PHYSICAL REVIEW B VOLUME 31, NUMBER 10 15 MAY 1985

Evidence of orientation independence of band offset in AlGaAs/GaAs heterostructures

W. I. Wang, T. S. Kuan, E. E. Mendez, and L. Esaki
IBM Thomas J. Watson Reserach Center, Yorktown Heights, New York 10598
(Received 4 February 1985)

The valence-band offset between GaAs and AlGaAs has been found to be independent of crystal orientation, as deduced from measurements of the two-dimensional hole densities in $Al_{0.26}Ga_{0.74}As$/GaAs heterojunctions. An analysis of the charge transfer yields a valence-band offset of 0.39 ± 0.02 of the energy-gap difference.

Band alignments at semiconductor heterojunctions are fundamental parameters of these interfaces and are important for device models.[1-3] The band offsets of many heterojunctions have been studied by x-ray photoelectron spectroscopy (XPS),[4-6] by optical absorption and luminescence experiments,[7,8] by current-voltage and capacitance-voltage measurements,[9-13] and by the charge-transfer method.[14] Several theories[15-17] appeared to be in agreement with selected experimental results. Most of the theories involve only bulk material properties, and many calculations deal with the band offset of the (110) orientation. However, experiments are usually performed on different orientations, e.g., mostly on the (110) orientation for XPS measurements involving III-V compounds, and on the (100) orientation for electrical and optical measurements. To our knowledge, the theories give no specific evidence nor arguments about the orientation dependence of the band offset. There have been reports[4,6] on the orientation dependence of the band offset for the Ge/GaAs heterojunction. However, the Ge/GaAs heterojunction involves the combination of a polar and a nonpolar semiconductor in addition to the interdiffusion problem. It is our opinion that heterojunction theories should be based on data taken from device quality interfaces. To what extent the Ge/GaAs system being measured represents a device quality interface is largely unknown. In this Rapid Communication, we present our results on the valence-band offset for AlGaAs/GaAs (100) and (311) heterojunctions as deduced from the charge-transfer method, which relates the carrier density in the GaAs channel to the impurity distribution in the AlGaAs. Our results, based on samples with hole mobilities among the highest reported for semiconductors, suggest that the band offset is orientation independent.

The p-type modulation-doped AlGaAs/GaAs structures were grown by molecular-beam epitaxy on undoped liquid-encapsulated Czochralski-grown semi-insulating GaAs substrates. The orientation of the (100) and (311) substrates was checked by x-ray back Laue reflection to be accurate within 1°. The heterostructure consisted of (1) a 1-μm GaAs buffer layer with p-type background doping in the 10^{14}–10^{15}-cm^{-3} range, (2) an undoped AlGaAs spacer layer with thickness of either 20.1 or 29.2 nm, (3) a p-AlGaAs layer doped with Be to a concentration of 1.2×10^{18} cm^{-3}, and (4) a very thin (~ 5 nm) layer of GaAs for surface protection. We have checked that the Be atoms are incorporated on group III (Ga or Al) lattice sites as simple substitutional acceptors. We chose (311) for this study because (311) is one of the simplest high index plane, consisting of equal densities of single-dangling and double-dangling sites. The details of the crystal growth and surface structures are outside the scope of this paper and will be reported elsewhere.[18] The AlAs mole fraction was calibrated to be 0.26 ± 0.02 by photoluminescence and beam flux measurements. In every sample, the doped AlGaAs was thick enough not to be completely depleted. Indium-cadmium dots were alloyed to form Ohmic contacts for van der Pauw–Hall measurements. Sheet carrier concentrations and Hall mobilities were measured at liquid-helium temperature (4.2 K) both in the dark and with the sample exposed to light. No persistent photoconductance was observed, in marked contrast to the situation for n-type modulation-doped structures. Owing to the very low mobilities (< 200 $cm^2 V^{-1} s^{-1}$) of holes in p-AlGaAs, parallel conduction has no influence on our measured two-dimensional (2D) channel hole densities. The experimental results are shown in Table I. As is already evident from the data, the sheet carrier densities are the same for both (100) and (311) orientations; therefore, the band offset must be the same for both orientations.

The valence-band offset of the p-type samples is estimated from the measured hole densities and spacer thicknesses following a standard procedure, as outlined, for example, in Ref. 19, to assure that the Fermi levels line up across the interface. This is illustrated in the energy band diagram of Fig. 1. The valence-band offset ΔE_v is the sum of the subband energy E_0, the Fermi energy E_F, the potential drop across the undoped spacer layer V_{sp}, the potential drop across the doped space-charge layer V_1, and the Be acceptor binding energy E_{ab}. E_0 is calculated self-consistently, using a local-density approximation for many-body effects[20] and assuming a parabolic, isotropic valence-band effective mass of 0.4 m_0. The Be acceptor binding energy is taken to be 35 meV, and the $Al_{0.26}Ga_{0.74}As$ dielectric constant is taken to be 12.3. The density of fixed "depletion" charges in the GaAs is assumed to be 7×10^9 cm^{-2}, corresponding to 10^{14} compensating donor impurities per cm^3 in the GaAs accumulation layer. With these assumptions the calculated

TABLE I. Sample characteristics of modulation-doped $Al_{0.26}Ga_{0.74}As$/GaAs heterostructures.

