 - \vec{S}_i) - (\alpha - \alpha')(\hat{\zeta}_i)[\hat{\zeta}_i.(\vec{S}_0 - \vec{S}_i)]$$

Where $S_o$ and $S_i$ are the displacements of the reference atom and ith atom.

$\hat{\zeta}$ is the unit vector along the line joining the reference atom to the ith atom.

By using above equation a dynamical matrix of 6x6 is formed and is given by the solution of characteristic equation

$[d(k) - m\omega^2 I] = 0$

Where D(k) is (12x12) dynamical matrix in case of wurtzite phase, as wurtzite structure has four atoms per unit cell and I is unit vector. The obtained dynamical matrix of (12 x 12) is solved at center of the zone to get relation between some vibrational frequencies and force constants. The following relations between force constants and some important vibrational frequencies are obtained.

$$\frac{4}{3}(\alpha_1 + 2\alpha_1') = \frac{m_1 m_2}{m_1 + m_2}\omega^2_{E_1(TO)}$$

$$\frac{4}{3}(\alpha_1 + 2\alpha_1') + 2(4\alpha_2 + 2\alpha_2') = m_2\omega^2_{A_1(TO)}$$

$$4(\alpha_2^2 + 25(\alpha_2')^2 + 10\alpha_2\alpha_2 - \alpha_1^2) + \frac{16}{3}(\alpha_1 + 2\alpha_1')(\alpha_2 + 5\alpha_2' + \alpha_1) - \left(\frac{4}{3}(\alpha_1 + 2\alpha_1') + 2\alpha_1 + 10\alpha_2'\right)(m_1 + m_2)\omega^2_{E_2^h} + m_1 m_2\omega^4_{E_2^h} = 0$$

$$\alpha_2 + 5\alpha_2' + \alpha_1' = \frac{m_1}{2}\omega^2_{E_2^l}$$

Here $m_1$ and $m_2$ are the mass of X (Al, Ga, B and In) and N atom respectively. By using the experimental values of the zone centre frequencies, $m_1$ and $m_2$ as the input parameter the above equations are solved to calculate force constants at zone centre of the binaries. To calculate the force constants for ternary alloys Vegard's law is used and the involved four force constants and mass of constituent atoms (P and Q) for any ternary alloy $P_xQ_{1-x}N$ are obtained by using Vegard's law as given below.

$$\alpha_{P_xQ_{(1-x)}N} = x\alpha_{PN} + (1-x)\alpha_{QN} \qquad 5.1$$

$$m_{P_xQ_{(1-x)}} = xm_P + (1-x)m_Q \qquad 5.2$$

Where $m_P$ and $m_Q$ are the masses of P (P = Al, Ga, In) and Q (Q = Al, Ga, In) and $\alpha_{PN}$ and $\alpha_{QN}$

Table I

Force constants for wurtzite ternary alloy $Al_xGa_{1-x}N$

| Alloy | Composition (x) | Force Constant ($10^4$ dyne $cm^{-1}$) | | | | Mass of $Al_xGa_{1-x}$ ($10^{-24}$gm) |
|---|---|---|---|---|---|---|
| | | $\alpha_1$ | $\alpha_1'$ | $\alpha_2$ | $\alpha_2'$ | |
| $Al_xGa_{1-x}N$ | 0.0 | 10.5253 | 2.8951 | 0.0933 | 0.2703 | 116.39 |
| | 0.2 | 10.81086 | 2.98002 | 0.21736 | 0.2583 | 102.125 |
| | 0.4 | 11.09642 | 3.06494 | 0.34142 | 0.2463 | 87.858 |
| | 0.6 | 11.38198 | 3.14986 | 0.46548 | 0.2343 | 73.592 |
| | 0.8 | 11.66754 | 3.23478 | 0.58954 | 0.2223 | 59.326 |
| | 1 | 11.9531 | 3.3197 | 0.7136 | 0.2103 | 45.06 |

