Staggered to straddling band lineups in InAs/Al(As, Sb)

S. Bhargava, H.-R. Blank, E. Hall, M. A. Chin, H. Kroemer, and V. Narayanamurti[a)]
Department of Electrical and Computer Engineering, University of California, Santa Barbara, California 93106

(Received 15 July 1998; accepted for publication 17 December 1998)

Ballistic electron emission spectroscopy (BEES) has been used to study both the conduction and valence band offsets between InAs and AlAsSb. With the addition of As to AlSb, the conduction band offset between it and InAs has been found to decrease despite the increase in the band gap. The resulting increase in the valence band causes the InAs/Al(As, Sb) band lineup to change from a staggered (type II) to a straddling (type I). Both room-temperature and low-temperature (77 K) BEES spectra have been taken to determine the band offsets. © *1999 American Institute of Physics.* [S0003-6951(99)01408-4]

The advent of ternary semiconductors has opened up the field of device growth, for it allows for the lattice matching and the control of band lineups over a much wider range. Most of the work to date in the III–V compound semiconductors has been accomplished through use of dual-cation compounds. However, the III–V dual-anion compound $AlAs_xSb_{1-x}$ is of great interest, for it is a high-band-gap material system that can be grown lattice matched to a variety of substrates, such as GaAs, InP, InAs, and GaSb.[1] The high band gaps of $AlAs_xSb_{1-x}$, ranging from ~1.6 (AlSb) to 2.2 eV (AlAs), make $AlAs_xSb_{1-x}$ very attractive for the fabrication of heterojunctions with large band offsets allowing for high carrier confinements. Recent work[1] at UCSB has demonstrated the strong sensitivity of structural and electrical quality on growth parameters and substrate temperature. $AlAs_xSb_{1-x}$ has successfully been used as the barrier material for midinfrared lasers,[2–5] in InAs-based heterostructure field-effect transistors,[6,7] and InP-based optoelectronics.[8–10]

The InAs/AlSb system exhibits a straddling (type II) band lineup, with a conduction band offset between InAs and AlSb (1.35 eV) bigger than the difference in band gaps (1.28 eV), and an AlSb valence band edge above the InAs valence band edge. From measurements on InAs/GaAs[11] and GaAs/AlAs,[12] transitivity dictates that InAs/AlAs will from a staggered (type I) band lineup. In the present work, we use ballistic electron emission spectroscopy (BEES) to determine band offsets between InAs and three concentrations of AlAsSb: 0% As, 16% As (lattice matched to InAs), and 56% As (lattice matched to InP) and to investigate the transition between the staggered and straddling regimes.

BEES is a three-terminal modification of a scanning tunneling microscope (STM) in which the STM tip, acting as an emitter, injects hot carriers into a thin (<100 Å) Au metal (base) layer grown on a semiconductor.[13,14] Since the attenuation length of these injected electrons in Au is ~125 Å,[15] they will travel ballistically through the metal until they reach the Schottky Barrier (SB). Some of the carriers will have sufficient energy and appropriate momenta to overcome the Schottky Barrier and will be collected at the semiconductor contact (collector). BEES is performed by pausing the STM tip during a topographic scan, and measuring the collector current, I_c, as a function of the tip-base voltage, V_t. When V_t becomes greater than the SB, a threshold in I_c is observed. A key point to note is that during the acquisition of the spectroscopic data, BEES's three-terminal capability allows for the energy bands in the metal semiconductor region to remain unchanged. BEES has been shown to give accurate measurements of band offsets.[12]

The molecular beam epitaxy (MBE) samples consisted of 20 Å InAs on 4000 Å Al(As)Sb grown upon the appropriate GaAs substrate (n^+ for conduction band and p^+ for valence band measurements). The layer structure and the energy band diagram for the InAs/AlSb sample are shown in Fig. 1. Using a shadow mask, 65 Å of Au were thermally evaporated in 1 mm dots at a background pressure of 2×10^{-7} Torr, as in typical device fabrication procedures. The thin metal and the InAs cap layers allow for the injected carriers to travel ballistically through *both* the Au and the InAs until the InAs/Al(As, Sb) interface is reached. Therefore, the energy of the electrons at that interface corresponds directly to the applied tip-to-base voltage. Since the InAs layer is thin in comparison to the Al(As, Sb) layer and InAs conduction band edge is beneath the Fermi level, the major-

