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Mid-infrared to ultraviolet optical properties of InSb grown on GaAs by molecular beam epitaxy

Vijay Richard D’Costa, Kian Hua Tan, Bo Wen Jia, Soon Fatt Yoon, and Yee-Chia Yeo

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Mid-infrared to ultraviolet optical properties of InSb grown on GaAs by molecular beam epitaxy

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Spectroscopic ellipsometry was used to investigate the optical properties of an InSb film grown on a GaAs (100) substrate, and to compare the optical properties of InSb film with those of bulk InSb. The film was grown by molecular beam epitaxy under conditions intended to form 90° misfit dislocations at the InSb-GaAs interface. The complex dielectric function obtained in a wide spectroscopic range from 0.06–4.6 eV shows the critical point transitions $E_0$, $E_1$, $E_1 + \Delta_1$, $E_0'$, and $E_2$. The amplitudes, energy transitions, broadenings, and phase angles have been determined using a derivative analysis. Comparing film and bulk critical point results reveal that the epitaxial film is nearly relaxed and has bulk-like optical characteristics. © 2015 AIP Publishing LLC.

I. INTRODUCTION

InSb offers the highest electron and hole mobilities among group III–V semiconductors. It also possesses a small bandgap $E_g$ of ~0.2 eV, which makes it suitable for mid-infrared optical devices. These unique properties make InSb highly desirable for integrating with Si for future optical and electronic devices. Since GaAs is nearly lattice-matched to Ge, integration of GaAs with Ge-buffered Si is possible and has been reported.1–4 Growth of high quality InSb films on GaAs is challenging due to large lattice mismatch of about ~14.6%. One approach to overcome mismatched epitaxy is to relieve strain energy through the formation of an interfacial misfit (IMF) dislocation array.5–7 IMF is attractive because the misfit dislocations (90°) are confined to the film-substrate interface and the subsequent growth follows a layer-by-layer strain-free epitaxy. IMF has been observed in a variety of III–V materials deposited on GaAs (001) substrate under specific growth conditions when it is energetically favorable to form 90° misfit dislocations instead of 60° misfit dislocations.8

Existence of 90° misfit dislocation array was reported for the growth of InSb on GaAs (001).9,10 The InSb films produced by Williams et al.9 showed threading dislocations and stacking faults in the film in addition to the 90° misfit dislocations at the interface. Kiel et al.10 fabricated higher quality InSb films and also carried out a detailed study of the interface by cross-sectional transmission electron microscopy (XTEM). The spacing between the misfit dislocations was found to have an average value of ~3 nm. This value nearly matches the expected periodicity of ~3.1 nm for pure 90° misfit dislocations at the InSb/GaAs. The theoretical misfit spacing value for pure 60° misfit dislocations is ~1.6 nm. However, the bulk of the InSb film still showed defects such as dislocation tangles and threading dislocations in addition to the presence of a rough interface with a ripple period of 40–50 nm. Their work suggests that there is some room for improvement of material quality of InSb film grown on GaAs.

The optical and electronic properties of InSb films formed by IMF need to be evaluated to assess their suitability for various device applications, in particular, around the bandgap region which lies in the mid-infrared energy range. The dielectric response from mid-infrared to ultraviolet and the critical points $E_0$, $E_1$, $E_1 + \Delta_1$, $E_0'$, and $E_2$ in crystalline InSb can be investigated using spectroscopic ellipsometry. The critical parameters include amplitudes, broadening parameters, phase angles, and energy transitions which provide valuable information about the electronic bandstructure of a material, and can be obtained using a derivative analysis of the complex dielectric function.11–13

There are reports on the determination of visible-UV dielectric function and critical point parameters associated with $E_1$, $E_1 + \Delta_1$, $E_0'$ and $E_2$ in bulk InSb11–17 and in InSb film on sapphire.18 These include even a temperature dependent investigation of $E_1$, $E_1 + \Delta_1$, $E_0'$ and $E_2$ critical points in bulk InSb.11,13 Spectroscopic ellipsometric investigation of the infrared dielectric function around $E_0$ as well as the critical point parameters has not been reported for bulk samples. A systematic study of critical point parameters in InSb film grown on GaAs has not been reported.

