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# Determination of the conduction-band structure of InSb subject to mechanical strain from measurements of the reflectivity spectrum

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The measurement of the effect of mechanical strain on the reflectivity spectrum in the plasma region of $n$-type InSb has been performed. The results allow the determination of the stress dependence of the electronic states at $\Gamma$ according to the theory described in the preceding paper [see also W. Howlett and S. Zukotynski, Phys. Rev. B **16**, 3688 (1977)]. We determine the deformation potentials to be $c = -7.0$ eV, $b = -1.7$ eV, $n = -5.1$ eV, in satisfactory agreement with previous work.

## I. INTRODUCTION

In the previous paper[1] (hereafter denoted I) it was shown that the reflectivity spectrum in the plasma region was a sensitive tool for studying the deformed-conduction-band structure[2] of the III-V semiconductors. Here we apply this analysis to experiments we have carried out in $n$-type InSb subject to uniaxial compression. [D. Aspnes and M. Cardona have recently studied the corrections to the band structure of deformed semiconductors associated with the interaction with the $\Gamma_{15}$ and $\Gamma_{12}$ bands. They found these corrections to be of major significance in GaAs and Ge. It appears that, due to its small energy gap, these contributions are not very important in InSb. Also, the expressions that they derive yield parabolic bands and therefore are of very limited application in the case of InSb (private communication).]

In Sec. II the experiment is described in detail. The strain dependence of the electrical conductivity is determined in Sec. III directly from the experimental results according to the method proposed in Paper I. The deformation potentials of the electronic states at $\Gamma$ are then computed and reconciled with previous determinations of these quantities.

## II. MEASUREMENT OF THE SHIFT OF THE REFLECTIVITY SPECTRUM OF $n$-TYPE InSb SUBJECT TO MECHANICAL STRAIN

$n$-type samples of InSb were obtained from Monsanto Co. in the form of single crystals oriented on (110) and (001) planes. The orientation was checked by the back-reflection Laue method and found to be accurate to within 1%. The same method was used to find the $\langle 110\rangle$, $\langle 100\rangle$, and $\langle 111\rangle$ axes in these planes. Typical sample size was $13\times5\times1$ mm. The long direction became the axis of stress, the large face the reflecting plane. This face was lapped, polished, and finally etched, whereas the back side was left relatively rough to prevent multiple reflections.

The samples actually came from three different batches of material, hereafter labeled 1, 2, and 3. The average carrier concentrations were $0.63\times10^{18}$, $1.2\times10^{18}$, and $1.8\times10^{18}\,\mathrm{cm}^{-3}$, respectively. Individual batches were quite homogeneous.

The reflectivity in the plasma region was measured at room temperature using a double-beam Perkin-Elmer infrared spectrophotometer equipped with an expanded sample compartment for reflectance measurements. The angle of incidence was 13°, and the radiation was polarized either along the axis of stress [transverse electric mode (TEM)], or perpendicular to it in the plane of incidence [transverse magnetic mode (TMM)]. For the samples described above, the reflectivity spectrum exhibited a minimum of about 5% around 20 $\mu$m. For higher wavelengths, the reflectivity increased rapidly, while for lower wavelengths it increased slowly to a constant value of about 33%.

Mechanical strain was produced by uniaxial compression. A squeezing assembly was designed so as to minimize off axial strains. Typical samples withstood up to 250 MPa.

Three different ways of characterizing the change in the reflectivity spectrum produced by uniaxial deformation were used. The first was the shift in frequency $\omega_m$ of the reflectivity minimum. The main problem with this technique was the difficulty in pinpointing the relatively shallow minimum with sufficient resolution so as to detect the shift produced by uniaxial strain. Also water-vapor absorption bands frequently distorted the actual minimum.

