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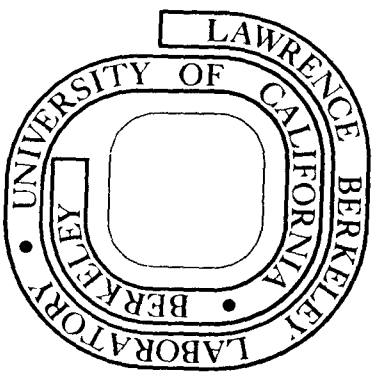

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ANGLE-RESOLVED PHOTOEMISSION MEASUREMENTS OF BAND DISCONTINUITIES IN THE GaAs-Ge HETEROJUNCTION*

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ABSTRACT

The conduction and valence band discontinuities for the (110) GaAs-Ge heterojunction have been measured as ΔE_c = 0.50 eV and ΔE_v = 0.25 eV by the angle-resolved ultraviolet photoemission (ARUPS) technique. These values are in good agreement with the theoretical predictions of Pickett, et al.

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During the past ten years, much effort has been devoted to understanding the physical properties of Schottky barriers and heterojunctions.[1] In both systems, the main effects originate at the interface; for example, it is well known that Schottky barrier heights, as measured by capacitance voltage (C-V) or current-voltage (I-V) characteristics, are nearly independent of the metal's work function for covalent semiconductor-metal pairs. Several theoretical models have been suggested to account for this pinning of the Fermi energy (E_f).[2-4] Recent results obtained with surface-sensitive techniques such as ultraviolet photoelectron spectroscopy (UPS),[5,6] partial yield spectroscopy,[7] and electron energy-loss spectroscopy,[8] however, seem to indicate that no single theory will explain the data for all Schottky barrier devices.

For semiconductor-semiconductor heterojunctions, as with Schottky barriers, the most serious problems arise from the misfit which necessarily occurs when materials of unequal lattice parameters are interfaced. The dangling bonds arising at the interface could be expected to provide electrically active states serving either as charge traps, in which case a modified band profile could result, or as recombination states which could affect the transport properties of the junction. The wide application of heterojunctions in electronic devices suggests that a better knowledge of their interface states would be useful for the "tailoring" of such devices. Nevertheless, up to now only one surface-sensitive experiment has been reported for such heterojunctions,[9] and that work did not establish the magnitudes of the conduction and valence band discontinuities at the interface, but only showed their

orientational dependence, which is a consequence of the dipole-like potential produced by the interface.

These discontinuities may, however, be determined from angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) data. Briefly, the method consists of detecting electrons which have been photoejected from the surface of one semiconductor single crystal which is covered with overlayers of a second semiconductor of various thicknesses; as the overlayer is produced, the top of the valence band (called here the "valence band maximum", VBM) will shift at the surface relative to E_f. Since the escape depth of electrons at these energies may be expected to be of the order of 10Å,[10] the data obtained for thicknesses of such magnitude reflect the electronic structure of the heterojunction at the surface and in its first few bulk layers. By increasing the overlayer thickness, it should be possible to observe a saturation in the substrate band bending; for overlayers of sufficient thickness (i.e., several times the inelastic mean free path), no photoemission from the substrate should be detectable, and the overlayer band bending should become observable.

The band scheme usually employed to describe a semiconductor-semiconductor heterojunction is shown in Fig. 1. In part (a), the energy levels are shown for two non-interacting (separated) materials; the characteristic parameters are the band gaps (E_g), electron affinities (χ), and positions of the Fermi levels relative to the bulk valence or conduction band energies (δ). As shown in part (b), the formation of the heterojunction leaves these parameters invariant, but the

charge flow across the junction, induced by the difference in chemical potential of the two materials, results in the equalization of the Fermi levels and a concomitant bending of the bands at the interface, given by V_D^1 and V_D^2. The discontinuities in the valence and conduction bands, ΔE_v and ΔE_c, are given by

$$\Delta E_v + \Delta E_c = \Delta E_g \quad , \tag{1}$$

while the relation

$$E_f^2 - E_f^1 = V_D^1 + V_D^2 \equiv V_D \tag{2}$$

describes the band bending. The partitioning of the induced potential into V_D^1 and V_D^2 is determined by the doping of the semiconductors, with the bending being larger for the less conducting material. As is clear from the figure, a simple equation obtains for the conduction band discontinuity:

