Effects of strain and confinement on the emission wavelength of InGaAs quantum dots due to a GaAsN capping layer

Stefan Birner¹, Oliver Schumann², Lutz Geelhaar² and Henning Riechert²

For optical fiber applications quantum dot (QD) lasers emitting at 1.3 and 1.55 µm are of great interest because of predictions for improved laser properties like lower threshold current density and reduced temperature sensitivity compared to quantum wells. A lot of investigations have been made to expand the emission wavelength of QDs towards 1.3 µm. This is done mainly by lowering the growth rate, embedding the QDs into an InGaAs quantum well or stacking of QDs. Another successful approach to reach 1.3 µm on GaAs substrates is the incorporation of nitrogen into the material surrounding the QDs where nitrogen reduces the lattice constant and, thus, also reduces the overall compressive strain in the sample formed due to the larger lattice constant of the QD material. These prospects have recently encouraged some investigations to examine the influence of nitrogen incorporation into the surrounding matrix material. The use of GaAsN as a capping layer for the QDs allows a wavelength extension of more than 100 nm. This wavelength extension is often attributed to the relief of the strain inside the QDs which is ascribed to strain compensation. However, we showed through our simulations that the opposite is the case. Although the GaAsN matrix leads to a reduction in the hydrostatic strain in the material surrounding the QDs, the hydrostatic strain inside the QDs increases. This strain inside the QDs can strongly change their emission wavelength. Therefore, exchanging the GaAs capping layer with a material of different lattice constant is expected to allow a tailoring of the emission wavelength of the QDs.

In addition, the electronic confinement of the QD, *i.e.* the height of the potential barrier formed by the conduction and valence band offsets of the QD and of the matrix material due to the different band gaps has an important influence on the emission wavelength as well. Increasing or decreasing the confinement results in a blueshift or redshift of the emission wavelength, respectively. Fig. 1 shows the conduction and valence band profile for two different matrix materials together with a sketch of the QD structure.



Fig. 1:

Conduction and valence bands as obtained from the simulations with a nitrogen content of 1.2% in the 10 nm thick GaAsN layer above the InGaAs quantum dot (QD) and the reference structure without nitrogen. The band structure is taken along a line in growth direction through the center of the QD. One can clearly see that the confinement of the electrons is reduced significantly due to the incorporation of nitrogen around the QD. The wetting layer (WL) consists of $In_{0.25}Ga_{0.75}As$ whereas the In content in the QD varies linearly from 25% to 100% at the top.

¹phone:+49-89-289-12752, fax:+49-89-12737, email: stefan.birner@nextnano.de ²Infineon Technologies AG Our experiments and simulations showed that a GaAsN capping layer grown on InGaAs QDs induces a strong redshift of the emission wavelength and extends it beyond 1.3 μ m (Fig. 2). In order to understand this behavior, we investigated this effect systematically by changing the nitrogen content in the GaAsN layer, varying the thickness of this layer and by embedding a GaAs spacer layer between the GaAsN layer and the QDs. We simulated the band structure and the electron and hole energy levels based on 6×6 **k**•**p** calculations including strain, deformation potentials and piezoelectric effects using the 3D device simulator next**nano**³ [1]. The QDs in our simulations have the shape of a symmetric truncated pyramid and the geometrical and alloy profile parameters for modeling the QDs were taken from XSTM measurements of our grown samples. The wetting layer underneath the QD is 2 nm thick and has an In content of 25% whereas the In content inside the QD varies linearly from 25% at the bottom to 100% at the top of the QD.

By means of our simulations we have shown that the strain inside the QDs is almost unaffected by the incorporation of moderate amounts of nitrogen (~ 1-2%) into the GaAs capping layer and cannot explain the observed increase of the emission wavelength. Instead, we conclude from comparisons between experimental data and simulations that the extension of the wavelength is caused by the strong reduction of the conduction band energy in the GaAsN layer (with respect to GaAs) and the hence resulting reduction of the confinement of the electron wavefunction in the QDs. The origin of the reduction of the conduction band energy is a special feature of the so-called *diluted nitride* semiconductor material GaAsN where the incorporation of small amounts of nitrogen leads to the formation of a narrow impurity band that lies energetically above the conduction band. The coupling of this impurity band to the conduction band leads to a reduction of the conduction band energy and thus to a decrease in the band gap energy. We modeled this band gap reduction by appropriate bowing parameters that were extracted from the widely accepted band-anticrossing model for diluted nitrides.

Furthermore, we showed both experimentally and by means of simulations that the insertion of a GaAsN layer below the QDs yields only a very small change in wavelength in contrast to the GaAsN capping layer.



Fig. 2:

Emission wavelength of the QDs at 300 K as a function of the thickness of the GaAsN_{1.2%} capping layer. The squares correspond to the experimental and the triangles to the simulated data. We varied the thickness of the GaAsN layer from 0 to 20 nm. A strong redshift of the emission wavelength is observed for increasing thickness of the GaAsN capping layer. At a thickness of about 10 nm, this redshift

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