Electronic States in Cylindrical Core-Multi-Shell Nanowire

A. O. Rudakov\textsuperscript{a} and I. A. Kokurin\textsuperscript{a,b,c,*}

\textsuperscript{a} Institute of Physics and Chemistry, Mordovia State University, Saransk, 430005 Russia
\textsuperscript{b} Ioffe Institute, St. Petersburg, 194021 Russia
\textsuperscript{c} St. Petersburg Electrotechnical University “LETI”, St. Petersburg, 197376 Russia
*e-mail: kokurinia@math.mrsu.ru

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Abstract—The recent advances in nanowire (NW) growth technology have made possible the growth of more complex structures such as core-multi-shell (CMS) NWs. We propose the approach for calculation of electron subbands in cylindrical CMS NWs within the simple effective mass approximation. Numerical results are presented for GaAs/Al\textsubscript{0.3}Ga\textsubscript{0.7}As radial heterostructure with AlGaAs-core and 4 alternate GaAs and AlGaAs shells. The influence of an effective mass difference in heterolayers is discussed.

Keywords: nanowire, radial heterostructure, core-multi-shell, electronic states

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1. INTRODUCTION

The recent progress in nanowire (NW) growth technology gives an opportunity to made the NW-based complex structures with so-called axial [1] and radial (core-shell) heterostructuring. Now there is a possibility to grow a large number of shells (see, for instance, reviews [2, 3] and references therein). Such structures known as core-multi-shell (CMS) NWs attract attention of researchers due to interesting properties and possible applications.

Due to a special geometry and the possibility to govern carrier states by means of external fields (electric, magnetic or deformation) the devices based on NW-structures [4] are very attractive for modern electronics and photonics. For example, there are lasers [5, 6] and light-emitting diodes [7] with CMS NW as a work item.

The carrier mobility can increase in CMS structures [8] comparative to continuous NW, that means the possibility of conductance quantization in such structures. Thus, CMS NWs are good candidates for utilizing as the working part of field effect transistors including spin ones.

The realization of multiple quantum wells in CMS NWs can lead to the spatial separation between the electron and hole, that allows one to control the lifetime of indirect excitons [9], which can travel over large distances before recombination, and cool down close to the lattice temperature and below the temperature of quantum degeneracy.

Thus, there is a need to know electron and hole subband spectrum in such structures. Here we develop a simple approach to find electronic states in III–V CMS NW with zinc-blende crystal lattice within single band effective mass approximation (EMA).

2. HAMILTONIAN AND NUMERICAL DIAGONALIZATION

Now we propose the approach for calculation of electron subband spectrum of CMS NWs (see Fig. 1a). We use a single-band envelope function approximation (EFA) to find electronic states in cylindrical CMS NW with zinc-blende crystal structure (starting from bulk \Gamma\textsubscript{6}-band states with scalar effective mass).

In cylindrical NW there are translational and rotational invariance, that means the following form of envelope wavefunction

\[ \psi_{mnk}(r, \varphi, z) = R_{mn}(r) \frac{1}{\sqrt{2\pi}} e^{\text{imp}} \frac{1}{\sqrt{L}} e^{ikz}, \]  

where \( L \) is the NW length, \( k \) is the longitudinal momentum, \( m = 0, \pm 1, \pm 2, ..., n = 1, 2, 3, ... \). The energy spectrum of one-dimensional (1D) subbands is given by

\[ E_{mn}(k) = \epsilon_{mn} + \frac{\hbar^2 k^2}{2m^*}, \]  

where \( m^* \) is the scalar conduction band effective mass, and \( \epsilon_{mn} \) is the energy of 1D-subband bottom.

For the case of uniform cylindrical NW of radius \( R \) applying zero boundary conditions (hard-wall poten-
We can find the Hamiltonian $H_0 + V(r)$ matrix in basis (3). It will contain $\epsilon_{mn}^0$ in diagonal and matrix elements of (5)

$$V_{l}^{mn} = V_0 \sum_{i=1}^{2} \int_{r_i}^{r_{i+1}} dr R_{lm}^0(r) R_{mn}^l(r)$$

in all positions. Where $r_i (i = 1–5)$ is the radius of $i$th radial heterointerface, and $r_0 = 0, r_5 \equiv R$. In chosen basis the matrix elements $V_{l}^{mn}$ can be found analytically [10], but we do not write them here due to their cumbersome form.