$$\Delta E_c = (\delta_1 + V_D^1) - (E_g^2 - \delta_2) + V_D^2 \quad . \tag{3}$$

Thus, a determination of V_D will also allow the calculation of ΔE_c. This has typically been done in the past by analyzing the C-V characteristics of the heterojunction,[1] according to the relationship

$$1/C^2 \sim (V_D - V) \quad . \tag{4}$$

Such results have frequently been explained by equating the conduction band discontinuity at the interface to the difference in electron affinities,

$$\Delta E_c \cong \chi_2 - \chi_1 \quad , \tag{5}$$

but the validity of this approach has been questioned by several authors, who have proposed different theoretical models.[11-14] For the (110) interface of the GaAs/Ge heterojunction, the predictions of the self-consistent pseudopotential method of Ref. 14 and the electron affinity difference method are given in Table I, along with C-V results.[15] The variation in the C-V data seems to indicate that such measurements must be made in conjunction with microscopically sensitive techniques in order to fully characterize the interface.

We report here the first ARUPS determination of the GaAs/Ge (110) heterojunction discontinuities. The experimental apparatus was described earlier.[16] Briefly, electrons were photoejected by 21.2 eV (HeI) photons from an in situ cleaved n-type GaAs (110) single crystal (carrier concentration of 8×10^{14} cm^{-3} by Hall effect measurements) which was subsequently covered by evaporative deposition with successively thicker overlayers of Ge. The electrons were energy analyzed using a cylindrical mirror analyzer with a resolution of 0.07 eV. During the depositions the temperature of the substrate was held at the epitaxial growth temperature[17] of 420°C, with a base pressure of 2×10^{-10} torr. ARUPS spectra were taken for various Ge coverages, ranging from a fraction of a monolayer to ca. 20 monolayers; coverages were determined by calibrating the oven with a piezoelectric thickness monitor, and one monolayer was defined as 8.85×10^{14} atoms cm^{-2}, in conformity with previous work.[5]

Selected results are shown in Fig. 2, where the spectra for clean and Ge-covered GaAs are presented for normal emission; these spectra are hereafter referred to as 0 to 6. The position of E_f was determined

by measuring the photoemission edge of a tantalum strip which was in electrical contact with the GaAs.[6] The small peak just to the left of E_f is due to emission from the Ga 3d core level, excited by 40.8 eV (HeII) photons which are a subsidiary component of the spectrum of the discharge lamp used. The separation of this peak and E_f decreases with Ge coverage, indicating a change in the relative separation, near the interface, of E_f and the valence band. Accordingly, we have aligned the spectra 0 to 4 by keeping fixed the Ga 3d peak position; the zero of energy is set as the Fermi level for the clean GaAs sample. Spectra 5 and 6, having thick Ge overlayers, have been aligned by keeping constant the VBM, a procedure which is sufficient for our purpose of obtaining shifts in E_f. A weak 3d signal was also observed for the spectrum 5 coverage at non-normal emission, and was used to confirm the alignment.

For the Ge covered surfaces, E_f is displaced from the zero of energy as shown in Fig. 2. This displacement is summarized in Fig. 3 where we have plotted the Fermi level position, relative to E_f for clean GaAs, as a function of overlayer thickness. A saturation value of the band bending is reached for very low coverages; this behavior was observed by Gregory and Spicer for the GaAs-Cs Schottky barrier.[5] For such layer thicknesses, most of the photoelectrons observed are originating in the GaAs, and the saturation value thus corresponds to the maximal GaAs band bending. For the spectra incorporating thick Ge overlayers, we see a further movement of E_f towards the VBM. This new saturation value is representative of the Ge half of the heterojunction; in fact,

the photoelectron escape depth is sufficiently short as to preclude, with the coverages employed in these spectra, observation of the substrate bands. From Fig. 3, we may immediately deduce that ΔE_v = 0.25 eV and, with ΔE_g = 0.75 eV, we obtain from Eq. (1) that ΔE_c = 0.50 eV. These results, which qualitatively agree more closely with the values of Ref. 14 than with those obtained by the use of Eq. (5), seem to indicate that equating ΔE_c to the electron affinity difference is a poor approximation, and that a better knowledge of the interface physical properties should be obtained through the use of more sophisticated theoretical models which include the possibility of relaxation at the interface.