Table II
Force constants for wurtzite ternary alloy $In_xGa_{1-x}N$

| Alloy | Composition (x) | Force Constant ($10^4$ dyne $cm^{-1}$) | | | | Mass $In_xGa_{1-x}$ ($10^{-24}$gm) |
|---|---|---|---|---|---|---|
| | | $\alpha_1$ | $\alpha_1'$ | $\alpha_2$ | $\alpha_2'$ | |
| $In_xGa_{1-x}N$ | 0.0 | 10.5253 | 2.8951 | 0.0933 | 0.2703 | 116.39 |
| | 0.2 | 1026008 | 2.65586 | 0.05014 | 0.25638 | 131.462 |
| | 0.4 | 9.994716 | 2.41662 | 0.0698 | 0.24462 | 146.534 |
| | 0.6 | 9.729424 | 2.17738 | 0.03618 | 0.22854 | 161.606 |
| | 0.8 | 9.464132 | 1.93814 | -0.0793 | 0.21462 | 176.678 |
| | 1 | 9.1992 | 1.6989 | -.1225 | 0.2007 | 191.75 |

## III. RESULTS AND DISCUSSIONS

It is clear from table I and II that as the dopant concentration increases (decreases) the mass of mixture $Al_xGa_{1-x}$ ($In_xGa_{1-x}$) decreases (increases) and force constants increases (decreases). The larger magnitude of force constants depicts the stronger inter atomic interaction and vice versa. It is clear from figure I that as the concentration of dopant i.e. Al increases in $Al_xGa_{1-x}N$ the magnitude of optical phonon frequencies ($E_2$(high), $E_1$(TO) and $A_1$(TO)) at zone centre increases while in $In_xGa_{1-x}N$ as the concentration of dopant increases the magnitude of all the optical phonon frequencies ($E_1$(TO), $A_1$(TO) and $E_2$(high)) at zone centre decreases which is in harmony with the fact that the stronger interaction leads to greater value of the optical phonon frequency and vice versa (Sinha et al., 2009). It is observed for both the ternary alloys that the optical phonon modes show linear variance the concentration of dopant from one end member to other end member. This shows that these alloys exhibit one mode behavior throughout the whole range of concentration. This variation of optical phonon modes with concentration is in agreement with existing results for $E_1$(TO) and $A_1$(TO) for $Al_xGa_{1-x}N$ (Liu et al., 1998). In graph I the solid lines represents the results of this work while the circles represent the results of (Ibanez et al., 2008) and rectangles represent results of (Liu S et al., 1998).

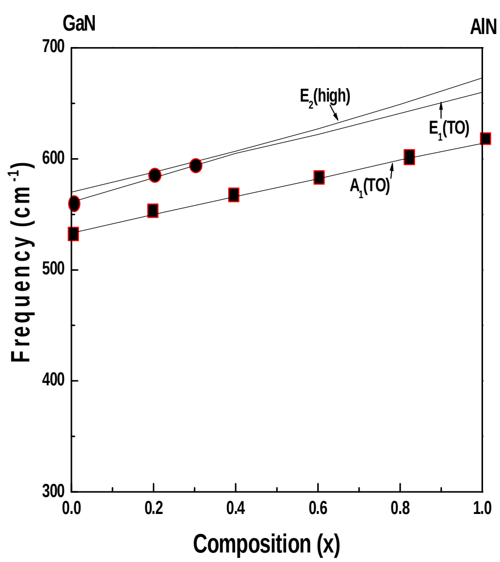


Figure I One mode behavior of wurtzite ternary alloy $Al_xGa_{1-x}N$.

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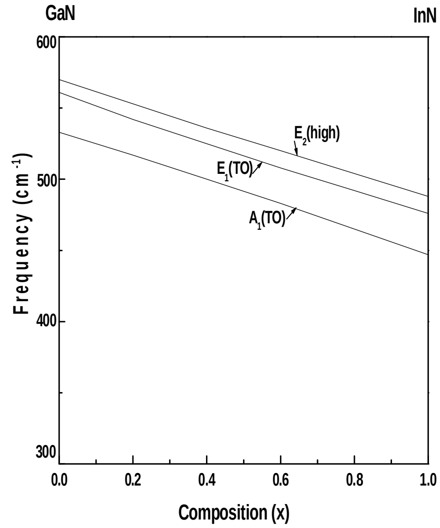


