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Si/InP(110) heterojunction

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An investigation of the morphology and energy levels at the Si/InP(110) interface for Si overlayers up to 12 monolayers thick was performed with use of photoemission, Auger-electron spectroscopy, and low-energy electron diffraction. Changes in the heterojunction morphology were observed by growing the interface at two temperatures, 20 and 280 °C. The intensity of the substrate core levels for both growth temperatures indicates laminar growth of the Si overlayer with some In and P included with the overlayer. At 280 °C growth temperatures, the substrate atoms are present in the overlayer in larger amounts. Examination of the chemical shifts in the In 4*d* core level which are resolved for the room-temperature Si/InP(110) interface shows two distinct contributions and indicates either surface segregation or intermixing of In. At higher growth temperatures, the In 4*d* peak is broader and may be due both to intermixing and to surface segregation. The P and Si $L_{2,3}VV$ signals indicate no bonding changes involving those species; however, the P 2*p* peak shifts in a way inconsistent with what is believed to be the band bending, and thus must be involved in a different chemical environment. Band-bending changes cease at low coverages such that the conduction-band minimum of InP is 0.4 eV from the Fermi level at the interface. The rapid stabilization is consistent with the defect model. The band-bending position is determined from the In 4*d* peak at low coverages and is difficult to determine at higher coverages since both the In 4*d* and P 2*p* peaks have chemically shifted components. Higher-temperature growth of the overlayer mostly changes the degree of intermixing of overlayer and substrate atoms. It does not affect the electrostatic dipole at the interface, and affects the heterojunction discontinuity only slightly. The valence-band discontinuity is 0.56 and 0.46±0.1 eV for the 20 and 280 °C growths, respectively. These values are in agreement with those in the literature.

INTRODUCTION

For this heterojunction system, Si evaporated on clean cleaved InP(110), the valence-band discontinuity, and Fermi level position at the interface have been presented earlier[1] as part of a broad survey of these two parameters for many systems. Other properties of the interface are also of concern from a fundamental point of view; for instance, the degree of epitaxy, abruptness, and the chemical reaction extent and type. These phenomena and others in the Si/InP(110) system are studied using photoemission, Auger spectroscopy, and low-energy electron diffraction (LEED).

Growth temperature (either 20 or 280 °C) is used as an additional parameter to control the properties of the interface. Measurement of the photoemission core-level energies of the overlayer and the substrate shows no change of the electrostatic dipole across the interface when the growth temperature is changed. Modification of the local atomic structure at the interface can be accomplished by changes in the growth temperature, and these may in principle change the charge transfer across the interface.[2,3]

Finally, a comparison with the quantum dipole theory is made, not only with regard to the prediction of the valence-band discontinuity for this system, but also with regard to the semiempirical prediction of this parameter from the values of metal semiconductor diode barrier heights formed between metals and the semiconductors of this heterojunction. In this way a better basis of understanding of the Si/InP heterojunction for device design[4] and fundamental studies is made available.

EXPERIMENTAL

Photoemission using the Mg $K\alpha$ line (1253.6 eV), the He resonance lamp (21.2- and 40.8-eV photon energy), Auger spectroscopy, and LEED were used to study the interface. The experiments were performed in a chamber with a base pressure of 6×10^{-11} Torr, and the ion gauge was not used during sample analysis to avoid exciting any residual oxygen (since excited oxygen has a higher sticking probability). Gold was evaporated on a molybdenum substrate for Fermi level calibration. The sample was cleaved *n*-type InP(110) with 5×10^{17} cm^{-3} Sn doping and was outgassed at 315 °C for 1 h prior to the 280 °C growth to expel any bulk hydrogen.[5] One monolayer (ML) is defined as the number of sites on the InP(110) surface and is 8.2×10^{14} atoms/cm.[2] The silicon overlayer was evaporated using an electron beam heated silicon crystal.

