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Empirical expression for the composition and temperature dependence of the energy gap in InAlSb

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HIGHLIGHTS

- An empirical expression for the energy bandgap versus composition and temperature for $In_{1-x}Al_xSb$ was proposed.
- Mesa type InAlSb photodiodes were fabricated on the epitaxial layer grown by MBE.
- The InAlSb bandgap was investigated through the spectral response measurement in a wide temperature range of 77–260 K.
- A good agreement between the theoretical and the experimental was obtained.

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ABSTRACT

An empirical expression for the energy bandgap as a function of alloy composition x and temperature for $In_{1-x}Al_xSb$ was reported. The $In_{1-x}Al_xSb$ epitaxial layers were grown by molecular beam epitaxy (MBE) on InSb(100) substrate, utilizing a p^+–p^+–n–n^+ structure. High resolution X-ray diffraction was used to characterize the epitaxial layers. The Al composition of 2.8% was obtained by assuming the Bragg's formula and Vegard's law. Spectral response measurement of the diodes has been employed to investigate the temperature dependence of the band gap of $In_{1-x}Al_xSb$ alloys in the range between 77 K and 260 K. The calculated results for energy gap of InAlSb were in good agreement with the available data and our experimental observation.

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1. Introduction

As photovoltaic infrared photodetectors can offer faster response times, higher sensitivity and high-temperature operations, dual band detections, there has been exciting progress in the development of photovoltaic infrared detectors during the past few years [1,2]. $In_{1-x}Al_xSb$ is an exceedingly crucial ternary semiconductor that demonstrates widespread application in the fabrication of specialized high-speed electronic and optoelectronic devices [3,4]. It provides a convenient strain-compensating barrier material for mid-IR interband cascade lasers and other antimonide device structures. Recently the first InSb nBn devices based on unipolar InSb/InAlSb/InSb structure were fabricated and preliminary electrical characterizations were reported [5–7]. The use of epitaxial $In_{1-x}Al_xSb$ on a heavily doped InSb substrate can more effectively control the thermal generation of charge carriers as the detector temperature rises above 110 K with reduced cooling [3]. To fully characterize the InAlSb/InSb heterostructure, a detailed understanding of the band gap dependence of the $In_{1-x}Al_xSb$ alloy on temperature and aluminum concentration is considerably indispensable.

In the past several years, extensive studies of the energy gap of InAlSb versus temperature and component have been conducted. The commonly accepted data on band gap of $In_{1-x}Al_xSb$ alloys were obtained by Agaev and Bekmedova [8], who yielded a linear variation of the direct energy gap with composition from 10% to 60% at 300 K. Subsequent electroreflectance measurements at room temperature by Isomura et al. determined the bowing parameter $c = 0.43$, which is then commonly referenced [9]. However, Komkov [10] accomplished the fundamental studies of the absorption edge and refined the dependence of the band gap on the composition of the $In_{1-x}Al_xSb$ alloy, determining the bowing parameter to be 0.32 eV, which is by 0.11 eV smaller than that of Isomura et al. In the other work [11], the energy gap for the $In_{1-x}Al_xSb$ alloy system was determined in the Al concentration range of 0–0.25 by transmission spectroscopy at both 300 K and 4.2 K. Recently, Fairs [12] investigated the electronic and optical properties of $In_{1-x}Al_xSb$ ternary alloys using the empirical pseudopotential method (EPM) under the virtual crystal approximation (VCA) that takes into

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account the effect of compositional disorder. The extent of the direct-to-indirect band gap transition was examined and found to be at an Al content of $x = 0.73$, which corresponds to an energy band- gap of 1.65 eV.

In the present work, we developed an empirical relation for E_g as a function of both T and x, in terms of the temperature-dependent energy gap of the two constituents, InSb and AlSb. It is, however, assumed that the bowing parameter c is independent of temperature. Then, in order to reveal the temperature dependence of the energy gap, we reported the use of a Fourier transform infrared spectrometer (FTIR) to measure the spectral response of the InAlSb mesa diodes, which differs from previously reported works. High-resolution X-ray diffraction (HRXRD) was used to confirm the material quality and characterize the Al component. Comparison between calculated results and the experimental observation was performed to examine the validity of this empirical expression. An excellent consistency was found between the theoretical and experimental results.

2. Experiments

The samples were grown on 2 in. InSb(1 0 0) wafers using a VG V80H MBE system, equipped with valved cracker cells for antimony, indium, and aluminum, respectively. The substrates misoriented by 2° toward the (1 1 1)B plane were degenerately doped to $2 \times 10^{18}\ \text{cm}^{-3}$ using tellurium, to induce a Moss-Burstein shift, so that they can become transparent across the mid-infrared wavelength range. We grew InAlSb layers with a thickness of d_{InAlSb} = 6 μm, utilizing a p^+–$\underline{p}^+$–n–n^+ structure, where $\underline{p}^+$ is a 10 nm thick InAlSb barrier layer with Al-content of approximately 10%. The epitaxial material dopants were tellurium and beryllium for n-type and p-type behavior, respectively. The electrically active doping levels were approximately $1 \times 10^{18}\ \text{cm}^{-3}$, $1 \times 10^{15}\ \text{cm}^{-3}$, and $1 \times 10^{18}\ \text{cm}^{-3}$ for the n^+, n and p^+ regions, respectively.

