Proposal for III-V ordered alloys with infrared band gaps

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It is shown theoretically that the recently observed spontaneous ordering of III-V alloys that yields alternate monolayer $(1\bar{1}1)$ superlattices provides the opportunity for achieving infrared band gaps in systems such as $(InAs)_1(InSb)_1$ and $(GaSb)_1(InSb)_1$. A substantial reduction in the *direct* band gap is predicted to result from the *L*-point folding that repel the Γ band-edge states.

Substantial effort has recently been focused on developing semiconductor materials for infrared (IR) devices in [redacted] of intersubband absorption in tunnelling III-V superlattices,[2] four general physical principles have been previously [redacted]

(i) *Bulk alloying.* In this simple approach one uses the fact that alloy band gaps vary smoothly and continuously with composition (often with a parabolic deviation from [redacted] CdTe) semiconductors that produces a $(SG)_{1-x}(LG)_x$ alloy with a desired IR gap.

(ii) *Superlattice quantum confinement without strain.* The basic idea here is to take a semiconductor with a very [redacted] larger gap (LG). For small layer thicknesses (*p*,*q*), quan- [redacted] LG = CdTe by Schulman and McGill[3] and by Smith *et al.*[4] and examined experimentally, e.g., by Reno and Faurie.[5]

[redacted] gap and small lattice constant (SGSL) and layer it coherently with a material having a larger gap and larger lattice constant (LGLL), forming a strained-layer $(SGSL)_p/$ [redacted] interface, thus lowering its Γ conduction-band minimum. At the same time, tetragonal *compression* of SGSL in the perpendicular direction splits its VBM, raising the energy of the upper split components. Both effects act to reduce [redacted] $x>0.61$. Since quantum confinement effects at small (*p*,*q*) act in the opposite direction, increasing the band gap, rel- [redacted] herently the misfit strain limits the maximum thickness that can be used.

(iv) *Superlattice-induced band inversion.* The basic [redacted] of the constituents (AC) is lower in energy than the VBM of the other (BC); in this type of band lineup, the super- [redacted] stituents. This approach has been proposed by Arch *et al.*[8] for AC = InAs and BC = GaSb. Like in (iii) above, here, [redacted] II" band arrangement, thick layers deteriorate severely the intensity of optical absorption due to increased separation between electrons and holes. To reduce the layer thickness [redacted] Mailhiot[9] for AC = InAs and BC = $Ga_{1-x}In_xSb$. This system was grown successfully by Chow *et al.*[10] where far-infrared photoluminescence was observed.

We discuss here a different principle of achieving in- [redacted] point) folds into the Brillouin zone center. This leads to a [redacted]

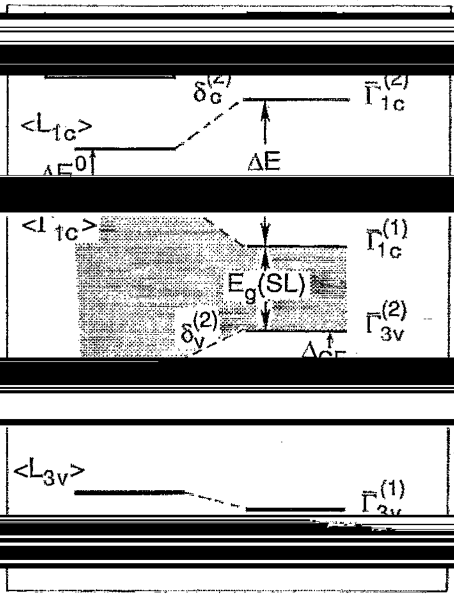


FIG. 1. Schematic plot of energy level shift at $\bar{\Gamma}$ of a typical III-V alloy [redacted]

[redacted] turned on. Values in parenthesis are for unrelaxed structures.

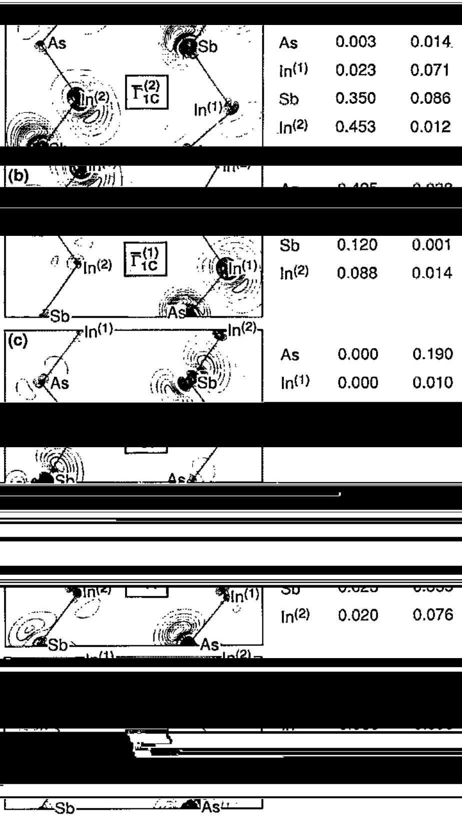
	GaAs/InAs	GaAs/InSb	GaAs/GaSb	InAs/InSb
$\Delta E^0 = \langle L_{1c}\rangle - \langle T_{1c}\rangle$	0.99	0.68	0.47	1.0
$\Delta E = \bar{\Gamma}^{(2)}_{1c} - \bar{\Gamma}^{(1)}_{1c}$	1.43 (1.22)	1.22 (1.02)	1.77 (1.28)	1.84 (1.39)
$R = \Delta E - \Delta E^0$	0.44 (0.23)	0.54 (0.34)	1.30 (0.81)	0.84 (0.39)

reduces the direct band gap, thus overwelming the opposite [redacted]