The second method measured the change in frequency $\omega_0$ ($\omega_0/\omega_m \simeq 0.95$) of an isoreflectivity point. The reflectivity changed rapidly around $\omega_0$, and so although the resolution of the system was not a critical factor, the response time was. Fortunately, $\omega_0$ could be chosen so as to eliminate water-vapor absorption. The third method measured the

TABLE I. Shift of reflectivity spectrum with uniaxial stress $\sigma_u$.

| Sample designation | Batch No. | Measurements method | Frequency of min. ($cm^{-1}$) | Min. Refl. | $\omega_0/\omega_m$ | Axis of stress | Reflecting plane | $\frac{\partial(\Delta\omega/\omega_m)}{\partial\sigma_u}$ or $\frac{\partial(\Delta\omega/\omega_0)}{\partial\sigma_u}$ TEM | $10^{-4}\frac{\partial R}{\partial\sigma_u}$ $(MPa)^{-1}$ TMM |
|---|---|---|---|---|---|---|---|---|---|
| *G* | 1 | 1 | 580 | ... | ... | ⟨100⟩ | (011) | 0.61 ±0.06 | −0.46 ±0.04 |
| *S* | 2 | 1 | 490 | ... | ... | ⟨100⟩ | (011) | 0.59 ±0.05 | −0.44 ±0.04 |
| 3 set 2 | 2 | 1 | 490 | ... | ... | ⟨100⟩ | (011) | 0.44 ±0.03 | −0.31 ±0.20 |
| *Sα* | 2 | 1 | 490 | ... | ... | ⟨110⟩ | $(1\bar{1}0)$ | 0.36 ±0.04 | −0.51 ±0.05 |
| 11*A P*26 | 3 | 1 | 395 | ... | ... | ⟨110⟩ | (001) | 0.37 ±0.05 | −0.15 ±0.02 |
| 11*B*3 | 2 | 2 | 495 | ... | 0.973 | ⟨100⟩ | (011) | 0.45 ±0.02 | −0.39 ±0.03 |
| 11*B*2 | 2 | 2 | 492 | ... | 0.975 | ⟨100⟩ | (011) | 0.44 ±0.04 | −0.41 ±0.04 |
| 11*A*2 | 2 | 2 | 490 | ... | 0.970 | ⟨100⟩ | (011) | 0.38 ±0.05 | −0.39 ±0.05 |
| 3 set 2 | 3 | 2 | 400 | ... | 0.950 | ⟨100⟩ | (011) | 0.61 ±0.03 | −0.64 ±0.03 |
| 5 | 2 | 2 | 485 | ... | 0.950 | ⟨110⟩ | $(1\bar{1}0)$ | 0.22 ±0.04 | −0.35 ±0.05 |
| 2*B* | 2 | 2 | 490 | ... | 0.960 | ⟨110⟩ | $(0\bar{1}0)$ | 0.32 ±0.05 | −0.35 ±0.06 |
| 10*B* | 3 | 2 | 395 | ... | 0.950 | ⟨110⟩ | (001) | 0.33 ±0.05 | −0.11 ±0.02 |
| 7 set 2 | 3 | 2 | 395 | ... | 0.950 | ⟨110⟩ | (001) | 0.30 ±0.04 | −0.19 ±0.03 |
| 8*A* | 3 | 2 | 400 | ... | 0.950 | ⟨110⟩ | (001) | 0.37 ±0.04 | −0.15 ±0.02 |
| 5*C* | 3 | 3 | 397 | 0.045 | 0.93 | ⟨111⟩ | $(1\bar{1}0)$ | 2.6 ±0.2 | −3.5 ±0.3 |
| 8*A* | 3 | 3 | 408 | 0.050 | 0.93 | ⟨110⟩ | (001) | 2.9 ±0.2 | −1.1 ±0.1 |
| 7 | 2 | 3 | 490 | 0.045 | 0.95 | ⟨110⟩ | $(1\bar{1}0)$ | 4.2 ±0.3 | −3.2 ±0.3 |

change in reflectivity at fixed frequency $\omega_0$ ($\omega_0 \simeq 0.95\omega_m$). In these measurements a lock in amplifier was integrated into the system and introduced a substantial improvement in resolution. For this reason method III had the highest accuracy of the three.

For each polarization mode, the quantities measured as a function of uniaxial compression $\sigma_u$ for methods 1 to 3 are, respectively, $\Delta\omega/\omega_m$, $\Delta\omega/\omega_0$, and $\Delta R(\omega_0)$. Measurements were taken at about 20-MPa intervals. For each technique a statistically significant linear relationship was found.