The numerical diagonalization was performed for CMS NW with 45 nm radius and the widths of well and barrier regions depicted in Fig. 2 (transparent and shaded areas, respectively). The finite barriers are of 230 meV height, that approximately corresponds to conduction band offset at heterointerface GaAs/Al$_x$Ga$_{1-x}$As with $x = 0.3$ [11]. Effective mass was chosen as in GaAs, $m^* = 0.067 m_0$. We used a finite dimension Hamiltonian of $40 \times 40$ dimension, that gives the perfect precision (better than 0.1%) for first 10 subbands in each block with fixed $m$. Besides 1D-subband bottoms the coefficients $C_{l}^{mn}$ was found giving coordinate dependence of wavefunction in accordance with Eqs. (1), (6), (3).

3. DISCUSSION

The results of numerical diagonalization for first ten 1D-subband bottoms are depicted in Fig. 2 as well as corresponding probability densities $|\Psi|^2$ found from Eqs. (6), (3). One can see an expected behavior of wave function: for low-lying states belonging to the family with the same $m$ the ground and first excited state wave functions are predominantly localized in different wells. For high-lying subbands wave func-
tions will have nodes inside each well region. As in uniform NW the subband ground state corresponding to higher $|m|$-value has a higher energy. However, relative position of subband with $m$ and subband with $m+1$ crucially depends on $V_0$ and relation between $r_r$.

Till now we supposed the equal effective masses both in wells and in barriers. In real structures it is necessary also to take into account a difference of effective masses in different cylindrical layers. In Al$_x$Ga$_{1-x}$As with $x = 0.3$ the effective mass value is $0.092m_0$ [11]. This difference does not distort the translational and rotational symmetry of the structure. However, in this case the motion along and across CMS NW is not formally separated. This means that Hamiltonian matrix remaining diagonal in $m$ and $k$ will parametrically depend on these quantum numbers. In order to include difference in masses into our scheme we have to replace the constant potential $V_0$ in the barrier region (see Eq. (5)) by the following operator

$$\tilde{V}(r) = \frac{\hbar^2}{2m_A} \left( \frac{1}{m_A} \frac{\partial^2}{\partial r^2} + 1 \frac{\partial}{\partial r} - \frac{m^2}{r^2} - k^2 \right) + V_0,$$  

where $m_A$ and $m_B$ are effective masses in wells and barriers, respectively.

The spectral problem in this case can be solved in the same manner but with two differences: (i) the matrix elements of $V(r)$ can be found only numerically; (ii) in order to find $E_{ml}(k)$ one have to diagonalize total Hamiltonian at each $k$ value, giving $\epsilon_{ml}$ to be the function of $k$. This leads to change in subband bottom energy and renormalization of effective masses in different subbands and nonparabolicity as well due to different penetration of wave function into the barriers. These results will be published elsewhere.

4. CONCLUSION

We proposed the approach for calculation of conduction band states in CMS NW. The numerical results for five radial-layer GaAs/Al$_{0.3}$Ga$_{0.7}$As CMS NW of 45 nm radius are presented. This approach can be easily generalized to describe hole states in complex valence band or multiband Hamiltonian in CMS NW of narrow-gap semiconductor.

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

REFERENCES

1. G. Nylund, K. Storm, S. Lehmann, F. Capasso, and L. Samuelson, Nano Lett. 16, 1017 (2016).
2. C. M. Lieber and Z. L. Wang, MRS Bull. 32, 99 (2007).
3. M. Royo, M. De Luca, R. Rurali, and I. Zardo, J. Phys. D: Appl. Phys. 50, 143001 (2017).
4. O. Hayden, R. Agarwal, and W. Lu, Nano Today 3, 12 (2008).
5. D. Saxena, N. Jiang, X. Yuan, S. Mukkapati, Y. Guo, H. H. Tan, and C. Jagadish, Nano Lett. 16, 5080 (2016).
6. T. Stettner, P. Zimmermann, B. Loitsch, M. Döblinger, A. Regler, B. Mayer, J. Winnerl, S. Matich, H. Riedl, M. Kaniber, G. Abstreiter, G. Koblmüller, J. J. Finley, Appl. Phys. Lett. 108, 011108 (2016).
7. K. Tomioka, J. Motohisa, S. Hara, K. Hiruma, and T. Fukui, Nano Lett. 10, 1639 (2010).
8. S. Funk, M. Royo, I. Zardo, D. Rudolph, S. Morkötter, B. Mayer, J. Becker, A. Bechtold, S. Matich, M. Döblinger, M. Bichler, G. Koblmüller, J. J. Finley, A. Bertoni, G. Goldoni, and G. Abstreiter, Nano Lett. 13, 6189 (2013).
9. L. V. Butov, Superlatt. Microstruct. 108, 2 (2017).
10. A. P. Prudnikov, Y. A. Brychkov, and O. I. Marichev, Integrals and Series: Special Functions (Gordon and Breach, New York, 1986), Vol. 2.
11. I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, J. Appl. Phys. 89, 5815 (2001).