Influence of aspect ratio on the lowest states of quantum rods

M. Willatzen*, B. Lassen*, R. Melnik* and L. C. Lew Yan Voon†

*Mads Clausen Institute for Product Innovation, University of Southern Denmark, Grundtvigs Allé 150, DK-6400 Sønderborg, Denmark

†Department of Physics, Worcester Polytechnic Institute, 100 Institute Road, Worcester, MA 01609

Abstract. The lowest valence-band states of $In_{0.53}Ga_{0.47}As$ quantum rods with infinite barriers are studied using a four-band Burt-Foreman model. Special emphasis is given to the study of quantum-rod shape dependency and consequences for the aspect ratio at the crossing of the lowest two states. The nonseparability of the problem leads to complex ground-state envelope function (and level crossing) and demonstrates the difference between (infinite) quantum-wire structures and finite quantum-rod structures. Finally, calculations are presented for $In_{0.53}Ga_{0.47}As$ quantum-rod structures embedded in InP. It is found that the aspect ratio at crossing of the two lowest states depends on the quantum-rod radius with InP finite barriers.

INTRODUCTION

A resurgence of interest in quantum wires (QWR's) and quantum rods (QR's) has happened recently due in part to new growth techniques for making free-standing and colloidal structures, [1] and also due to the observation of linearly-polarized photoluminescence in InP nanowires [1] and CdSe QR's [2, 3] and the insensitivity of the interband transition energies on the length of the QR's. [2, 4] Evidently, an understanding of and control over these properties is necessary in order to make use of these nanostructures, e.g., as biological labeling and optoelectronic devices. Nevertheless, the theoretical study of these near-band-edge states is still at a primitive stage. Previous results by Hu *et al.* [2], using empirical pseudopotential theory revealed that a level crossing takes place between the two top valence-band states; however, they considered a rather artificial structure with cylindrical quantum rods embedded in a spherical dot. We present in this paper calculations of the energy levels of the lowest valence-band states of cylindrical QR's as a function of the aspect ratio by varying the cylinder rod length keeping the diameter constant. We also verify that a crossing of the lowest two states depends on the choice of barrier material and (for finite barriers in general) on the quantum-rod radius. This is done by computing energy levels of (a) $In_{0.53}Ga_{0.47}As$ quantum-rod structures with infinite barriers, and (b) $In_{0.53}Ga_{0.47}As$ quantum-rod structures with InP finite barriers using the Burt-Foreman model and following the method of Sercel and Vahala [5].

THEORY

The band structure of the cylindrical quantum-rod structures is calculated using a four-band $k \cdot p$ theory within the axial approximation, following the method of Sercel and Vahala. [5] It involves expressing the $k \cdot p$ Hamiltonian in terms of cylindrical polar coordinates ρ, ϕ, z and noting that a good quantum number (due to axial symmetry) is the projection of the total angular momentum (of the envelope function and Bloch state) along the rod axis (labeled z):

$$F_z = L_z + J_z, \tag{1}$$

where the angular momentum L_z of the envelope function can only take integer values, and the J_z values belong to the $J = \frac{3}{2}$ subspace of heavy-holes (HH's) and light-holes (LH's).

There is a double degeneracy with respect to the sign of F_z due to the presence of time-reversal symmetry and inversion symmetry. Two new features we have introduced into the Sercel–Vahala theory are the use of the Burt-Foreman Hamiltonian [6, 7] (instead of the Luttinger-Kohn one originally used by Sercel and Vahala) and the implementation of confinement. The latter is done exactly as a coupled ρ–z problem, rather than the decoupling assumed by, e.g., Katz *et al.* [4]. The calculations are performed using the finite element method (FEM). Since the FEM is a variational reformulation of the problem interfaces do not need special treatment. Partial differential equations are solved in weak form by integrating equations such that slope discontinuities are captured and the correct result is found even with a fairly sparse grid [8].