It has recently been noted[12] that numerous III-V alloys exhibit in vapor phase growth *spontaneous* long-range ordering in the form of monolayer $(AC)_1/(BC)_1$ superlattices in the (111) orientation (the "CuPt-like structure"). [redacted] CuPt ordering are given in Ref. 12. In all cases, ordering occurred as a result of *homogeneous* alloy growth *without* [redacted] $\langle\Gamma\rangle + \langle L^{111}\rangle$. The folded zincblende states at this wave vector are coupled in the superlattice by the perturbing potential $\delta V(\mathbf{r}) = \delta V^{(\text{chem})} + \delta V^{(\text{size})}$ that has the symme- [redacted] size mismatch. This potential couples the alloy states and leads to a "level repulsion" between them, whereby superlattice states are displaced relative to the unperturbed (virtual crystal) states. For example, the $\bar{\Gamma}$-folding alloy states $\langle\Gamma_{1c}\rangle$ and $\langle L_{1c}\rangle$ couple through δV, producing the super- [redacted] The lowering of the CBM will be denoted (Fig. 1) as [redacted] mutually repelled (Fig. 1). The increase in the energy of [redacted] mum at X is considerably higher in these systems[14] than $\bar{\Gamma}^{(1)}_{1c}$, the former will not be discussed here.

To quantify the extent of level repulsion, we denote by ΔE^0 the $\langle L_{1c}\rangle - \langle\Gamma_{1c}\rangle$ energy difference *before* coupling [redacted]

ence between the superlattice states $\bar{\Gamma}^{(2)}_{1c}$ and $\bar{\Gamma}^{(1)}_{1c}$. Table I [redacted] approximation (LDA), as implemented by the semirelativistic linearized augmented plane-wave (LAPW) method.[15] In all cases we have assumed that the superlattice is matched to a substrate whose lattice constant is the [redacted] bution to R. This can be exemplified by the results for [redacted]



[redacted] $(InAs)_1(InSb)_1$ in CuPt-like structure, plotted in the (110) plane. The contour step size is 4×10^{-3} e/au.^{3} Charges are normalized to 2 e/cell. [redacted] decomposed charge (in units of e) for these states, where $In^{(1)}$ and $In^{(2)}$ [redacted]

[redacted] ature direct band gaps [Eq. (4)] for the four systems forming CuPt-like structure. The numbers in parenthesis are cystal field (denoted Δ_{CF} in Fig. 1) averaged values. The last row gives the change in the spin-orbit splitting $\delta\Delta_0$ relative to their respective averaged binary values. To include spin-orbit interactions, subtract 1/3 $\delta\Delta_0$ from E_g(SL). All energies are in eV.

	GaAs/InAs	GaSb/InSb	GaAs/InSb	InAs/InSb
E_g(binary)[a]	1.52/0.42	0.81/0.24	1.52/0.81	0.42/0.24
E_g(SL)[b]	0.55 (0.58)	0.09 (0.12)	0.27 (0.36)	−0.28 (−0.20)
$\delta\Delta_0$	−0.01	−0.01	0.08	0.08

[redacted]

InAs/InSb: we find that without structural relaxation [where $\delta V(\mathbf{r}) = \delta V^{(\mathrm{chem})}(\mathbf{r})$] band coupling gives $R = 0.39$ eV, while after relaxation $\delta V^{(\mathrm{size})}(\mathbf{r})$ further in- [redacted]

the various states, as illustrated in Fig. 2 for $(\mathrm{InAs})_1/$ [redacted]

valence-band maximum $\bar{\Gamma}_{3v}^{(2)}$ is found to be localized systematically on the heavy atom semiconductor, while the [redacted]

enhances substantially both the wave function localization and the mixing of s character into the valence-band-edge states [Fig. 2(d)] that are pure p states in the cubic binary [redacted]

tems $\delta\Delta_0 \lesssim 0$, while for common-cation systems the negative bowing ($\delta\Delta_0 > 0$) is sizable.

[redacted]

dicted SL gap" E_g (SL) by subtracting the calculated level shifts (Fig. 1) from the experimental[16] (exptl) average of the gaps of the *constituents*

[redacted]

(iii) above would therefore suggest that these SL's will have a larger band gap than the bulk constituent with the [redacted]

ergy denominators[11] ΔE^0 (Table I), consistent with a perturbation theory description. Indeed, since the L_{1c} level is closer in most alloys to Γ_{1c} than is X_{1c}, the level repulsion [redacted]

Our semirelativistic calculations predict that in the [redacted]

given composition x one has additional control over the band gap through variations of the growth parameters that [redacted]

[1]See reviews by R. Triboulet, Semicond. Sci. Technol. 5, 1073 (1990) and in *Materials for Infrared Detectors and Sources*, edited by R. F. C. [redacted]
[4]D. L. Smith, T. C. McGill, and J. N. Schulman, Appl. Phys. Lett. 43, 180 (1983).
[redacted]
Stein, Appl. Phys. Lett. 52, 831 (1988).
[8]D. K. Arch, G. Wicks, T. Tonaue, and J.-L. Staudenmann, J. Appl. Phys. 58, 3933 (1985).
[9]D. L. Smith and C. Mailhiot, J. Appl. Phys. 62, 2545 (1987); C. Mailhiot and D. L. Smith, J. Vac. Sci. Technol. A 7, 445 (1989).
[redacted]
Sci. Technol. B 8, 710 (1990).
[redacted]
[16]*Landolt-Bonstein: Numerical Data and Functional Relationships in Science and Technology*, edited by O. Madelung, M. Schulz, and H. [redacted]

binary constituents (Table II) and $b \approx 0.6$ eV (Ref. 16) is the bowing

[redacted]