In conclusion, we have demonstrated the viability of ARUPS as a structure-sensitive tool, on the microscopic level, for determining band discontinuities in semiconductor-semiconductor heterojunctions, and have obtained results for the GaAs/Ge (110) couple which suggest the need for further theoretical work. A paper which describes our data in more detail is currently under preparation.

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TABLE I

BAND DISCONTINUITY RESULTS (eV)		
Method	ΔE_v	ΔE_c
ARUPS[1]	0.25	0.50
EPM[2]	0.35	0.40
C-V[3]	0.60-0.19	0.15-0.56
Eq.(5)	0.69	0.06

[1]This work.
[2]Ref. 15.
[3]Ref. 14.

FIGURE CAPTIONS

Figure 1. Band scheme (a) before and (b) after the formation of a semiconductor-semiconductor heterojunction. The ordinate is the relative energy, and the abscissa the position in real space, with x = 0 at the interface. See text for explanation of symbols. The figure is drawn so that GaAs would qualitatively correspond to material 1, and Ge to material 2.

Figure 2. Spectra at normal emission and 21.2 eV photon energy of clean (dotted) and Ge covered (solid) (110) GaAs. The magnified portion of spectrum 0 shows the Ga 3d peak due to 40.8 eV radiation. Approximate coverages are as given.

Figure 3. Plot of the separation of the Fermi levels for clean GaAs and for Ge covered GaAs, as a function of overlayer thickness.