The slopes $\partial(\Delta\omega/\omega_m)/\partial\sigma_u$, $\partial(\Delta\omega/\omega_0)/\partial\sigma_u$, and $\partial R(\omega_0)/\partial\sigma_u$ as well as 95% confidence intervals were obtained by a least-squares analysis for the two directions of polarization. The results of this analysis for each of the samples measured are found in Table I. It should be noted that the results were generally quite reproducible on successive runs on the same sample. Samples from a particular batch and with the same strain-polarization configuration gave fairly consistent results. Variations were observed in going from one batch to another.

## III. ANALYSIS OF EXPERIMENTAL RESULTS

Equations (I-1)–(I-6), (I-17), (I-26), and (I-45) permit the calculation of the unstressed Fermi level $\epsilon_{F0}$ and carrier concentration $N_0$ from any two measurements of the reflectivity spectrum (for example, the minimum reflectivity and the frequency $\omega_m$ at which it occurs). The unstressed band parameters were taken as $E_g = 0.00767$ a.u.,[3,4] $\Delta = 0.031$ a.u.,[5] $P^2 = 0.403$ a.u.[3] The results for typical samples in each batch are shown in Table II. The four functions $a_1, \ldots, a_4$ describing the ac conductivity under deformation were subsequently computed from (I-39)–(I-44) and are also given in Table II.

To conform with the analysis in I, it is necessary to diagonalize the conductivity $\hat{\sigma}$ for uniaxial compression. The strain tensor $\hat{\epsilon}$ was computed in Ref. 6 for uniaxial compression along the ⟨100⟩, ⟨110⟩, and ⟨111⟩, crystallographic directions. Using these results, the components of $\hat{\sigma}$ can be explicitly calculated from (I-45) and the eigenvalue problem solved. For each of the three uniaxial compressions considered above one finds that the stress axis is a principal axis, with the other two orthogonal principal directions lying in the plane perpendicular to the stress axis. For ⟨110⟩ uniaxial stress, the two principal directions in this plane are ⟨001⟩ and $\langle 1\bar{1}0\rangle$, while for ⟨100⟩ and ⟨111⟩ stress the two eigenvalues in this plane are degenerate. To conform with the notation in I, $Z$ denotes the stress axis, $Y$ is normal to the reflecting

TABLE II. Fermi level, carrier density, functions $a_i$ for each sample batch calculated from the reflectivity spectrum in the plasma region.

| | Batch 1 | Batch 2 | Batch 3 |
|---|---|---|---|
| $\omega_m(\mathrm{cm}^{-1})$ | 580 | 490 | 400 |
| $k_f$(a.u.) | 0.019 8 | 0.017 2 | 0.014 1 |
| $\epsilon_f$(a.u.) | 0.008 51 | 0.007 02 | 0.005 29 |
| $N(\mathrm{cm}^{-3})$ | $1.83\times10^{18}$ | $1.16\times10^{18}$ | $0.626\times10^{18}$ |
| $a_1$(a.u.) | 0.244 | 0.239 | 0.227 |
| $a_2$(a.u.) | −1.92 | −1.93 | −1.94 |
| $a_3$(a.u.) | −11.8 | −15.2 | −21.5 |
| $a_4$(a.u.) | 38.2 | 41.5 | 47.0 |

plane, and $X$-$Z$ forms the reflecting plane (with the plane of incidence being $X$-$Y$). Hence, for the experimental configurations already described, the $X, Y, Z$ directions always form the eigenvectors of $\hat{\delta}$ (or $\hat{I}/I_0$). The eigenvalues are all linear in $\sigma_u$ and one can write

$$\frac{\partial(\Delta\hat{I}_{ii}/I_0)}{\partial\sigma_u} = a_1 f_1 + a_2 f_2 + a_3 f_3 c + a_4 f_4 b + a_4 f_5 n, \quad i = x, y, \text{or } z. \tag{1}$$

$a_1, \ldots, a_4$ are given in Table II, $c$, $b$, and $n$ are the deformation potentials, and $f_1, \ldots, f_5$ are functions of the elastic compliances $s_{11}, s_{12}, s_{44}$,[7] and depend on the stress axis as well as the principal axis under consideration. The $f_i$ for the different experimental configurations are given in Table III.

