Dynamical analysis of low-energy-electron-diffraction intensities from InSb(110)

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Dynamical calculations of the intensities of normally incident low-energy electrons diffracted from InSb(110), performed using a matrix inversion method, are reported for structures resulting from (i) a kinematical search, (ii) a dynamical search, and (iii) energy-minimization calculations. The model structures considered in all three cases embody distortions of the uppermost three atomic layers of InSb from their truncated bulk geometries. The dynamical calculations are compared with elastic-low-energy-electron-diffraction intensities measured for 14 beams with a sample temperature of T = 150 K. This comparison leads to the selection of the mostprobable surface structure for InSb(110) as one in which the top layer undergoes both a rigid rotation of 28.8° and a 0.05 Å relaxation toward the substrate. The Sb atoms in the top layer move outward and the In atoms inward, giving a relative vertical shear of 0.78 Å. In the second layer, the In move outward 0.09 Å and the Sb inward 0.09 Å. This surface atomic geometry is nearly identical to that which we reported earlier for covalently-bonded GaAs(110) but somewhat different from the reported for ZnTe(110) which exhibits a slightly more ionic bonding. We infer, therefore, that highly covalent zinc blende-structure compound semiconductors exhibit reconstructions of their (110) surfaces characterized by (i) large bond rotations in the uppermost layer, with the anion moving outward and cation inward, (ii) small bond-length alterations except for possible 4-5% contractions of the back bonds between the outermost anion and the cation in the layer beneath, and (iii) distortions from the bulk geometry which penetrate at least two atomic layers in from the surface.

I. INTRODUCTION

Atomic geometries for the (110) surfaces of zinc blende structure compound semiconductors, especially GaAs(110), have been extracted via the analysis of several different spectroscopic measurements, including elastic-low-energy-electron-diffraction (ELEED) intensities, 1-12 angular integrated ultraviolet photoemission spectra (UPS),^{9,13,14} angle-resolved ultraviolet photoemission spectra (ARUPS),¹⁵⁻¹⁷ polarization-dependent angle-resolved photoemission spectra (PARUPS),^{16,18} and the electron paramagnetic resonance (EPR) of adsorbed O₂ species.¹⁹ Moreover, three procedures for determining these atomic geometries via minimization of surface energy functionals have been proposed.²⁰⁻²² It has been demonstrated that, for the extensively examined case of GaAs(110), all of these methodologies lead to compatible surface structures within their inherent uncertainties.²³ In this paper we report the extension of ELEED intensity analyses to the case of InSb(110) and the comparison of the resulting atomic geometry both with that predicted by Chadi's energy-minimization procedure²¹ and with those of GaAs (110), $^{10, 11, 23}$ ZnTe(110), 12 and ZnO $(10\overline{10})$. $^{24, 25}$ Since no surface-structure determinations utilizing other methods have reported for InSb(110), we cannot yet compare our atomic geometry with those determined by the other methodologies as was done in the case of GaAs(110).^{11,12}

Perhaps the most significant conclusion emanating from our structure determination is the near identity of the reconstructions of GaAs(110) and InSb(110) measured relative to the bulk lattice constant of each material [which is 15% greater for InSb than for GaAs (Ref. 26)]. Since the bonding ionicities of the two materials are nearly equal,²⁷ this conclusion is consistent with the hypothesis^{2,28} that the character of the bonding of a compound semiconductor is a major factor in the determination of the atomic geometry of its nonpolar surfaces.

Our analysis also is directed toward clarifying two technical issues which have arisen in the applications of ELEED intensity analysis to the determination of the structure of the nonpolar surfaces of compound semiconductors. First, we examine the sensitivity of the methodology to relaxations parallel to the surface. For GaAs(110) both "bond-relaxation"¹⁶ (or "normaldisplacement"¹¹) and "rotational-relaxation"¹⁶ (or "bond-rotation"¹¹) models have been consid-

