XXXII Panhellenic Conference on Solid State Physics and Materials Science
Conference Center "Carolos Papoulias", 18-21 September 2016, Ioannina, Greece

Finite Element Analysis of Quantum Nanostructures

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The elastic stress-strain fields build-up in III-V compound semiconductor nano-heterostructures, due to lattice mismatch, have a significant effect on their optoelectronic properties, for example the induced changes of levels in the conduction and valence bands and thus, affect the performance of III-V based microelectronic devices. Hence, we have used the Finite Element Method (FEM), in order to obtain an accurate description of the induced stress-strain fields. FEM is a versatile and efficient simulation technique, which can be applied in nanostructures of any geometrical shape, providing the right selection of the appropriate elastic constants. Here, FEM analysis is employed to simulate elastic strain fields, directional deformation and stresses in different quantum nanostructures, where the lattice misfit between the heterostructures is simulated in the framework of thermo-elasticity theory. In particular, we present FEM calculations for three different nanostructure geometries: (111)-oriented GaAs/$Al_xGa_{(1-x)}$As core-shell nanowires (NWs), (111)-oriented GaAs NWs comprising two consecutive $In_xGa_{(1-x)}$As quantum wells, and (211)-oriented InAs/GaAs surface and buried quantum dots (QDs). The effects of the chemical composition of the active regions and size of the heterostructures are studied. Specifically, for the GaAs/$In_xGa_{(1-x)}$As NWs the In concentration varied from 0.25 to 1, while for GaAs/$Al_xGa_{(1-x)}$As core-shell NWs the Al concentration varied from 0.2 to 0.65, respectively. In the latter case, shell-to-nanowire (S/NW) relative diameter ratios of 0.45 to 0.65 were studied and the results were compared with experimental and molecular dynamics results. FEM simulations showed that the strain distribution within the nanostructures is sensitive to both their chemical composition, as well as their size.

Acknowledgements
Work supported by the Research Projects for Excellence IKY/Siemens.