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Theoretical studies of surface phonon polariton in wurtzite AlInN ternary alloy

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ABSTRACT

In this study, we report the surface phonon polariton (SPP) characteristics of wurtzite structure aluminium indium nitride ($Al_xIn_{1-x}N$) ternary alloys over the whole Al composition range. An anisotropic model is used to simulate the surface polariton (SP) dispersion curves of the $Al_xIn_{1-x}N$ ternary alloys. The characteristics of these dispersion curves are discussed in detail and the effects of the composition dependence of the $Al_xIn_{1-x}N$ on the SPs are illustrated and explained. Moreover, the relevant experimental information from the attenuated total reflection (ATR) method is also presented, namely, the corresponding ATR spectra are simulated based on the standard matrix formulation. Through this study, it has been found that the SPP mode of the wurtzite $Al_xIn_{1-x}N$ exhibits mixed-mode behaviour.

1. Introduction

In recent years, group III-nitride semiconductors such as AlN, GaN and InN and their ternary compounds, such as $Al_xGa_{1-x}N$, $Ga_xIn_{1-x}N$, and $Al_xIn_{1-x}N$, have become alternative materials for optoelectronics as light-emitting diodes (LEDs), high efficiency solar cells and laser diodes (LDs) [1,2]. This is due to their direct band-gap and the ability to control their band-gap in a wide range. For example, the $Al_xIn_{1-x}N$ ternary alloy has the widest band-gap among the III-nitride group, which varies from 0.6 to 1.1 eV in InN [3] to 6.2 eV in AlN [4]. Subsequently, $Al_xIn_{1-x}N$ can be used as an active layer for LEDs and LDs in the spectral region from ultraviolet to near infrared (IR). In addition, it is reported that $Al_xIn_{1-x}N$ is lattice-matched to GaN or $Ga_xIn_{1-x}N$, which can be used as cladding layer for a LD structure with minimal strain [5].

Among the III-nitride ternary alloys, $Al_xIn_{1-x}N$ has received less attention than $Al_xGa_{1-x}N$ and $Ga_xIn_{1-x}N$. Even though the first growth of $Al_xIn_{1-x}N$ was approximately 30 years ago [6], there have been only a few publications on the growth of $Al_xIn_{1-x}N$, its band-gaps and electrical properties [7–11] and its fundamental optical properties such as phonon behaviour [12,13]. The relatively low amount of work on this material has been mainly due to the difficulty of growing $Al_xIn_{1-x}N$. According to Matsuoka [7], the tendency towards instability for III-nitride ternary compounds is greater if the value of each interaction parameter is higher. The principle is shown by the theoretical interaction value of $Al_xIn_{1-x}N$, which is much higher than the others. Consequently, good quality $Al_xIn_{1-x}N$ samples are difficult to grow.

Until now, the fundamental surface phonon polariton (SPP) characteristics of $Al_xIn_{1-x}N$ have remained unclear. Because the knowledge of the SPP modes is fundamental to the understanding of the behaviour of the coupling effect between the photon and the surface phonon, it is also important for designing devices on surfaces, such as photonic devices [14,15] as well as for near-field microscopy [16,17] and reflection-type sensors in the mid-IR region [18]. Hence, from both the fundamental physics point of view and the potential applications of the nitrides as semiconductors, there is an absolute need for thorough studies on the fundamental properties of these materials.

Over the past twenty years, studies on the SPP of the GaAs/AlAs superlattice [19] and GaAs/$Al_xGa_{1-x}As$ multiple-quantum-well structures [20] have been reported. However, only a small number of studies have reported on the SPP for binary, ternary and quaternary III-nitride compound semiconductors. The SPP of wurtzite GaN [21–24] and AlN [25] has been studied by means of both experimental and theoretical work. For InN, theoretical work on SPP has been published by Ng et al. [26]. Meanwhile, very recently, SPP studies of the ternary compounds of $Al_xGa_{1-x}N$ [24,27] and $In_xGa_{1-x}N$ [28] and the quaternary compounds $Al_xIn_yGa_{1-x-y}N$ [29] have been reported.

In this paper, theoretical studies on the SPP characteristics of wurtzite structure $Al_xIn_{1-x}N$ semiconductor are reported. The surface polariton (SP) dispersion curves of wurtzite $Al_xIn_{1-x}N$ 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.

2. Theory

Generally, SPP is an interface mode and it depends on the optical properties of at least two dielectric media, where phonon-polaritons propagate along a direction perpendicular to the surface normal. Its

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amplitude attenuates in going from surface to bulk [30]. It is an elementary excitation resulting from the coupling of an IR photon (with transverse magnetic mode) with a transverse-optic (TO) phonon in polar crystals. Typically, the frequency of this surface mode falls in the mid-IR region. Another unique characteristic of the SPP is that it can propagate through the forbidden band of the bulk polariton (BP) modes (i.e., the interval between the TO and longitudinal-optic (LO) phonon frequencies) and results in surface-enhanced IR absorption. Fig. 1 shows the schematic diagram of the dielectric function and the differential between the dispersion of BP and SPP of cubic structure [31]. The shaded area is the forbidden band for the BP, which is between the frequencies of TO and LO. The dielectric function between the TO and the LO phonon frequencies is negative. Typically, SPP mode can be measured by the ATR method [32]. The unique characteristic of the ATR method is the evanescent wave that can propagate through the forbidden band which can directly excite the SPP [20,30,33].