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ered.^{10, 11, 16, 19, 20} Although, for GaAs(110), the bond-rotated structures appear to be superior to the normal-displacement ones, this result generally has been displayed in the literature only in terms of structures differing both in perpendicular and parallel atomic positions.^{10, 11, 16} In this paper we evaluate the sensitivity of our ELEED intensity analysis to atomic displacements parallel to the surface by comparing structures differing only in these coordinates, thereby, revealing a precision of $\Delta d_{\parallel} \sim 0.1$ Å for dynamical calculations. This precision is rather greater than that associated with the $\Delta d_{\parallel} \sim 0.5$ Å uncertainty characteristic of kinematical analyses.^{29,30} Second, we consider the issue of establishing the presence of subsurface relaxations. In particular, we show that achieving adequate descriptions of certain beams requires these relaxations, and hence we are confident that they occur for InSb(110) as well as for GaAs(110). We infer, therefore, that highly covalent zinc blende-structure compound semiconductors exhibit reconstructions of their (110) surfaces characterized by (i) large bond rotations in the uppermost layer, with the anion moving outward and cation inward, (ii) small bond-length alterations, except for possible contractions by as much as 5% of the back bonds between the uppermost anion and the cations in the layer beneath, and (iii) distortions from the bulk geometry which penetrate at least two atomic layers in from the surface.

We proceed by first indicating our experimental procedures in Sec. II. Then in Sec. III, we describe the nature of our model calculations. In Sec. IV, we discuss the structure determination as well as the sensitivity of the computed intensity profiles to atomic motions parallel to the surface. In Sec. V, we summarize our results.

II. EXPERIMENTAL PROCEDURES

The low-temperature ($T \sim 150$ K) ELEED intensities analyzed in our study of InSb(110) were obtained using a standard Physical Electronics Industries LEED system¹² embodying a custom-adapted manipulator. Specifically, we modified the Physical Electronics Industries S/N-504-6-174 manipulator to cool the sample via a copper braid connecting a small liquid-nitrogen resevoir to a copper block on the sample holder. All metal junctions were copper brazed for good thermal conduction. The flexible copper braid had the minimum length to allow the necessary freedom of rotation for the sample holder in the vacuum. The crystal itself was tightly mounted on a piece of Mo foil, one end of which had a good thermal contact with the copper block. Alumel and chromel thermocouple wires were spot-welded on the back side of the Mo foil. Using pressurized liquid nitrogen, we could keep the temperature of the sample

stable during the data-taking process. The temperature of Mo foil in steady state was about 125 K, as shown by the thermocouple reading. Consequently, we believe that the surface of the crystal was cooled to at least 150 K. Since the measured ELEED intensities were compared with rigid-lattice model calculations, the precise value of the sample temperature is not important for our analysis.

The InSb sample was purchased from General Diode Corporation. The (110) surface was prepared by conventional cutting-polishing-etching sequences, consisting of mechanical polishing with 5μ SiC powders and chemical etching with a solution of 0.2% bromine in methanol. The crystal was then mounted on the Mo foil and placed in the vacuum chamber. The surface was cleaned by argon-ion bombardment (1.0 keV, 6 min) and reordered by thermal annealing (T - 640 K, 75 min). After this treatment, Auger profiles were taken to verify that the surface was contaminant-free and stoichiometric within the accuracy of Auger electron spectroscopy (AES) technique ($\sim 0.1\%$).

The condition of normal incidence was checked by the symmetry of the spot pattern, i.e., by verifying



FIG. 1. Schematic indication of the surface atomic geometry and the associated ELEED normal incidence spot pattern for the (110) surface of InSb. The symbols utilized in Table I are defined in the upper panel of the figure. The numerical values shown are taken from panel (c) of Table I. that the intensity of the (hk) beam is equal to that of the $(\bar{h}k)$ beam. The dimensions of the LEED pattern revealed no significant deviation of the surface unit mesh from that expected of a truncated bulk crystal described by the atomic geometries given by Wyckoff.²⁶ A schematic diagram of the surface atomic geometry, including the unit mesh dimensions, is presented in Fig. 1 in which the normalincidence spot pattern also is indicated.

