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Stress reduction and electric properties of InSb thin films grown by metalorganic vapor phase epitaxy on sapphire substrates with an InAs buffer layer

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ABSTRACT

InSb thin films were grown by metalorganic vapor phase epitaxy using an InAs buffer layer on sapphire (0001) substrates. The stresses and strains in InSb were controlled by the thickness of the InAs buffer layer, and it was found that with decreasing compressive stress in InSb, the crystalline quality and the electrical properties improved. The thermoelectric properties of InSb were assessed and it was found that the power factor of InSb with a thickness of 5 μm reached as high as 5.8×10^{-3} W/mK^2 at 600 K.

1. Introduction

The narrow-gap III-V semiconductor, InSb, has been used in detectors of infrared radiation and also in Hall elements [1]. Recently, the high potential of InSb for thermoelectric applications has been reported [2,3]. InSb layers have conventionally been grown on semi-insulating (SI) GaAs substrates because the lattice mismatch between InSb and GaAs is small compared with that between Si substrates, as shown in Table 1, and because the parasitic capacity can be reduced when an insulating substrate is used. Nevertheless, even when using GaAs, the lattice mismatch is as high as 14.6%, which leads to the generation of defects in the interface between InSb and the GaAs substrate. On the other hand, we have focused our attention on the much smaller lattice mismatch between InSb and sapphire, which is 3.7%, as shown in Table 1. InSb growth on a sapphire (0001) substrate along the [111] direction is most probable [4] as shown in Fig. 1. In fact, a peak from InSb (111) by $2\theta/\omega$ X-ray diffraction was dominant. Consequently, the coordinates must be transformed from the [001] direction to the [111] direction. The stresses and strains investigated in our study were calculated using the transformed coordinates.

2. Experiments

The InAs and InSb thin films studied here were grown on sapphire (0001) substrates by metalorganic vapor phase epitaxy (MOVPE). To evaluate the thermoelectric properties of InSb thin films, the films were characterized in terms of the biaxial strain and stress and the electrical properties. The strains in InAs and InSb were estimated by $2\theta/\omega$ X-ray diffraction analysis at (111) diffraction planes, and their stresses were calculated using relationship (1). The electrical properties were studied using Hall measurements.

The large mismatch of lattice constants between InSb and GaAs induces a high density of misfit dislocations at the InSb/substrate interface [5], which leads to the degeneration of the crystal quality and electrical properties of InSb layers. In particular, extraordinarily large carrier accumulation [6] occurs at the interface between InSb and GaAs, and causes unacceptable current leakage in the InSb layer. Moreover, sapphire is a dielectric material, and when it is used as a substrate for electronic devices, it plays an important role in reducing the parasitic capacity. The use of an insulating substrate is essential particularly for thermoelectric materials because carrier injection from the substrate occurs when a non-insulating substrate is used at high temperatures.

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Table 1
Lattice constants and lattice mismatches for InSb with various substrates [8].

	Cubic (001)	Cubic (111)		Mismatch
	a (Å)	a (Å)	c (Å)	%
InSb	6.478	4.581	7.480	–
InAs	6.058	4.284	6.995	6.9
GaAs	5.653	3.997	6.528	14.6
Si	5.431	3.841	6.271	19.3
	Hexagonal (0001)			Mismatch
	a (Å)	c (Å)		%
Al_2O_3	4.758	12.991		3.7

3. Results and discussion

Fig. 2 shows the InAs thickness dependences of the full width at half maximum (FWHM) of the rocking curve (Y-axis, closed circles) and the compressive stress (R-axis, closed triangles) for InSb thin films of 0.5 μm thickness. The thicknesses of the InAs layers were 6, 15, 30, and 60 nm. With increasing thickness of the InAs buffer layer, the compressive stress in InSb increases, and accordingly, the FWHM at the (111) diffraction plane increases. This result means that the InAs layer buffers the stress in the InSb layer by accommodating the stress in the InAs itself.

The stresses (σ_{ij}) depend only on the strains (ϵ_{kl}) by the following expression.

$$\sigma_{ij} = c_{ijkl}\epsilon_{kl} \tag{1}$$

Here, the coefficients c_{ijkl} are the elastic constants and are expressed as follows in the [111] direction for a cubic system [7].

$$(C') = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} + (2C_{44} - C_{11} + C_{12}) \times \begin{bmatrix} \frac{1}{2} & -\frac{1}{6} & -\frac{1}{3} & 0 & \frac{1}{3\sqrt{2}} & 0 \\ -\frac{1}{6} & \frac{1}{2} & -\frac{1}{3} & 0 & -\frac{1}{3\sqrt{2}} & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & 0 & -\frac{1}{3\sqrt{2}} \\ \frac{1}{3\sqrt{2}} & -\frac{1}{3\sqrt{2}} & 0 & 0 & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & -\frac{1}{3\sqrt{2}} & 0 & -\frac{1}{6} \end{bmatrix} \tag{2}$$