Orientation	Spacer (nm)	Sheet density (cm^{-2})	4.2-K mobility ($cm^2 V^{-1} s^{-1}$)
(100)	20.1	2.62×10^{11}	9.28×10^4
(311)	20.1	2.60×10^{11}	1.16×10^5
(100)	29.2	1.72×10^{11}	8.88×10^4
(311)	29.2	1.79×10^{11}	7.4×10^4

 ©1985 The American Physical Society

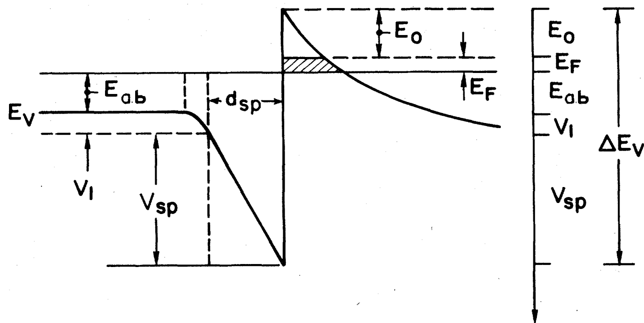

FIG. 1. Schematic illustration of the band diagram showing quantities that were used for the calculation of the valence-band offset. d_{sp} is the thickness of the undoped spacer layer.

valence-band offset is 126 ± 4 meV. The energy-gap difference between $Al_{0.26}Ga_{0.74}As$ and GaAs is 324 meV, so the valence-band offset is 0.39 ± 0.02 of the energy-gap difference. Our results are consistent with the recently determined band offset for this heterojunction.[8, 11-14] In our estimation of the valence-band offset, errors connected with the calculation of hole energies, e.g., the choice of effective mass in the simple model we use and the approximation used for many-body effects, are hard to estimate because of the complicated valence-band structure[21] in this system, but are thought to be very small. In any event, the absolute energy of the valence-band offset would not affect our conclusion drawn from the present experiment; i.e., we observed the same sheet carrier density for both (100) and (311) heterojunctions; therefore, the valence-band offset must be the same for both orientations.

Among the various heterojunction theories, Tersoff's[17] is in closest agreement with the available experimental data.[22] His theory is based on the dielectric screening of quantum dipoles at the heterointerface. Our result of the orientation-independent band offset is consistent with the physical basis of his theory, i.e., the dielectric response is isotropic and orientation independent.

We thank J. Karasinsky for x-ray orientation of the crystals, and to E. Wilkie for polishing the substrates. We are indebted to F. Stern for providing results of his calculations and to J. Tersoff for helpful discussions. This work was sponsored in part by the U.S. Army Research Office.

[1]A. G. Milnes and D. L. Feucht, *Heterojunctions and Metal Semiconductor Junctions* (Academic, New York, 1972).
[2]M. L. Cohen, Adv. Electron. Electron. Phys. **51**, 1 (1980).
[3]H. Kroemer, Surf. Sci. **132**, 543 (1983).
[4]R. W. Grant, J. R. Waldrop, and E. A. Kraut, Phys. Rev. Lett. **40**, 656 (1978).
[5]A. D. Katnani and G. Margaritondo, Phys. Rev. B **28**, 1944 (1983).
[6]R. S. Bauer and H. W. Sang, Jr., Surf. Sci. **132**, 479 (1983).
[7]R. Dingle, W. Wiegmann, and C. H. Henry, Phys. Rev. Lett. **33**, 827 (1974).
[8]R. C. Miller, D. A. Kleinman, and A. C. Gossard, Phys. Rev. B **29**, 7085 (1984).
[9]H. Kroemer, W. Y. Chien, J. S. Harris, and D. Edwall, Appl. Phys. Lett. **36**, 295 (1980).
[10]C. M. Wu and E. S. Yang, J. Appl. Phys. **51**, 2261 (1980).
[11]T. W. Hickmott, P. M. Solomon, R. Fischer, and H. Morkoc, J. Appl. Phys. **57**, 2844 (1985).
[12]J. Batey, S. L. Wright, and D. J. DiMaria, J. Appl. Phys. **57**, 484 (1985).
[13]D. Arnold, A. Ketterson, T. Henderson, J. Klem, and H. Morkoc, Appl. Phys. Lett. **45**, 1237 (1984).
[14]W. I. Wang, E. E. Mendez, and F. Stern, Appl. Phys. Lett. **45**, 634 (1984).
[15]W. A. Harrison, J. Vac. Sci. Technol. **14**, 1016 (1977).
[16]W. R. Frensley and H. Kroemer, Phys. Rev. B **16**, 2642 (1977).
[17]J. Tersoff, Phys. Rev. B **30**, 4874 (1984).
[18]W. I. Wang (unpublished).
[19]F. Stern, Appl. Phys. Lett. **43**, 974 (1983).
[20]F. Stern and S. Das Sarma, Phys. Rev. B **30**, 840 (1984).
[21]V. Ekenberg and M. Altarelli, Phys. Rev. B **30**, 3569 (1984).
[22]W. I. Wang and F. Stern (unpublished).