RESULTS

The relative intensity profiles of the substrate photoemission and Auger signals are shown[6] in Fig. 1. The upper panel is for the 20 °C growth temperature and the lower for 280 °C. The Si 2*p* intensity was used to calibrate the coverage to previous studies[7] and is not shown. An

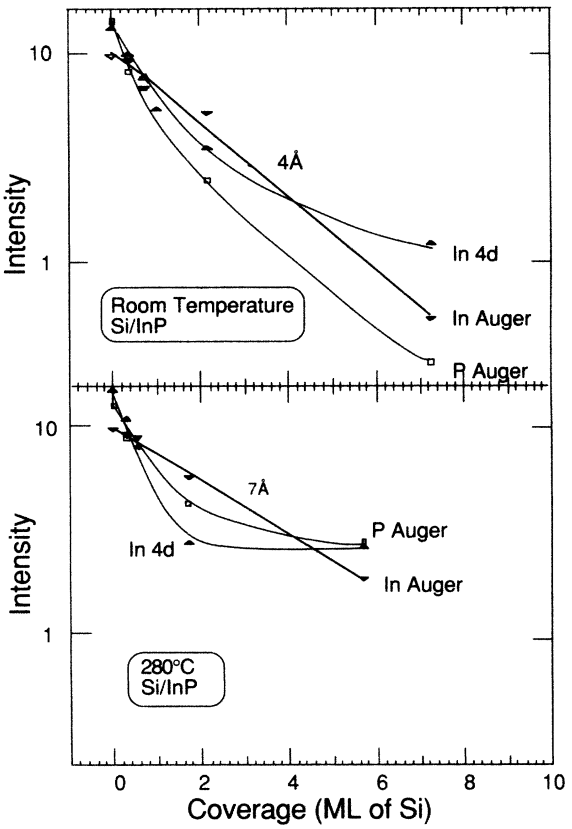

FIG. 1. Photoemission (XPS and He-resonance lamp) core-level areas and Auger derivative-mode peak-peak intensities are shown for the various electron emission versus overlayer thickness.

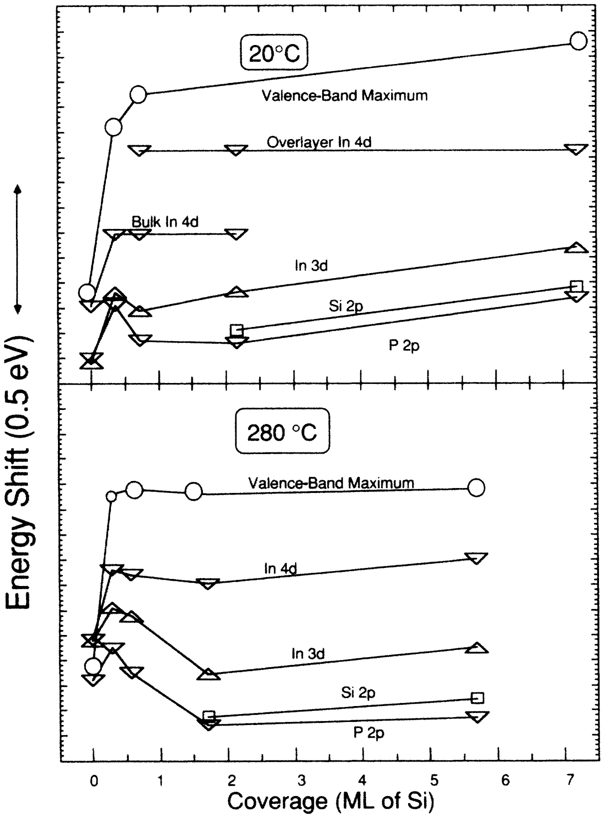

FIG. 2. Energy positions of the substrate and overlayer cores and the valence band.

