Tuning the piezoelectric fields in quantum dots: Electronic and optical properties of [*N*11] grown nanostructures

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Recent advances in growth techniques have made semiconducting quantum dots (QD) and quantum wires grown along [*N*11] directions a reality [1]. In contrast to the traditional (001) orientation, this geometry enables significant piezoelectric fields in the case of polar semiconductors crystallizing in the zincblende structure, such as GaAs, InAs and their alloys. These fields lead to a quantum confined Stark effect, which efficiently affects the optical properties of (*N*11) oriented devices. Consequently, an increasing number of experimental studies has been devoted to such promising systems. However, due to the complex geometry of (*N*11) oriented structures only few theoretical investigations have been performed in this domain.

We theoretically studied the elastic deformation and piezoelectric fields in InAs quantum dots grown on (*N*11) GaAs substrates within the continuum elasticity theory. Our model QD has the shape of a symmetric truncated tetrahedral pyramid, its height is 4 nm and it is located above a 1 nm InAs wetting layer. Particular attention was given to the influence of substrate orientation on both the volume deformation of the dot and the strain-induced piezoelectric field due to the non-zero shear strain. The influence of the piezoelectric fields on the electron and hole ground states for an (*N*11) QD was investigated within the envelope function approach using a position dependent effective mass tensor for the highest valence band obtained from the strain dependent Bir-Pikus 6×6 **k·p** Hamiltonian. All calculations were performed using the next**nano**[3] device simulator that has been developed at the Walter Schottky Institute [2].

Heterostructures made of materials with different lattice constants are subjected to elastic deformations. This volume deformation of the crystal is represented by the hydrostatic strain $\mathrm{Tr}(\boldsymbol{\varepsilon}_{ij})$ and depends strongly on the orientation of the substrate as shown in Fig. 1 for a pyramidal shaped InAs quantum dot embedded in a GaAs matrix. As these quantum dots differ with respect to their strain fields, different piezoelectric potentials act on them (see Fig. 2) that alter the conduction and valence band edges. We note that the piezoelectric field has the highest magnitude for the (111) growth direction. The field gets smaller with increasing *N* and finally vanishes for the case of [100] growth direction (not shown here). Due to the nature of the piezoelectric effect, the sign of the piezoelectric charge depends on the atomic composition of the

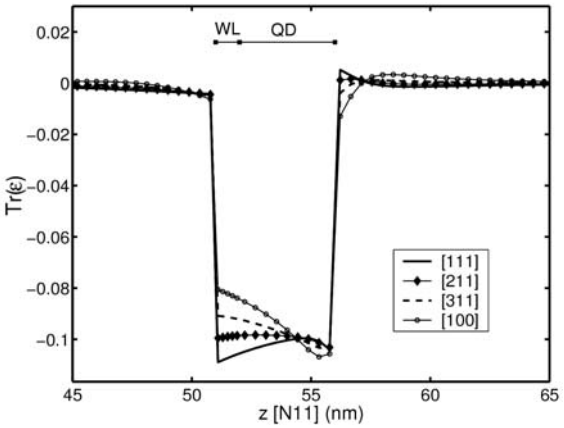

Fig. 1: *The hydrostatic strain along the fourfold QD symmetry axis for four different orientations of the substrate (111), (211), (311) and (100). The 1 nm InAs wetting layer (WL) and the InAs QD (height 4 nm) locations are indicated.*

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interface. We thus have to distinguish between the substrate's Ga planes, referred to as (*N*11)A, and the As planes, referred to as (*N*11)B. From a computational point of view, these two cases differ in the sign of the piezoelectric constant. There are two reasons for the piezoelectric charge existence, namely the discontinuity of the piezoelectric constant at the interface and the non-zero gradient of strain. We find that the piezo charge distribution in (*N*11) QDs has a dipole symmetry rather than a quadrupole symmetry as was found for (100) oriented dots [3].

Our study enables us to consider two effects on the electron and hole states, namely the effect of strain and the effect of piezoelectric charge. The effect of strain in our model does not depend on the substrate termination type but the piezo effect does. The electron and hole eigenstates were obtained as the solutions of the one-particle Schrödinger equation. In order to investigate the role of the piezoelectric field, we calculated the fundamental transition energy without any piezoelectric field and with the field, for both the A and B type substrate. We found that the fundamental transition energy can either be reduced or enlarged by the piezoelectric field. This is because the electric field can increase or decrease the spatial separation of the electron and hole wavefunctions that already exists due to the non-symmetric strain pattern. Its influence on the eigenfunctions is larger in the case of (*N*11)A substrate than in the case of (*N*11)B substrate (not shown here). The opposite is true for the eigenenergies, the corresponding energy shift is plotted in Fig. 3. We see that the effect has different sign depending on the substrate termination, and different magnitude which increases as the [*N*11] growth direction deviates from [100] towards [111] direction.
Our calculations demonstrate that by varying the growth direction and the substrate termination type, it is possible to tailor the built-in electric field, and thus the optical transition energy of these QD systems. [4]

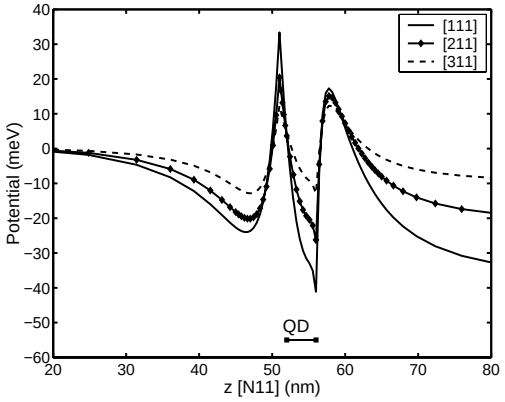

Fig. 2: *The piezoelectric potential along the QD symmetry axis calculated for three different orientations of the substrate; (111)A, (211)A and (311)A. The QD location is shown.*

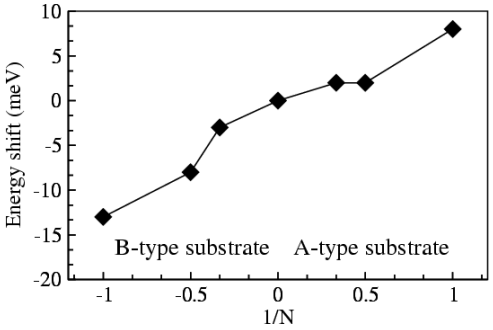

Fig. 3: *The fundamental transition energy shift due to the piezoelectric effect with respect to the case of no piezo effect. The axis of abscissae indicates the substrate orientation. Positive numbers correspond to (N11)A substrate, negative numbers to (N11)B.*

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[2] next**nano**³ - next generation 3D nanodevice simulator
The software is available from www.wsi.tum.de/nextnano3 and www.nextnano.de.
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