In this paper, we investigate the electronic bandstructure of InSb grown on GaAs using spectroscopic ellipsometry from 0.06 to 4.6 eV at room temperature. The growth of InSb on GaAs by molecular beam epitaxy (MBE) is optimized using IMF arrays. The amplitudes, energy transitions, broadenings, and phase angles are obtained for the critical points $E_0$, $E_1$, $E_1 + \Delta_1$, $E_0'$ and $E_2$ using a derivative analysis. The critical point parameters obtained for the film are in good agreement with the bulk values indicating a crystalline and nearly relaxed film.
II. GROWTH DETAILS AND STRUCTURAL CHARACTERIZATION

Heteroepitaxial InSb layer was grown on a (001) semi-insulating GaAs substrate using a solid source MBE equipped with arsenic (As) and antimony (Sb) valved crater sources. The crater temperature of the Sb source was set at 900°C to produce predominately Sb and Sb$_2$ fluxes. The GaAs substrate was pre-heated to 580°C to remove the native oxide. This was followed by the deposition of a 100 nm-thick GaAs buffer at 580°C to smoothen the surface. The substrate temperature was then lowered to 540°C under the As overpressure and annealed at the same temperature for 600 s without As overpressure. Subsequently, the substrate temperature was reduced to 310°C and the wafer was exposed to Sb flux for 240 s. The annealing of the wafer at 540°C and its exposure to Sb flux for 240 s are found to be critical for the formation of a single monolayer of Sb atoms on the surface of the substrate prior to InSb growth. It minimizes the formation of 60° misfit dislocation at the surface. A ~300 nm thick InSb layer was subsequently grown by opening the indium shutter.

The structural quality of the sample was investigated by high-resolution X-ray diffractometry (HR-XRD) and XTEM. Figure 1(a) shows the (004) ω-2θ curve for the InSb film. The peak at lower ω angle corresponds to InSb layer. The full-width-half-maximum (FWHM) of InSb film peak is ~185 arcseconds. Such small values of FWHM are observed typically only in films at least a micrometer thick. Reduction of FWHM in micrometer thick films is attributed to improvement in crystalline quality, particularly in the top portion of the film that is far from the highly defective film-substrate interface. The out-of-plane lattice constant of InSb film was obtained from the symmetric (004) ω-2θ curve. ω-2θ curves corresponding to asymmetric reflections (115) and (115) were acquired to obtain the in-plane lattice constant. The in-plane strain ε$_{||}$ in the InSb film is ~0.1% indicating that the film is nearly relaxed (~99.3%). The lattice mismatch between the InSb film and GaAs substrate is relieved through the formation of misfit dislocation array at the interface. The XTEM image of the sample as shown in Fig. 1(b) indicates the presence of an IMF layer. The misfit spacing is found to be ~3.2 nm, which nearly matches the theoretical value of ~3.1 nm. The threading dislocation density in the film estimated from TEM images is <$10^{10}$ cm$^{-2}$. In addition, atomic force microscopy (AFM) showed that the root mean square (RMS) roughness of InSb film is ~1 nm.

III. ELLIPSOMETRY AND CRITICAL POINT ANALYSIS PROCEDURES

J. A. Woollam’s infrared variable angle spectroscopic ellipsometer (IR-VASE) and a variable angle spectroscopic ellipsometer (VASE) were used for acquisition of ellipsometric angles Ψ and Δ. The data were acquired at two angles of incidence, 65° and 75°, from 480 to 3630 by 8 cm$^{-1}$ (0.06 to 0.45 eV) and 1.2 to 4.6 by 0.01 eV on the IR-VASE and VASE, respectively. A reference InSb substrate was characterized along with the InSb film grown on GaAs. Fig. 2(a) shows the experimental and the model pseudo-dielectric function for InSb film sample in the IR energy range. Pseudo-dielectric function denotes the dielectric response of the entire sample (overlayer-film-substrate). The visible-UV pseudo-dielectric function for InSb film is shown in Fig. 3(a). $E_0$, $E_1$, $E_2$, and $E_3$ are observed in the visible-UV pseudo-dielectric function. $E_0$ is masked by the presence of interference oscillations in the infrared range. The feature around 1.5 eV in the visible-UV dielectric function also corresponds to an interference oscillation.

