Motivation

→ GaP:N as novel material for light emitters/detectors in the visible spectral range
→ crossover from indirect to direct material theoretically predicted
→ strong decrease of the band-gap energy with increasing nitrogen concentration experimentally observed

Results

→ growth of GaP$_N$ ($y < 0.10$) single layers and GaP$_x$Ga$_{1-x}$N$_y$superlattices on GaP substrates with orientations (001), and (001) with 5° off towards [110]
→ increased N-incorporation on miscut substrates
→ photoluminescence (PL): redshift of PL-peak with increasing y, y-disappearance of phonon replicas for y > 0.0135 as possible hint for indirect to direct crossover
→ transmission (TM): redshift of N-induced absorption tail with y, absorption peaks due to excitation bound to NN-pairs
→ ellipsometry (MIR): detection of a GaP$_{0.97}$N$_{0.03}$ (366 cm$^{-1}$) and a GaN$_{0.97}$N$_{0.03}$ (450 cm$^{-1}$) like phonon; linear increase of the amplitude of the GaN-like phonon open possibility to measure y independently
→ ellipsometry (MIR-UV-VUV): detection of 6 critical point transitions at the Γ point (E$_{\Gamma}$, E$_{\Sigma}$, E$_{\Delta}$, and along the $[111]$, $[110]$, and $[100]$ directions) $\Delta E$ to $\Sigma$ and $\Delta$, respectively; blueshift of E$_{\Gamma}$, $\Sigma$, and $\Delta$ with y, and small y-dependence of all other detected CPs indicate that the direct $\Gamma$, $\Sigma$, and $\Delta$ transitions do not show the N-induced redshift of the absorption tail

GaP$_N$ single layers

→ GaPN single layers
→ high-resolution x-ray diffraction
→ GaP$_N$ (y = 0.06%)
→ GaP$_N$ (y = 0.009%)

GaP/GaP MQW's

→ GaP$_{0.97}$N$_{0.03}$ (366 cm$^{-1}$) and a GaN$_{0.97}$N$_{0.03}$ (450 cm$^{-1}$) like phonon; linear increase of the amplitude of the GaN-like phonon open possibility to measure y independently
→ increased N-incorporation on miscut towards [110] miscut compared to (001) GaP substrates
→ increased gas-phase composition of Ga$_2$N$_3$N$_y$ compared to the growth of Ga$_2$N$_3$N$_y$N$_z$ due to the higher P partial pressure

Photoluminescence

→ impurity limit ($y = 0.006$%): luminescence due to excitons bound to NN-pairs with corresponding photon replicas
→ redshift of PL-peak with increasing y
→ $y \leq 0.015$: luminescence of PL peaks disappears
→ possible explanation: $0.06 \leq y \leq 2.85$%: luminescence due to N-cluster states with more than two nitrogen atoms
→ $y \leq 0.015$: luminescence of PL peaks decreases with increasing nitrogen concentration
→ redshift of the absorption tail with increasing y
→ interaction between NN-pairs and formation of N-cluster with more than two N atoms leads to increasing broadening and decreasing amplitude of NN-peaks, respectively
→ redshift of absorption tail might be explained by a superposition of N-cluster states

Phonon Properties

→ method: mid-infrared spectroscopic ellipsometry
→ we detect a GaP-like (E$_{\Omega}$, $\Omega$ = 366 cm$^{-1}$; $\Omega$ = 403 cm$^{-1}$) and a GaN-like (E$_{\Omega}$, $\Omega$ = 485 cm$^{-1}$; $\Omega$ = 450 cm$^{-1}$) phonon band
→ $\Omega$ is redshifted with increasing y as a result of tensile strain and alloying
→ the TO-frequencies of the TO$_1$ and TO$_2$ at $y = 0.03$ are nearlyunchanged with increasing $y$ for $x$, the effects of alloying and biaxial tensile strain-compensate
→ $\Omega$ $\approx$ (494 ± 54) cm$^{-1}$ agrees well with the calculated local-mode frequency of N in GaP$_y$ ($\Omega$ = 495 cm$^{-1}$), extended linear diatomic chain model), and with several experimental results for N-doped GaP$_{1-y}$N$_y$ ($\Omega$ $\approx$ 494 cm$^{-1}$) and (y = 0.03) blueshifted with increasing y and accounts for the increasing amplitude of $\Omega$ with increasing y (figure 4) for the GaN-like phonon
→ linear increase of $\Omega$ with $y$ (d$\Omega$/dy = 2.75 ± 0.25 cm$^{-1}$) gives possibility to measure the nitrogen concentration in GaP$_x$N$_y$ independently

Optical Properties of GaP$_{1-y}$N$_y$

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N-N pairs in GaP$_x$N

→ N is a prevalent impurity in GaP and causes binding states within the band gap of the host material
→ electron is bound in the shortrange potential of two nitrogen atoms (distance $\Delta d_{NN}$, below), binding energy decreases with increasing distance $\Delta d_{NN}$ ($< 0.03$)
→ N-N complex acts as an ionized acceptor ($i \approx 8$)

Critical points

→ method: near-infrared to vacuum-ultraviolet spectroscopic ellipsometry
→ all critical points (CPs)-energies are affected by the combined effects of tensile strain, which should result in a redshift of CPs, and of alloying (linear interpolation to the CP energies of [GaP-N$_y$], quantitative calculations of both effects is difficult because there is a lack of CP-energies of [GaP-N$_y$], and a lack of determination potentials of both, GaP and $\Delta$-GaP
→ blueshift of critical points $E_{\Omega}$ and $E_\Sigma$ with $y$, due to dominating influence of alloying ($\Delta E_{\Omega}$ and $\Delta E_\Sigma$) in contrast to redshift of the absorption tail and the PL peak
→ small redshift of CP $E_\Delta$ with $y$, due to dominating influence of tensile strain
→ no shift of CP $E_\Sigma$ and $E_\Delta$ with $y$ due to compensation of both effects
→ direct $\Gamma$-, $\Sigma$-, and $\Delta$-transitions do not follow the nitrogen-induced unusual behavior of the absorption tail in agreement with recent pseudopotential impred calculations by P. R. Kent et al. [Phys. Rev. Lett. 86, 2641 (2001)]