

Using superlattice ordering to reduce the band gap of random (In,Ga)As/InP alloys to a target value via the inverse band structure approach

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Thermophotovoltaic (TPV) devices are intended to absorb photons from hot blackbody radiating objects, often requiring semiconductor absorbers with band gap of ~ 0.6 eV. The random $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloy lattice matched $x_{\text{In}}=0.53$ to a 001 InP substrate has a low-temperature band gap of 0.8 eV, about 0.2 eV too high for a TPV absorber. Bringing the band gap down by raising the In concentration induces strain with the substrate, leading to a two-dimensional (2D) \rightarrow three-dimensional (3D) morphological transition occurring before band gaps suitable for TPV applications are achieved. We use the inverse band structure approach, based on a genetic algorithm and empirical pseudopotential calculations, to search for *lattice-matched* InAs/GaAs multiple-repeat unit structures with individual layer thicknesses lower than the critical thickness for a 2D \rightarrow 3D transition. Despite the fact that quantum confinement usually *increases* band gaps, we find a quantum superlattice structure with the required *reduced* gap and a significant optical transition that matches all target requirements. This is explained by the predominance of potential-energy level anticrossing effects over

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strates $n = 5$. One thus needs to consider a more complicated material search problem, allowing for multiple-repeat unit structures $AC_n/BC_m/AC_p/BC_q \dots$. Thus, our problem can be articulated as a search for $InAs_n/GaAs_m/InAs_p/GaAs_q \dots$ multiple-repeat units that: i) have a target band gap of 0.6 eV at low T , ii) have an overall composition that warrants the lattice matching on an InP substrate (53% of In), and iii) have individual InAs and GaAs layers not thicker than the critical thicknesses for the 2D \rightarrow 3D morphological transition (5 MLs).

mum of the structure shown in Fig. 4 c along the 001 direction. It can be seen that both wave functions present the greatest contributions in the InAs-rich segment of the multiple-repeat structure, resulting in a spatially direct band gap. The CBM spreads along all of the InAs-rich segment, while the VBM is more concentrated in the middle part of the InAs-rich segment. As Fig. 4 d shows, the GaAs-rich region constitutes a barrier for both electrons and holes, as it should be expected. The whole band-offset profile shows a type-I-like character, with electron and holes effectively confined in the InAs-rich segment. The thin GaAs monolayers in between InAs-rich segments play the role of strain relievers in the InAs-rich segments and have small influence on the intensities of the CBM and VBM squared wave functions, as can be seen in Figs. 4 a and 4 b . The same role is played by the thin InAs layers in the GaAs-rich part of the structure. Thus, the intercalation of thin GaAs and InAs layers in the InAs-rich and GaAs-rich segments, respectively, reduce the internal strain between the stacking layers of the superlattice while keeping an effective type-I band offset, reducing the band gap to a 0.6 eV target gap. The calculated dipole matrix element square for the VBM \rightarrow CBM transition in the best-matched structure shown in Fig. 4 c is significant, with the transition probability being around 30% of that for the bulk GaAs. Different from the bulk, there is a difference in intensity between the transitions with parallel and perpendicular polarizations. The transitions with perpendicular polarizations 110 directions are 10^2 times stronger than that for parallel 001 polarization. This should be expected once both VBM and CBM levels are concentrated in the InAs-rich layers, which reduces the probability of transitions between InAs and GaAs along the 001 growth direction.

In conclusion, we applied the IBS method in the search for InAs / GaAs structures that lattice match to a 001 InP substrate and have a target band gap of 0.6 eV. We found that a complex multiple-repeat unit satisfies the requirements imposed by the target band gap and the critical thickness of the individual InAs and GaAs layers. The final IBS structure has a spatially direct band gap and a significant VBM \rightarrow CBM dipole matrix element square.

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⁷It is possible to grow mismatched In_{0.08}As_{0.84}n_{811T}.00T4Teo1T810T1TT4T44TeM