The experimental results can be analyzed to give $\partial(\Delta I_{ii}/I_0)/\partial\sigma_u$ directly. For the TEM $\partial(\Delta I_{zz}/I_0)/\partial\sigma_u$ can be determined unambiguously from the change of the reflectivity spectrum. $\partial(\Delta I_{xx}/I_0)/\partial\sigma_u$ can also be determined directly from the TMM results as long as one neglects the contribution from $\partial(\Delta I_{yy}/I_0)/\partial\sigma_u$. For an angle of incidence of 13°, a rough calculation shows this approximation to be justified. Each of the 17 samples in Table II were analyzed in this way, and the results averaged for samples from the same batch and having a common measurement technique and stress-polarization configuration. These computations were based on the theory of I and relied essentially on a numerical rather than an analytical analysis. The results are presented in Table IV.

It should be pointed out that these calculations have neglected the effect of changes in the lattice dielectric constant $\hat{\kappa}$ and carrier relaxation time $\tau$ due to strain. While the dependence of $\hat{\kappa}$ on strain has not been studied for InSb, the work on GaAs would suggest[8] that at most 10%, and usually much less, of the observed shift of the reflectivity spectrum could be attributed to the change in $\hat{\kappa}$. From (I-48)for a minimum reflectivity of 5%, one finds $\omega_m\tau \simeq 15$. From arguments in I one would expect that the carrier scattering does not affect the optical properties at these frequencies. An approximate calculation puts an upper limit of 5% on the contribution of changes in $\tau$ with strain to the shift of the reflectivity spectrum.

Tables III and IV, along with Eq. (1), can be used to determine the deformation potentials $c$, $b$, and $n$ for InSb. It is obvious that there is more data in Table IV than is needed to uniquely determine $c$, $b$, and $n$. The last three columns of Table IV give the values of the deformation potentials that are obtained for each row.

The results in Table IV corresponding to method No. 3 [change in $R(\omega_0)$] allow two independent determinations of $n$. We get two very consistent values: $n = -5.1$ eV and $n = -5.0$ eV. The remaining data in Table IV allows only one more independent determination of $n$ and yields a value about 30%

TABLE III. Functions $f_i$ for uniaxial stress along the ⟨100⟩, ⟨110⟩, and ⟨111⟩ directions.

| Axis of stress | Principal axis | $f_1$ | $f_2$ | $f_3$ | $f_4$ | $f_5$ |
|---|---|---|---|---|---|---|
| ⟨100⟩ | ⟨100⟩ | $-(s_{11}+s_{12})$ | $-s_{11}$ | $-(s_{11}+2s_{12})$ | $-2(s_{11}-s_{12})$ | 0 |
| | ⊥ to ⟨100⟩ (cylindrical symmetry) | $-(s_{11}+2s_{12})$ | $-s_{12}$ | $-(s_{11}+2s_{12})$ | $(s_{11}-s_{12})$ | 0 |
| ⟨110⟩ | ⟨110⟩ | $-(s_{11}+2s_{12})$ | $-\frac{1}{2}(s_{11}+s_{12})-\frac{1}{4}s_{44}$ | $-(s_{11}+s_{12})$ | $-\frac{1}{2}(s_{11}-s_{12})$ | $-\frac{1}{4}s_{44}$ |
| | ⟨1$\bar{1}$0⟩ | $-(s_{11}+2s_{12})$ | $-\frac{1}{2}(s_{11}+s_{12})+\frac{1}{4}s_{44}$ | $-(s_{11}+2s_{12})$ | $-\frac{1}{2}(s_{11}-s_{12})$ | $\frac{1}{4}s_{44}$ |
| | ⟨001⟩ | $-(s_{11}+2s_{12})$ | $-s_{12}$ | $-(s_{11}+2s_{12})$ | $(s_{11}-s_{12})$ | 0 |
| ⟨111⟩ | ⟨111⟩ | $-(s_{11}+2s_{12})$ | $-\frac{1}{3}(s_{11}+2s_{12})-\frac{1}{3}s_{44}$ | $-(s_{11}+2s_{12})$ | 0 | $-\frac{1}{3}s_{44}$ |
| | ⊥ to ⟨111⟩ (cylindrical symmetry) | $-(s_{11}+2s_{12})$ | $-\frac{1}{3}(s_{11}+2s_{12})+\frac{1}{6}s_{44}$ | $-(s_{11}+2s_{12})$ | 0 | $\frac{1}{6}s_{44}$ |

