$In_xGa_{1-x}As$–$In_yGa_{1-y}As$ strained-layer superlattices: A proposal for useful, new electronic materials

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Strained-layer superlattices grown from lattice-mismatched layers of InGaAs are proposed as useful electronic materials with tailorable electronic properties. The first study of the electronic properties of these structures has been carried out. Band-gap energies are calculated as a function of layer thicknesses and compositions. The results demonstrate for the first time that the lattice constant, band gap, and transport properties of ternary strained-layer superlattices can be independently varied. This new capability could permit InGaAs strained-layer superlattices to significantly broaden the range of applications associated with the InGaAs ternary compound.

Strained-layer superlattices (SLS's) are high-quality superlattices grown from lattice-mismatched materials. The layers in these structures are kept sufficiently thin to ensure that the lattice mismatch is totally accommodated by layer strains,[1–3] so that misfit defects are not generated. Semiconductor SLS's form a new class of materials with interesting and potentially useful properties. For example, an intervening SLS can be used to improve the quality of materials which must be grown over (dislocated) graded layers due to the lack of a conveniently available, lattice-matched substrate.[4,5] This structural property is a consequence of the strains in the SLS layers.

Recently, the first theoretcial[6,7] and experimental[8–10] studies of the electronic properties of SLS's have been carried out. These studies have emphasized the potential of SLS's as useful electronic materials. SLS's allow great flexibility in the tailoring of their electronic properties through the choice of layer materials and layer thicknesses.[6–8] Although these studies have been carried out for SLS's in the GaAsP ternary system, new SLS structures can be grown from a wide variety of lattice-mismatched materials. In this Brief Report, we propose SLS's made from mismatched layers of InGaAs as new and useful electronic materials, and we present the first results on the electronic properties of these structures. Theoretical values of the band gaps of these $In_xGa_{1-x}As$–$In_yGa_{1-y}As$ SLS's are calculated as a function of layer thicknesses and layer compositions. The results provide the first demonstration of the capability of independently varying three material properties (lattice constant, band gap, and perpendicular transport) in ternary strained-layer superlattices.

In order to correctly calculate the energy levels of SLS's it is, in general, necessary to include the appreciable shifts and splittings of the bulk energy bands due to the layer strains.[6] This is in contrast to the case of conventional lattice-matched (e.g., AlGaAs) superlattices, for which strain effects are negligible. For (100) oriented SLS's, the layer strains can be resolved into hydrostatic and (100) uniaxial components.[6,7] These strains affect the InGaAs SLS band gaps by shifting the bulk conduction-band minima of the layers (which form the quantum wells associated with the SLS conduction-band minimum) and by splitting the degeneracy of the bulk valence-band maxima (which form two sets of quantum wells associated with the SLS valence-band maxima). It should be noted that the strain-induced shifts of the bulk (Γ) conduction-band minima of these SLS layers are qualitatively different from those of the previously studied GaP-GaAsP SLS system[7] (in which the bulk conduction-band minima occur at X). These effects have been incorporated into an effective-mass (Kronig-Penney) model. The bulk (unstrained) InGaAs material parameters used in this work are given in Table I. The shifts in the conduction-band minima and valence-band maxima energies of InGaAs per unit strain are calculated by using the experimental parameters of Ref. 11 and the calculated hydrostatic and uniaxial strain components of the layers.[12] Valence-band offsets for the strained $In_xGa_{1-x}As$–$In_yGa_{1-y}As$ heterostructures are obtained by shifting the unstrained band offsets [taken

TABLE I. Values of effective masses and unstrained band minima energies (without valence-band offsets) for bulk $In_xGa_{1-x}As$.

