Barrier Localization in the Valence Band of Modulated Nanowires

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Abstract. We present evidence that the phenomenon of inversion recently discovered in a one-band model [L. C. Lew Yan Voon and M. Willatzen, J. Appl. Phys. **93**, 9997 (2003)] is much more general and is present in both multiband theories and in the excited states. A critical radius of around 15 Å (7 Å) is obtained for holes in InGaAs/InP (GaAs/AlAs) modulated nanowires.

INTRODUCTION

A new type of nanostructures, so-called nanowire superlattices or modulated nanowires, has recently been grown [1, 2, 3, 4]. Material systems studied so far include GaAs/GaP [1], Si/SiGe [2], InAs/InP [3], and ZnSe/CdSe [4], and typical dimensions have been radii of 200–400 Å. It is speculated that these structures might find applications as nano bar codes, waveguides, lasers, and LEDs, and that nanowire superlattices are an improvement over plain nanowires. Due to the large radii of the structures grown so far, there is not yet any experimental evidence of novel quantum phenomena in these structures. Here, we are reporting a unique kind of wave function localization due to the longitudinal modulation using a multiband $\mathbf{k}\cdot\mathbf{p}$ theory, whereby the bound states are localized in the barrier layer below a so-called critical radius. We had earlier predicted the phenomenon in the conduction band on the basis of a one-band model [5] and studied the impact of symmetry [6, 7, 8].

THEORY

The valence-band structures of the modulated nanowires with zincblende constituents and with an [001] wire axis were calculated using a four-band $\mathbf{k}\cdot\mathbf{p}$ theory within the axial approximation, following the method of Vahala and Sercel [9]. It involves expressing the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian in terms of cylindrical polar coordinates ρ, ϕ, z and noting that a good quantum number 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). The total wave function is then written as

$$\psi(\mathbf{r}) = \sum_{J_z} f_{J_z}(\rho, z) e^{i(F_z - J_z)\phi} |\frac{3}{2} J_z\rangle, \tag{2}$$

where $f_{J_z}(\rho, z)$ are the envelope-function components. Two new features of our theory are the use of the Burt-Foreman Hamiltonian [10] (instead of the Luttinger-Kohn one) and the presence of confinement along the wire axis.

CALCULATIONS AND RESULTS

The coupled differential equations were solved using the finite-element method. We represented the superlattice structure by using a finite number of periods; it turns out that only a couple of periods are necessary for convergence.

Calculations have been carried out for GaAs/AlAs and $In_{0.53}Ga_{0.47}As$/InP modulated nanowires with layer thicknesses of 20–50 Å and a circular cross-section with radii ranging from 5 Å to 15 Å. The sum squared of the envelope function components for two different radii for GaAs/AlAs ($In_{0.53}Ga_{0.47}As$/InP) nanowires with layer widths of 50 Å (20 Å) are shown in Fig. 1 (Figs. 2–3); the occurence of the inversion is evident in both cases

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(the regions of highest probability densities are the small darkest ones — dark red if in color). In the case of $In_{0.53}Ga_{0.47}As/InP$, Fig. 2 is for the ground state, while Fig. 3 is for the second excited state; it turns out that the critical radius is about the same for the first excited state and the ground state.

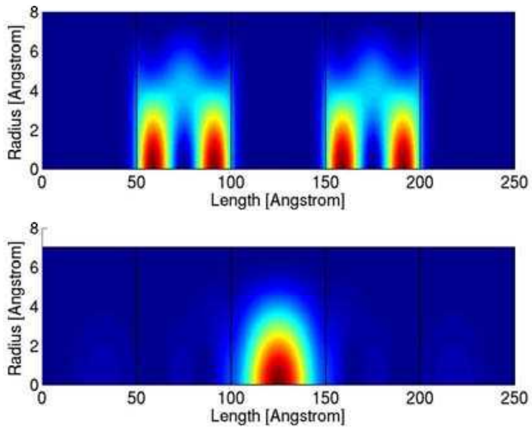

FIGURE 1. Probability density for GaAs/AlAs above and below critical radius.

