Digest Journal of Nanomaterials and Biostructures Vol. 10, No. 2, April - June 2015, p. 489 - 495

THE EFFECT COMPOSITION DEPENDENCE OF SURFACE PHONON POLARITON MODE IN WURTZITE $In_xGa_{1-x}N$ ($0 \le x \le 1$) TERNARY ALLOY

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This study reports the theoretical study of the influence composition dependence of the surface phonon polariton (SPP) mode in wurtzite structure α-InxGa1−xN ternary alloy over the whole structure range. The effects of the alloy composition x on the location of SPP mode are identified. An anisotropic model is used to simulate the surface polariton (SP) dispersion curves of the $In_xGa_{1-x}N$ ternary alloys. The characteristics of these dispersion curves are explained and the effects of the composition dependence of the $In_xGa_{1-x}N$ on the SPs are clarified. Moreover, The obtained results have been compared with the calculated *p*-polarised IR attenuated total reflection (ATR) spectra produced by standard matrix formulation.Through this study, it has been found that the SPP mode of the wurtzite $In_xGa_{1-x}N$ shows one-mode behavior. Finally, the composition dependence of the SPP mode with bowing parameter of -23.126 cm^{-1} is determined.

(Received February 15, 2015; Accepted May 6, 2015)

Keywords: Surface phonon polariton (SPP); Attenuated total reflection(ATR); Indium gallium nitride α- $In_xGa_{1-x}N$ ternary alloy

1. Introduction

Currently the wide-gap GaN-based nitride semiconductors attract a great deal of attention in research and development, because of their useful technological applications in light-emitting diodes in the near-UV-blue-green spectral region [1], and their potentialities for use in the hightemperature electronics [2] In recent years, many groups have focused their attention on the In-rich nanostructures in InGaN epilayers [3–10]. the $In_xGa_{1-x}N$ ternary system is interesting because it is the most important and indispensable material used for the active layer in blue and green light emitting diodes and lasers.[11−13] Many researching works devoted to $In_xGa_{1-x}N$ has been directed towards the understanding of its optical and electronic properties. In spite of huge efforts, research on its fundamental surface properties (surface phonon polariton (SPP) mode) is still has not received sufficient attention. Recently, SPP properties in ternary mixed crystals have been widely investigated. [14−17] In this paper, theoretical studies on the SPP characteristics of wurtzite structure $In_xGa_{1-x}N$ semiconductor are reported. The surface polariton (SP) dispersion curves of wurtzite $In_xGa_{1-x}N$ semiconductors are simulated by an anisotropic model. The results are compared with the calculated *p*-polarised IR attenuated total reflection (ATR) spectra generated by standard matrix formulation. The influence of the alloy composition x on the SPP mode of the α-$In_xGa_{1-x}N$ ($0 \le x \le 1$) semiconductors is also investigated. This is crucial because knowledge of the alloying effects on the SPP modes is essential for understanding the behaviour of the photon–phonon coupling.

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2. Theory

Let us consider the SP dispersion relation of the anisotropic crystal. We assume that the opticalc-axis of the crystal is parallel to the surface normal (caxis || z) and perpendicular to the direction of propagation (caxis ⊥ x). Therefore, the theoretical SP dispersion curve at the interface between wurtzite $In_xGa_{1-x}N$ semi-infinite crystal and vacuum can be expressed by [18]

$$k_x(\omega) = \frac{\omega}{c}K_x(\omega) = \frac{\omega}{c}\left[\frac{\varepsilon_{\|}(\omega)-\varepsilon_{\|}(\omega)\varepsilon_{\perp}(\omega)}{1-\varepsilon_{\perp}(\omega)\varepsilon_{\|}(\omega)}\right]^{1/2}, \quad (1)$$

