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Zone centre Phonon Mode Behavior of cubic phase of Ternary Nitrides

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Abstract
We have studied the phonon mode behavior of the ternary $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ at zone centre using de Launey Angular force constant model. The phonon frequency at zone centre has been found for $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$. The In and Al content of the alloy is in the range $0<x<1$. The one mode behavior has been observed and it is found that for $In_xGa_{1-x}N$ continuous decreases in phonon frequency with the increase in the content of In and for $Al_xGa_{1-x}N$ increase in phonon frequency is reported with decrease 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

Introduction

The group III-V(AlN, BN, GaN and InN) and II-VI (SiC) are considered as third generation semiconductor materials after first generation of semiconductor elements Si and Ge and second generation semiconductor compounds InP and GaAs (1). The potential applications of these materials are these are used in LEDs and LDs. But the power of LEDs and LDs based on II-VI materials decrease when emitted wavelength decreases to blue region. Also life time for green LDs is one hour and 100 hours for green LEDs. This prevents the commercialization of these. On the other hand III-V nitrides are the hot spots for the researchers in semiconductor materials research and applications [2]. The main interaction of these materials is due to their wide direct band gap, which can also be varied according to the requirement by alloying. By alloying with suitable composition band gap can be varied from 0.7-0.9 eV (for InN) region to 6.3 eV for GaN(3,4), which will cover light emitting area from infra-red, visible and UV region.

By using alloy of GaN doped with with suitable composition of Al or In can be used for preparing LEDs and electronic devices according to use [9]. GaN based semiconductor materials have high thermal conductivity, large electron drift velocity, resistance to high voltage, useful at high temperature. A large conduction band offset can be achieved in Al- based devices, which make it useful in telecommunication applications [4]. By changing the composition of the dopant the molecular weight and lattice constant changes, which causes change in binding energy, refractive index and electron mobility [5]. Group-III nitrides are also good materials high power and high temperature microelectronic devices due to their high melting point [6]. Apart from the other applications these materials have some interesting properties like easy cleavage of cubic structure, high quality, cheap, conductive substrates and possibility of high doping level [7]. Due to all above application and properties these materials can meet the next generation of electronic equipment demands of small size, high frequency, work in extreme conditions, high power and high efficiency [1].

Due to such important properties of these materials of utmost importance of researchers theoretically and experimentally. There are few studies of these materials on basis of Raman spectroscopy and by molecular beam epitaxy [8]. A. L K Teles [9] studied the The electronic, structural, and thermodynamic properties of cubic (*zinc blende*) group-III nitride ternary $In_xGa_{1-x}N$ and quaternary $Al_xIn_yGa_{(1-x-y)}N$ alloys by combining first-principles total energy

calculations and cluster expansion methods. Tabata et al[10] study the phonons of zinc blende $In_xGa_{1-x}N$ ($0<x<0.31$) layers are observed through first-order micro-Raman scattering experiments Guo et al [11] studied the Al, Mg doped GaN (sphalerite structure) electronic structures and optical properties. Xing et al [12] studied Mn doped GaN (sphalerite structure) of the electronic structures and optical properties. Despite the already existent experimental work on ternary *InGaN* alloys. But there is lack of knowledge of basic properties of these materials important for material characterization such as phonon frequency and its dependence on alloy composition. In the present study we have reported the zone centre phonon frequency of the GaN doped with Al and In with varying composition 0<x<1 by using the de launey angular force constant model. The zone centre phonon frequency of these alloys is studied and results are found in excellent agreement with existing experimental and theoretical results with large range of composition.

Methedology

In this study by using de Launey Angular force constant model we have calculated the zone centre frequency of the In and Al doped GaN with composition (0<x<1). Here we will consider two parts of the interaction: 1) Central interaction (ion-ion radial interaction), which act along the line joining the two neighbors. 2) Angular force which depends upon the angle which the line joining the moving atoms to its neighbors makes with the equilibrium position of the line. These forces are considered for nearest and next nearest neighbors. We shall let α_1 and α'_1 denote the force constant associated with central force and angular force of the nearest neighbor, while α_2 and α'_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

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

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 (6x6) dynamical matrix and I is unit vector. The matrix is expanded at long wavelength limit, results in the formulation of the relation between measured elastic constants, four unknown force constants and experimental value of the zone centre frequency. The relations thus obtained are as given

$$\frac{4}{3}\left(\alpha_1 + 2\alpha_1'\right) = \left[\frac{mM}{(2m+M)}\right]\omega_0^2 \quad \text{----------(1)}$$

$$aC_{11} = \frac{1}{3}\left(\alpha_1 + 2\alpha_1'\right) + 4\left(\alpha_2 + \alpha_2'\right) \quad \text{----------(2)}$$

$$aC_{12} = \frac{1}{3}\left(\alpha_1 - 4\alpha_1'\right) + 2\left(\alpha_2 - 5\alpha_2'\right) \quad \text{----------(3)}$$

$$aC_{44} = \frac{1}{3}\left(\alpha_1 + 2\alpha_1'\right) + 2\left(\alpha_2 + 3\alpha_2'\right) - \frac{\left(\left(\alpha_1 - \alpha_1'\right)^2\right)}{\left(3\left(\alpha_2 + 2\alpha_1'\right)\right)} \quad \text{-----(4)}$$