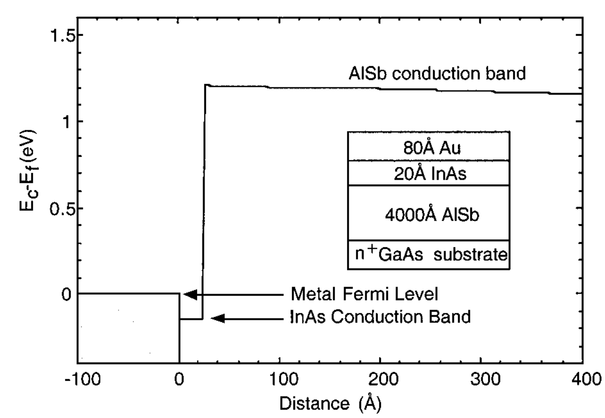

FIG. 1. Calculated band profile and structure for Au/InAs/AlSb measurement. For AlAsSb, a 4000 Å AlAsSb layer was used instead of AlSb.

[a)]Present address: Division of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138. Electronic mail: venky@deas.harvard.edu

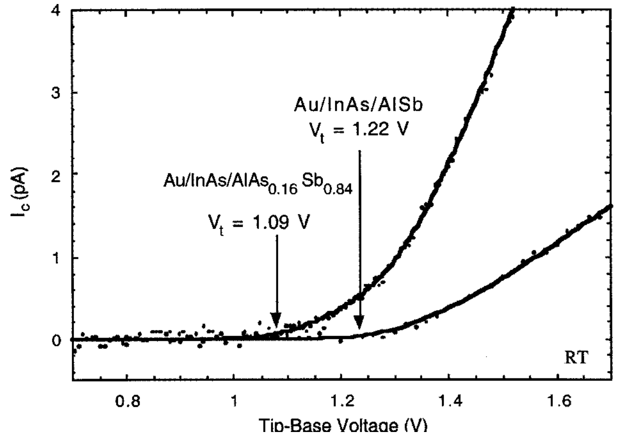

FIG. 2. Representative BEES spectra for Au/InAs/AlSb and Au/InAs/$AlAs_{0.16}Sb_{0.84}$.

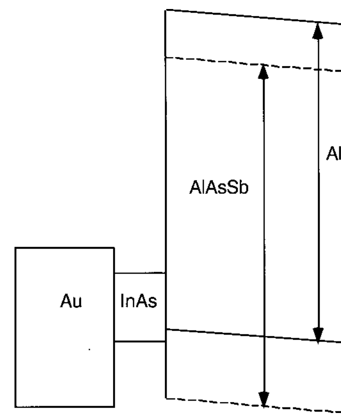

FIG. 3. Band Positioning of the InAs and Al(As)Sb depicting the staggered (AlSb) and straddling (AlAsSb) band lineups.

ity of the band bending occurs in the Al(As, Sb), not the InAs. The injected carriers will reach the collector contact only if they have enough energy to overcome the Al(As)Sb barrier. Therefore, the height measured in the BEES spectra corresponds directly to the maximum in the band edge (at the InAs/Al(As, Sb) interface). Numerical values for the thresholds were obtained through fitting to the theoretical Bell–Kaiser model.[15] Previous work by the authors[12] has shown that taking quantum mechanical reflection at the barrier causes a modification of about 20 meV in the absolute value of the threshold. The relative changes in the threshold as a function of composition are model independent.