Where $k_x(\omega)$ is the wave vector of the SP along the *x* direction ; $K_x(\omega)$ is the dimensionless quantity; ω is the angular frequency of the SP and *c* is the velocity of light in vacuum ($3 \times 10^8 cm^{-1}$). The symbols $\varepsilon_{\|}(\omega)$ and $\varepsilon_{\perp}(\omega)$ denote the dielectric function parallel (‖) and perpendicular (⊥) to the *c*-axis, respectively. In this work, the dielectric functions, $\varepsilon_{\|}(\perp)$, for the studied structures have been modelled based on a damped harmonic oscillator model. By considering the anisotropy structure of the semi-infinite bulk crystal, the expression for $\varepsilon_{\|(\perp)}$ is given by [19]

$$\varepsilon_{\|(\perp)}(\omega) = \left(\varepsilon_{\infty}\frac{\omega_{LO}^2-\omega^2-i\omega\gamma_{LO}}{\omega_{TO}^2-\omega^2-i\omega\gamma_{TO}}\right)_{\|(\perp)}. \quad (2)$$

Here ,ε_{∞} is the high-frequency dielectric constant, and $\omega_{LO(TO)}$ and $\gamma_{LO(TO)}$ are, respectively, the LO (TO) phonon frequency and the phonon damping. The dielectric functions in Eq.(2) are used to describe the behaviour of the zone-centre phonon modes of binary semiconductors.Because the behaviour of phonon modes of the ternary alloys is complicated and because they have been found to exhibit either one-, two- or mixed-mode behaviour, Eq.(2)is not suitable for the case $In_xGa_{1-x}N$ ($0<x<1$). Nevertheless, the dielectric constant for a ternaryalloy $A_xB_{1-x}C$ as a function of alloy composition *x* can be simplified as [20]:

$$\varepsilon(A_xB_{1-x}C)_{\|,\perp} = x\varepsilon(AC)_{\|,\perp} + (1-x)\varepsilon(BC)_{\|,\perp}, \quad (3)$$

Where $\varepsilon(AC)_{\|(\perp)}$ and $\varepsilon(BC)_{\|(\perp)}$ are, respectively, the dielectric constants parallel (perpendicular) to the *c*-axis for AC and BC binary compounds. The corresponding ATR spectra for the studied structure have been calculated. The simulation of *p*-polarised IR ATR follows the Otto configuration [21] In contrast to that of the SP dispersion curves, there are three layers to consider: the prism, the vacuum and the $In_xGa_{1-x}N$ layers. The

calculation of the ATR spectrum is based on the standard matrix formulation, as described by Dumelow et al.[19].

In this work, the parameters used to calculate the SP dispersion curves and the ATR spectra for the $In_xGa_{1-x}N$ ($0 \le x \le 1$) ternary alloys are obtained from Refs. [22–25] and listed in Table 1. For the SP dispersion curves, the phonon lifetime was set as infinite (damping =0) to reveal all the SP branches. For the ATR spectra, all of the damping parameters were set at 5. Note that larger damping values may cause some dips to disappear due to the broadening effects.

