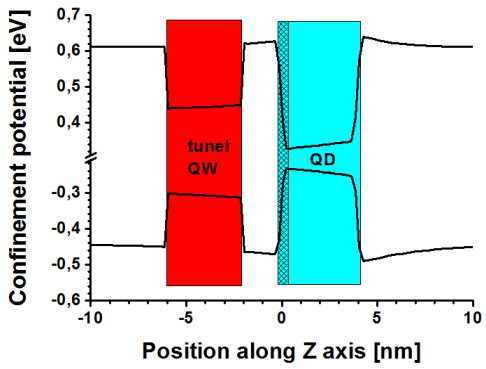
Electronic Structure Calculations of InP-Based Coupled Quantum Dot – Quantum Well Structures

Janusz Andrzejewski [1]

[1] *Laboratory for Optical Spectroscopy of Nanostructures, Department of Experimental Physics, Wrocław University of Technology, Wyb. Wyspiańskiego 27, 50-270 Wrocław, Poland*

The hybrid quantum-mechanical systems combining structures of various dimensionalities are of interest due to still not fully explored electronic, kinetic and optical properties. This in turn makes them prospective in many electronic or optoelectronic applications, with the flag example of quantum dot (QD) – quantum well (QW) tunnel injection lasers [1]. Hereby, we theoretically analyze the electronic structure of a coupled tunneling system considered as to be grown on InP substrate and made of InAs self-assembled QDs or quantum dashes and auxiliary $In_{0.53}Ga_{0.47}As$ quantum well, both separated and cladded in-between the lattice-matched AlGaInAs barriers. The QD electronic levels have been tuned so to get the ground state emission wavelength at the third telecommunication window of 1.55 μm. The typical energy band profile through the center of the QD is presented in the Figure, where the effect of strain distribution slopping the confinement potential is visible.



For the calculations, the own program based on eight-band k·p theory has been used [2]. It has several functionalities necessary for proper calculation of this rather complicated quantum structure. The program is able to calculate the energy levels of a QW in 3D geometric numerical box and it can simultaneously handle QDs of even large sizes with different shapes. The computations are very efficient due to employing especially developed and original preconditioner for calculating the inner eigenvalues of the multi-band k·p models. In addition, the nonlinear piezoelectric effect is included. The realistic morphological parameters and compositional gradients are possible to be taken into account [3].

As the efficient carrier tunnel injection scheme in lasers is based on LO-phonon-assisted tunneling of carriers from a QW to QDs in which the lasing transition occurs, the electronic structure should be so, that the lowest conduction band state and the highest valence band state of the entire system should both be QD-like, and the next higher energy conduction and valence band states should be QW-like. In order to fulfill this condition in the investigated structure the width of the QW and the sizes of the QD have been changed. In order to fulfill the above mentioned requirements, the following has been obtained: (i) the QW width should be in the range of 4÷5 nm; (ii) it is not possible to obtain the proper levels layout for large and asymmetric nanostructures; (iii) smaller symmetric or slightly asymmetric dots/dashes (e.g. 12 x 25 nm) offer to achieve the assumed electronic features. Eventually, the simulations have indicated that the energy levels layout is very sensitive to the band offsets, even in their narrow range values well accepted in the literature.

[1] T. Chung et al. *J. Appl. Phys.* **79**, 4500 (2001).
[2] J. Andrzejewski, *J. Comp. Phys.* **249**, 22 (2013).
[3] A. Maryński et al. *J. Appl. Phys.* **114**, 094306 (2013).