abrupt laminar interface will give exponential decay of substrate intensity, and will yield a straight line on this graph. The P Auger and In 4*d* photoemission data are surface sensitive, with kinetic energies of 120 and 18 eV, respectively. At low coverages, laminar growth is observed at both temperatures, but some In and P is observed, however, near the overlayer surface at higher coverages. At 280 °C there is more In and P in the overlayer. From the intensity data alone, it cannot be determined whether the excess In and P is intermixed in the overlayer, or surface segregated. The data does indicate, however, that islands of Si are not formed below 2 ML since the intensity decays rapidly until that coverage. It is unlikely that islands of Si begin to form above that coverage since already at 2 ML, for topological reasons, there is Si bonded to Si. However, islands of In cannot be ruled out. The increase in growth temperature has increased the intermixing at the interface and brought noticeably more P into the overlayer (in addition to the valence-band changes which will be discussed later).

The core-level and valence-band maximum energy shifts are shown in Fig. 2. From this figure the energy shift of each core level can be obtained, and the positions of the core levels relative to each other for each sample are preserved. Thus the Si 2*p* has the same energy relative to the P 2*p* and In 3*d*, and no measurable change in electrostatics has occurred between the two growth tempertures. For the room temperature In 4*d*, two energies are shown, one for the bulk and one for the overlayer (where they can be resolved). At low coverages, this core level best represents the band bending because it is obtained at high resolution so the chemical shift is resolved, and the kinetic energy is most accurately calibrated. The valence band has a different energy position relative to the Si 2*p* for the respective samples, indicating a change in the nature of the valence-band maximum. An idealized line shape formed from a Lorentzian convolved with a Gaussian was optimized in energy, width, and intensity to the core-level data. The Lorentzian represents the intrinsic line shape of the core level and is due to the limited lifetime of the hole remaining after the photo-excitation of the electron. The Gaussian represents approximately the instrumental resolution and is a convolution of the intensity distribution of the x-ray source or the He-resonance lamp with the electron analyzer throughout. This approximation can be checked by fitting the Fermi edge of gold or silver (which has an intrinsic broadening of kT or about 0.026 meV, much less than the instrument width) to a Gaussian convolved with a step function. The results show a reasonably good fit and the approximation of the instrument response as a Gaussian is justified. The centroid of the peak, represented in Fig. 2, is shown with a vertical offset which is equal for the two panels so that direct comparison can be made. The valence-band maximum energy shown in the figures is the extrapolation of the top of the valence band to zero emission, as usual, because the spectral intensity at the valence-band maximum varies over energies larger than the instrumental resolution.

Low-energy electron diffraction patterns at primary beam energies between 50 and 150 eV were monitored to observe the order of the growing layer. At 0.3 ML, the LEED was clearer for the 280 °C growth (and it was 1×1 for both growth temperatures). At 0.7 ML, only a few diffuse dots on a bright background in the 1×1 pattern were still visible at both growth temperatures. If the Si were islanding the LEED pattern would remain to higher coverages, since the substrate pattern of the sea would be observed around the islands. Thus the LEED shows that the growth was laminar for at least the first layer, in agreement with the photoemission and Auger intensity data. Also, the first layer is nonepitaxial and randomized on the surface, otherwise some LEED pattern would remain. In general, a LEED pattern tends to remain even if there are only patches of epitaxial area, or if there is even a mild tendency for atomic alignment with the substrate. Thus the Si is not bonding in equivalent sites on the surface. From the LEED results alone, it is shown that the growth of the first layer is laminar and disordered and all following layers are disordered.

Increasing the growth temperature increases the amount of In and P in or on the overlayer. The valence-band maximum evolves at about the same rate for both growth temperatures (it has reached its final position by 0.7 ML) indicating that interface width is narrow (albeit intermixed) and about the same for both temperatures.

After deposition of 0.3 ML of silicon, the valence-band maximum changes dramatically and moves up in energy by about 0.4 eV more than the change in band bending! (See Fig. 3.) The valence-band maximum (shown more clearly in the inset) is at higher energy for the room-temperature growth, which is interpreted as the result of changing overlayer properties, and not a change in band alignment. The valence-band position is stable after 1 ML. This rapid change and stabilization is consistent with results for other heterojunction systems like Ge/GaAs(110) (Ref. 8) and indicates that the heterojunction properties of the interface are formed by this low coverage. The escape length of the electrons from the top of the valence band at 15-eV kinetic energy is nearly as surface sensitive as the In 4*d*. The rapid valence-band stabilization gives another indication of the upper limit of the width of the interface, consistent with the intensity data.