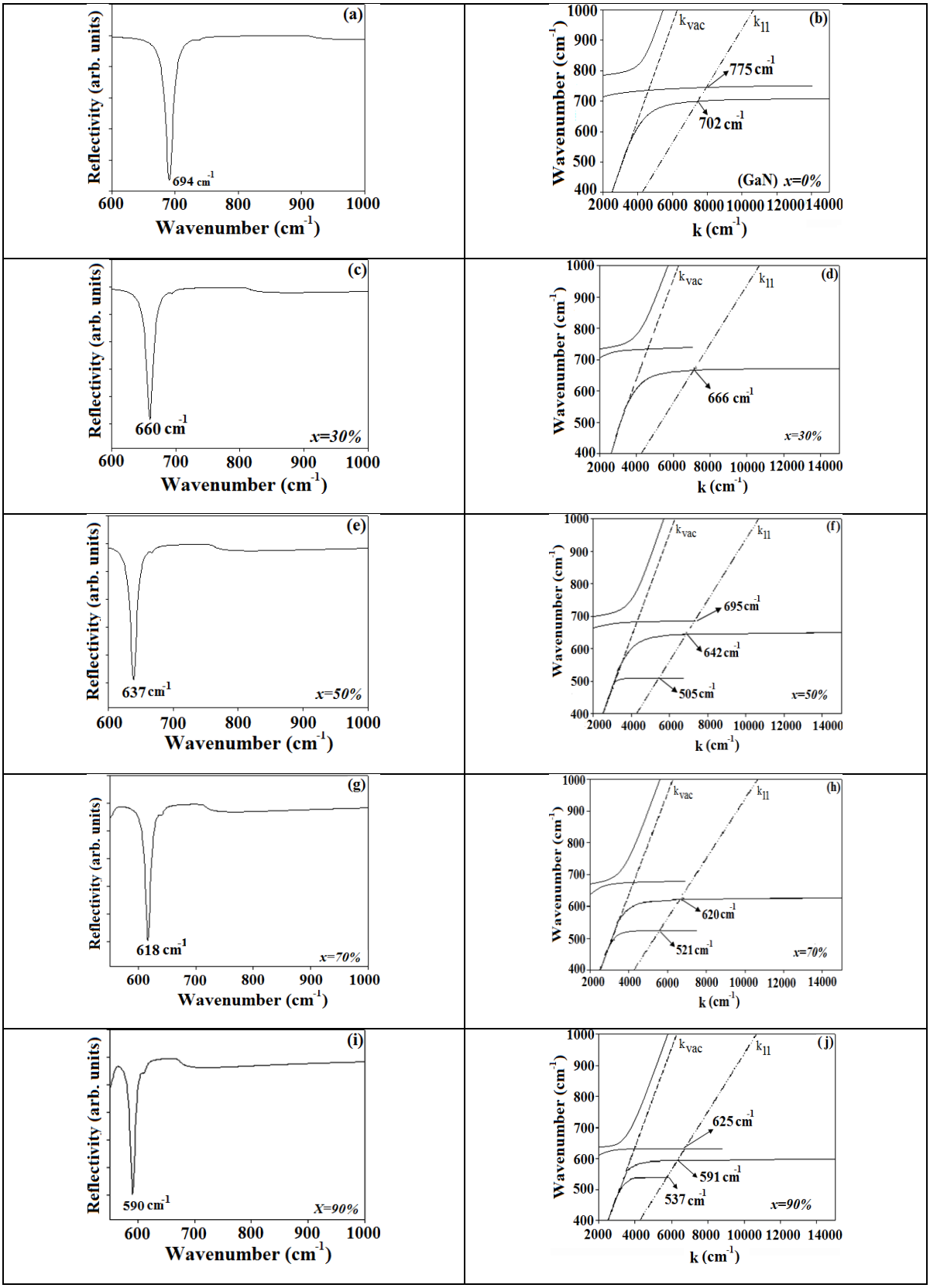
Table 1: Parameters used to calculate $\varepsilon(In_xGa_{1-x}N)_{\|,\perp}$, surface polariton dispersion curves and p-polarised IR ATR spectra of wurtzite $In_xGa_{1-x}N$ ($0 \le x \le 1$) semiconductor.

Binary compound	$\omega_{TO,\|}$ (cm^{-1})	$\omega_{LO,\|}$ (cm^{-1})	$\varepsilon_{\infty,\|}$	$\omega_{TO,\perp}$ (cm^{-1})	$\omega_{LO,\perp}$ (cm^{-1})	$\varepsilon_{\infty,\perp}$
GaN	532[a]	734[a]	5.31[b]	559[a]	741[a]	5.14[b]
InN	447[c]	586[c]	8.10[d]	476[c]	593[c]	8.34[d]

[a]Taken from Davydov et al.[24].
[b]Taken from Yu et al.[25].
[c]Taken from Davydov et al.[22].
[d]Taken from Abbar et al.[23].

