Design and Fabrication of Nitride Heterostructures for Intersubband Applications

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Abstract. Models based on the effective-mass approximation and Schrödinger-Poisson calculations were used to design AlN/GaN multiple quantum well structures for intersubband transitions. The structures were grown by molecular beam epitaxy and the surface morphology and the structural quality were investigated. GaN waveguides were fabricated using standard cleanroom techniques. This report is concerned with the various challenges encountered when trying to fabricate quantum cascade lasers based on group III-nitrides. The challenges are discussed in the light of our results.

Keywords: QCL, GaN, short wavelength

1. Introduction

Photonic devices with intersubband transitions have several advantages over the common interband ones. The main application of intersubband devices is for quantum cascade lasers (QCL). Such lasers constitute a large research field and about 20 companies worldwide are involved in commercial enterprises concerning QCLs. The common use is for lasers within the mid-IR spectral range, 5-25 µm, for spectroscopy and chemical detection of trace elements in liquids and gases. Large research efforts are made to extend the applications to shorter or longer wavelengths. These spectral ranges depend on the applications. The mid-IR is for detection, and spectroscopy, of chemical compounds. Far-IR, λ > 50 µm is for THz-applications. There is a new spectral area of interest for λ < 5 µm (short wavelengths). Commercial QCLs are available from 3.25 µm and up. This shortest wavelength represents the vibration frequency of one of the lightest organic molecules: C-H. In a range below this, 1.55 – 3.25 µm, we have telecommunication either in traditionally fibres, in plastic fibres or in free space. A new rapidly expanding application area for the short wavelengths is countermeasures for airplanes.

Existing QCLs are made of AlGaAs/GaAs, InGaAs/InAlAs/InP, InGaAs/AlAsSb/InP or InAs/AlSb/InAs. The parameters that determine the properties of the device are the material combination giving the conduction band edge offset, the layer compositions and thicknesses and the strain due to lattice constant mismatch. The theoretical limit for λ in the InAs/AlSb material is ~2.7 µm. Additionally the intensity in QCLs is reduced with reduced wavelength. For shorter wavelengths we need a material heterostructure with larger band offset, which is fulfilled in AlN/GaN. In the nitrides, however, a new parameter is incorporated; the polarization, which provide an electric field across the individual layers, cf. Fig. 1.

Fabricating intersubband devices based on group III-nitrides, eg. GaN and related alloys, is challenging with respect to epitaxy, design and device processing [1-6]. Substrates, such as sapphire and SiC, are commonly employed in nitride epitaxy due to the lack of commercially available nitride substrates that have

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both a sufficiently high structural quality and a large area. The consequence of heteroepitaxy on dissimilar substrates, is a high defect density in the (Al,Ga)N/GaN structures due to the large lattice mismatch between substrate and layer. This high defect density has a negative impact on the device performance. The intrinsic internal electric fields across heterostructures grown along the c-direction represent a challenge since these electric fields may effect both electron confinement and efficient current injection. The target emission wavelength for nitride intersubband structures is between 1.55 and 3 µm [7-9]. This target wavelength requires 0.5-1.5 nm wide barriers and homogeneous and abrupt AlN/GaN heterointerfaces. This is challenging from an epitaxial point of view since a very precise control over the layer thickness must be maintained throughout the full quantum cascade laser (QCL) structure [10-13] which can consist of 15-75 (Al,Ga)N/GaN periods [14,15]. To achieve efficient n-type doping of Al\textsubscript{x}Ga\textsubscript{1-x}N alloys with a high Al-content is yet another challenge [16].

In this report we outline the various challenges related to the fabrication of nitride-based QCL structures, which we have investigated. Based on the effective-mass approximation and self-consistent Schrödinger-Poisson calculations we have modelled an AlN/GaN QCL structure.

2. Modelling

The intrinsic electric fields across heterostructure layers, shown along the c-direction in Fig. 1, influence the electron confinement due to the QW distortion. The short 1.55 - 3 µm wavelengths require 0.5-1.5 nm wide homogeneous barriers with abrupt AlN/GaN heterointerfaces. Intersubband transitions were calculated in systems with two or three energy levels [17-18]. This design was used as the basis for our experiments to cast light over the challenges related to device simulation, epitaxy, characterization and device processing [19]. In Fig. 1 the principal function of a simple 2-level QCL-structure is shown when under bias. The electron is injected in the ground state of the first deep QW and relaxes to a state in the neighbouring deep QW before this is emptied. The energy difference in the diagonal transition represents the emission wavelength. Details of the band structure calculations are shown in [17].