TABLE IV. Determination of $\partial(\Delta I_{ii}/I_0)/\partial\sigma_u$ and deformation potentials.

| Batch No. | Measurement technique | No. of samples | Axis of stress | Plane of reflection | $10^{-4}\frac{\partial(\Delta I_{zz}/I_0)}{\partial\sigma_u}$ ($MPa^{-1}$) | $10^{-4}\frac{\partial(\Delta I_{xx}/I_0)}{\partial\sigma_u}$ ($MPa^{-1}$) | $c$ (eV) | $b$ (eV) | $n$ (eV) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | ⟨100⟩ | (011) | 1.22 | −0.94 | −6.9 | −1.2 | ··· |
| 2 | 1 | 2 | ⟨100⟩ | (011) | 1.04 | −0.79 | −6.4 | −1.0 | ··· |
| 2 | 2 | 3 | ⟨100⟩ | (011) | 0.83 | −0.84 | −6.2 | −0.90 | ··· |
| 3 | 2 | 1 | ⟨100⟩ | (011) | 1.12 | −1.02 | −7.5 | −1.3 | ··· |
| 2 | 1 | 1 | ⟨110⟩ | (1$\bar{1}$0) | 0.71 | −1.04 | | | |
| 2 | 2 | 2 | ⟨110⟩ | (1$\bar{1}$0) | 0.55 | −0.66 | −6.6 | −1.2 | −3.1 |
| 3 | 1 | 1 | ⟨110⟩ | (001) | 0.73 | −0.31 | | | |
| 3 | 2 | 3 | ⟨110⟩ | (001) | 0.63 | −0.30 | | | |
| 3 | 3 | 1 | ⟨110⟩ | (1$\bar{1}$0) | 1.23 | −0.96 | −7.0 | −2.3 | −5.1 |
| 3 | 3 | 1 | ⟨110⟩ | (001) | 1.17 | −0.48 | | | |
| 3 | 3 | 1 | ⟨111⟩ | (1$\bar{1}$0) | 1.23 | −0.96 | −7.2 | ··· | −5.0 |

lower. We tended to discount this determination because of the experimental superiority of method No. 3 and take $n=-5.1$ eV.

The average values of $c$ and $b$ are −7.0 and −1.7 eV. In these averages we have double weighted values arising from method No. 3 as a somewhat arbitrary way of quantifying our feelings on the relative merits of the three methods.

Thus the values of the deformation potentials of InSb found by this work are

$$c=-7.0 \text{ eV}, \quad b=-1.7 \text{ eV}, \quad n=-5.1 \text{ eV}.$$

We place an upper limit of 15% on the uncertainty in these results arising from the dependence of $\hat{\kappa}$ and $\tau$ on deformation.

## IV. COMPARISON WITH PREVIOUS WORK

Earlier works[6,9] have also used the shift of the plasma minimum with uniaxial stress to determine the deformation potentials of InSb. In this work, with the use of I, we have treated the Maxwell equations in a more rigorous manner, although for an angle of incidence of 13° this has little effect on the numerical values of the deformation potentials which are found. We have also extended the technique so as to describe other changes in the reflectivity spectrum—a distinct advantage experimentally. Two major differences in the theory underlying the analysis of the experimental results also exist between this work and Refs. 6 and 9. These are

(i) The deformed conduction band is modeled according to the recent calculation in Ref. 2, rather than the one performed by Bir and Pikus.[10] There are two major differences between these works which both affect the analysis of the experimental results. They are (a) The deformed band structure of Ref. 2, as opposed to Ref. 10, contains certain strain-dependent terms which do not involve $c$, $b$, and $n$. These terms in fact involve the matrix element $P^2$ and turn out to be substantial for the narrow gap III-V semiconductors for sufficient depth into the band. (b) The calculation in Ref. 2 is independent of the relative size of $E_g$ and $\Delta$. However, Ref. 10 applies only in the limits $E_g \ll \Delta$ or $E_g \gg \Delta$. In InSb, $E_g \simeq \frac{1}{4}\Delta$, so the condition $E_g \ll \Delta$ is only nominally satisfied.