The data acquisition required about two weeks during which the base pressure of the vacuum system stayed in the 10^{-10} Torr range. The spots of the LEED pattern always looked sharp and bright. The intensities were recorded with a Gamma Scientific spot photometer. The intensity data presented herein are averages over three separate runs of the measured intensities for each beam. This procedure was adopted because smaller structural features in the intensity profiles varied from one run to another, although the main features of these profiles deviated from the averages shown by less than $\pm 10\%$. Data were collected for 14 beams, i.e., those with the beam indices $(10) = (\overline{10}), (01), (0\overline{1}), (11) = (\overline{11}),$ $(1\overline{1}) = (\overline{11}), (20) = (\overline{2}0), (02), (0\overline{2}), (21) = (\overline{2}1),$ $(12) = (\overline{1}2), (2\overline{1}) = (\overline{21}), (1\overline{2}) = (\overline{12}), (13) = (\overline{13}),$ and $(1\overline{3}) = (\overline{13})$. These 14 normal-incidence intensity profiles, taken at $T \sim 150$ K, are the experimental ELEED intensities upon which our structure analysis is based.

III. MODEL CALCULATIONS

An approximate multiple-scattering model of the diffraction process, described previously,¹¹ was used to perform our calculations of the ELEED intensities. In this model, which is embodied in a series of computer programs, the scattering species are represented by an energy-dependent phase shifts in terms of which the ELEED intensities from the surface are computed. The scattering amplitudes associated with the uppermost three atomic layers are evaluated exactly, as are those of each of the individual atomic layers beneath. The interference between the upper three layers and the various layers in the substrate is calculated kinematically as described by Meyer et al.¹¹ Convergence tests¹¹ revealed that the consideration of a slab of six atomic layers and the use of six phase shifts for each scatterer yield predicted intensities which are generally accurate to within a few percent, so these parameters were adopted for the calculations presented herein.

The electron-ion core interaction is described by a one-electron muffin-tin potential. The one-electron crystal potential is formed from a superposition of overlapping ionic (e.g., $In+Sb^{-}$) charge densities.³¹ The local Slater approximation³² is used for the exchange potential. The bulk crystal structure (see Fig. 1) is that given by Wyckoff.²⁶ We use the muffin-tin

radii $r_{MT}(In) = 1.36$ Å, $r_{MT}(Sb) = 1.44$ Å, as determined from crystal potential crossover. The Wigner-Seitz radii are $r_{WS}(In) = 1.95$ Å and $r_{WS}(Sb) = 2.06$ Å. Once the crystal potential V, in a given Wigner-Seitz cell has been obtained, the potential is reduced to muffin-tin form as described by Duke *et al.*³¹ The resulting phase shifts are shown in Fig. 2.

The electron-electron interaction is incorporated via a complex inner potential³³ with constant real part V_0 and an imaginary part characterized by the inelastic collision mean free path λ_{ee} .³⁴ We selected $V_0 = 8 \text{ eV}$ and $\lambda = 8 \text{ Å}$ in order to align the major features in the calculated and observed intensity profiles. The modest reproducibility of smaller structural features in the measured intensities and of the large number of structural parameters which exert a significant influence on the calculated intensity profiles conspire to render ineffectual efforts to improve upon this procedure by the automated *R*-factor methods which have proved useful for metal surfaces.³⁵

The consequences of thermal lattice vibrations are neglected in the calculations reported herein which are performed for a rigid lattice of scatterers. The major reason for this approximation is our experience with GaAs(110).¹¹ In that case we found that includ-



FIG. 2. Phase shifts for the In⁺ and Sb⁻ species resulting from the use of Slater exchange, overlapping atomic potentials, muffin-tin radii of 1.36 Å for In and 1.44 Å for Sb, and an average potential of V = -15.8 eV in the muffin-tin region.

ing larger atomic vibrations of the surface relative to the bulk atomic species led to serious discrepancies in the description of high-order beams. Moreover, if the surface and bulk vibrational amplitudes are equal, their inclusion into the model calculation acts primarily to reduce uniformly all of the calculated inten-



FIG. 3. Comparison of calculated (solid curves, six phase shifts) and measured (dashed curves) intensities of the (01) beam of normally incident electrons diffracted from InSb(110). Curve (a): the measured intensity at T = 150 K (dashed curve) and the calculated intensity (solid curve) using the bulk geometry of Wyckoff (Ref. 26) and the threelayer "normal-displacement" reconstruction of Yeh et al. (Ref. 30) for a rigid-lattice model. Curve (b): same as curve (a), but evaluated using the "rotationally-relaxed" structure shown in panel (b) of Table I, and a rigid lattice. Curve (c): same as curve (a) but evaluated using the twolayer "best-fit" reconstruction described in Table I [panel (c)] and a rigid lattice. Curve (d): same as curve (c), but evaluated using the single-layer structure described in Table I [panel (d)] and a rigid lattice. Curve (e): same as curve (a), but evaluated using the three-layer reconstruction of Chadi (Ref. 21) described in Table I [panel (e)] and a rigid lattice.

