Electronic structure and optical transitions in InAsSb/InGaAs quantum dots

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Self-assembled InAsSb/InGaAs quantum dots are candidates for optical detectors and emitters in the 2-5 micron band with a wide range of applications for atmospherical chemistry studies. While photoluminescence peaks at wavelengths as high as 2.2 μm have been measured in InAsSb dots [1], the present study aims at determining the maximum wavelength theoretically achievable. The energy band gap of unstrained bulk $InAs_{1-x}Sb_x$ is smallest for x=0.62 but biaxial strain for bulk $InAs_{1-x}Sb_x$ grown on $In_{0.53}Ga_{0.47}As$ shifts the energy gap to higher energies and the smallest band gap is reached for x=0.51 (Fig. 1), which seems therefore to be the preferred concentration for long wavelength optical devices. We next examine how the electronic confinement in the quantum dots modifies these simple considerations. We have calculated the electronic structure of lens shaped $InAs_{1-x}Sb_x$ quantum dots with diameter 37 nm and height 4 nm embedded in a $In_{0.53}Ga_{0.47}As$ matrix of thickness 7 nm and lattice matched to an InP buffer (Fig. 2). The relaxed atomic positions were determined by minimizing the elastic energy obtained from a valence force field description of the inter-atomic interaction. The electronic structure was calculated with an empirical tight binding approach with the parameters obtained from Ref. [2]. Figure 3 shows the variation of the energy gap in the quantum dot as a function of the Sb concentration. For concentrations larger than x=0.5, the electrons are not confined in the dot, which results from the conduction band edge in the $InAs_{1-x}Sb_x$ being at higher energy than in the $In_{0.53}Ga_{0.47}As$ matrix. The bulk conduction and valence band edges in Figure 4 clearly illustrate that the InSb/ $In_{0.53}Ga_{0.47}As$ heterostructure is of type II. We will further show the variation of the exciton energy and oscillator strength as a function of Sb concentration throughout the region where the electron is confined in the $In_{0.53}Ga_{0.47}As$ buffer material.

[1] Y. Qiu and D. Uhl, Appl. Phys. Lett. 84, 1510 (2004).
[2] J.M. Jancu, R. Scholz, F. Beltram and F. Bassani, Phys. Rev. B 57, 6493 (1998).

A full journal publication of this work will be published in the Journal of Computational Electronics.

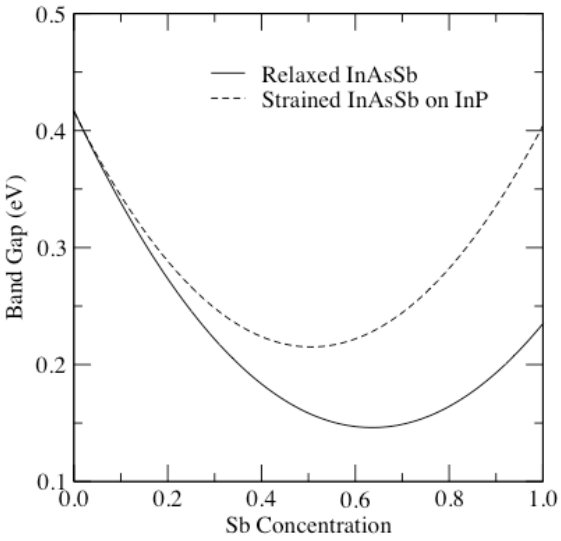

Figure 1: Bulk energy band gap for unstrained and InP lattice matched $InAs_{1-x}Sb_x$ as obtained from experimental band gaps, deformation potentials and elastic constants.

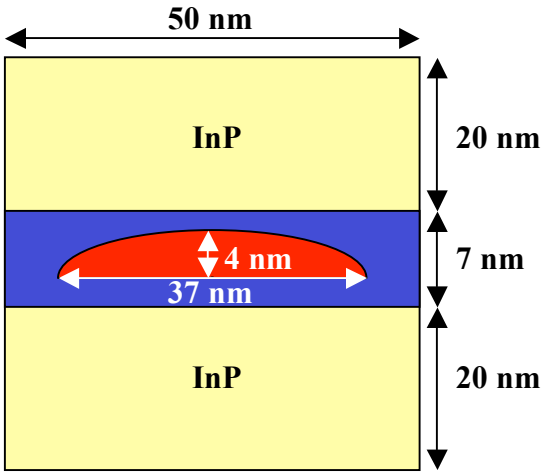

Figure 2: Simulation cell for an $InAs_{1-x}Sb_x$ quantum dot embedded in an $In_{0.53}Ga_{0.47}As$ matrix.

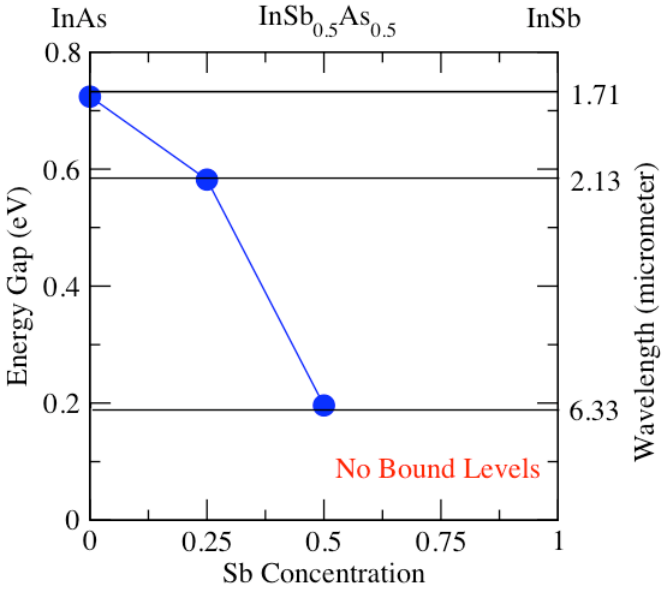

Figure 3: Energy gap in an $InAs_{1-x}Sb_x$/ $In_{0.53}Ga_{0.47}As$ self-assembled quantum dot as a function of Sb concentration.

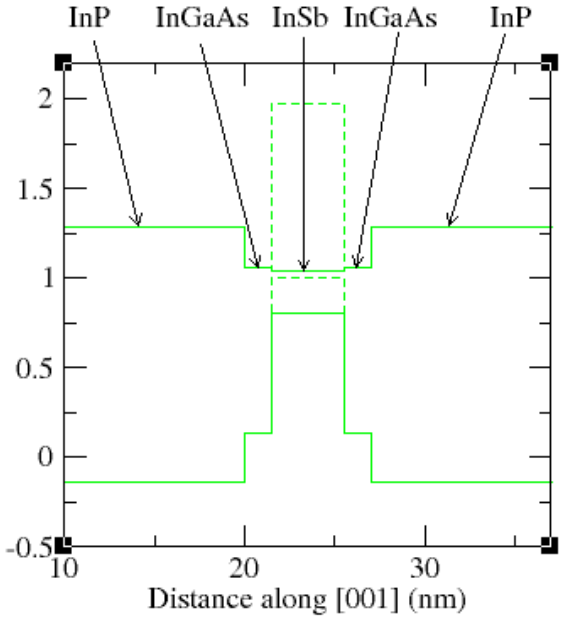

Figure 4: Bulk conduction and valence band edges for unstrained (solid lines) and lattice matched (dashed lines) InSb on $In_{0.53}Ga_{0.47}As$ and InP.

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