Band minima	m^*/m_e[a]	Energy (eV)
Γ_e	$0.067-0.044x$	$1.424-1.601x+0.536x^2$
Γ_v	0.61	0.0

[a]Based on values given in P. Lawaetz, Phys. Rev. B 4, 3460 (1971).

from electron affinity data to be $\Delta E_v = 0.235(x-y)$] by the strain-induced shifts of the ionization potential.[13]

Results are given in Fig. 1 for the calculated band gaps (E_g) of GaAs–$In_xGa_{1-x}As$ (100) SLS's as a function of the calculated SLS lattice constant in the planes parallel to the interfaces ($a^{\parallel}$). Expressions for $a^{\parallel}$ as a function of superlattice structure are given in Refs. 3 and 6. The different curves are for SLS's with different layer thicknesses. The $a^{\parallel}$ values are varied by changing the $In_xGa_{1-x}As$ composition from the limiting case of $x=0.0$ to $x=0.25$. These compositions correspond to lattice mismatches of $\leq 1.8\%$. For comparison, the corresponding result for the InGaAs ternary is also included. It can be seen from Fig. 1 that the SLS E_g decreases with increasing layer thickness d, for fixed $a^{\parallel}$ (fixed x). This dependence is due to the usual quantum size effects which become important in this layer thickness regime. For fixed d, the SLS E_g decreases with increasing x. This dependence results from the bulk E_g dependence of the $In_xGa_{1-x}As$ layers (which determine the bottoms of the quantum wells) on x. More importantly, these results show that for a given $a^{\parallel}$, a range of SLS band gaps is obtained. Thus it is possible to vary the InGaAs SLS band gap independently of lattice constant, in contrast to the behavior of the bulk InGaAs ternary itself. This capability is one example of the tailorability of SLS properties.

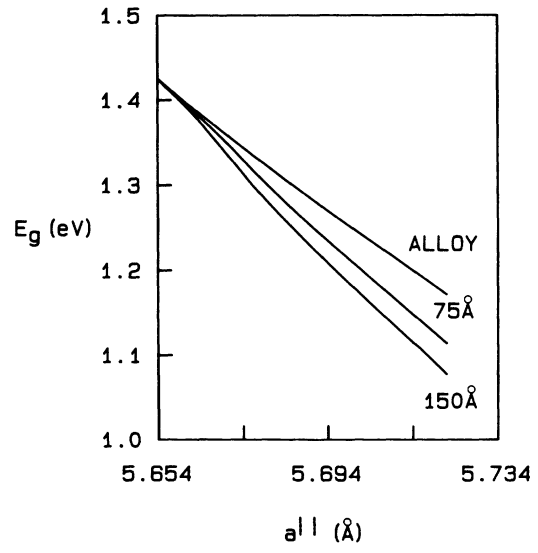

FIG. 1. Calculated band gaps of GaAs–$In_xGa_{1-x}As$ (100) SLS's as a function of SLS lattice constant in the planes parallel to the interfaces. The various curves are the results for SLS's with different layer thicknesses (all of these structures have equal GaAs and InGaAs layer thicknesses). The lattice constant is varied by varying x. The gap vs lattice constant curve for bulk InGaAs is also included for comparison.

Although only one set of discrete E_g vs $a^{\parallel}$ lines is given in Fig. 1, it is possible to get a continuous range of E_g for each $a^{\parallel}$. In Fig. 2, this is illustrated for a set of $In_xGa_{1-x}As$–$In_yGa_{1-y}As$ (100) SLS's with fixed $a^{\parallel}$ (lattice matched to the alloy $In_{0.3}Ga_{0.7}As$). For these structures, x is varied independently ($x \geq 0.3$), and a y value is chosen ($y \leq 0.3$) for each x value such that $a^{\parallel}$ is kept fixed. The different curves are for SLS's with different layer thicknesses. Figure 2 illustrates that both layer composition and layer thickness can be used to vary the SLS band gap. Note that there are many different structures with both the same lattice constant $a^{\parallel}$ and the same E_g. This makes possible the capability of varying other SLS properties independently of both E_g and $a^{\parallel}$. For example, the component of carrier effective mass perpendicular to the SLS interfaces can be affected by the SLS bandwidths which, in turn, are influenced by the SLS layer thicknesses. Calculated values of these effective-mass components for the structures in Fig. 2 indicate that over a factor of 100 variation in mass values can be obtained. In general, these SLS's have four parameters to vary (layer thickness and composition of each type of SLS