Room-temperature BEES measurements were performed on five Au/InAs/AlAsSb (three *n*-type and two *p*-type) samples with As concentrations of 0%, 16%, 56%. Figure 2 shows two representative BEES spectra of InAs/AlSb and InAs/$AlAs_{0.16}Sb_{0.84}$. The observed BEES thresholds decrease as the As concentration is increased. At the higher As concentrations, the material is becoming highly strained (~3% lattice mismatch for the 56% sample). Even though the BEES current was therefore smaller, it was more than adequate to make the offset measurements. The highly strained InAs cap layer can cause extra charged states at the InAs/AlAsSb which can trap and reduce the BEEM current significantly since only a few pA are measured. In addition, the BEES thresholds for each sample increased as the temperature was decreased from RT to 77 K. These values are shown in Table I. From previous BEES measurements on Au/InAs/AlSb, the Au Fermi level is pinned 130 meV in the InAs conduction band.[16] To deduce the conduction band offset (CBO) between InAs and Al(As)Sb, the 130 meV value is added to the appropriate BEES thresholds.

This decrease in the thresholds and the conduction band offsets comes in strong contrast to the expected increase in the band gap in going from AlSb to AlAsSb.[17] Since the band-gap increase must be absorbed as a sum of the changes in the conduction and valence bands, with respect to the InAs conduction band edge, an increase in the valence band offset for InAs/$AlAs_xSb_{1-x}$ must therefore be concluded.

In the case of InAs/AlSb, the AlSb valence band could not be probed by BEES as it lies higher in energy than the AlSb valence band (staggered band lineup). Since the InAs/AlSb valence band offset must increase (from the *n*-type results), the $AlAs_xSb_{1-x}$ valence band will become visible as x is increased (Fig. 3). At As concentrations of 0.16 and 0.56, BEES could be performed and Fig. 4 shows a low-temperature (90 K) spectrum obtained on the $x=0.16$ valence band offset (DE_v) sample. Using the 77 K InAs band gap of 0.40 V,[18] DE_v's of 0.33 and 0.75 V are obtained between InAs/$AlAs_{0.16}Sb_{0.84}$ and InAs/$AlAs_{0.56}Sb_{0.44}$. This extrapolation requires the assumption that Au/InAs Fermi level pinning position remains independent of temperature.[19]

Low-temperature measurements were also performed on the three *n*-type samples to give a more complete understanding of the band structure. The BEES thresholds are expected to follow the band-gap dependence and are therefore expected to increase as the temperature is decreased. As seen in Table I, each of the three *n*-type concentrations exhibited an 80–100 meV threshold increase at low temperature. The low-temperature conduction band offsets are again calculated by adding the 130 meV from the observed BEES thresholds.

TABLE I. Measured BEES results (thresholds and conduction band offsets) on Au/InAs/Al(As)Sb samples.

Material	*n*-type RT	RT DE_c	77 K *n*-type	LT DE_c	77 K *p*-type
InAs/AlSb	1.22 V	1.35 V	1.31 V	1.44 V	⋯
16% As	1.09 V	1.22 V	1.19 V	1.32 V	−0.86 V
56% As	1.02 V	1.15 V	1.10 V	1.23 V	~−1.28 V

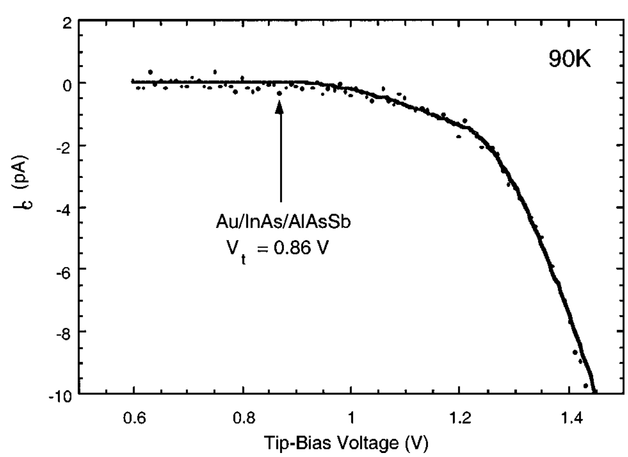

FIG. 4. BEES spectra obtained for measuring the valence band offset between InAs and $AlAs_{0.16}Sb_{0.84}$. A threshold value of 0.86 eV is obtained yielding a DE_v of 0.37 V.

