Modeling of purely strain-induced GaAs/InAlAs quantum wires

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Cleaved edge overgrowth (CEO) quantum wires (QWRs) at the intersection of two perpendicular quantum wells (QWs) where the (100) QW and the (011) QW are of type I, thus allowing for electron and hole confinement, have shown to provide enhanced exciton binding energies and a concentration of the oscillator strength. At the T-shaped intersection a one-dimensional QWR running along the direction perpendicular to the (0-11) plane is formed because electron and hole wave functions can expand into a larger volume. For clear one-dimensional characteristics at room temperature, a large energy separation between the constituting two-dimensional QWs and the QWR is needed. The optimization of this confinement energy was sought by a variety of groups using unstrained and strained structures. Here, we theoretically studied strained QWR structures that were grown using the CEO technique and consist of a single QW only. Strong carrier confinement is achieved purely by lateral strain variation within the QW which is promising for the development of room temperature devices. In the first growth direction an InAlAs layer serves as the stressor material. Growing a GaAs QW directly on the cleaved (011) plane in a second growth step results in a strongly strain modulated T-shaped structure.

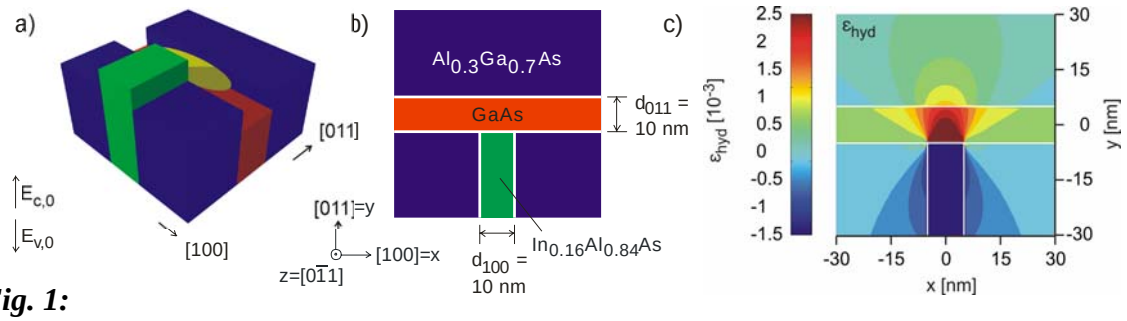

Fig. 1:
a) Conduction $E_{c,0}$ (or valence $E_{v,0}$) band edge without considering strain effects. The position of the wave function is indicated. b) Schematic of the strained T-shaped QWR structure. The 10 nm GaAs QW is grown on the cleaved edge of a strained $In_{0.16}Al_{0.84}As$ barrier. c) The hydrostatic strain (trace of the strain tensor, i.e. relative change in volume) has its maximum at the intersection, where it leads to a reduced band gap which is the requirement for confining the charge carriers. Thus, the QWR is formed in the GaAs QW due to the tensile strain field induced by the $In_{0.16}Al_{0.84}As$ layer.

In the sample sketched in Fig. 1b), the $In_{0.16}Al_{0.84}As$ barrier layer (width 10 nm) has a larger lattice constant than $Al_{0.3}Ga_{0.7}As$ and thus is subject to tensile strain in the [100] direction, which is transmitted to the overgrown GaAs QW (width 10 nm) where a QWR is formed at the lateral positions of the stressor layers. Since this direct growth on the cleaved edge leads to strong strain modulations, large confinement energies were predicted for such structures. Here, we present results of computations with the nano device simulator next**nano**[3], which was used for the optimization of the sample layout. The strain tensor was calculated by minimizing the elastic energy within continuum elasticity theory, where the unit cells were allowed to deform in the (*x*,*y*) plane only. Along the translationally invariant *z* direction the lattice commensurability constraint forced the InAlAs layer to