Using $C_{11} = 67.2$ GPa, $C_{12} = 36.7$ GPa, and $C_{44} = 30.2$ GPa [8],

$$(C') = \begin{bmatrix} 82.2 & 31.7 & 26.7 & 0 & 7.1 & 0 \\ 31.7 & 82.2 & 26.7 & 0 & -7.1 & 0 \\ 26.7 & 26.7 & 87.1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 20.2 & 0 & -7.1 \\ 7.1 & -7.1 & 0 & 0 & 20.2 & 0 \\ 0 & 0 & 0 & -7.1 & 0 & 25.2 \end{bmatrix} (\text{GPa}) \tag{3}$$

The above effect of the InAs buffer layer was reflected in the electrical properties. Fig. 3 shows the InAs thickness dependence of the electron mobility (Y-axis, closed circles) and the carrier concentration (R-axis, closed triangles) of the same InSb films as those in Fig. 2. With increasing InAs buffer layer thickness, the electron mobility in InSb decreased, and the carrier concentration in InSb increased and then saturated. This saturation of the carrier concentration is considered to be due to the carrier accumulation effect, which has been reported in InSb films grown on hetero-substrates [5,6]. Our result shows that such carrier accumulation in InSb was reduced when the stress in InSb was reduced.

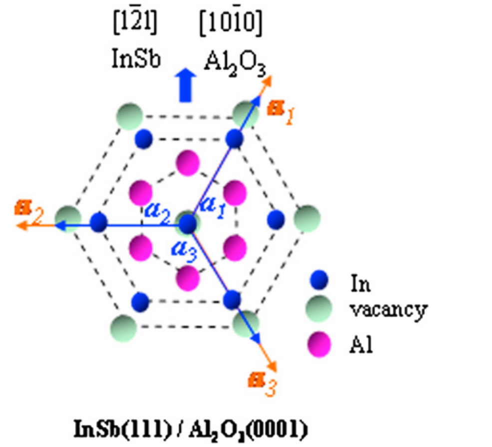

Fig. 1. Lattice direction between InSb(111) and Al_2O_3(0001) planes.

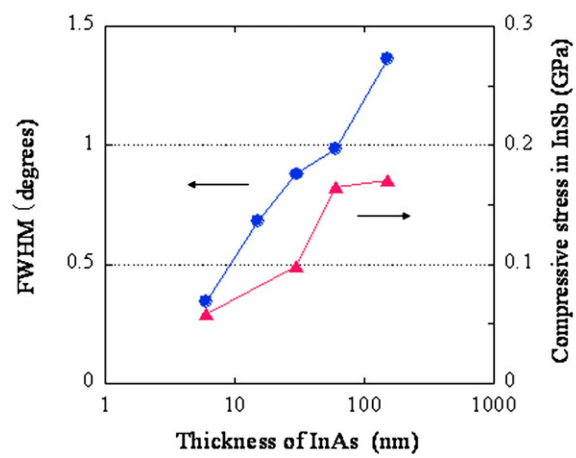

Fig. 2. InAs thickness dependences of FWHM of rocking curve (Y-axis) and compressive stress (R-axis) for InSb thin films of 0.5 μm thickness.

Fig. 4 shows the InSb thickness dependence of the FWHM of the rocking curve in the (111) plane. The thickness of the InAs buffer layer was fixed to 15 nm. With increasing InSb thickness, the FWHM of InSb decreased. The results shown in Figs. 2–4 suggest that a reduction of stress in InSb leads to an improvement of the crystalline quality and electrical properties.

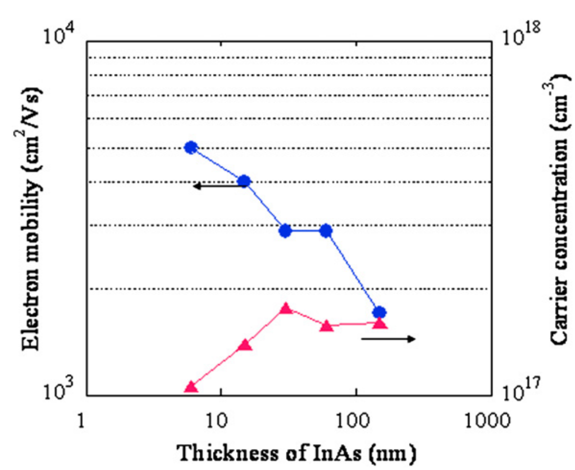

Fig. 3. InAs thickness dependences of electron mobility (Y-axis) and carrier concentration (R-axis) for InSb thin films of 0.5 μm thickness.