To further investigate the optical response of InSb layer in detail, the film sample was modeled as a three-layer structure consisting of a bottom-most GaAs substrate, InSb film, and a...
surface layer. The surface film was modeled as an InSb-oxide layer in the visible-UV range.\(^2\) It was described as a rough layer in the infrared range where oxide optical constants are not available. The dielectric function of GaAs substrate used in the modeling was obtained by characterizing it separately. The visible-UV complex dielectric function of InSb film is modeled using four, Kramers-Kronig consistent, parameteric oscillators\(^23\) which describe the four critical point transitions \(E_1, E_1 + \Delta_1, E_0,\) and \(E_2\). The mid-infrared data were analyzed separately using a model containing an \(E_0\) critical point structure. The overlayer thickness (oxide or roughness), the InSb film thickness, and the InSb parametric optical constants were obtained simultaneously using standard ellipsometric data fitting procedures. With the layer thicknesses determined, dielectric function of InSb film was then extracted on a wavelength-by-wavelength basis.\(^23\) The dielectric function obtained in this manner is termed as point-by-point dielectric function. For the bulk InSb sample, essentially the same procedure was used to obtain parametric and point-by-point dielectric functions, using just an overlayer-substrate model.

Point-by-point and model infrared dielectric functions obtained for the InSb film are shown in Fig. 2(b). The direct bandgap \(E_0\) is now seen in the imaginary part of infrared dielectric function, revealing its square root dependence on photon energy. Fig. 3(b) shows point-by-point and model dielectric functions in the visible-UV range. The excellent agreement between the point-by-point and model dielectric function confirms the Kramers-Kronig consistency of the point-by-point function. The amplitude of \(E_2\) peak in the dielectric function of InSb film is \(\sim 21.8\) at \(3.87\) eV, which is close to the value of \(22.0\) obtained by Bermudez and Ritz\(^1\) for bulk InSb, whose surface was cleaved and maintained in ultrahigh vacuum. Using chemical etching, Aspnes and Studna\(^1\) achieved a value of \(21.3\) for the amplitude of \(E_2\) peak.

Point-by-point dielectric function is preferred to parameterized dielectric function for numerical derivative analysis.\(^23\) Although the oscillator model provides a very good fit to the raw data, small discrepancies may result near the critical points which can be amplified while calculating derivatives of the parameterized dielectric function. The visible-UV dielectric function with an energy step size of \(0.01\) eV is differentiated using 13 Savitzky-Golay smoothing coefficients for second-order derivatives with a polynomial of order 5. The derivatives of the experimental dielectric function were fitted using an analytic expression\(^23\)

\[
\frac{d^2\varepsilon_{\text{visible-UV}}}{dE^2} = \sum_j A_j e^{i\Phi_j} \left[ (E - E_j + i\Gamma_j) \right]^{-1/2},
\]

where \(A_j\) is the amplitude for transition \(j\), \(\Phi_j\) is the phase angle, \(E_j\) is the critical point energy and \(\Gamma_j\) is the broadening parameter. The summation covers the four transitions \(E_1, E_1 + \Delta_1, E_0,\) and \(E_2\). Although numerical differentiation of model is desirable in addition to numerical differentiation of experimental data,\(^23\) we ensured that the number of smoothing coefficients was carefully chosen to enhance the signal to noise ratio without distorting the sharp features in experimental data relative to unsmoothed data.

First-order numerical derivatives are used in the determination of direct bandgap \(E_0\) of InSb. The mid-infrared data with \(1\) meV energy step size were smoothed using 13 Savitzky-Golay coefficients corresponding to a polynomial of order 4. The first derivative of infrared dielectric function was fitted using an analytic lineshape given by\(^23\)

\[
\frac{d\varepsilon_{\text{IR}}}{dE} = A_0 \frac{E_0^3}{E^3} \frac{E_0 E_0^4}{(E - E_0 + i\Gamma_0)^{3/2}},
\]

where \(A_0\) is the amplitude, \(\Phi_0\) is the phase angle, and \(\Gamma_0\) is the broadening parameter for \(E_0\) critical point. \(A_0\) is the magnitude of the low-energy pole, which accounts for absorption outside of the infrared range.

The derivatives of the imaginary and real parts of the dielectric function were fitted simultaneously by a least-square procedure which uses the Levenberg-Marquardt algorithm.\(^25\) The critical point analysis for an InSb film is shown in Figs. 4 and 5. The sharp features in the visible-UV derivative spectra in Fig. 4 correspond to critical points \(E_1, E_1 + \Delta_1, E_0,\) and \(E_2\). A fit using Eq. (1) gives all the critical point parameters associated with these four critical points. The main derivative feature in the infrared range in Fig. 5(a) and 5(b) corresponds to \(E_0\), critical point with its associated parameters given by Eq. (2). The \(E_0\) feature can be clearly seen in the first-order derivatives, and nearly identical parameters are obtained with and without smoothing operation. On the contrary, \(E_0\) feature in the second-order derivatives appears to be overwhelmed by noise in the experimental data. We needed about 21 smoothing coefficients corresponding to a polynomial of order 5 to obtain good signal to noise ratio for second-order derivatives. \(E_0\) obtained from first-order derivatives lies within the experimental error (\(3\) meV) of the energy value obtained using second-order derivatives.

