PHYSICAL REVIEW 8 VOLUME 50, NUMBER 11 15 SEPTEMBER 1994-I

Type-II-+type-I transition in (GaX)„/(InX)„(001) superlattices (X=P, Sb) as a function of period n

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Coherently strained GaX/InX interfaces (X=P, Sb) lattice matched to a (001)-oriented substrate are pre-dicted to have a type-I band-gap alignment, with both the valence-band maximum and the conduction-band
minimum

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(a) GaP/InP (001) (b) GaSb jlnSb (001)
VBM

Ga a)

CBM CBlvl

Ga

gi
1'Ga)

I ~Sb~lI

6)g I Hg

FIG. 2. Wave-function amplitudes lP;(r)l (i is VBM, CBM) in the (011)plane of (a) (GaP)t/(InP)t (001) and (b) (GaSb)t/(InSb)t (001)

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localization. A reasonable rule for common-anion superlat-tices is that the I -like CBM will be localized on the cation sublattice with lower atomic s-orbital energy, while the I -like VBM will be localized on the cation sublattice with

higher atomic p-orbital energy. The LDA calculated orbital energies of the Al, Ga, In, Zn, Cd, and Hg atoms are plotted in Fig. 4. As we can see, e4,(Ga)&e5,(in), and e4~(Ga) & e5„(ln). Since the band-edge states of ultrathin GaX/InX (X=P, As, or Sb) superlattices originate from the I states of the binary constituents, our rule predicts that the CBM will be localized on GaX, while the VBM will be localized on InX (type-II alignment). This prediction is con-sistent with our explicit calculations for GaP/InP and GaSb/InSb systems, and with the results of Magri' for (GaAs)t/(InAs), (111) superlattices and of Taguchi and Ohno' for (GaAs), /(InAs)t (001) superlattices. These au-thors find that the CBM wave function of these systems has a larger amplitude on the GaAs layer. Our model predicts that in GaX/AlX (X=P, As, Sb) short-period superlattices the VBM wave function and the I'-like CBM wave function will be both localized on GaX, whereas in InX/AIX superlattices

the I'-like band-edge states will be both localized on InX. Also, common-anion II-VI ultrathin superlattices are pre-dicted to be type-I (see Fig. 4); this prediction is consistent with the results of Beavis et al. for CdTe/HgTe superlat-
tices.

In conclusion, we have shown that atomic orbitaI energies determine wave-function localization at the band edges of ultrathin (n =1—3), lattice-matched GaP/InP (001) and GaSb/InSb (001) superlattices, leading to a type-II alignment with the VBM on In and the CBM on Ga. On the other hand, as n~~ we have a type-I heterojunction with both the VBM and the CBM localized on In. Thus, for these systems, a type-Il~type-I transition of a novel type is expected as the period of the superlattice increases, and is predicted to occur around n=4. This result suggests that if we have some thin Ga-rich and In-rich domains in composition-modulated

alloy, '

then electrons will prefer Ga sites while holes will
prefer In sites.

This work was supported by the U.S. Department of En-ergy, OER-BES, Grant No. DE-AC02-83-CH10093.

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