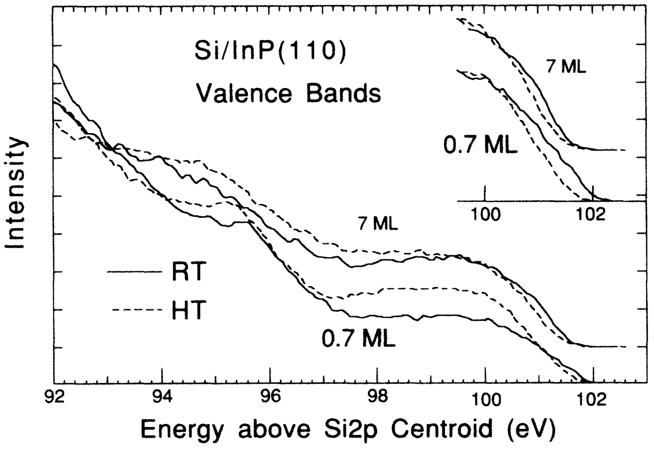

FIG. 3. Valence bands energy distribution curves (EDC) are shown for room-temperature growth (solid lines) and 280 °C growth (dashed lines) at 0.7 ML of Si coverage (lower curves) and 7 ML (upper curves). Band-bending differences have been removed by referencing the spectra to the energy position of the Si 2*p*.

At 7 ML the valence-band maximum energy measured with respect to the Si 2*p* core levels is at a higher kinetic energy position for the room-temperature growth than for the 280 °C growth. The valence-band maxima are shown in Fig. 3 where the energy scale is relative to the Si 2*p* centroid. And yet the overlayer core level is at the same position relative to the P 2*p* substrate core level. These observations indicate that the nature of the valence-band maximum is different for the 280 °C growths and will be discussed further later.

The high resolution, surface sensitive In 4*d* emission (18-eV kinetic energy) is obtained using the He *II* resonance at 40.8-eV photon energy and shows excess intensity at the highest coverage, indicating indium surface segregation or intermixing on/in the overlayer. The energy distribution curves for the In 4*d* core level for the room-temperature growth in Fig. 4 clearly show the initial band-bending change due to Fermi level pinning. At higher coverages of 0.3 and 0.7 ML, no further band bending occurs and the data can be well represented by a shifted overlayer contribution at about 0.35 eV shallower in binding energy which appears and eventually is the only visible component, since the bulk contribution is reduced in intensity. At 0.7 ML, the peak is too broad to contain one component. Metallic In islands usually cause the In 4*d* to shift by larger amounts which changes as the cluster forms and the screening changes, but these islands cannot be ruled out here. Only one bonding environment of the In in the overlayer is likely—otherwise the In 4*d* would likely show more than one shifted component at high coverage. The bulk contribution to the In 4*d* disappears exponentially with coverage but with a short characteristic length. At higher coverages Si either modifies the environment of the bulk In or intermixes with it. This is consistent with the LEED and intensity results, and shows an intermixing of one or two atomic layers at the interface.

The 280 °C growth In 4*d* curves show unresolved chemical shifts (Fig. 4, right panel). This is apparent from the curve for 7 ML which shows a broader width from additional emission at the shallow binding energy side. Surface segregation of In cannot be ruled out, as before, but in addition, In may be dispersed throughout the overlayer with varying amounts of P in the local bonding configuration. The exact bonding configurations are not known.