Here m is the mass of Y_xGa_{1-x} (Y = In or Al) $(xM_Y+(1-x)M_{Ga})$and M being mass of N. a is the lattice parameter and C_{11}, C_{12} and C_{44} are the elastic constants. By using experimental values of the zone centre frequency [13] and elastic constants as given in [14,15] the force constant has been calculated and are given as

Table1 Force constants for ternary alloy$In_xGa_{1-x}N$

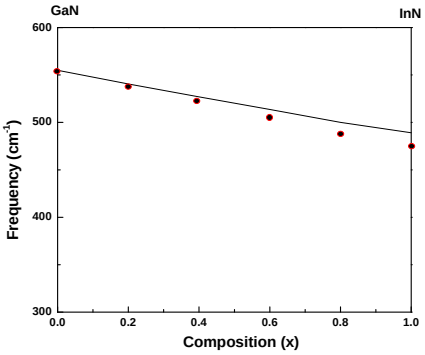
Composition (x) in alloy $In_xGa_{1-x}N$	Force Constant (10^4 dyne cm^{-1})				
	α_1	α_1'	α_2	α_2'	Mass
0.0	14.06	0.98	1.95	0.15	116.39
0.2	13.49	0.99	1.87	0.13	131.462
0.4	12.92	1.01	1.74	0.09	146.534
0.6	12.35	1.01	1.71	0.08	161.606
0.8	11.78	1.02	1.63	0.06	176.678
1	11.22	1.04	1.55	0.04	191.75

Table 2 Force constants for ternary alloy $Al_xGa_{1-x}N$

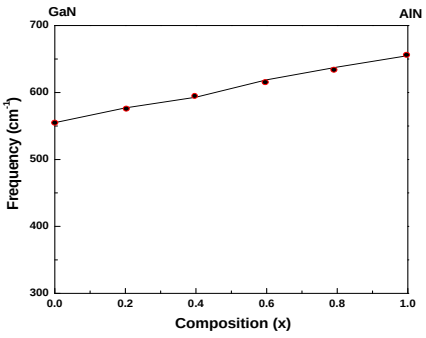
Composition (x) of alloy $Al_xGa_{1-x}N$	Force Constant (10^4 dyne cm^{-1})				
	α_1	α_1'	α_2	α_2'	Mass
0.0	14.06	.98	1.95	.1	116.3
0.2	14.31	1.01	1.99	.1	102.1
0.4	14.56	1.04	2.02	.1	87.85
0.6	14.81	1.08	2.08	.1	73.59
0.8	15.06	1.11	2.12	.1	59.32
1	15.32	1.5	2.17	.15	45.06

Results and discussion

The phonon behavior of ternary alloy system falls into two types, one mode and two mode behavior. One mode behavoiur means have only one set of frequencies and that show linear dependence on composition from one binary to other binary. While materials showing two mode behavior do not exhibit linear depenmdence on the composition (10). The optical phonon frequencies of $In_xGa_{(1-x)}$ N epitaxial layers grown by molecular beam epitaxy (MBE) were experimentally studied recently measured by Raman spectroscopy [16].



Graph 1 Phonon mode behavior of ternary $Al_xGa_{1-x}N$



Graph 1 Phonon mode behavior of ternary $Al_xGa_{1-x}N$

It was found that the phonons exhibit a one-mode type behavior and their frequencies show linear dependence on the alloy composition [9]. In graph 5.2 the solid lines represents the results of this work while the black circles represent the results of Santos et al [4]. This shows that materials exhibit one mode behavior for the whole range of the composition which is in agreement with other reported results [4][18]. In graph 2 the solid lines represents the results of this work while the black circles represent the results of Harima [18]. It is clear from the graphs that both the alloys show one mode behavior and zone centre phonon frequency varies continusely with the composition, which is in excellent agreement with the existing experimental and theoretical results [7], [14], [19]. Also it follows the well known fact that frequency is inversely proportional to the mass. If we compare the both the ternaries it is found that in $In_xGa_{(1-x)}N$ the frequency decreases with increase in composition of In while in case $Al_xGa_{(1-x)}N$ the frequency increases with increase composition of dopant (Al) As the composition of In (in alloy $In_xGa_{(1-x)}N$) increase mass of the alloy increases and clear from the graph that frequency decreases. So it is clear that frequency of GaN can be increased or decreased by doping with suitable composition of the In or Al.

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