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InAsSb/InAs: A type-I or a type-II band alignment

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Su-Huai Wei and Alex Zunger
National Renewable Energy Laboratory, Golden, Colorado 80401 (Received 14 June 1995)

Using first-principles band-structure calculations we have studied the valence-band alignment of
InAs/InSb, deducing also the offset at the InAsl „Sb„/InAsl „Sb~ heterostructure. We find the follow-ing: (i) Pure InAs/InSb has a "type-II broken gap" alignment both with and without strain. (ii) For Sb-
rich InAsl „Sb /InSb heterostructures, the unstrained band alignment is type II; both epitaxial strain
and CuPt ordering enhance the type-II character in this Sb-rich limit. (iii) For As-rich
InAs/InAs, Sb„heterostructures the top of the valence band is always on the alloy layer while the
conduction-band minimum can be localized either on the alloy layer (type-I) or on the InAs layer (type-II), depending on the balance between concentration, strain, and degree of ordering/phase separation. In this case, epitaxial strain enhances the type-II character, while ordering enhances the type-I charac-
ter. Our results are compared with recent experimental observations. We find that the type-I behavior
noted for some As-rich InAs/InAsl Sb„ interfaces and the type-II behavior noted in other such sam-
ples could be explained in terms of the dominance of ordering and strain effects, respectively.

I. INTRODUCTION

InAs& Sb /InAs&» Sb» semiconductor alloys and
heterojunctions have been studied as potential IR detec-
tors and emitters' '

. While the InAs, „Sb alloy sys-
tem provides the lowest band gap attainable within the
family of bulk III-V semiconductors [145 meV at
x =0.634 (Ref. 13)], this value is not small enough to produce the 10—12p absorption (124—103 meV) needed
in far-infrared detection. Two strategies present them-
selves: one can either change the growth conditions to promote CuPt ordering of the InAs& Sb„alloy, '

thus

reducing its band gap. Alternatively, one can form a
heteroj unction between an arsenide-rich and an
antimonide-rich alloy with a type-II band alignment, in
which case the effective band gap is smaller than either of
the constituents. The latter approach has been proposed'
and tested '

for Sb-rich heterojunctions. The
InAs0, 3Sbos~/InSb strained-layer superlattices, for ex-
ample, was found to have a

type-I

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Kronig-Penney model was used to extract values of the band offset. The best fit (to two emission lines) corre-sponded to a band

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III. METHOD OF CALCULATION OF BAND OFFSET
BETWEEN ALLOY CONSTITUENTS

tice constant, bulk modulus, and band-gap deformation
potential despite E &0 and E'""'&0. Furthermore.
to obtain the conduction-band offset under different

strain conditions we use the relation AE, =DE —AE„,
where hE =Eg" (e) E—s" (e) is the strain-dependent
LDA-corrected band-gap difference between AD =InAs and AC=InSb. The band gap Es(e) for compound AC and strain e is given by

So far we explained the method of calculating band ofFsets between the binary constituents. To obtain the valence-band offset between alloy constituents
InAs, Sb /InAs& Sb, we assume that at a given sub-
strate with lattice constant a„ the valence-band energy
varies with composition x as

E„(a„x)=E,(a„O)+xbE,(a„InAs/InSb)

b, x—(1—x).
where, Es"LD~(e) is the LDA calculated band gap for compound AC under strain e, and Es",„~,(0) is the experi mentally measured' zero-strain band gap at T=0. We
assume that the LDA correction [terms in the square bracket of Eq. (2)] is strain independent. For InAs the LDA correction is 1.11 eV, while for InSb it is 1.00 eV. This method of band-offset calculation has been used in

the past to compute the unrelaxed valence-band offsets of
numerous semiconductor heterojunctions, ' ' yielding
reasonable agreement with experiment, e.g.,

Here b,E„(a„ InAs/InSb) is our LDA calculated
valence-band ofFset between the pure binaries (Sec. II),
strained on the substrate with lattice constant a,. The
coefficient b, is the bowing parameter of the top of the al-loy valence band. In general, b, is negative and its mag-
nitude is much smaller than the total band-gap bowing
b. The valence-band offset between InAs& Sb„and
InAs, Sb is EE,(a„x/y) =E„(a„y) E,(a„x—), which
can be

Th85 Tf 456.67 558.3T BT /Xi23ro/XET10.27 Tf 136.4081/Xi2 9.81 Tf 312.89 491.89 sce-bandp3 /Xi2 9.81 Tf 360 481.22BT /Xi235D(4)8.68 Tf 235.33 482 ET BT beTd (bulk)T/Xi2 8.86 Tf 52 547.relatioET x—)

ca7

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negativT /X256.6373te

3030ET BT /Xi2 /XfaT 2 8.96 Tf 312.78 5 558.565(30ETTj ET B T BT /Xi2 9.85 Tf.22 515.6 Td)Tj30j5(with)Tjhow/Xi2 9.49 Tf 312.263.33 T13Td (29T ET BT 4a Fc2 9.26 Tf 423.657.89 662D

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C. Effects of strain on the oRset between the pure compounds

For the biaxially compressed layer (InSb), the VBM is a heavy-hole (hh) (—',,+—,

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