The Auger signals from the $L_{2,3}VV$ Si and P transitions can be informative with regard to chemistry and are shown in Fig. 5. This data was taken in the derivative mode with incident electrons of 2 keV. The 7 ML curve is shown with a reduced amplitude. The line shapes remain narrow for all overlayer coverages. The Si $L_{2,3}VV$

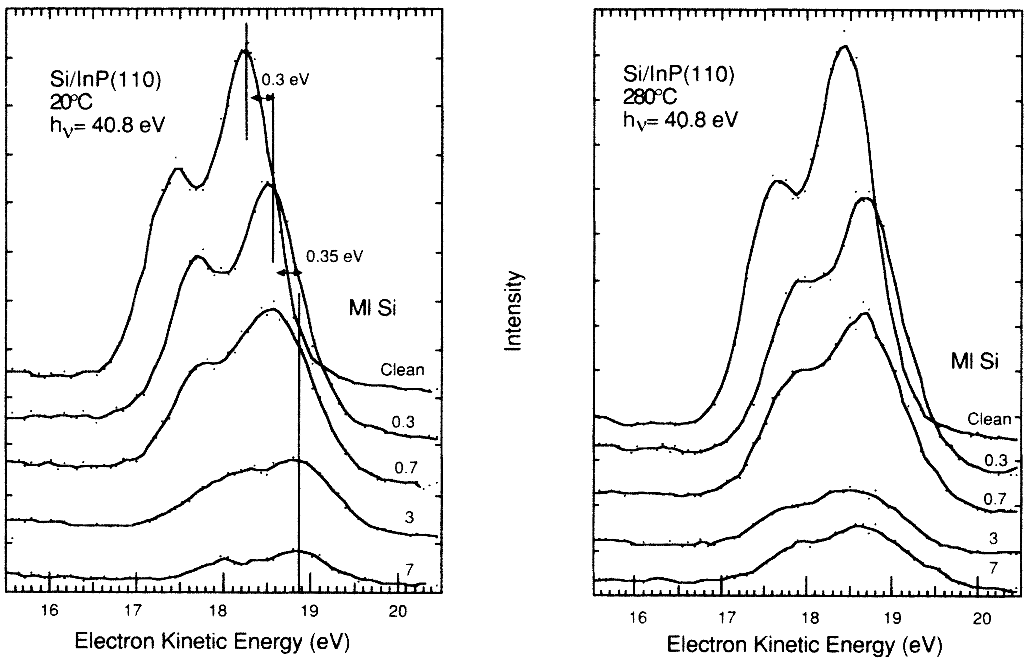

FIG. 4. In $4d$ core level taken at $h\nu = 40.8$ eV are for 20 °C (left) and 280 °C (right) growth are shown here. The data are shown with dots, and a 0.15 eV FWHM Gaussian smoothing is shown with a solid line.

has been used to study the products of chemical reactions for silicides and the higher kinetic energy dip of the derivative spectra shows a splitting when the Si valence electrons bond differently, i.e., is in a metal-rich silicide.[9] The interpretation has been extended to the P Auger[10] so that a splitting indicates a new hybridization and new compound formation. The simple Auger line shapes observed for Si and P indicate that probably no new hybridization is being formed.

The P $2p$ core level observed with photoemission broadens at 0.6 ML from a combination of bulk and intermixed components but then narrows again as the overlayer forms. The low-resolution, bulk sensitive 1117-eV emissions do not resolve the components. Using the increased width at intermediate coverage and the increasing P $2p$—bulk In $4d$ energy difference, we conclude that the P $2p$ is chemically shifted (in addition to the resolved shifts of the In $4d$).

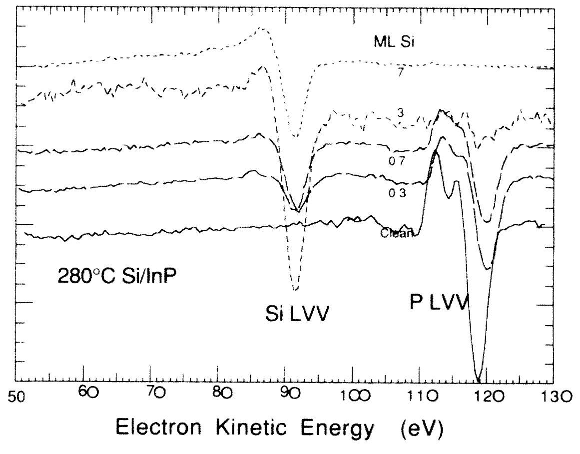

FIG. 5. P and Si $L_{2,3}VV$ Auger signals for the 280 °C growth are shown with a vertical offset for display.

