Computer simulations of electron transport through a nanowire quantum dot

D. Łapa, A. Sowa and J. Adamowski∗

Faculty of Physics and Applied Computer Science,
AGH University of Science and Technology,
Al. Mickiewicza 30, 30-059 Kraków, Poland
∗e-mail: adamowski@ftj.agh.edu.pl

Semiconductor nanowires, as quasi-one-dimensional conductors, are very promising candidates for constructing nanodevices of future electronics and quantum computing. Recently, the nanowires with single [1] and multiple [2] quantum dots (QDs) have been studied. The nanowire QDs can be used to control the resonant electron tunneling through the semiconductor nanodevices. The present paper is addressed to the electron tunneling through the nanowire with the single QD, which has been fabricated from the InP/InAs/InP double barrier heterostructure grown within the InAs nanowhisker [1]. This nanostructure forms a resonant tunneling diode (RTD) nanodevice with current-voltage characteristics typical to the conventional RTD layer structures. The nanowire RTD [1] is characterized by a pronounced current peak, an extremely large peak-to-valley ratio (50:1), and a negative differential resistance.

We present the results of calculations by a transfer matrix method for the one-dimensional electron transport through the double barrier nanostructure. Instead of the commonly used rectangular approximation of the double barrier potential, we approximate it by the two-center power-exponential potential [3], which takes into account a different softness of the potential barriers. A necessity of using the soft potential barrier results from the interface smoothness (non-perfect sharpness) that has been recently studied for GaAs/AlGaAs nanostructures [4]. The application of the potential with a variable softness allows us to model the realistic profile of the QD confinement potential. The InAs/InP interface exhibits a smearing extending up to 3 lattice spacings [1], moreover, the strain field acts near the interface. The calculations have been performed for the double-barrier potential with the different softness from the soft (double Gaussian) to the hard (rectangular-like) potential. We have also studied the effect of a spacer, which separates the double-barrier nanostructures from the contacts. We have calculated a transmission coefficient as a function of energy of incident electrons and a current as a function of bias voltage. The transmission maxima agree very well with energy levels of quasi-bound states, that have been calculated by an imaginary time-step method. Each maximum of the transmission coefficient results in a peak of the current on the bias voltage scale. We have found that the positions of transmission maxima shift towards higher energies if the confinement potential becomes more soft, which results from the corresponding increase of the confinement energy. This leads to the shift of the position of current peak towards the higher voltage. The best agreement with the experimental data [1] has been found for intermediate softness of the confinement potential with all other nanodevice parameters fixed at nominal values.