Let us consider the SP dispersion relation of the anisotropic crystal. We assume that the optical c-axis of the crystal is parallel to the surface normal ($c_{axis} \parallel z$) and perpendicular to the direction of propagation ($c_{axis} \perp x$). Therefore, the theoretical SP dispersion curve at the interface between wurtzite $Al_xIn_{1-x}N$ semi-infinite crystal and vacuum can be expressed by [30]:

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

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 (3×10^8 cm^{-1}). The symbols $\varepsilon_{\parallel}(\omega)$ and $\varepsilon_{\perp}(\omega)$ denote the dielectric function parallel ($\parallel$) and perpendicular ($\perp$) to the c-axis, respectively.

In this work, the dielectric functions, $\varepsilon_{\parallel(\perp)}$, 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 $\varepsilon_{\parallel(\perp)}$ is given by [19]:

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

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 of $Al_xIn_{1-x}N$ ($0<x<1$). Nevertheless, the dielectric constant for a ternary alloy $A_xB_{1-x}C$ as a function of alloy composition x can be simplified as [34]:

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

where $\varepsilon(AC)_{\parallel(\perp)}$ and $\varepsilon(BC)_{\parallel(\perp)}$ 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 [32] and the experimental setup is given elsewhere [22]. In contrast to that of the SP dispersion curves, there are three layers to consider: the prism, the vacuum and the $Al_xIn_{1-x}N$ 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 $Al_xIn_{1-x}N$ ($0\le x\le1$) ternary alloys are listed in Table 1. These parameters were obtained from Davydov et al. [35], Abbar et al. [36], Haboek et al. [37] and Persson et al. [38]. 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 $\varepsilon(Al_xIn_{1-x}N)_{\parallel,\perp}$, surface polariton dispersion curves and p-polarised IR ATR spectra of wurtzite $Al_xIn_{1-x}N$ ($0\le x\le1$).

Binary compound	$\omega_{TO,\parallel}$ (cm^{-1})	$\omega_{LO,\parallel}$ (cm^{-1})	$\varepsilon_{\infty,\parallel}$	$\omega_{TO,\perp}$ (cm^{-1})	$\omega_{LO,\perp}$	$\varepsilon_{\infty,\perp}$ (cm^{-1})
InN	447[a]	586[a]	8.10[b]	476[a]	593[a]	8.34[b]
AlN	610[c]	891[c]	4.72[d]	670[c]	912[c]	4.53[d]

[a] Source from Davydov et al. [35].
[b] Source from Abbar et al. [36].
[c] Source from Haboek et al. [37].
[d] Source from Persson et al. [38].

3. Results and discussion

Fig. 2 shows the theoretical SP dispersion curves (left-hand-side) with p-polarised IR ATR spectra (right-hand-side) for $Al_xIn_{1-x}N$ with Al composition $x = 0$, 0.2, 0.4, 0.6, 0.8 and 1. The interval used in this work was 0.2 cm^{-1}. Also shown in the theoretical SP dispersion curves are the light wave in vacuum ($k_{vac}(\omega) = \omega/c$) and the light

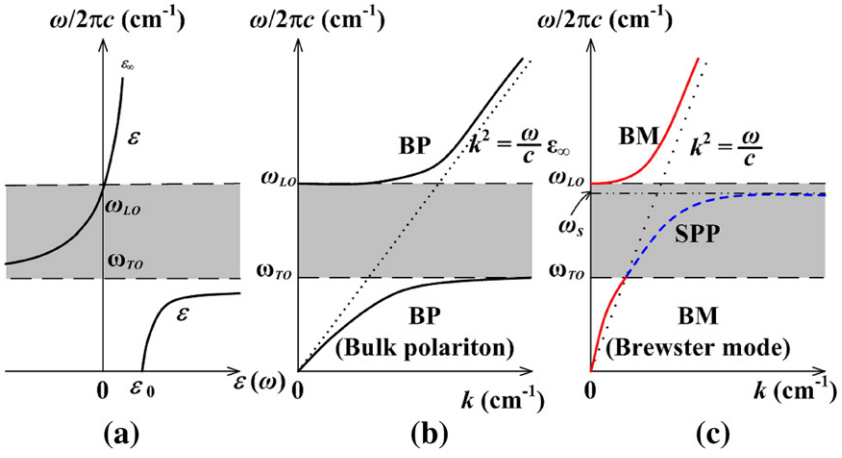

Fig. 1. Schematic diagram of the dielectric function and the differential between the dispersion of bulk polaritons and surface phonon polaritons of cubic structure [31].