The measured offsets are ∼100 meV above what would be expected from simple linear extrapolation between InAs/AlAs and InAs/AlSb. This includes the estimated expansion of the band gaps at lower temperatures (∼200 meV). This suggests the bowing of the band gaps as a function of concentration and strain effects arising from lattice mismatching.

In summary, BEES has been used to measure the InAs/Al(As, Sb) band offsets as a function of As concentration. BEES's ability to follow both the conduction and valence band offsets allow us to follow their positions with relative ease. We have found with the addition of As to AlSb, the band lineup between InAs and Al(As, Sb) changes from straddling (type II) to staggered (type I).

The authors would like to thank J. English for his technical support. This work was partially funded through AFOSR Grant No. 442520-2537. They would also like to acknowledge the Deutsche Forschungsgemeinschaft and the NSF Science and Technology Center for Quantized Electronic Structures.

[1] H.-R. Blank, S. Mathis, E. Hall, S. Bhargava, A. Behres, M. Heuken, H. Kroemer, and V. Narayanamurti, J. Cryst. Growth **187**, 18 (1998).
[2] H. K. Choi, G. W. Turner, and Z. L. Liau, Appl. Phys. Lett. **65**, 2251 (1994).
[3] A. A. Allerman, R. M. Biefeld, and S. R. Kurz, Appl. Phys. Lett. **69**, 465 (1996).
[4] K. Xie, J. H. Zhao, Y. Shi, and H. Lee, IEEE Photonics Technol. Lett. **8**, 667 (1996).
[5] Y. H. Zhang, H. D. Le, D. H. Chow, and R. H. Miles, Semicond. Sci. Technol. (to be published).
[6] C. R. Bolognesi, E. J. Caine, and H. Kroemer, IEEE Electron Device Lett. **15**, 16 (1994).
[7] B. Brar and H. Kroemer, IEEE Electron Device Lett. **16**, 548 (1995).
[8] O. Blum, I. J. Fritz, L. R. Dawson, and T. J. Drummond, Electron. Lett. **31**, 1247 (1995).
[9] B. Lambert, Y. Toudic, Y. Rouillard, and M. Gauneau, Appl. Phys. Lett. **66**, 442 (1995).
[10] O. Blum, K. M. Geib, M. J. Hafich, and J. F. Klem, Appl. Phys. Lett. **68**, 3129 (1996).
[11] T.-H. Shen, M. Elliott, R. H. Williams, and D. Westwood, Appl. Phys. Lett. **58**, 843 (1991).
[12] J. J. O'Shea, E. G. Brazel, M. E. Rubin, S. Bhargava, M. A. Chin, and V. Narayanamurti, Phys. Rev. B **56**, 2026 (1997).
[13] W. J. Kaiser and L. D. Bell, Phys. Rev. Lett. **60**, 1406 (1988).
[14] For a recent review of BEEM, see L. D. Bell and W. J. Kaiser, Annu. Rev. Mater. Sci. **26**, 189 (1996).
[15] L. D. Bell and W. J. Kaiser, Phys. Rev. Lett. **61**, 2368 (1988).
[16] S. Bhargava, H.-R. Blank, V. Narayanamurti, and H. Kroemer, Appl. Phys. Lett. **70**, 759 (1997). To minimize variations in the Fermi level pinning the InAs surface treatment was kept the same in the present experiments.
[17] An estimate of the band gap of AlAsSb is made by using a linear extrapolation of the AlSb and AlAs values. The same technique is used to estimate the offsets between InAs/AlAsSb.
[18] Y. Lacroix, C. A. Tran, S. P. Watkins, and M. W. Thewalt, J. Appl. Phys. **80**, 6416 (1996).
[19] H. Kroemer (private communication).