sities.¹¹ Consequently, given our present ignorance of the vibrational amplitudes near the surface of InSb(110), the most prudent decision for the analysis of low-temperature ELEED intensity data seems to be to neglect thermal vibrations entirely until their magnitudes become established more firmly. On the basis of calculated³⁶ bulk vibrational amplitudes for InSb and GaAs and of the similarity between T = 318and 150 K measured intensities for GaAs (Ref. 11) this approximation appears adequate for low-order beams although marginal for higher-order beams like the (13) and (13) beams. We argue in Sec. IV, however, that this uncertainty in the analysis of the higher-order beams does not seriously impair our structure determination.

IV. STRUCTURE DETERMINATION

The starting point of our structure determination is the consideration of two previously-proposed atomic



FIG. 4. Same as Fig. 3, only for the (10) beam.

4 Å	ositions (e symbo	of the atou Is defining	ms in the u g the structu	ppermost t ures are de	hree atomic t fined in the u	oilayers for th uppermost pa	hose recon inel of Fig.	structed sur 1. All dist	rfaces of InS ances are gi	b(110) for w ven in Å.	hich calcula	ted ELEED	intensities are	shown in
ayer		Sb	Ц	Δ۱, ۱	$\Delta_{2,1}$	Δ _{3,1}	T'21p	Γ'εζρ	4.,	d12,y	รี	In ₁ -Sb ₁ % bond length change	In ₁ -Sb ₁ % bond length change	In ₂ -Sb ₁ % bond length change
3 2 1		10.080 10.060 10.050	10.750 10.060 10.050	0.830	-0.120	0.100	1.481	2.401	4.858	3.239	27.1°	4.31	-18.80	0.57
3 5 1		10.080 10.060 10.050	10.750 10.060 10.050	0.830	-0.120	0.100	1.481	2.401	5.088	3.858	30.9°	0.01	-2.25	-6.45
3 2 1		10.177 10.090 0.0	10.604 10.090 0.0	0.781	-0.180	0.0	1.597	2.381	5.059	3.823	28.8°	0.01	0.92	-4.49
351		10.177 0.0 0.0	10.604 0.0 0.0	0.781	0.0	0.0	1.687	2.291	5.059	3.823	28.8°	0.01	-1.06	-1.63
3 2 1		10.188 10.069 10.023	10.504 10.080 10.046	0.692	-0.149	0.069	1.707	2.417	5.045	3.636	25.7°	-0.55	-2.26	-0.83

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geometries for InSb(110). The proposed geometry resulting from a kinematical analysis of CMTA room-temperature ELEED intensity data by Yeh et al.³⁰ is given in panel (a) of Table I. In their analysis only displacements of the scatterers normal to the surface of InSb(110) were considered because of the well-established^{6, 23, 37} insensitivity of kinematical analyses to relaxations parallel to the surface. The second initially-considered structure is that predicted by Chadi²¹ on the basis of his energyminimization methodology which worked so well for GaAs(110).²³ This structure is specified in panel (e) of Table I. Inspection of Table I reveals that these two structures deviate from each other in both the perpendicular and parallel relaxations of the uppermost anion and cation by more than the usuallyquoted^{9, 10, 33} accuracy of $\Delta d \sim 0.1$ Å for an ELEED



FIG. 5. Same as Fig. 3, only for the (11) beam.

structure determination. Consequently, we performed a search of the structural parameter space in the vicinity of both geometries in an effort to resolve this apparent discrepancy between the proposed structures.

We describe the results of this search by proceding in steps. First, we examine the extent to which the two initial structures lead to a satisfactory description of the measured intensities. Second, we consider various routes toward improving the correspondence between the calculations and the measurements, illustrating the highlights of the end results of each route. Finally, we assess the precision of the final "best-fit" structure emanating from this procedure.

