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Phonon frequency variations in high quality $InAs_{1-x}Sb_x$ epilayers grown on GaAs

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ABSTRACT

Undoped $InAs_{1-x}Sb_x$ epilayers with different compositions ($0.55 \leq x \leq 0.78$) were grown by molecular beam epitaxy on semi-insulating GaAs (1 0 0) substrates. The quality of the samples was determined by high resolution X-ray diffraction (HRXRD) rocking curves and the lattice dynamics were studied by using Raman spectroscopy at room temperature. Optical phonon frequency range shows strong two-mode phonon behavior for all compositions. With an increase in the Sb composition, InAs-like longitudinal-optical (LO), and transverse-optical (TO) phonon peaks exhibit a blue shift whereas a red-shift was observed for InSb-like LO phonon peak. Moreover, transverse-acoustic (TA) and mixed mode InSb-like 2IA/2TA phonon modes were identified successfully. HRXRD results revealed that the best full width at half maximum value reported up to now was achieved for the sample with a composition of $x = 0.55$ and thickness of 550 nm.

1. Introduction

Sb-based group III–V compounds has received much interest in recent years as an alternative to HgCdTe (MCT) for many device applications such as night vision, medical imaging, sensitive pollution gas monitoring, etc [1–4]. Although MCT is a crucial material, especially for medium- and long-wavelength infrared photodetectors, there are still some challenges in terms of lack of stability and non-uniformity over a large area due to Hg vapor pressure. Besides, MCT based detectors only work under cryogenic conditions and they are high cost materials. In order to overcome those difficulties, Sb-based III–V materials have been investigated as an alternative material system [5]. Among them, $InAs_{1-x}Sb_x$ ternary compound has been one of the most popular material systems.

Although Sb-based material systems are grown on GaSb substrates mostly, due to the costs and available substrate sizes, GaAs substrate is a promising alternative for those material systems. However, the lattice mismatch between $InAs_{1-x}Sb_x$ and GaAs ($7.2\% < \Delta a/a < 14.6\%$) causes the growth of high-quality $InAs_{1-x}Sb_x$ on GaAs to be a challenging issue [6]. Moreover, the band gap difference between GaAs and $InAs_{1-x}Sb_x$ results in a different optical absorption which causes a variation in substrate temperature during growth. Namely, following $InAs_{1-x}Sb_x$ layer formation the substrate temperature increases due to a higher absorption even though the substrate heater kept at the same temperature. Hence, it should be monitored continuously during the growth and controlled by decreasing the substrate heater temperature to compensate the increase in substrate temperature. Together with lattice mismatch this undesired effect has a deleterious impact on the quality of the epi-crystals. Consequently, studies on growing high quality $InAs_{1-x}Sb_x$ epilayers still conserves challenging issues to achieve high quality epi-crystals.

It is well known that Raman spectroscopy is a strong technique to understand the lattice vibrations of various material systems [7]. The first Raman spectroscopy study of $InAs_{1-x}Sb_x$ alloys on InAs and InSb substrates performed by Cherng et al. reported "one-mode" phonon behavior for $x \leq 0.6$ composition and "two-mode" phonon behavior for larger values [8]. Then, a similar study for $InAs_{1-x}Sb_x$ alloys grown with different composition on GaAs substrate by MBE were carried out by Li et al. and "two-mode" phonon behavior was observed [9]. However, very few studies are reported up to now and new studies are very crucial to improve the crystal quality and increase the knowledge about those ternary alloys.

This study presents Raman spectroscopy results of $InAs_{1-x}Sb_x$ epilayers grown on GaAs substrates together with high resolution X-ray diffraction (HRXRD) measurements. HRXRD results indicated high quality epi-crystals and "two-mode" phonon behavior was clearly presented in all grown ternary samples, as expected. Besides, InAs-like LO, InAs-like TO, InSb-like LO, and mixed mode InSb-like 2IA(K) peaks were identified as a function of Sb composition.

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2. Experimental

A set of samples (S1, S2, S3, S4, and S5) were grown on epi-ready semi-insulating GaAs (1 0 0) substrates using Veeco GEN20MC solid-source MBE system. Substrate temperature was measured by using an IRCON pyrometer which is calibrated against the GaSb $(1\times3)\rightarrow(2\times5)$ surface reconstruction transition [10]. Prior to the growth, native oxide was desorbed from the GaAs surface under As_2 overpressure at 600–605 °C. After oxide desorption, GaAs substrate temperature decreased to the growth temperature (around 450 °C) under As_2 overpressure. At the growth temperature, In cell shutter was opened while As beam flux was available to initiate the $InAs_{1-x}Sb_x$ layer growth and waited for 10 s. Subsequently, Sb cell shutter and valve were opened. Undoped $InAs_{1-x}Sb_x$ epilayers were grown for 100 min under different As and Sb beam equivalent pressure (BEP) ratios to acquire different As and Sb compositions.

The Raman spectra were obtained at room temperature by using Bruker Optics FT-Raman Scope III system. As an excitation source, 532 nm laser line was focused on the sample with 100X microscope objective in a backscattering geometry. The incident light power was kept at 2 mW. The signals were collected by a charge-coupled device (CCD) detector with 25×1000 μm aperture.

HRXRD measurements were performed by PANalytical X′Pert PRO X-ray diffraction system. To determine composition of alloys, (0 0 4) HRXRD rocking curve measurements were obtained using the Cu Kα radiation and a four bounce Ge (4 0 0) hybrid monochromator/detector setup with a fixed divergence slit of 1/8°. The HRXRD measurements were conducted at a voltage of 45 kV and a current of 40 mA.