IV. RESULTS AND DISCUSSION

A. \(E_1\) and \(E_1 + \Delta_1\) transitions

The critical point parameters obtained for \(E_1\) and \(E_1 + \Delta_1\) for InSb film and InSb substrate samples are
TABLE I. Critical point parameters associated with $E_1$ and $E_1 + \Delta_1$ transitions for the InSb film.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>InSb film</th>
<th>Bulk InSb</th>
<th>Other reports</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$ (eV)</td>
<td>1.862 ± 0.002</td>
<td>1.857 ± 0.002</td>
<td>1.872, a 1.845, b 1.86 c</td>
</tr>
<tr>
<td>$A_{E_1}$</td>
<td>4.6 ± 0.3, 4.0 d</td>
<td>5.1 ± 0.3, 4.0 d</td>
<td></td>
</tr>
<tr>
<td>$\Gamma_{E_1}$ (eV)</td>
<td>0.054 ± 0.002</td>
<td>0.050 ± 0.002</td>
<td>0.05 c</td>
</tr>
<tr>
<td>$\Phi_{E_1}$ (radians)</td>
<td>1.39 ± 0.06</td>
<td>1.41 ± 0.05</td>
<td>1.48 c</td>
</tr>
<tr>
<td>$E_1 + \Delta_1$ (eV)</td>
<td>2.367 ± 0.008</td>
<td>2.362 ± 0.006</td>
<td>2.374, a, 2.362, b, 2.36 c</td>
</tr>
<tr>
<td>$\Delta_1$ (eV)</td>
<td>0.505 ± 0.008</td>
<td>0.505 ± 0.006</td>
<td>0.502, a, 0.517, b, 0.50 c</td>
</tr>
<tr>
<td>$A_{E_1 + \Delta_1}$</td>
<td>2.8 ± 0.5, 2.7 d</td>
<td>3.0 ± 0.4, 2.7 d</td>
<td></td>
</tr>
<tr>
<td>$\Gamma_{E_1 + \Delta_1}$</td>
<td>0.080 ± 0.008</td>
<td>0.071 ± 0.006</td>
<td>0.072 c</td>
</tr>
<tr>
<td>$\Phi_{E_1 + \Delta_1}$ (radians)</td>
<td>1.5 ± 0.2</td>
<td>1.5 ± 0.1</td>
<td>1.57 c</td>
</tr>
</tbody>
</table>

aExperimental values from Ref. 14.
bExperimental values from Ref. 13.
cExperimental values from Ref. 11.
dTheoretical values obtained using Eqs. (4) and (5).

The amplitudes of $E_1$ and $E_1 + \Delta_1$ transitions denoted by $A_{E_1}$ and $A_{E_1 + \Delta_1}$, respectively, are summarized in Table I along with their ratio $A_{E_1}/A_{E_1 + \Delta_1}$. We obtain $A_{E_1}/A_{E_1 + \Delta_1} \sim 1.6$ and 1.7 for film and bulk InSb, respectively, which is in good agreement with the experimental ratio$^{10}$ of ~1.8 reported for bulk InSb. This can be also compared with the theoretical ratio obtained from $k.p$ theory. The theoretical expressions for $A_{E_1}$ and $A_{E_1 + \Delta_1}$ are given by$^{11}$

$$A_{E_1} \simeq \frac{44(E_1 + \Delta_1)}{3a_0E_1^3},$$

$$A_{E_1 + \Delta_1} \simeq \frac{44(E_1 + 2\Delta_1)}{3a_0(E_1 + \Delta_1)^3},$$

where $a_0$ is the lattice constant of InSb. The $k.p$ theory predicts the amplitude ratio to be ~1.5. This is consistent with the experimental amplitude ratios obtained for bulk InSb and InSb film.