The band bending at low coverages is best obtained from the In $4d$ because the bulk component is resolved. The band bending is stable after the first evaporation, and in analogy with the metal overlayer studies, the Fermi level is said to be pinned. (See Fig. 6.) Using the clean surface to obtain the InP valence-band-maximum—to —In $4d_{3/2}$ energy (which averages 17.44 ± 0.05 eV for five cleaves) and then using the bulk portion of the In $4d$ at low coverages, we find the Fermi level is pinned for both temperatures at about 0.4 eV below the conduction-band maximum of the InP. (Previously,[1] a value of 0.7 eV was found.)

The rapid pinning shown in Fig. 6 is not in disagreement with the defect model.[11] The first absorbed atoms (<0.7 ML) generate structural defects in the substrate whose in-gap states pin the Fermi level. From the data obtained here, it cannot be demonstrated that in-gap defect states from the overlayer did not cause the pinning, but note that the pinning position corresponds to approximately mid-gap in the Si, whereas a cleaved Si crystal pins at 0.3 eV above the valence-band maximum.

The valence-band discontinuity is determined[1] by taking the valence-band maximum E_v change and subtracting the band-bending change. The E_v change is found by extrapolating the valence-band edge to zero emission for the clean surface and the fully formed heterojunction. Thus

$$\Delta E_v = E_{v,\text{final}} - E_{v,\text{clean}} - \Delta E_{BB} .$$

This standard technique has been applied many times before, and represents the valence-band discontinuity

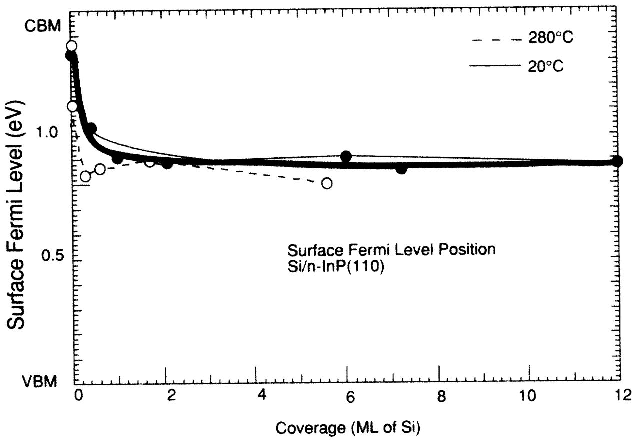

FIG. 6. Fermi-level position is shown for various coverages of Si. The conduction-band minimum (CBM) and valence-band maximum (VBM) refer to the substrate. Three experiments are shown, two at 20 °C (filled circles) and one at 280 °C (open circles).

which photoemission measures.[12] This measurement is represented in Fig. 7. The pinning position represented by the In $4d$ is slightly different for the two growth temperatures. The heterojunction valence-band discontinuity is obtained from the valence-band maximum changes subtracting the band bending, and these values are shown on the figure. This figure is analogous to Fig. 6 except that it represents the changing energy levels where the Fermi level is fixed, and it allows for the changing valence-band maximum of the overlayer.

The valence-band discontinuity which we obtain is 0.56 and 0.46 eV for the 20 and 280 °C temperatures, respectively. The absolute uncertainty is about ±0.1 eV. This value is in good agreement with the 20 °C value of 0.57 eV obtained earlier,[1] but different from theoretical predictions for crystalline interfaces from the universal parameter tight binding theory[13] and the quantum dipole model[14] which give $\Delta E_v = 0.14$ and 0.40 eV, respectively.