The analysis outlined above was carried out using all 14 measured beams. One of these, the (21) beam, was examined in a preliminary report of this work,²⁹ and hence is not reconsidered here. Two others, the (20) and $(0\overline{2})$ beams, neither were analyzed earlier for GaAs $(110)^{11}$ nor were very useful in discriminating between structures. Hence, we do not show their intensities. Finally, although we



FIG. 6. Same as Fig. 3, only for the $(0\overline{1})$ beam.

did not expect the (13) and $(1\overline{3})$ beams to be described well by a rigid-lattice calculation, we include the analysis of the (13) beam for completeness. Thus, we present calculations for the (01), $(10) = (\overline{10}), (11) = (\overline{11}), (0\overline{1}), (1\overline{1}) = (\overline{11}), (02),$ $(12) = (\overline{12}), (2\overline{1}) = (\overline{21}), (1\overline{2}) = (\overline{12}), and$ $(13) = (\overline{13})$ beams in Figs. 3-12. A typical sensitivity analysis for the (21) beam is illustrated in Fig. 13. These calculations and data constitute the synopsis which we present explicitly herein of those on which we based our structure determinations.

We begin by comparing the measured intensities with those predicted for the structure of Yeh *et al.*³⁰ [panel (a) in Figs. 3–12] and of Chadi²¹ [panel (e) in Figs. 3–12]. The structure of Yeh *et al.*,³⁰ gives poor agreement with the observed intensities for the (11) (Fig. 5), the (11) (Fig. 7), the (02) (Fig. 8), and the (21) (Fig. 10) beams. Similarly, the structure of Chadi²¹ gave poor agreement with the measurements for the (01) (Fig. 3), the (10) (Fig. 4), the (11) (Fig. 7), and the (02) (Fig. 8), beams. On balance, neither structure gives better correspondence with the experimental data than the other, and neither yields as good a correspondence as that achieved earlier for GaAs(110).¹¹

In order to determine how much of the difference between the Chadi and Yeh intensity profiles is due to vertical motions, and how much due to motions in a plane parallel to the (110) surface, we examined the modification of the structure of Yeh et al.³⁰ described in panel (b) of Table I. This structure is the "rotationally relaxed" (i.e., no bond length changes occur in the first layer) structure which yields the same vertical shears as that of Yeh et al. From comparison with the measured intensity [compare panels (a) and (b), Figs. 3-12] we see that this "rotationally-relaxed" structure is distinctly superior to the "normal-displacement" structure of Yeh et al. This result is especially evident in the $(1\overline{1})$ (Fig. 7) and (02) (Fig. 8) beams, although most beams are improved in the rotationally relaxed structure. As expected,^{23, 37} this conclusion supplements the kinemati-



FIG. 7. Same as Fig. 3, only for the $(1\overline{1})$ beam.



FIG. 8. Same as Fig. 3, only for the (02) beam.

cal results, discussed by Yeh *et al.*,³⁰ in which these relaxations have little effect on the correspondence between the kinematically-calculated and the measured intensities.

Having determined that "rotationally-relaxed" structures are superior to the "normal-displacement" structures, at least for the structure discussed, we next explored rotation angles of the top layer, ω_1 , in the range $25.7^{\circ} < \omega_1 < 30.9^{\circ}$, i.e., the range bounded by the structures of Yeh *et al.*³⁰ and Chadi,²¹ with corresponding first-layer vertical shears in the range $0.69 < \Delta_{1,1} < 0.88$ Å, and with the second-layer reconstruction as given by Yeh *et al.* Good agreement between the calculated and measured intensities was obtained for an intermediate bond-rotation angle of 28.8°, approximately half way between those angles corresponding to the structures of Yeh *et al.* and Chadi, respectively [panel (c), Figs. 3–12, and Table I].

Although the initially considered structures differed little in their second-layer distortions, we examined second-layer shears in the range $0 < \Delta_{2,1} < 0.2$ Å

(Fig. 1), and found that a value of $\Delta_{2,1} = 0.18$ Å, 50% larger than that of Yet *et al.*,³⁰ is preferred if the top layer is contracted only 0.05 Å toward the substrate, instead of the 0.15 Å contraction proposed by Yeh *et al.* This structure also is closer to the contraction of 0.03 Å resulting from the energy minimization calculation,²¹ which used a 25.7° top-layer rotation.

