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Negative band gap bowing in epitaxial InAs/GaAs alloys and predicted band offsets of the strained binaries and alloys on various substrates

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We use pseudopotential theory to provide (1) the band offsets of strained GaAs and InAs on various substrates and (2) the energies $E_v(x)$ and $E_c(x)$ of the valence and conduction bands of $In_xGa_{1-x}As$ alloy, as a function of composition. Results are presented for both the bulk alloy and for the alloy strained on InP or GaAs. We predict that while $E_c(x)$ bows downward for relaxed bulk alloys, it bows upward for strained epitaxial alloys. The calculated alloy offsets are used to discuss electron and hole localization in this system. © *2002 American Institute of Physics.*
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InAs and GaAs are the building blocks of a diverse range of systems,[1] including short-period superlattices $(InAs)_n/(GaAs)_m$ of the binary constituents, bulk alloys $In_xGa_{1-x}As$, epitaxial alloys that are coherently grown on a substrate (InP or GaAs), alloy superlattices or quantum wells $(In_xGa_{1-x}As)_p/(InP)_q$, and GaAs-embedded InAs quantum dots. A central quantity that controls many of the optical and transport properties of such systems are the band-edge energies E_v and E_c of the valence (v) and conduction (c) states, as a function of composition, strain, and material dimensionality. Two things are known about these quantities. First, the relative band offset E_v(InAs/GaAs) and E_c(InAs/GaAs) between the *end-point binary compounds* can be obtained either from direct photoemission[2] or transport[3] measurements or can be calculated using accurate first-principles calculations (summarized for all III–V's and all II–VI's in Ref. 4). Second, the pressure dependence of the band gap $E_g=E_c-E_v$ (summarized in Ref. 5 for all zincblende semiconductors) are also known. What is generally not known directly about these quantities is: (i) the *relative* offset $E_{v,c}(In_xGa_{1-x}As/In_yGa_{1-y}As)$ as a function of *alloy composition*, and, (ii) the *absolute* pressure, or strain dependence of the *individual* band-edge energies E_v, and separately E_c. But knowledge of these quantities is crucial because the relative alloy band-edge offset and their absolute pressure dependence decides the confinement of holes or electrons in heterostructures made of strained alloy wells and barriers.

Alloy offsets, e.g., the offset between $In_xGa_{1-x}As$ and InP or GaAs, are generally unknown via direct measurements and are usually treated as an adjustable parameter (along with other quantities) when measured interband transition energies are fit to simple, effective-mass based models.[6–8] Such fits produce a disappointingly large range of alloy band offsets. It is generally unknown how much of the uncertainty results from fundamental limitations in the underlying (effective-mass) physical model used in the fit and how much should be attributed to interdependence between the fitting parameters of the model (e.g., uncertainties in the strain-modified effective masses lead to uncertainties in the fitted band offsets). It is not uncommon to encounter equally precise optical measurements on InAs/GaAs systems, inter-

offsets between the end-point binaries InAs/GaAs using the first-principles local density method, as implemented via the linear augmented plane wave (LAPW) approach.[15] Reference 4 and references therein describe how one deduces from LAPW calculations the position of core levels of GaAs, InAs, and GaAs/InAs heterojunction relative to the respective band edges and how these quantities gives the band offsets. To first order, the calculated offset is unaffected by the ''local density approximation (LDA) band gap error.'' Figure 1 shows our resulting band-edge energies for GaAs and InAs versus strain, where we combined our calculated LDA band offsets with the measured band gaps of the binaries. The band-edge energies are given as absolute energies with respect to the intrinsic vacuum level as zero. We see that the unstrained, ''natural'' valence offset (central panel of Fig. 1) is rather small (52 meV) but it increases rapidly with strain. This is shown more clearly in Fig. 2 which depicts the offsets on three specific (001) substrates. On the GaAs substrate, the heavy-hole (hh) offset is 383 meV, the light-hole (lh) offset is 198 meV (hole localized on InAs) and the conduction band offset is 693 meV. On the InAs substrate, we have a reversal of hole states, with lh above hh, giving a negative hh offset of -261 meV, while the lh offset is 279 meV (hole localized on GaAs). The conduction band offset is now reduced to 289 meV. On the intermediate InP substrate, we have a hh offset of 316 meV, a lh offset of only $249-316 = -76$ meV (hole localized on GaAs), and an intermediate conduction band offset of 465 meV. The calculated conduction band offset on GaAs substrate (693 meV) compares well with the most recent experimental determination[3] (690 meV)