Figure II One mode behavior of wurtzite ternary alloy $In_xGa_{1-x}N$

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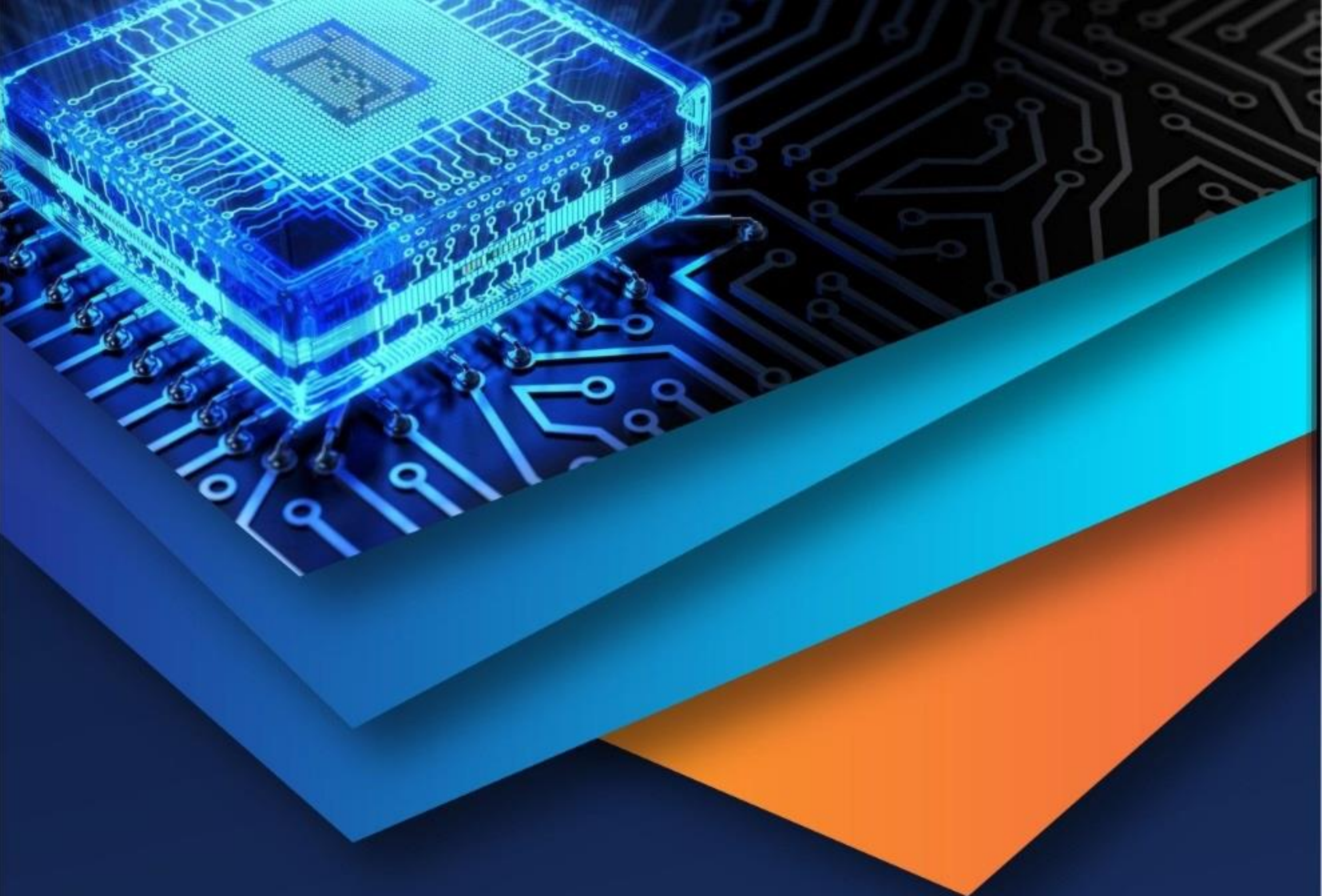

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