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NUMERICAL RESULTS AND DISCUSSIONS

Our results reveal that the two lowest energy levels converge to within 1 meV as a function of the quantum-wire length for a given diameter when the former is approximately 6 times larger than the latter. Of course, this value increases for the higher valence-band energy levels. However, if one is interested in the first state only it can be concluded that the quantum rod behaves like an infinite quantum wire above an aspect ratio of approximately 1:6.

This ratio is higher than that given by Katz *et al.* [4] since they did not require the same accuracy in convergence. In actual fact, their resolution is of the order of tens of meV only. Furthermore, the energy difference we find between the result at an aspect ratio of 1:2 and the converged value is approximately 15 meV. Hence, the variation is outside the resolution of the experiment of Katz *et al.* [4].

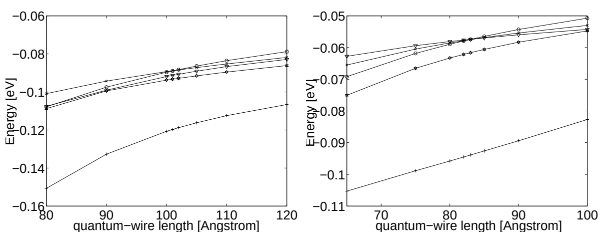

FIGURE 1. Uppermost valence-band structure of $In_{0.53}Ga_{0.47}As$ quantum rods as a function of rod length (all structures correspond to a diameter of 100 Å). Infinite barrier assumption (left) and InP barriers (right).

In Figure 1 (left), we plot the first six energy levels in the valence band near the crossing of the two lowest states slightly above a quantum-wire length of 100 Å in the case with infinite barriers. This value is computed for a diameter of 100 Å, however, our results show that the crossing does not change with the diameter if the aspect ratio is kept constant. In other words, the eigenvalues are related by a constant if the problem is scaled as a whole. In actual fact, inspection of the Hamiltonian and the boundary-conditions reveals this scaling property for infinite barriers. For the range shown [80-120 Å], the variation in energy is seen to be about 20 meV. The plotted curves with line codings: cross, circle, and plus correspond to $|F_z| = 1/2$ while the others (triangle and star) correspond to $|F_z| = 3/2$. Evidently, the nature of the groundstate is $|F_z| = 1/2$ below and above the aspect ratio at crossing.

In Figure 1 (right), we plot the first six energy levels in the valence band near the crossing of the two lowest states in the case with InP barriers for a quantum-rod of radius 50 Å. The aspect ratio at crossing now takes place near 84 Å and the range plotted is from 65 Å to 100 Å. Another significant change with finite InP barriers is that now the uppermost valence-band is a $|F_z| = 3/2$ ($|F_z| = 1/2$) state at aspect ratios below (above) the aspect ratio at crossing. Hence, the presence of a barrier region strongly affects the symmetry and structure of the eigenstates. Again, this complex behaviour is a result of the nonseparability of the problem. In addition, our calculations confirm that the aspect ratio at level crossing depends on the radius of the quantum rod with finite barriers. This is expected theoretically since the mathematical problem for the finite barrier problem does not obey the simple scaling principle applying to the corresponding infinite-barrier problem. Indeed, for a quantum rod of radius 50 (75) Å the aspect ratio at level crossing is 0.84 (0.93).

CONCLUSIONS

An aspect ratio of approximately 1:6 for the convergence of the lowest two states of a QR to within 1 meV is found using FEM calculations based on a Burt-Foreman formulation of the Sercel-Vahala method. A level crossing of the lowest two states is confirmed for our cylindrical QR based upon cubic InGaAs materials. Finite barrier calculations reveal that the aspect ratio at level crossing depends on the radius of the quantum rod and the barrier material. Also, the nature of the two uppermost levels depends strongly on the presence of a barrier material. This is verified by comparing model results obtained using infinite barriers and InP finite barriers.

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