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Theoretical modelling of InGaAs quantum rods: terahertz intraband absorption and its dependence on rod height

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Abstract. The electronic structure and the intraband optical properties of self-assembled quantum rods were analysed using a theoretical model based on strain-dependent eight-band $\mathbf{k} \cdot \mathbf{p}$ method. It was found that the intraband optical absorption spectrum for the radiation polarised in the growth direction has one strong peak caused by the transition from the ground state to the state confined in the rod with one node in the growth direction. On the other hand the absorption of in-plane polarised radiation is weaker and is determined by the transitions to mixed quantum well - quantum rod states. The most prominent transitions fall into the technologically relevant terahertz region of the electromagnetic spectrum and can be tailored by engineering the quantum rod height.

1. Introduction

Self-assembled semiconductor quantum dots have attracted a lot of interest in the past decades due to their applications in electronic and optoelectronic devices, which are expected to exhibit better performance than similar devices based on quantum wells. Typical self-assembled quantum dots grown in Stranski-Krastanov mode have height-to-diameter aspect ratio significantly smaller than one. Novel quantum nanostructures, so called quantum rods or quantum posts [1, 2, 3, 4] have recently been realised. Such structures were obtained by the alternating deposition of very short (of the order of monolayer) layers of InAs and GaAs. Subsequent intermixing of InAs and GaAs leads to the InGaAs quantum rod with large height-to-diameter ratio. The height of these structures, and consequently their aspect ratio, can be tailored by the number of deposited layers in contrast to conventional quantum dots where it is more difficult to control the geometry. It is therefore of great importance to develop a theoretical description of electronic and optical properties which would enable the optimisation of quantum rod structures. Initial work in this area was focused on the calculation of energy levels and interband optical properties [1, 2, 5]. In this work, we focus on intraband optical properties, which are of particular interest since the transitions are in the technologically relevant terahertz region and can be adjusted by the height of the quantum rod.

2. Theoretical Considerations

The electronic structure of quantum rods was modelled using the eight-band envelope function $\mathbf{k} \cdot \mathbf{p}$ model [6, 7, 8, 9, 10]. Strain distribution was taken into account using the continuum mechanical model [11]. Numerical calculation of the components of the strain tensor was performed using the finite element method [12]. Rods of cylindrical shape were considered and the axial approximation [13] was introduced. In such a way, the problem was reduced from a three dimensional one to a two dimensional one. The Hamiltonian eigenvalue problem was then solved using the orthonormal function expansion method where the basis was formed from the direct product of Bessel functions in the radial direction and the plane waves in the growth (z) direction. The cylindrical symmetry of the rods introduces a good quantum number of the z -component of the total quasi-angular momentum m_f which takes the half-integer values [13, 14]. The optical transition selection rules then allow only the transitions with $\Delta m_f = 0$ in the case of z -polarised radiation and $|\Delta m_f| = 1$ for x -polarised radiation.

The structures at low temperatures were considered here and therefore it was assumed that only the ground state in the conduction band is significantly occupied. The intraband optical absorption spectrum was therefore calculated by adding the contributions from the transitions from the ground state to each of the excited states. The inhomogeneity of the quantum rod ensemble was taken into account by assuming a Gaussian lineshape with a standard deviation equal to 10% of the transition energy for each of the transitions.

3. Numerical Results and Discussion

The quantum post geometrical parameters and material composition were taken in accordance with experiments from the literature. The diameter was taken to be equal to 10 nm [1]. The height of the rod was varied from 20 nm to 40 nm, which is the typical range of quantum rod heights [1, 2], with a step of 5 nm. The InAs/GaAs short-period superlattice, away from the quantum rod, becomes an InGaAs quantum well layer with an In composition of 16% [1] during the growth of the structure. The In content in the quantum rod is approximately 45% [1]. Such a structure is schematically shown in the bottom part of Fig. 1.

The energy level diagram and the wavefunctions of the most relevant states for the transitions from the ground state are shown in top part of Fig. 1 for the 30 nm high rod. The absorption of z -polarised radiation from the ground state, which has no nodes, is strongest to a state which has one node in the z -direction. This state arises due to quantum confinement effect in the z -direction and its energy is therefore directly determined by the rod height. As a consequence, the intraband optical absorption spectrum of the z -polarised radiation can be directly tailored by the quantum rod height, as can be seen from Fig. 2. For the largest quantum rods (40nm), when the height is significantly larger than the diameter, this state is the first excited state. Therefore, the absorption spectrum for z -polarised radiation is then fully determined by the transition from the ground to first excited state. This situation is dual to the situation in conventional flat-shaped quantum dots where the absorption spectrum of x - polarised radiation is dominated by the transition to the pair of first excited states [13]. In these dots the first excited state arises due to confinement in the lateral direction and therefore it is x - rather than z -polarised radiation that can excite the electron from the ground state.