![Figure 1. QCL-design based on a diagonal transition for high quantum efficiency. The initial well on the right hand side enhances the injection and lowers the internal voltage drop over the active structure.](image)

3. Experiment

Our structures were grown in a Gen-II plasma-assisted molecular beam epitaxy (MBE) system using Al- and Ga-solid sources. Active nitrogen was obtained from an SVT radio frequency N-plasma source. The heterostructures were deposited on c-sapphire substrates as well as 3-4 µm thick GaN(0001)/c-sapphire templates. The GaN template layers had a threading dislocation density of ~10\textsuperscript{8} cm\textsuperscript{-2} or more. All structures were grown at 800°C under Ga-stable conditions. The growth rate was 300 nm/h for both AlN and GaN.

The crystal quality was investigated with X-ray diffraction (XRD) by recording Ω-2Ω-scans across the (0002) reflection. The surface morphology was characterized by a Veeco Dimension 3000 atomic force
microscope (AFM) and a JEOL JSM-6301F scanning electron microscope (SEM). Cross-sectional transmission electron microscopy (TEM) was used to investigate the microstructure. Temperature dependent absorption measurements were previously performed to investigate the temperature stability of the absorption peak [18].

4. Results and discussion

Figure 2 shows an $\omega$-2$\Theta$ XRD scan across the GaN(0002) reflection from an intersubband superlattice structure consisting of 20 periods of 3.2 nm AlN and 2.1 nm GaN. The superlattice was grown on a 100 nm buffer on a GaN template. A 100 nm thick cap layer concluded the structure. The lower (red) curve denotes the simulated XRD profile whereas the upper (blue) curve denotes the experimental result. A relatively good match between experiment and simulation can be observed evidencing that the desired period thickness has been achieved. The inset in Fig. 2 displays a cross-sectional TEM micrograph obtained from a section of the superlattice. The bright layers correspond to the AlN barriers and the dark layers are the GaN wells. Both layers are sharp and homogeneous throughout the depicted section indicating a precise control over the epitaxial growth conditions and homogeneous atomic planes in the thin individual layers.

Crack formation is observed on sample surfaces as revealed by AFM. This is expected on structures grown on GaN buffer layers, which exert a tensile strain on the AlN barrier layers [20]. Temperature-dependent absorption measurements show that the redshift of the absorption peak is very small, only 15 $\mu$eV/K [18].

A waveguide for AlN/GaN based QCLs was designed and grown on c-sapphire. This structure consists of a 500 nm thick gain region sandwiched between 500 nm thick n-doped AlGaN injection and extraction layers but does not include an active region. The width of the waveguide is 8 $\mu$m and is located next to the 5
µm wide top metal contact. Injection occurs laterally and requires a second side contact. The white elliptical area indicates the well confined, guided low loss TM polarized mode (see the inset in Fig. 3). It has been shown that a single mode QCLs can be obtained using proper design parameters [21].

Figure 3. SEM micrograph of a GaN waveguide designed according to the QCL design shown in the inset. This structure was used to optimize the dry etching processing parameters and does not include any active region. Nearly vertical sidewalls and smooth surfaces can be observed. The white elliptical area in the inset indicates the guided low loss TM polarized mode. Proper design parameters are expected to yield a single mode QCL.

5. Conclusions

In this work we have focused on the challenges related to the fabrication of a nitride-based QCL emitting between 1.55 and 3 µm. To summarize, these challenges include the lack of large area native nitride substrates having a sufficiently low defect density, non-flat-band conditions due to the internal electric fields, crack-formation due to large lattice mismatch between structure and to substrate, weak intersubband luminescence and inefficient current transport through the heterostructures. We have highlighted and investigated the feasibility of several of the critical fabrication steps to obtain MBE-grown intersubband heterostructures. We have shown that a very precise control of the epitaxial process can be achieved. This is necessary for keeping the uniformity and homogeneity throughout the structure, which might consist ~150 periods. The obtained layers are sharp and homogeneous but the structures exhibit cracks. The intersubband transitions are insensitive to temperature as only a weak dependence of the absorption peak on temperature was observed. This speaks for the assumption that efficient and stable nitride QCLs can be made to operate without external cooling systems. Further, we have fabricated GaN waveguides suitable for a QCL.

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7. References