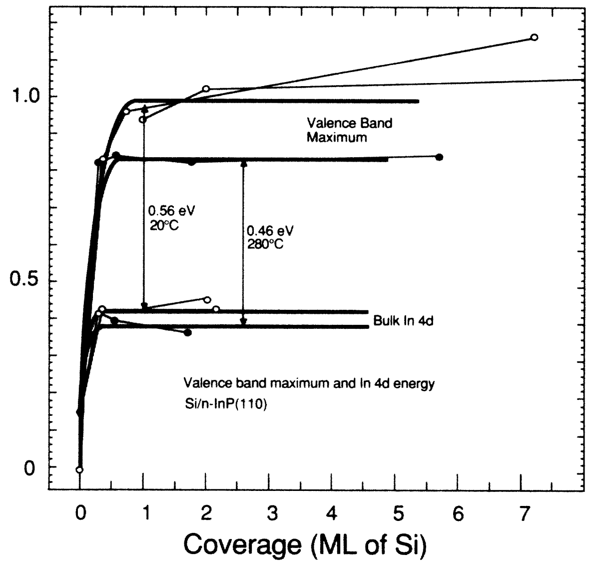

FIG. 7. The energy positions of the valence-band maximum (upper) and bulk In $4d$ (lower) are shown versus overlayer thickness. Both growth temperatures are shown. The In $4d$ initial energy was adjusted to correspond with the degree of initial pinning in this figure.

The slight difference in ΔE_v for the two growth temperatures is due to modifications of the valence-band maximum energy with respect to the core levels, and not due to band alignment changes: The overlayer Si $2p$ to bulk P $2p$ core-level energy difference gives no indication of a changed electrostatic interfacial dipole[2,3] (also see Figs. 2 and 3). The band bending is slightly different in the two cases but the energy difference in the core levels is constant for the various coverages in each sample and is the same for the two growth temperatures. This indicates no change in interfacial dipole when the growth temperature is changed, similar to previous results,[15,16] including when the atomic and chemical nature of the interface is

TABLE I. The Schottky barrier heights for n-type InP [N. Newman, T. Kendelewicz, L. Bowman and W. E. Spicer, Appl. Phys. Lett. **46**, 1176 (1985)] and for n-type Si [P. A. Tove, Surf. Sci. **132**, 336 (1983)] are in the left columns. Center columns have the interfacial Fermi-level position with respect to the valence-band maximum (and differ from the first columns by the band gap of the respective materials). On the right are the differences, which average 0.51 eV, which are a semiempirical prediction for the valence-band discontinuity of Si/InP. Most of these values are in good agreement with our experimental values for the valence-band discontinuity.

	Schottky barriers on InP and Si				
Metal	n-InP	n-Si	InP $E_F - E_v$	Si $E_F - E_v$	Predicted ΔE_v
Ag	0.50	0.7	0.85	0.4	0.45
Cr	0.45	0.6	0.9	0.5	0.4
Cu	0.42	0.63	0.93	0.47	0.53
Au	0.37	0.79	0.98	0.31	0.67
Pd	0.41	0.72	0.94	0.38	0.58
Mn	0.35	0.3	1.0	0.8	0.2
Sn	0.35	0.59	1.0	0.51	0.49
Al	0.33	0.5–0.7	1.02	~0.5	0.42
Ni	0.32	0.60	1.03	0.5	0.53 eV

modified.[17] Thus microscopic effects at the interface do not affect the band lineup. The core levels are not expected to be sensitive to changes in the valence-band structure, in particular the splitting of the valence-band maximum due to strain[18] and the properties of the overlayer. Thus we have an indication that the heterojunction valence band discontinuity in this system is composed not only of the usual rigid band alignment but also of changes in the overlayer valence band itself.