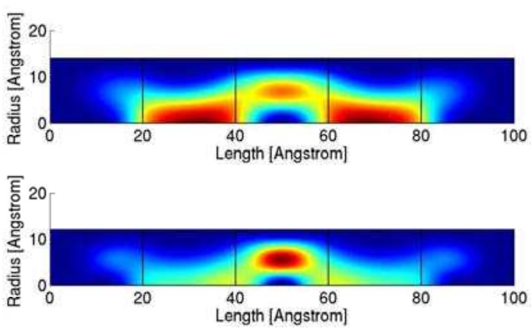

FIGURE 2. Probability densities for the ground state for $In_{0.53}Ga_{0.47}As/InP$ above and below critical radius.

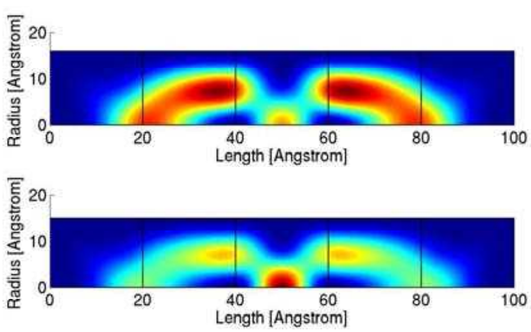

FIGURE 3. Probability densities for the second excited state for $In_{0.53}Ga_{0.47}As/InP$ above and below critical radius.

We have also calculated the critical radii using an analytical one-band model [5]; differences compared to the exact multiband results are of the order of 50%.

SUMMARY

- The existence of critical radii for the inversion of hole states in modulated nanostructures is demonstrated using a multiband calculation.
- There is a dependence of the critical radius on the layer widths.
- Excited states also display critical radii.
- The analytical one-band model is only semi-quantitatively accurate.
- It is proposed to observe the inversion via interband absorption or transport experiments in GaAs/AlAs modulated nanowires of diameters near 40 Å.

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REFERENCES

1. Gudiksen, M. S., Lauhon, L. J., Wang, J., Smith, D. C., and Lieber, C. M., *Nature*, **415**, 617–620 (2002).
2. Wu, Y., Fan, R., and Yang, P., *Nano Lett.*, **2**, 83–86 (2002).
3. Björk, M. T., Ohlsson, B. J., Sass, T., Persson, A. I., Thelander, C., Magnusson, M. H., Deppert, K., Wallenberg, L. R., and Samuelson, L., *Nano Lett.*, **2**, 87–89 (2002).
4. Solanki, R., Huo, J., Freeouf, J. L., and Miner, B., *App. Phys. Lett.*, **81**, 3864–3866 (2002).
5. Lew Yan Voon, L. C., and Willatzen, M., *J. App. Phys.*, **93**, 9997–10000 (2003).
6. Melnik, R., Willatzen, M., Lew Yan Voon, L. C., and Galeriu, C., "Finite element analysis of nanowire superlattice structures," in *Proc. ICCSA Montreal*, edited by C. T. V. Kumar, M. Gavrilova and P. L'Ecuyer, ICCS, Springer, 2003, vol. Part II, pp. 755–763.
7. Willatzen, M., Melnik, R. V. N., Galeriu, C., and Lew Yan Voon, L. C., *Mathematics and Computers in Simulations*, **65**, 387–397 (2004).
8. Galeriu, C., Lew Yan Voon, L. C., Melnik, R. N., and Willatzen, M., *Comp. Phys. Commun.*, **157**, 147–159 (2004).
9. Vahala, K. J., and Sercel, P. C., *Phys. Rev. Lett.*, **65**, 239–242 (1990).
10. Burt, M. G., *J. Phys. Cond. Mat.*, **11**, R53–R83 (1999).