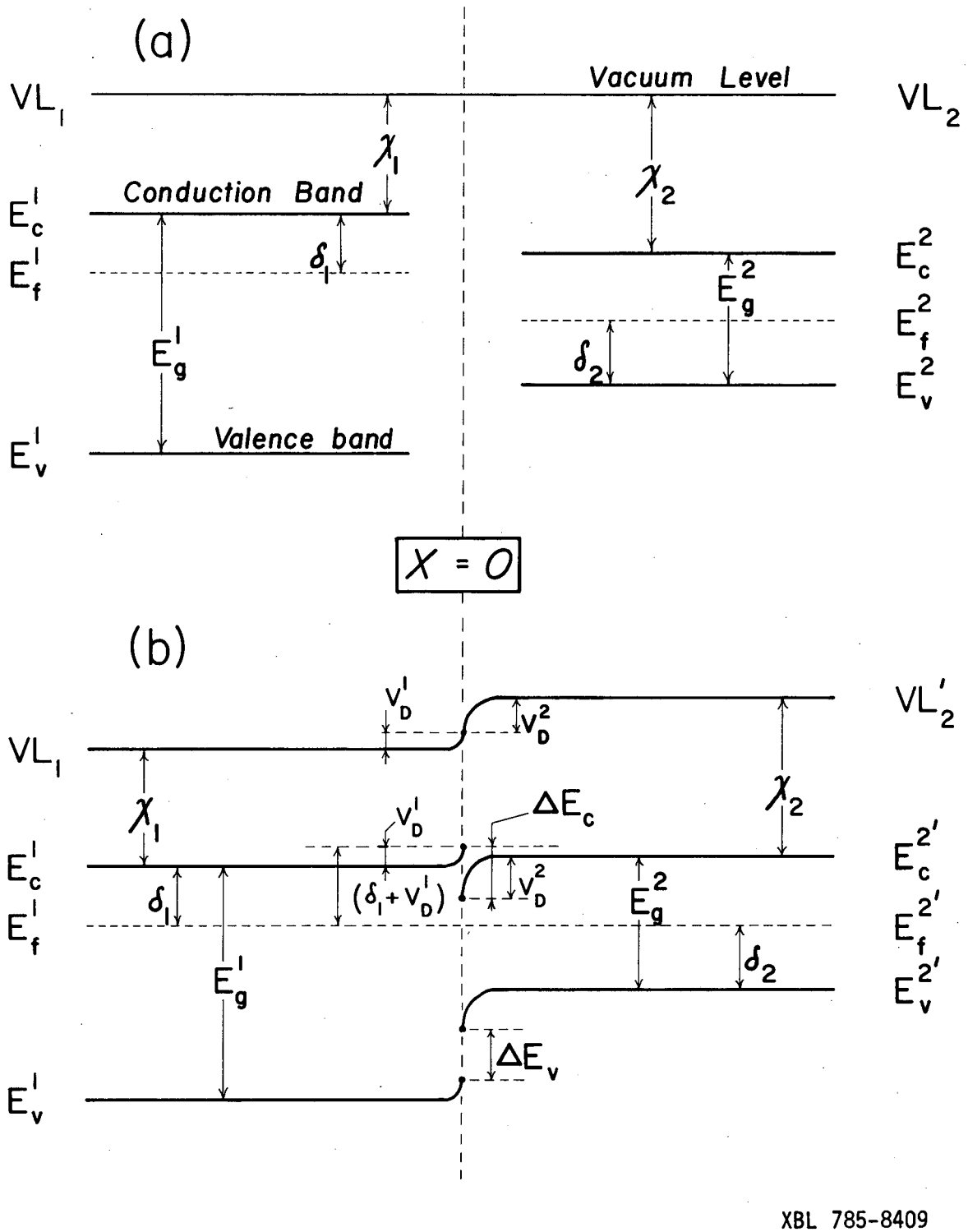

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Figure 1

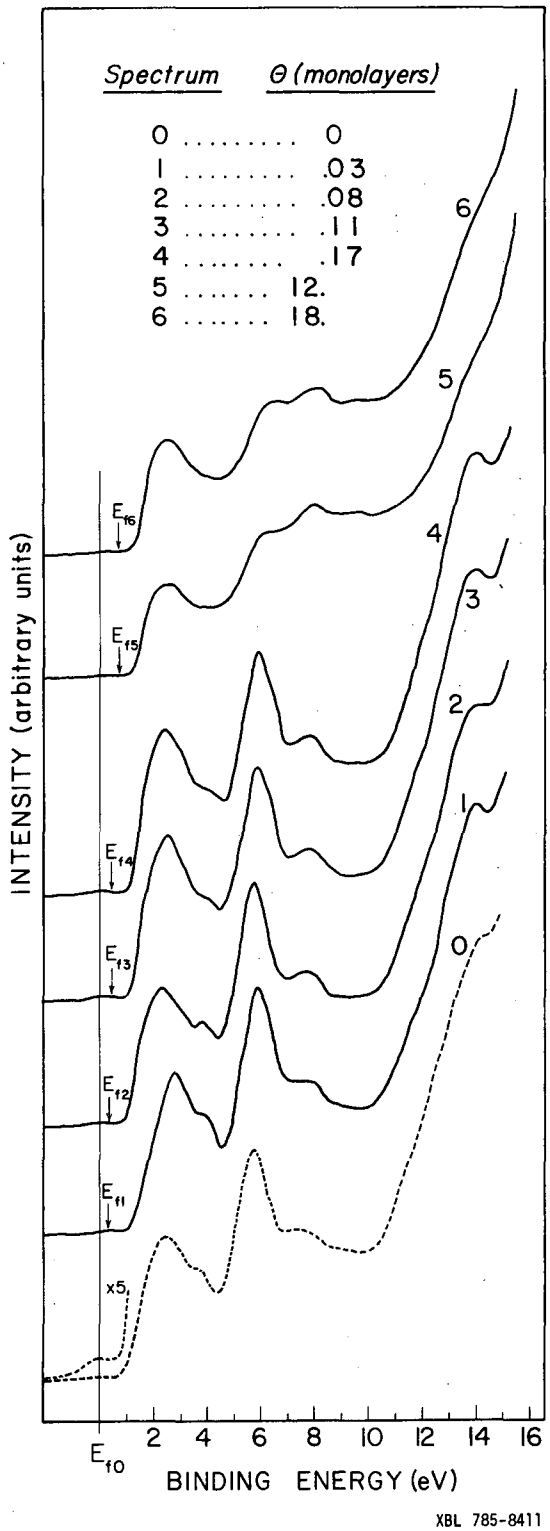
Spectrum
Θ (monolayers)
0 0
1 ..... .03
2 ..... .08
3 ..... .11
4 ..... .17
5 ..... 12.
6 ..... 18.
INTENSITY (arbitrary units)
BINDING ENERGY (eV)
E_f0
E_f1
E_f2
E_f3
E_f4
E_f5
E_f6
x5
0
1
2
3
4
5
6
2 4 6 8 10 12 14 16
XBL 785-8411