The spectroscopic ellipsometer WVASE32 M2000-F (J.A. Wollam Co. Inc.) based on phase modulation was employed in the wavelength region from 245 nm to 1 μm for the thickness determination of grown samples. The ellipsometric spectra were measured at an angle of incidence of 75º. A CCD detector was used in order to detect reflected light from sample. The measured data were fitted using the Levenberg–Marquardt least square algorithm with an average mean squared error (MSE) ranged from 3 to 4 nm for the measured thicknesses (550–592 nm).

3. Results and discussion

HRXRD measurements were conducted to determine the Sb composition as well as the quality of the epilayers. HRXRD rocking curves for five grown samples S1, S2, S3, S4, and S5 are presented in Fig. 1. The sharp peak observed at around 33.05 degree is from GaAs substrate where the peaks at around 28.22 and 30.56 degrees are associated with InSb and InAs, respectively. As expected, rocking curve peak positions of the $InAs_{1-x}Sb_x$ epilayers are sequentially located between InSb and InAs peaks depending on the Sb composition. Thicknesses of $InAs_{1-x}Sb_x$ epilayers were determined by spectroscopic ellipsometry and summarized in Table 1 including the HRXRD measurement results. It is very well known that HRXRD full width at half maximum (FWHM) is an indication of crystal quality. Comparing FWHM values obtained from our samples with the ones reported up to now indicate that all grown samples can be

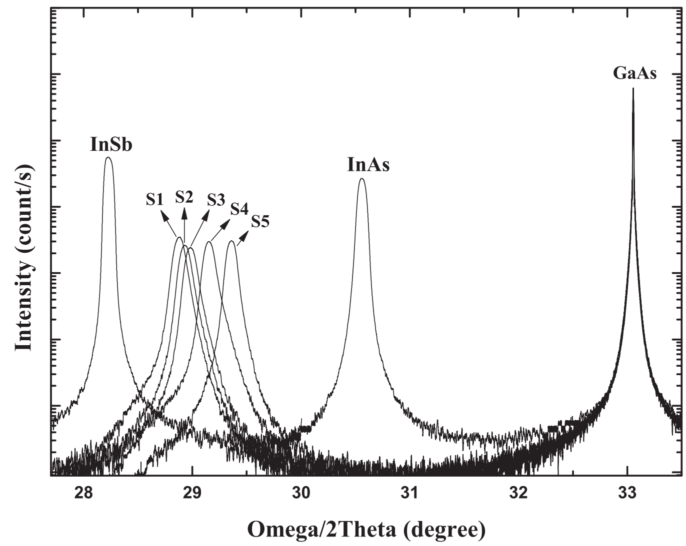

Fig. 1. X-ray diffraction spectra of $InAs_{1-x}Sb_x$, InAs, and InSb epilayers grown on GaAs substrate.

classified as high quality crystals [11–14]. Moreover, the achieved FWHM value for the sample S5 with a 550 nm thickness is the best value reported up to now.

In order to understand the lattice dynamics of the grown samples Raman spectroscopy was applied and Raman scattering spectra of samples with varying Sb composition are presented in Fig. 2 where, InAs and InSb were used as reference samples in order to present the complete picture. LO peaks for InSb and InAs are observed clearly at 189 and 230 cm^{-1} while TO peaks are identified at 178 and 216 cm^{-1}, respectively [15,16]. It was reported that $InAs_{1-x}Sb_x$ alloys have one- or two-mode phonon behaviors depending on the Sb composition [8,9]. As can be seen from Fig. 2, for all the studied ternary samples, two-mode phonon behavior is observed and the peaks are attributed to InAs- and InSb-like LO phonons. We designated the LO-peaks as LO_1 for InAs-like, LO_2 for InSb-like and the shoulder at the left hand side of the InAs-like peak as TO_1 phonon modes. The Raman spectra of grown samples at the lower wave number side (90 – 140 cm^{-1}) was observed as well and presented in Fig. 3. As can be seen from the figure, InAs has peaks at around 86, 106, 117, and 153 cm^{-1} that can be assigned as 2TA(L), 2TA($\Delta\rightarrow$K), 2TA(W), and 2IA(K), respectively [17]. Similarly, the observed peaks around 83, 118, and 135 cm^{-1} for InSb can be assigned as 2TA(X), 2IA(K) [17], and TO(Δ_3)–TA(Δ_3) [18], respectively. Finally, as in the case of InAs and InSb, the $InAs_{1-x}Sb_x$ alloys exhibit a mixed-mode peak that can be assigned as 2IA(K) closer to the InSb 2IA(K) peak due to the high Sb composition in the grown alloys.

All peak positions observed in the Raman spectra of grown alloys including reference samples are summarized in Fig. 4. The LO_1 peak intensity decreases with an increase in Sb content and a blue shift was observed in the phonon peak frequency. The peak positions of LO_1 phonons are fitted by linear least-squares method as;

$$\upsilon_{LO_1}\,(cm^{-1}) = 231 - 21_x$$

In addition to LO phonon peak, TO phonon modes were observed as a weak peak although they are forbidden from (1 0 0) surface may be due to the slight sample misalignment or perhaps because of the presence of disorder in structure [8]. Linear least-squares fitting for TO_1 phonon mode gives;

$$\upsilon_{TO_1}\,(cm^{-1}) = 281 - 18_x$$

Table 1
The summary of HRXRD and ellipsometry measurement results of $InAs_{1-x}Sb_x$ epilayers.

Sample	Peak position	Sb composition	FWHM (arcsec)	Thickness (nm)
S1	28.88	0.78	409.2	592
S2	28.93	0.76	406.2	571
S3	28.99	0.73	390.0	569
S4	29.15	0.65	382.7	567
S5	29.35	0.55	358.8	550

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