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adopt the lattice constant of $Al_{0.3}Ga_{0.7}As$. The new conduction and valence band edges were determined by taking into account the shifts and splittings due to the relevant deformation potentials. The strain-induced piezoelectric fields were obtained by solving Poisson's equation. Finally, the 2D single-band Schrödinger equation had to be solved for the electron and heavy hole eigenenergies and wave functions within effective-mass theory using the envelope function approximation in a self-consistent Schrödinger-Poisson cycle. For the electrons we assumed an isotropic effective mass tensor, whereas for the heavy holes an anisotropic effective mass tensor (GaAs: $m_{100} = 0.350\ m_0$, $m_{011} = 0.643\ m_0$) was derived from the Luttinger parameters. At the interfaces all material parameters varied steplike. Fig. 2 depicts the electron and hole probability densities in a strained $GaAs/In_{0.16}Al_{0.84}As$ QWR. The separation of the electron and hole wave functions, which unfortunately reduces the overlap integral that is important for optical transitions, is an effect of piezoelectricity. Neglecting the piezo effect results in symmetric probability densities as shown in Fig. 2a). It is important to realize that the confinement is purely due to strain. If the strain is neglected it is not possible to confine charge carriers at the T-shaped intersection. In Fig. 3 the calculated confinement energy, which is the difference between the electron-hole ground state transition energies of the QW and the QWR, is plotted and compared to experimental results of spatially resolved micro-photoluminescence measurements. While the rising of the confinement energy with increasing stressor layer thickness and increasing width of the overgrown QW is very well reproduced with our single-band approach, the calculated absolute values do not match the experimental data perfectly well. Confinement energies in the range of 50 meV with respect to the corresponding energy for the QW are obtained, which is approximately twice the value of k_BT at room temperature. To enhance the overlap of the electron and hole wave functions the $In_{0.16}Al_{0.84}As$ layer can be replaced by quaternary $In_{0.16}Al_{0.84-x}Ga_xAs$. With increasing x the band gap of the stressor layer gets smaller without relevantly changing the strain configuration. The simulations show that for x=0.7 the electron wave function is located closer to the center of the hole wave function than shown in Fig. 2.

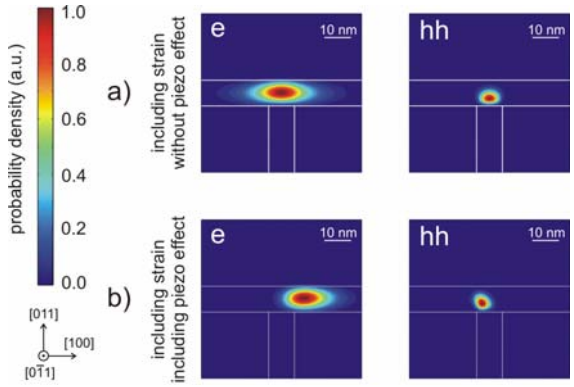

Fig. 2:
Contour plots of the calculated probability densities of the electron (e) and heavy hole (hh) wave functions. The units are scaled so that the maximum value equals 1.
a) without piezoelectric fields
b) including piezoelectric fields

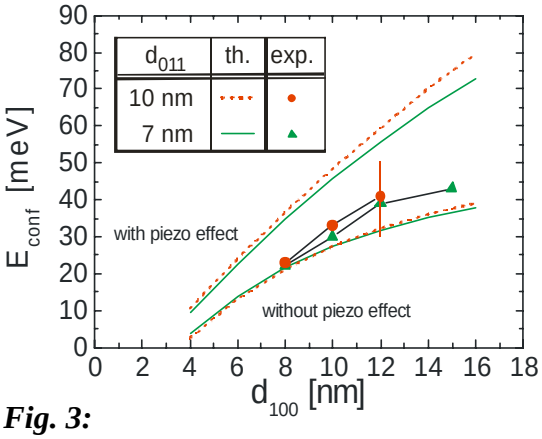

Fig. 3:
Theoretical (th.) and experimental (exp.) values of the confinement energies E_{conf} of strained $GaAs/In_{0.16}Al_{0.84}As$ QWRs where the thickness of the stressor layer and the QW were varied. The piezo effect clearly enhances the confinement energy.

[1] The next**nano**³ software package can be downloaded from www.wsi.tum.de/nextnano3. Support is available through www.nextnano.de.