In the growth processes, In, Sb_4, Al, Si and Be flows were formed by crucible sources with shutters. A V/III ratio of 4 and a growth rate of 0.5 monolayers per second were used in the growth reported in this article. Wafer temperature was determined via thermocouple readings which however have no direct contact with it. Thermocouple calibration was realized according to the known transition temperature between surface superstructures (4×4) and pseudo-(1×3) on InSb(1 0 0) which was equal to approximately 385 °C.

The crystalline quality of the epitaxial layers was assessed by using HRXRD, from which we can also determine the Al component by assuming Bragg's formula and Vegard's law. The X-ray radiation source was a copper tube (emitting $K_{\alpha 1}$ radiation at a wavelength of 1.54056 Å). The typical rocking curves for InAlSb/InSb are shown in Fig. 1, and the Bragg angle of InSb is 28.396°. Because of the low Al-content grown in the InAlSb film, the InSb substrate peak was close to the InAlSb epitaxial peak. The full width at half maximum (FWHM) of InAlSb epitaxial layers was approximately 0.036°, suggesting that the material was of good quality. The lattice parameters of unstrained InSb and AlSb are $a_{InSb} = 6.4794$ Å and $a_{AlSb} = 6.1355$ Å, respectively. We can obtain an Al composition of approximately 2.8%, based on the splitting between the alloy peak and substrate from Vegard's law. The deviation of two peaks of five different points on whole 2-in. wafer was measured. Thus, the Al compositional variations across the wafer with a standard deviation less than 5% could be achieved, which presented a high degree of uniformity.

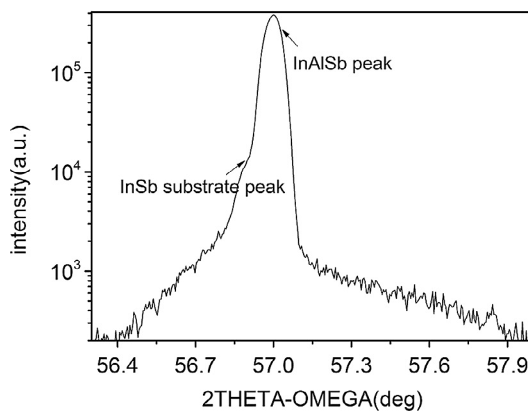

Fig. 1. X-ray diffraction rocking curve of InAlSb layers on InSb substrate at (0 0 4).

The preparation of the epitaxial InAlSb diodes was based on the well-established technology currently used for the fabrication of the bulk InSb detectors [13] except for the different p-n junction formation process. A dry chemical inductively coupled plasma (ICP) etching process was employed to form the mesas of the InAlSb diodes with the depths of ~4 μm. The surface was passivated by a native anodic oxidation layer and ZnS coating. The Au/Cr ohmic contacts were used as metallization electrodes of both the p and n regions. For the measurement, the diodes were assembled in a metal liquid nitrogen Dewar whose operating temperature can be easily monitored through the temperature controller. Here, we chose a diode size of 200 μm × 200 μm for the experiment.

The optical measurements were carried out with the use of a Bruker IFS 66/S FTIR spectrometer. The KBr and CaF_2 beamsplitters were the options installed in the interferometer and here we chose the latter one, since KBr is a highly hygroscopic material. The standard source for IFS 66/S is a globar for MIR spectroscopy and the interferograms were detected by a DLATGS detector with an integrated preamplifier.

3. Results and discussion

3.1. Calculations

The variation in the band-gap energy E_g with composition of a ternary alloy $A_{1-x}B_xC$ is assumed to fit a simple quadratic form [14]:

$$E_g(x) = ax + b(1-x) - cx(1-x) \tag{1}$$

where a and b are, respectively, the measured band gap at $x = 1$ and $x = 0$, c is known as the bowing parameter which accounts for the deviation from a linear interpolation between the two binaries BC and AC. Consequently, by using the value $c = 0.43$ from reference [9,12], Eq. (1) can be written for $In_{1-x}Al_xSb$ as a function of x and T as follows:

$$E_g(x,T) = E_g^{AlSb}(T)x + E_g^{InSb}(T)(1-x) - 0.43x(1-x) \tag{2}$$

Using the Varshni equation [15], $E_g(T) = E_g(0) - [\alpha T^2/(T+\beta)]$, we may obtain from Eq. (2)

$$E_g(x,T) = \left[E_g^{AlSb}(0) - \frac{\alpha^{AlSb}T^2}{T+\beta^{AlSb}}\right]x + \left[E_g^{InSb}(0) - \frac{\alpha^{InSb}T^2}{T+\beta^{InSb}}\right](1-x) - 0.43x(1-x) \tag{3}$$

Table 1
Values of material parameters [16] $E_g(0)$, α and β.

Material	$E_g(0)$ (eV)	α (10^{-4} eV/K)	β (K)
AlSb	2.386	4.2	140
InSb	0.235	3.2	170

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