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 $In_xGa_{1-x}As$ alloy lattice matched ($x_{In}=0.53$) 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) → 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 → 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 $(n \leq 5)$. One thus needs to consider a more complicated material search problem, allowing for multiple-repeat unit structures $(AC)_n/(BC)_m/(AC)_p/(BC)_q\cdots$. Thus, our problem can be articulated as a search for $(\mathrm{InAs})_n/(\mathrm{GaAs})_m/(\mathrm{InAs})_p/(\mathrm{GaAs})_q\cdots$ 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→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→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→CBM dipole matrix element square.

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