(ii) The ac conductivity under deformation has been calculated in I using a technique designed especially for energy bands containing only a small deviation from isotropy. No restrictions are imposed on the symmetry, algebraic form, $\vec{k}$ dependence, etc., of the term describing the deviation from isotropy. The method is ideal for the deformed conduction band in the III-V semiconductors. In Refs. 6 and 9 the ac conductivity was computed using a technique[11] devised for ellipsoidal bands of the form

$$\gamma(\epsilon)=\sum a_{\alpha\beta}k_\alpha k_\beta , \tag{2}$$

where $\gamma$ is an arbitrary function of energy and the $a_{\alpha\beta}$ are constants. Unfortunately, while the deformed conduction band of InSb can be placed in a form resembling (2), the $a_{\alpha\beta}$ are functions of energy. This suggests that one treat the $a_{\alpha\beta}$ as constants by evaluating them at $\epsilon_{f0}$. A substantial error is produced in this way, especially for small effective mass materials such as InSb.

The deformation potentials for InSb found in Ref. 6 are listed in Table V. There are discrepancies of the order of 100% and more with the values obtained in this work. A detailed quantitative analysis was performed in Ref. 12 which showed that the qualitative arguments presented above [(i) and (ii)] each accounted for approximately one half of the discrepancy.

TABLE V. Deformation potentials on InSb.

| Author (Ref.) | Method | $c$ (eV) | $b$ (eV) | $n$ (eV) |
|---|---|---|---|---|
| Keyes (13) | piezoresistance | −7.0 | ... | ... |
| Long (14) | piezoresistance | −7.2 | ... | ... |
| Potter (4) | piezoresistance | −7.0 | ... | ... |
| Abduvakhidov (15) | intrinsic carrier concentration | −6.5 | ... | ... |
| Bradley *et al.* (16) | optical energy gap | −7.1 | ... | ... |
| Volkov (17) | piezoresistance | −7.2 | −1.4 | −6.8 |
| Fischer (18) | tunnel current | −10 | −1.3 | −12.8 |
| Bir and Pikus (10) | piezoresistance | −7.2 | −0.6 | −8.0 |
| Valyasko (19) | photoconductivity | ... | −1.7 | −7.5 |
| Seiler *et al.* (20) | magneto-phonon oscillations | −6.1 | −2.0 | −8.1 |
| Benoît à la Guillaume *et al.* (21) | piezo emission | −7.0 | −2.9 | −8.5 |
| Pollak *et al.* (22) | magnetoreflectivity | ... | −2.0 | −8.5 |
| Cardona *et al.* (23) | piezobirefringence | ... | −1.8 | −10.8 |
| Smith *et al.* (24) | ultrasonic attenuation | −5.2 | ... | ... |
| Zukotynski and Howlett (6) | plasma minimum | −1.8 | −1.5 | −3.5 |
| Ranvaud *et al.* (25) | cyclotron resonance | −7.0 | −1.8 | −8.4 |

When the deformation potentials $c$, $b$, and $n$ determined in this work are compared with the remaining values shown in Table V, a quite satisfactory agreement is apparent. The scatter of values of $c$ in Table V is small and the agreement with our value of −7.0 eV is excellent. The dispersion of values of $b$ in Table V is quite large but our value of −1.7 eV appears to be quite consistent. Our value of $n = -5.1$ eV is somewhat lower than the values in Table V but, when the error limits are placed on our value and those in the table, the apparent discrepancy basically disappears.

It should be noted that, while the experimental methods listed in Table V are extremely varied, they all determine the deformation potentials from the strain dependence of the energy gaps at the Γ point. In the model proposed in Ref. 2 and used in this work, the strain dependence of the conduction-band eigenstate at arbitrary $\vec{k}$ is expressed in terms of the Γ-point deformation potentials. Thus the satisfactory numerical agreement between the values of the deformation potentials found in this work and those obtained by other methods (Table V) is strong evidence for the validity of the deformed conduction band model proposed in Ref. 2.

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