To support the case for second-layer distortions we show in panels (c) and (d) of Figs. 3–12, our best-fit structure, and the same structure with the second layer undistorted. While almost all of the beams are sensitive to our large second-layer shear of, $\Delta_{2,1} = -0.18$ Å, the (01), (11), and (21) beams are especially sensitive (Figs. 3 and 7 and Ref. 29, respectively). It should be noted that the (01) and (11) beams for GaAs(110) also were found to be the most sensitive to second-layer distortions,^{8,11} while the (21) beam was not examined for this effect. While the single-layer reconstruction gives a better description of a limited number of beams [compare panels (c) and (d), Figs. 3 and 12], the multilayer reconstruct



FIG. 9. Same as Fig. 3, only for the (12) beam.



FIG. 10. Same as Fig. 3, only for the $(2\overline{1})$ beam.

tion gives a better description overall.

Although both initially-considered structures for InSb(110)^{21,30} contain small third-layer reconstructions, we are unable to detect such small distortions, $|\Delta_{3,1}| < 0.1$ Å, because of their magnitude and the damping effects of inelastic collisions. This result is analogous to that obtained for GaAs(110).¹¹

It is noteworthy that most of the structures shown in Table I deviate from each other in the vertical displacements by less than the usually quoted^{5,9,10} accuracy of ELEED structure analyses, i.e., $\Delta d_{\perp} < 0.1$ Å. The significant structural results emanating from this dynamical multilayer analysis are the occurrence of second-layer reconstructions, and the clear indication of the superiority of bond-rotation models relative to normal-displacement models.

Finally, the values of the displacements of the surface species both parallel and perpendicular to the (110) surface are important in determining the magnitude of bond-length alterations associated with surface reconstructions. Consequently, we examined in some detail the precision with which our dynamicalintensity analysis specifies displacements parallel to the surface of the uppermost anion and cation. The beam which proved most sensitive to these relaxations is the $(2\overline{1})$ beam for which the results for Sb displacements are shown in Fig. 13. It is evident from this figure that for the $(2\overline{1})$ beam a small contraction of the length of the surface Sb-In bond at the expense of reducing the contraction of Sb back bonds to the layer beneath is preferred [panel (b) versus panel (c)]. This displacement cannot, however, be large [panel (a) versus panel (c)]. On balance, when all beams are considered the consequences of relaxing the Sb-In spacing parallel to the surface from the "best-fit" structure tend to be small and positive for $\Delta d_{\parallel} < 0.1$ Å and definitely deleterious both



FIG. 11. Same as Fig. 3, only for the $(1\overline{2})$ beam.



FIG. 12. Same as Fig. 3, only for the (13) beam.



FIG. 13. Sensitivity analysis for motion of the uppermost Sb species parallel to the surface as reflected in comparisons of calculated (solid lines) and measured (dashed lines) intensities of the $(2\overline{1})$ beam of normally-incident electrons diffracted from InSb(110). Panel (c) shows the best-fit structure given by panel (c) in Table I. Panels (a) and (b) show results for the top-layer Sb displaced parallel to the (110) plane towards the top-layer In by 0.2 and 0.1 Å, respectively. Panel (d) and (e) illustrate results for displacements in the opposite direction by 0.1 and 0.2 Å, respectively.

for larger contractions and for any expansions. We conclude from these studies that the precision of the analysis for motions parallel to the surface is about 0.1 Å and that the "best-fit" structure given in panel (c) of Table I lies near the inner extremity of allowed values of $\Delta_{1,y}$, with values more like $\Delta_{1,y} = 5.1$ Å being preferred.

V. SYNOPSIS

In this paper we report a surface-structure determination for InSb(110) via dynamical ELEED analysis.