The broadening parameters for $E_1$ and $E_1 + \Delta_1$ are slightly larger than the bulk values obtained in this work as well as those reported for bulk in literature. This might be attributed to the presence of threading dislocations and small compressive strain in the nearly relaxed films. The phase angles for $E_1$ and $E_1 + \Delta_1$ obtained for the film are in good agreement with the bulk values. We notice that the magnitude of phase angle for $E_1$ is slightly greater than that for $E_1 + \Delta_1$ for both our film and bulk, consistent with the finding for bulk InSb$^{11}$ at room temperature.
TABLE II. Critical point parameters associated with \( E_0 \) and \( E_2 \) transitions for the InSb film.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>InSb film</th>
<th>Bulk InSb</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_0 ) (eV)</td>
<td>( 3.14 \pm 0.14 )</td>
<td>( 3.14 \pm 0.14 )</td>
</tr>
<tr>
<td>( A_{E_0} )</td>
<td>( 1.7 \pm 0.1 )</td>
<td>( 1.6 \pm 0.1 )</td>
</tr>
<tr>
<td>( \Gamma_{E_0} ) (eV)</td>
<td>( 0.21 \pm 0.14 )</td>
<td>( 0.20 \pm 0.14 )</td>
</tr>
<tr>
<td>( \Phi_{E_0} ) (radians)</td>
<td>( -1.3 \pm 0.1 )</td>
<td>( -1.2 \pm 0.1 )</td>
</tr>
<tr>
<td>( E_2 ) (eV)</td>
<td>( 4.05 \pm 0.01 )</td>
<td>( 4.03 \pm 0.01 )</td>
</tr>
<tr>
<td>( A_{E_2} )</td>
<td>( 8.3 \pm 1.3 )</td>
<td>( 9.3 \pm 1.4 )</td>
</tr>
<tr>
<td>( \Gamma_{E_2} ) (eV)</td>
<td>( 0.16 \pm 0.01 )</td>
<td>( 0.16 \pm 0.01 )</td>
</tr>
<tr>
<td>( \Phi_{E_2} ) (radians)</td>
<td>( 2.7 \pm 0.2 )</td>
<td>( 2.7 \pm 0.2 )</td>
</tr>
</tbody>
</table>

*Experimental values from Ref. 32.

**Experimental values from Ref. 11.

B. \( E_0 \) and \( E_2 \) transitions

The critical points associated with \( E_0 \) and \( E_2 \) are summarized in Table II. \( E_0 \) corresponds to two doublets but is modeled as a single critical point in our analysis, because we are not able to resolve the weak internal doublet structures from this room temperature data. It has been reported that these features stay well resolved in the second derivative spectra up to 200 K. Low temperature investigation of \( E_0 \) in bulk InSb reveals all its associated features and is easier to track them up to room temperature. The \( E_0 \) transition value for the InSb film is consistent with the value we obtained for the bulk. The critical points associated with \( E_0 \) show much larger uncertainties compared to other critical points. This is reported to be true for even temperatures lower than room temperature.

Unlike \( E_0 \) critical point, \( E_2 \) critical point is a strong feature in the UV energy range. The energy transition value for the film is in good agreement with our bulk InSb value as well as the bulk values reported in literature. The broadenings and phase angles obtained for this critical point in InSb film agree well with the bulk values. The amplitude of the \( E_2 \) transition has not been reported but the value obtained for the film is consistent with the value we obtained for the bulk.

C. \( E_0 \) transition and absorption coefficient

The critical point parameters obtained for \( E_0 \) for InSb film and bulk InSb samples are summarized in Table III. The bandgap value from the first derivative analysis agrees well with the reported values for InSb obtained from absorption and photoluminescence measurements. The energy transition and phase angle for the film are in good agreement with the values obtained for bulk. The broadening parameter for the film is nearly three times larger than its counterpart in bulk. As pointed out for \( E_1/E_1 + \Delta_1 \) transition, this may be related to residual strain in the film as well as the presence of threading dislocations in bulk of the film. Also, the broadening parameter associated with \( E_0 \) might be more sensitive to threading dislocations and strain in comparison to \( E_1/E_1 + \Delta_1 \) transition.

V. CONCLUSIONS

In conclusion, we studied the optical properties of an InSb film grown on GaAs (001) using spectroscopic ellipsometry. The complex dielectric function of InSb film is determined from 0.06 to 4.6 eV. The critical points \( E_1, E_1 + \Delta_1, E_0, \) and \( E_2 \) are analyzed using a second derivative analysis of dielectric function. A first derivative analysis was used to obtain the critical point parameters associated with \( E_0 \). The results indicate that the film is of optical quality similar to bulk InSb and is nearly strain-free.

ACKNOWLEDGMENTS

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