On the other hand, when the absorption of x -polarised radiation in quantum rods is concerned, one would normally expect (in a quantum rod with infinite potential barrier) that it takes place to a state with one node in the lateral direction. In quantum rods that are narrow such a state should have an energy which is quite high and one would therefore expect that absorption of x -polarised radiation takes place at much larger photon energies than in the case of z -polarised radiation. However, this is not the case in the structure considered here, as can be seen from Fig. 2. One should note that the InGaAs quantum rod confinement potential is rather shallow, as can be seen from Fig. 1. Furthermore, the InGaAs quantum rod is embedded in an

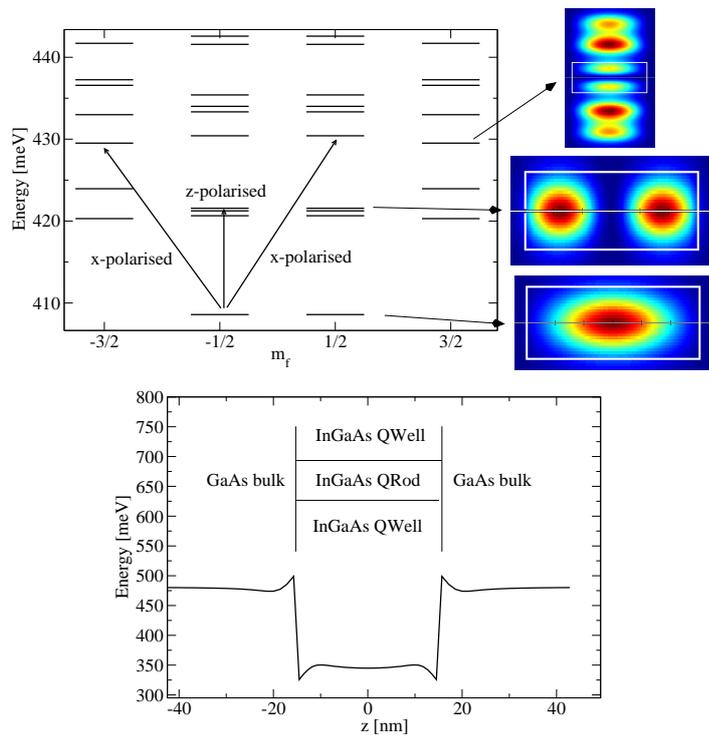


Figure 1. Top: Energy level diagram of the states with $|m_f| \leq 3/2$ for a 30 nm high quantum rod. The transitions that mostly determine the intraband absorption spectrum for incident x - and z -polarised radiation are marked. The contour plots of the wavefunctions of the states involved in these transitions are shown on the right. White lines represent the quantum rod boundary and its axis. Bottom: Effective on-axis potential profile and the schematic view of the structure.

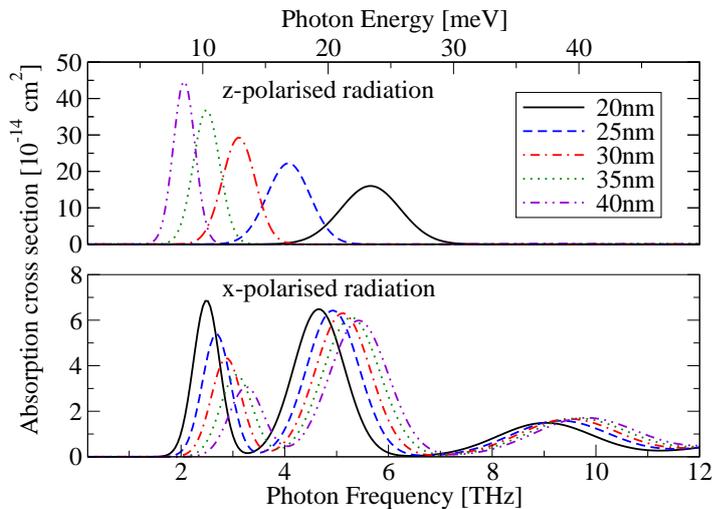


Figure 2. Intraband optical absorption cross section of quantum rods in the case of z - polarised radiation (top) and x -polarised radiation (bottom). The height of each of the quantum rods is indicated in legend.

InGaAs quantum well, which makes the lateral confinement even shallower. As a consequence, the rod with such a shallow potential cannot accommodate the state where the wavefunction has a node in the radial direction and is in the same time confined within the rod. In the rods considered here, the absorption of x -polarised radiation predominantly takes place to the states, such as the one illustrated in Fig. 1 in the case of the 30 nm rod. As can be seen from Fig. 1 the wavefunction of this state is not confined at all to the interior of the rod. This is therefore a mixed quantum rod - quantum well state, with no nodes in the z -direction. The position of such states with respect to the ground state is therefore much less affected by the quantum rod height than for the states with nodes in the z -direction. As a consequence, the shifts in the intraband optical absorption spectrum of x -polarised radiation are much smaller than in the case of z -polarised radiation. Furthermore, the absorption spectrum for x -polarised radiation

is much weaker than for z -polarised radiation, which is fully in-line with the delocalised nature of the excited state to which the absorption takes place.

4. Conclusion

To conclude, we have used the eight band $\mathbf{k} \cdot \mathbf{p}$ model to calculate the electronic and optical properties of a new class of semiconductor quantum nanostructures: self-assembled quantum rods. We found that the positions of the absorption peaks can be tailored by the choice of rod height. The rods respond quite differently to x - and z -polarised radiation. The most prominent transitions fall in the (2–6) THz spectral region which is the region where existing terahertz quantum cascade lasers operate. Consequently, the possibility is opened for integration of quantum rod terahertz detectors with quantum cascade lasers for terahertz sensing applications.

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