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Nonlinear Strain Models in the Analysis of Quantum Dot Molecules

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Abstract

Strain effects are fundamental to optoelectromechanical properties of low dimensional semiconductor structures such as quantum dots (QDs). Nevertheless, their influence is typically analysed with simplified linear models based on the minimisation of uncoupled, purely elastic energy functionals with respect to displacements. The applicability of such models is limited to the study of isolated idealised quantum dots, and both coupled and nonlinear effects need to be accounted for in the analysis of more realistic structures. The range of applicability of QD-based structures is growing rapidly and include photodectors, laser-based emitters, quantum computing elements, and nano-biological devices to name just a few. These new applications require revising conventional strain models which are becoming increasingly inadequate in the modelling and analysis of these structures.

In this contribution we provide a survey of the existing models and discuss the analysis of a WZ GaN/AlN quantum dot and a QD molecule comprising of an array of several quantum dots. We note that although ab initio atomistic models may be more accurate, being extremely computationally demanding, they are often unpractical for realistic applications mentioned above [1, 2]. In such hexagonal structures as we consider, piezoelectric (as well as spontaneous pyroelectric) polarization effects are strongly nonlinear which make it inadequate to apply methodologies based on superposition principles [3]. Moreover, strictly speaking, one has to account for the fact that built-in strain and electric field effects are not separate processes in such structures. First, we consider the application of a von Kármán nonlinear model to accommodate for the coupling between in-plane and out-of-plane strain contributions. Then, we discuss bandstructure calculation models in the spirit of a modified Rashba-Sheka-Pikus strain Hamiltonian and present some results of computational experiments with these models. Finally, we discuss the influence of different geometries on the optoelectromechanical properties of nanostructures, including recently reported by experimentalists solid-state rolled-up nanotubes [4].

References

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