The valence-band maximum has been shown to depend on the crystallinity of the overlayer[19] and strain across the interface.[18] Since the data here supplies no evidence of strain across the interface, and the overlayer is nonepitaxial and disordered for both growth temperatures, much of the change is probably due to the other properties of the overlayer itself.[20] In particular, microvoids and the consequent defects may be annealed out at the higher growth temperature.[21] Effects due to intermixing have not been systematically studied yet, but note that the higher temperature growth has more intermixing but a sharper valence-band maximum.

Agreement[22] between the quantum dipole theories[14] for the heterojunction valence-band discontinuity and experiment is better than that for any other available theory.[22] This agreement is evidence for similar phenomena in Schottky barriers[23] since the same basic phenomena of neutral points E_B and screening of energy differences by the dielectric constant are expected. But there is compelling evidence for the defect model at the early stages of interface information for both thin Schottky barriers and for heterojunctions.[24] In Schottky barriers, there is no evidence yet precluding the simultaneous operation of both the defect model and the quantum dipole model, in addition to the Schottky model.[25]

It has also been suggested[23] that the interfacial Fermi level (with respect to the valence-band maximum) for a particular metal on semiconductor A subtracted from that for semiconductor B has the same value as the valence band discontinuity for semiconductor A on B. This premise is checked for the present system. In the left-hand columns of Table I are shown the Schottky barrier heights for several metals on n-InP(110) and n-Si. These are converted to interfacial Fermi-level positions with respect to the valence-band maximum in the center columns. On the right is the difference in the center columns, which is the semiempirical prediction of the valence-band discontinuity for Si/InP. Focusing now on the right-hand column, one standard deviation for this distribution is 0.09 eV. It may be said that the values are roughly constant, although this is not conclusive, since the I-V values in the table are expected to be precise to about 0.02 eV. Neglecting the value for Mn, which is anomalously far from the mean, the average value of the predicted valence band discontinuity is 0.51 eV with the Si barrier larger than the InP, which is in good agreement with the experimental value obtained here.

CONCLUSION

We find that the room temperature Si/InP interface is essentially abrupt and laminar, although some In and P is in/on the overlayer Si. At 280 °C growth, the interface has more P and In intermixed in the Si, although the interfacial region is not significantly wider when the temperature is increased.

There is no change in the electrostatic dipole across the interface when the deposition temperature is changed, since we find no change in overlayer Si $2p$ core-level energy relative to the substrate core levels. There is, however, a small but significant change in the valence-band discontinuity measured from the valence-band maximum. The valence-band discontinuity is 0.56 and 0.46 eV from the room temperature and 280 °C growths, respectively, and the difference comes from changes in the valence bands and not changes in the atomic bonding electrostatic dipole at the interface. The slight change in valence-band maximum is attributed to the change in overlayer properties. The results of this study show that high-growth temperature molecular beam epitaxy studies and room-temperature heterojunction studies may give slightly different values for the heterojunction discontinuity because of the change in valence-band maximum energy when the growth temperature is changed.

The Fermi-level position is 0.4 eV below the conduction-band minimum for moderate coverages of Si, and is determined from the bulk In $4d$ at low coverages. Comparison with the quantum dipole model gave good agreement. The heterojunction discontinuity which the theory predicted from bulk properties of Si and InP differed significantly with the available data, and the semiempirical prediction using Schottky diodes to obtain the heterojunction discontinuity was good. Furthermore, the presence of defects which could pin the Fermi level was apparent.

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[5] Hydrogenation of the overlayer Si by heating the crystal could affect the valence-band maximum; hence this must be avoided. Aside from thoroughly outgassing the sample, no means are available to be sure hydrogen is not involved, since it has a low spectroscopic profile.

[6] The clean surface usually shows a higher intensity than when the surface has even a slight overlayer coverage, and this is because the sample alignment is performed on the clean surface, and the sample is returned as nearly as possible to the same coordinate settings for subsequent analysis. These settings are slightly different from the optimized ones, and thus the systematic lowering of the intensity after the initial alignment. Full alignment of all of the sample coordinates would increase the intensity but also reduce the dependability in the analysis position on the surface.

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