3. Results and discussion

Fig 1 shows the theoretical SP dispersion curves (right -hand-side) with *p*-polarised IR ATR spectra (left right-hand-side) for $In_xGa_{1-x}N$ with In composition x = 0, 0.3, 0.5, 0.7,0.9 and 1. Also shown in the theoretical SP dispersion curves are the light wave in vacuum ($k_{vac}(\omega)=\omega/c$) and the light wave in ATR prism ($k_{\|}(\omega)=k_{vac}(\omega)\, n_p \sin\theta$ where n_p is the refractive index of the ATR prism, and θ is the internal angle of incidence in the prism). Note that the $k_{\|}(\omega)$ lines in that figures were calculated using the values of n_p = 2.4 and θ =45°, that is, according to the common specifications for an ATR diamond prism [13]. The choice of this ATR prism depended on its transmission spectral range where the SPP mode should occur. Let us first examine the *p*-polarised IR ATR spectra. In general, the observed dip(s) is (are) the result of the resonance at a frequency where the wave vectors of the incident radiation and the surface polaritons SPs are matched. In other words, the observed dip(s) actually correspond to the crossing of the SP dispersion curves with the light waves in the ATR prism , $k_{\|}(\omega)$, which will be discussed later.


(a)
Reflectivity (arb. units)
694 cm-1
Wavenumber (cm-1)
(b)
kvac
k11
775 cm-1
702 cm-1
(GaN) x=0%
Wavenumber (cm-1)
k (cm-1)
(c)
660 cm-1
x=30%
(d)
666 cm-1
x=30%
(e)
637 cm-1
x=50%
(f)
695 cm-1
642 cm-1
505 cm-1
x=50%
(g)
618 cm-1
x=70%
(h)
620 cm-1
521 cm-1
x=70%
(i)
590 cm-1
X=90%
(j)
625 cm-1
591 cm-1
537 cm-1
x=90%

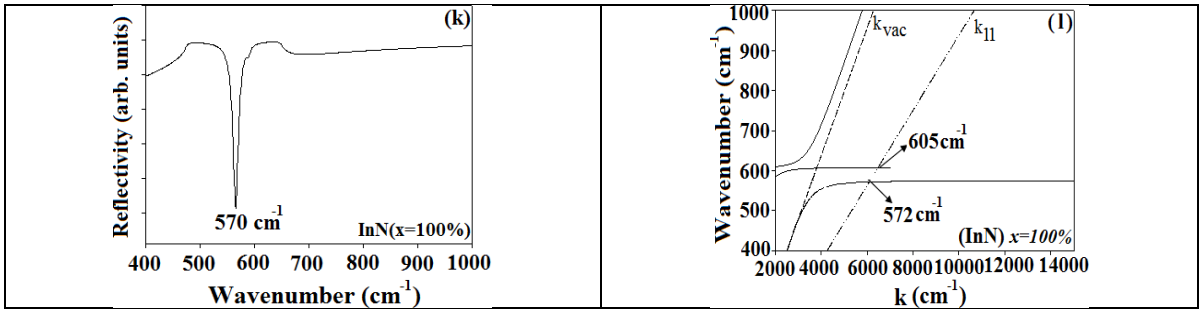


Fig. 1. Surface polariton theoretical dispersion curves (right-hand-side) with p-polarised IR ATR spectra (left-hand-side) for wurtzite for wurtzite $In_xGa_{1-x}N$ semiconductor with x =0, 0.3, 0.5, 0.7, 0.9 and 1. The light wave in vacuum and the light wave in attenuated total reflection crystal are indicated by $k_{vac}(\omega)$ and $k_{//}(\omega)$, respectively.

From Fig. 1, it can be seen that there is an absorption dip for the binary compounds of GaN (x=0) and InN (x=1). However, only the absorption dip that falls on the lower frequency is of special interest, as it corresponds to the SPP mode or the real surface mode[26,27] This correspondence is because its frequency is located both in the spectral range between the SPP modes of GaN and InN (i.e.,$SPP_{InN}<SPP_{InGaN}<SPP_{GaN}$) and in the dispersion curves where the SP branch persists as $k_x(\omega)$ approaches infinity.

To make sure the dips were a surface mode, *p*-polarised IR ATR spectra are compared with the SP dispersion curve. The SP dispersion curves of the $In_xGa_{1-x}N$ in Fig. 1 are the solutions for Eq. (1).