On the basis of our model calculations we conclude that the uppermost two atomic layers are reconstructed relative to the truncated-bulk structure²⁶ given by a unit mesh $a_x = 4.58$ Å, $a_y = 6.48$ Å and atomic positions $d_{1,12} = 2.29$ Å, $d_{y,1}$ (In) = 4.86 Å relative to antimony species at the origin of the unit mesh. Specifically, we find that $d_{\perp,12}(Sb) = 2.56 \pm 0.1 \text{ Å}, d_{\perp,23}(Sb)$ $= 2.20 \pm 0.1$ Å, $d_{\perp,12}(In) = 1.60 \pm 0.1$ Å, $d_{\perp,23}(In)$ = 2.38 ± 0.1 Å, and $\Delta_{y,1}(In) = 5.1 \pm 0.1$ Å. These tolerances include both the reconstruction proposed for InSb(110) by Chadi²¹ and the rotationally relaxed modification of the structure of Yeh et al.²⁶ because of our assessment of uncertainties in the analysis caused by ignorance of the electron-solid force law^{4,9,33} and the use of a limited data base.³³ Given our model force law and the data base reported herein, however, both of the previously proposed structures^{21, 20} can be rejected as incompatible with the data to within the precision of the present analysis. Thus, the tolerances specified above reflect our evaluation of the accuracy of the analysis rather than its precision as evident, e.g., from Figs. 3-13.

The preferred structure which we obtain for InSb(110), a 28.8° rotated top layer contracted downward 0.05 Å, with a 0.18 Å second-layer shear, is virtually identical to that found for GaAs (110); a 27.4° rotated top layer contracted 0.05 Å downwards, and a 0.12 Å second-layer shear. In fact, our structure is closer to that for GaAs(110) than that found by energy minimization.²¹ That the structures should be virtually identical is not surprising^{2, 28} given the comparably identical covalent character of their bonding.²⁷

From a comparison of the structures for GaAs(110) and InSb(110) via ELEED intensity analysis we conclude that reconstructions of the (110) surfaces of covalently bonded compound semiconductors probably exhibit two universal features: large bond rotations (i.e., $\omega_1 \sim 27^\circ$) of the uppermost layer in which the anion moves outward and cation inward, and smaller counter relaxations of the subsurface layer beneath. The precise extend of bondlength modification is unclear, however, due to the 0.1 Å uncertainties in the relaxation of the uppermost cations and anions. For both GaAs(110) and InSb(110) the "best-fit" structures exhibit bondlength changes of less than 1% except for a 4% contraction of the back bonds between the surface anion and the cations in the layer beneath. Our sensitivity analyses suggest, however, that more nearly equal contractions of (2-3)% of both the surface and back bonds of the uppermost anion provide a slightly improved description of the ELEED data for InSb(110). The distinction between these two structures lies outside either the accuracy or precision of the ELEED intensity analyses given to date, as does the determination of the existence of third-subsurface-layer reconstructions. Assessment of these finer details of the surface structure must await the acquisition and

analysis of larger ELEED intensity data bases, and a more precise specification of the atomic vibrations within the uppermost three atomic layers.

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- ¹A. R. Lubinsky, C. B. Duke, B. W. Lee, and P. Mark, Phys. Rev. Lett. <u>36</u>, 1058 (1976).
- ²C. B. Duke, A. R. Lubinsky, B. W. Lee, and P. Mark, J. Vac. Sci. Technol. <u>13</u>, 761 (1976).
- ³C. B. Duke, A. R. Lubinsky, M. Bonn, G. Cisneros, and P. Mark, J. Vac. Sci. Technol. <u>14</u>, 294 (1977).
- ⁴C. B. Duke, J. Vac. Sci. Technol. <u>14</u>, 870 (1977).
- ⁵P. Mark, G. Cisneros, M. Bonn, A. Kahn, C. B. Duke, A. Paton, and A. R. Lubinsky, J. Vac. Sci. Technol. <u>14</u>, 910 (1977).
- ⁶A. Kahn, G. Cisneros, M. Bonn, P. Mark, and C. B. Duke, Surf. Sci. <u>71</u>, 387 (1978).
- ⁷A. Kahn, E. So, P. Mark, and C. B. Duke, J. Vac. Sci. Technol. <u>15</u>, 580 (1978).
- ⁸A. Kahn, E. So, P. Mark, C. B. Duke, and R. J. Meyer, J. Vac. Sci. Technol. <u>15</u>, 1223 (1978).
- ⁹C. B. Duke, Crit. Rev. Solid State Mater. Sci. 8, 69 (1978).
- ¹⁰S. Y. Tong, A. R. Lubinsky, B. J. Mrstik, and M. A. Van Hove, Phys. Rev. B <u>17</u>, 3303 (1978).
- ¹¹R. J. Meyer, C. B. Duke, A. Paton, A. Kahn, E. So, J. L. Yeh, and P. Mark, Phys. Rev. B <u>19</u>, 5194 (1979).
- ¹²C. B. Duke, R. J. Meyer, A. Paton, P. Mark, E. So, and J. L. Yeh, J. Vac. Sci. Technol. <u>16</u>, 647 (1979).
- ¹³K. C. Pandey, J. L. Freeouf, and D. E. Eastman, J. Vac. Sci. Technol. <u>14</u>, 904 (1977).
- ¹⁴K. C. Pandey, J. Vac. Sci. Technol. <u>15</u>, 440 (1978).
- ¹⁵J. A. Knapp, D. E. Eastman, K. C. Pandey, and F. Patella, J. Vac. Sci. Technol. <u>15</u>, 1252 (1978).
- ¹⁶D. J. Chadi, J. Vac. Sci. Technol. <u>15</u>, 631,1244 (1978); Phys. Rev. B <u>18</u>, 1800 (1978).
- ¹⁷A. Huigser, J. Van Laar, and T. L. Van Rooy, Phys. Rev. Lett. A <u>65</u>, 337 (1978).
- ¹⁸G. P. Williams, R. J. Smith, and G. J. Lapeyre, J. Vac. Sci. Technol. <u>15</u>, 1249 (1978).
- ¹⁹D. J. Miller and D. Haneman, J. Vac. Sci. Technol. <u>15</u>, 1267 (1978).