Figure 2

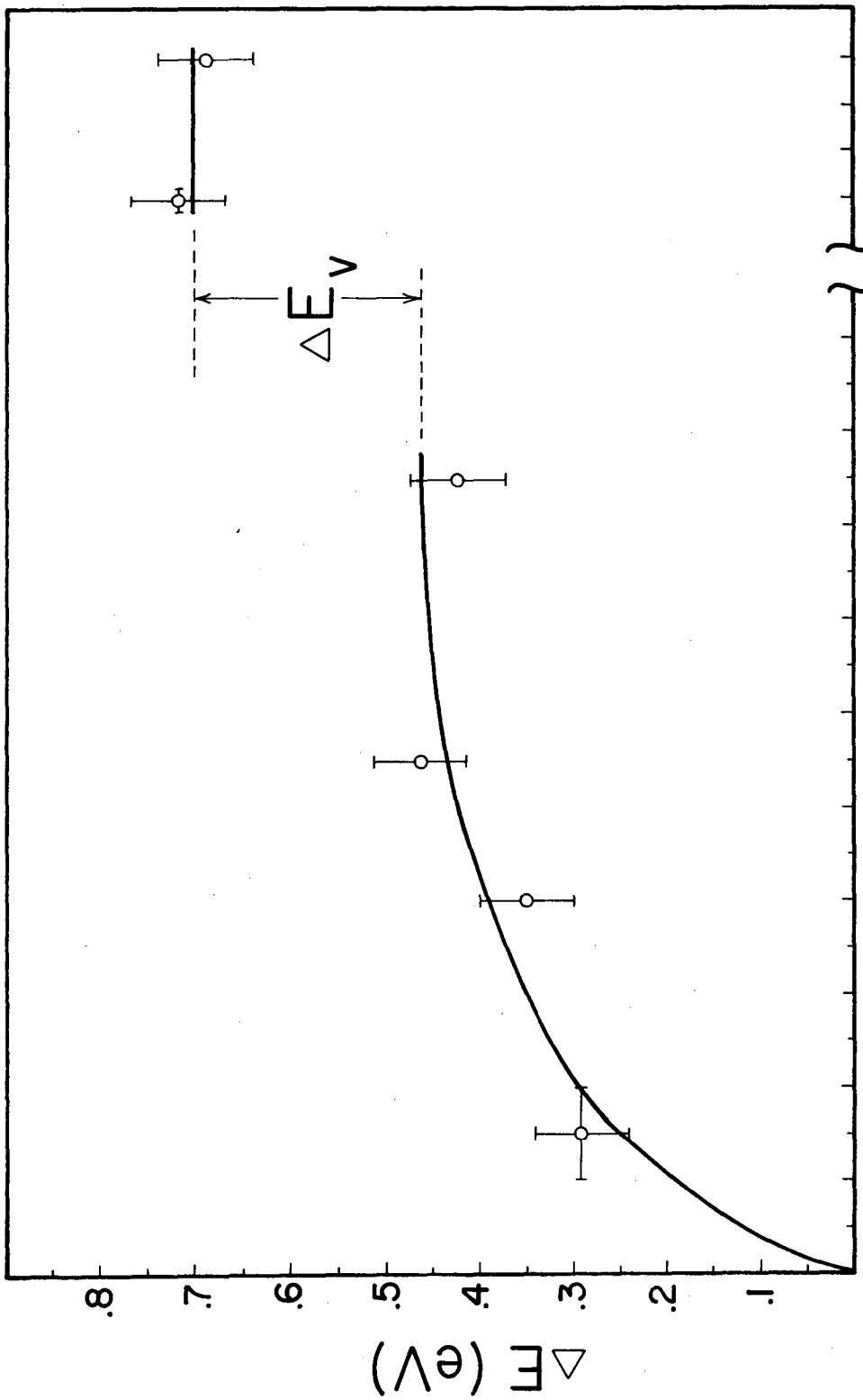

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Figure 3

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