By For ternary alloy $In_xGa_{1-x}N$ ($0 < x < 1$) samples, the number of intersecting points varies with the In composition. However, only the middle crossing point of the dispersion curves of $In_xGa_{1-x}N$ ($0 < x < 1$) is of special interest, as it corresponds to the SPP mode or the real surface mode.[28] This is because its frequency located both in spectral range between the SPP modes of lnN and GaN (i.e., SPP lnN < SPP InGaN < SPP GaN), and in the dispersion curves where the SP branch persist as k_x (ω) approaches infinity. Note that the other intersecting points are known as virtual surface mode [28] or pseudo SPP mode. [29] From the experimental point of view, these pseudo SPP modes are quite difficult to be observed because its spectral strength is weak as compared to that of the real surface mode.[17]

The positions labelled are the intersections of the SP dispersion curve with the $k_{||}$ lines and correspond to the SPP mode. From Fig. 1, it is found that the positions of the intersection points of the $k_{||}$ line and the SP dispersion curve do not well agree with the theoretical ATR spectra. This is mainly because the calculation of the SP dispersion curves does not account for the coupling effect of the ATR prism and the finite thickness of the air gap.

The frequency of the SPP mode of the $In_xGa_{1-x}N$ as a function of in composition x is plotted over the entire composition ranges ($0 \leq x \leq 1$) and is shown in Fig. 2. As the In composition x increases, it is found that the frequency of the SPP mode gradually decreases from that of InN ($x = 0$) to GaN ($x = 1$). These results indicate that the SPP mode of $In_xGa_{1-x}N$ is strongly dependent on the In composition x, and the behaviour of the SPP mode can be classified as one-mode behaviour.

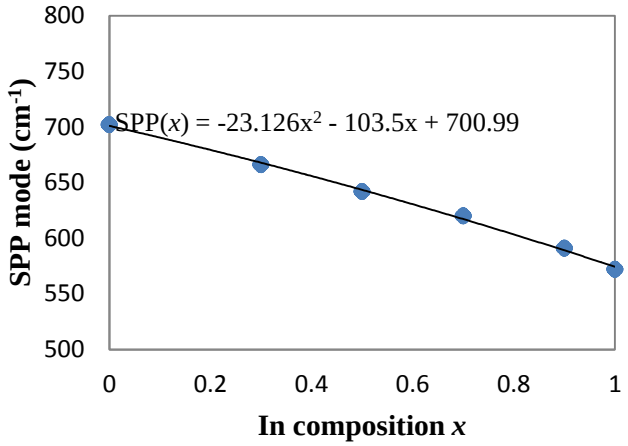


Fig. 2. Surface phonon polariton (SPP) mode of the $In_xGa_{1-x}N$ ($0 \leq x \leq 1$) semiconductors as a function of In composition. The solid line represents the best fit of the nonlinear interpolation of the data.

From the best fit of the nonlinear interpolation of these data, the composition dependence of the SPP mode (in cm^{-1}) of the α- $In_xGa_{1-x}N$ semiconductors over the entire composition range ($0 \leq x \leq 1$) can be expressed as:

$$\text{SPP } In_xGa_{1-x}N\ (x) = -23.126x^2 - 103.5x + 700.99 \quad (4)$$

From Eq. (4), it can be found that the SPP mode of the α- $In_xGa_{1-x}N$ exhibits the bowing factor for the theoretical of $-23.126cm^{-1}$. The negative sign indicates that the SPP modes of the alloy are larger than the linear interpolation result.

4. Conclusions

Theoretical SP dispersion curves and *p*-polarised IR ATR spectra for wurtzite structure $In_xGa_{1-x}N$ ($0 \leq x \leq 1$) alloys have been simulated using an anisotropic model. From the best fit of the nonlinear interpolation, the composition dependence of the SPP mode with an upward bowing parameter is theoretically obtained. The results revealed that the surface mode of the $In_xGa_{1-x}N$ alloys is strongly dependent on the In composition and its behaviour can be classified one-mode behaviour.

Acknowledgments

The authors would like to acknowledge Nano-Optoelectronics Research and Technology Laboratory, School of Physics and Universiti Sains Malaysia for financial support.

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