- ²⁰D. J. Miller and D. Haneman (unpublished).
- ²¹D. J. Chadi, Phys. Rev. Lett. <u>41</u>, 1062 (1978); Phys. Rev. B <u>19</u>, 2074 (1979).
- ²²W. A. Goddard III, J. J. Barton, A. Redondo, and T. C. McGill, J. Vac. Sci. Technol. <u>15</u>, 1274 (1978).
- ²³C. B. Duke, R. J. Meyer, A. Paton, P. Mark, A. Kahn, E. So, and J. L. Yeh, J. Vac. Sci. Technol. 16, 1252 (1979).
- ²⁴C. B. Duke, A. R. Lubinsky, S. C. Chang, B. W. Lee, and P. Mark, Phys. Rev. B <u>15</u>, 4865 (1977).
- ²⁵C. B. Duke, R. J. Meyer, A. Paton, and P. Mark, Phys. Rev. B <u>18</u>, 4225 (1978).
- ²⁶R. W. G. Wyckoff, Crystal Structures (Wiley, New York, 1963), Vol. I, p. 108.
- ²⁷J. C. Phillips, Rev. Mod. Phys. <u>42</u>, 317 (1970).
- ²⁸C. B. Duke, Mater. Sci. Eng. <u>25</u>, 13 (1976).
- ²⁹C. B. Duke, R. J. Meyer, A. Paton, J. L. Yeh, J. C. Tsang, A. Kahn, and P. Mark, J. Vac. Sci. Technol. (to be published).
- ³⁰J. L. Yeh, P. Mark, C. B. Duke, R. J. Meyer, and A. Paton (unpublished).
- ³¹C. B. Duke, N. O. Lipari, and U. Landman, Phys. Rev. B <u>8</u>, 2454 (1973).
- ³²J. C. Slater, Phys. Rev. <u>81</u>, 385 (1951).
- ³³C. B. Duke, Adv. Chem. Phys. <u>27</u>, 1 (1974); in *Dynamic Aspects of Surface Physics; Proceedings of the International School of Physics "Enrico Fermi"*, edited by F. O. Goodman (Editrice Compositori, Bologna, 1974), p. 99.
- ³⁴C. B. Duke and C. W. Tucker, Jr., Surf. Sci. <u>15</u>, 231 (1969).
- ³⁵M. A. Van-Hove, S. Y. Tong, and M. H. Elconin, Surf. Sci. <u>64</u>, 85 (1977).
- ³⁶J. F. Vetelino, S. P. Gaur, and S. S. Mitra, Phys. Rev. B <u>5</u>, 2360 (1972).
- ³⁷E. Y. So, Ph.D. thesis (Princeton University, 1979) (unpublished).