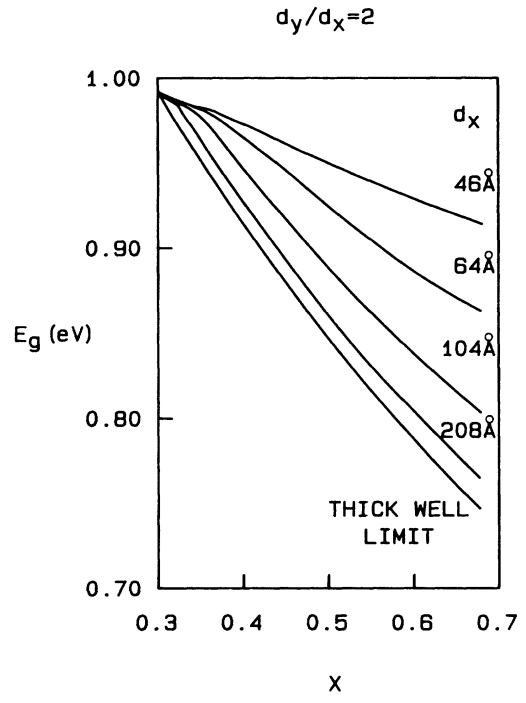

FIG. 2. Calculated band gaps of $In_xGa_{1-x}As$–$In_yGa_{1-y}As$ (100) SLS's with fixed lattice constant parallel to the interfaces (matched to $In_{0.3}Ga_{0.7}As$) as a function of x. For each x, y is chosen to keep the lattice constant fixed. The various curves are the results for SLS's with different thicknesses of the layer with composition x (all of these structures have layers with composition y that are chosen to be twice as thick as those with composition x).

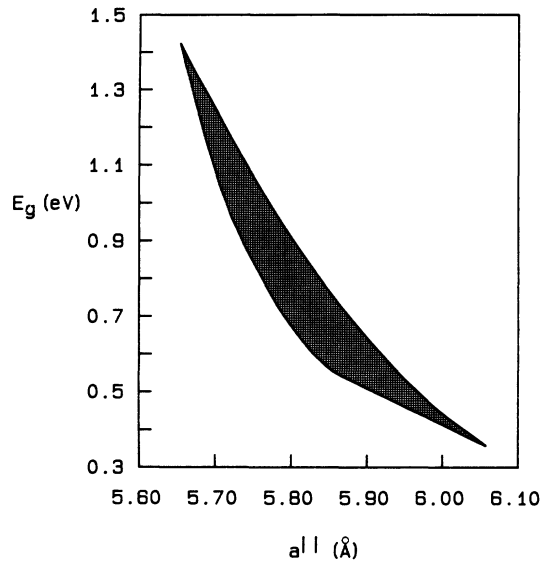

FIG. 3. Calculated range of band gaps vs parallel lattice constant for $In_xGa_{1-x}As$–$In_yGa_{1-y}As$ (100) SLS's obtained by varying layer thicknesses and layer compositions. The obtainable gaps are contained in the shaded area. The upper bound of this area coincides with the gap vs lattice constant curve for bulk InGaAs.

layer) so that, in principle, four material properties might be varied independently.

It is of interest to consider what range of band gaps is possible for InGaAs SLS's. The results of examining a large number of (100) SLS structures give a range of band gaps versus $a^{\parallel}$ represented by the shaded area in Fig. 3. The upper bound coincides with the E_g versus lattice constant curve for the InGaAs alloy. The range increases away from the end points (corresponding to bulk GaAs and InAs) and reaches a maximum of ~240 meV near $a^{\parallel}=5.80$ Å. We note that this range of E_g encompasses the wavelength ranges of interest for optical fiber communication. For each $a^{\parallel}$, the range of E_g corresponds to a new set of lattice-matched SLS materials. These SLS's can themselves be used as the "layers" in lattice-matched heterostructures of arbitrary layer thickness (for which lattice matching is still required to obtain high-quality structures). This capability could significantly expand the number of applications of the InGaAs ternary system.

In conclusion, SLS's grown from mismatched layers of InGaAs have been proposed as useful, new electronic materials with tailorable electronic properites. The first study of the electronic properties of these structures has been carried out. The dependence of the InGaAs SLS band gaps on layer compositions and layer thicknesses has been obtained, as well as the range of InGaAs SLS band gaps obtainable for each SLS lattice constant. The results show for the first time that three material properties (lattice constant, band gap, perpendicular transport) can be varied independently in ternary strained-layer superlattices.

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