Basic Semiconductor Physics
Band-structure effects in surface lateral superlattices

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In this work we study the physics of two-dimensional electron systems (2DESs) subjected to periodic potential modulations. For the first time we have employed a local doping method to fabricate such model systems, in which we are able to recover the known commensurability oscillations. Furthermore, using the cleaved-edge overgrowth technique, we fabricate ultra-precise modulated systems, that reveal previously unresolved quantum interference oscillations.

We fabricate lateral surface doped superlattices (LSDSLs) by heating the Zn:SiO₂ capped surface of a modulation doped heterostructure with the highly focused beam of an Ar⁺ laser. A non-linear thermally activated diffusion process results in local compensation doping of the initial n-type silicon doping layer by p-type zinc atoms. Laser writing an array of 10 µm long lines across a small Hall bar at low laser power yields LSDSLs with one-dimensional modulation. Measurement results of a sample with period $d = 300$ nm are shown in Fig. 1(a) for two temperatures. At magnetic fields below $B = 1$ T Weiss oscillations with their typical weak temperature dependence are clearly resolved as $1/B$ periodic oscillations in the longitudinal magnetoresistance. Two-dimensional LSDSLs are obtained by laser writing a 10 µm $\otimes$ 10 µm square array of dots in a small hall bar at high laser

Fig. 1: Low temperature magnetoresistance measurements of (a) a weakly doped one-dimensional LSDSL with period $d=300$ nm showing Weiss oscillations (arrows: theoretically expected minima location) (b) a strongly doped two-dimensional LSDSL with period $d=500$ nm showing antidot resistance oscillations

Fig. 2: Sample design. The modulated 2DES is induced upon application of a positive gate voltage.

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power. Clear resistance maxima are found at magnetic field strengths corresponding to electron cyclotron orbits around one and four antidots with d = 500 nm as indicated by arrows in Fig. 1(b), in agreement with a simple electron pinball model.

Lateral superlattices with unprecedented precision are obtained by periodically modulating the material composition directly adjacent to the 2DES using two subsequent orthogonal molecular beam epitaxy growth steps, as shown in Fig. 2. Fourier transformed low-temperature and electron density dependent magnetotransport data reveal oscillations, that we unambiguously relate to the artificial bandstructure with a semiclassical theory, as shown in Fig. 3. Magnetoresistance oscillations associated with areas $A_F^n$ in reciprocal space by means of Onsager’s relation originate from self-interference along closed electron orbits, in part made possible by magnetic breakdown. $A_F^0$, for example, corresponds to Shubnikov-de Haas oscillations of the undisturbed 2DES, and dominates at high magnetic fields. On the other hand, oscillations associated with areas $A_D^n$ are due to quantum interference between open electron paths. This process is reminiscent to the Aharonov-Bohm effect in real space: Electrons starting for example at point $P1$ can either travel along path $\alpha$ or path $\beta$ to arrive at point $P2$. Constructive interference between both paths leads to maximum backscattering probability, and resistance maximum, while destructive interference results in a resistance minimum. This theory establishes for the first time a direct theoretical relationship between Fermi surfaces and the well-known Weiss oscillations, here identified as difference area $A_D^l = A_F^0 - A_F^l$.

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Anisotropic quantum Hall systems at millikelvin temperatures

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One of the most amazing discoveries from the recent years of research on quantum Hall systems was the observation of a transport anisotropy in higher Landau-levels. This effect shows up only in very high-mobility samples above \(10^7 \text{ cm}^2/\text{Vs}\) and only at temperatures below 150 mK. The anisotropy was attributed to the formation of a striped phase, a new ground state competing with the fractional Laughlin and integer Hall states. In order to gain insight into the relation between the orientation of the proposed stripes and the crystal axes we investigate the influence of slightly misoriented wafers on the anisotropy.

We grow our high-mobility samples by GaAs/AlGaAs molecular beam epitaxy under ultra-high vacuum conditions based on very pure source materials. The two-dimensional system is created by a modulation doped GaAs/Al\(_x\)Ga\(_{1-x}\)As (\(x=0.3\)) single interface heterojunction with Si \(\delta\)-doping and a 800 Å spacer. We study growth on normal and intentionally misoriented (001)-GaAs wafers, which include miscut angles of 1°, 1.5° and 2° towards the (111) and (110)-planes. Square 4×4 mm\(^2\) samples are cleaved out of the wafers and contacted with In using Van der Pauw geometry. State of the art samples show mobilities beyond \(10^7 \text{ cm}^2/\text{Vs}\) at an electron sheet density of \(2.1 \times 10^{11} \text{ cm}^{-2}\) below 1.5 K.

The experiments are carried out in a optimized \(^3\)He/\(^4\)He dilution refrigerator, which allows for a base temperature of approximately 5 mK. We cool the electron gas via the wiring to the contacts by sintered silver heat exchangers. Analog lock-in technique with low excitation currents of 4 nA is used to measure the longitudinal or the Hall resistance while sweeping the magnetic field with a small rate of 5 mT/min.

Fig. 1. shows the anisotropy effect of a \(13.4 \times 10^6 \text{ cm}^2/\text{Vs}\) mobility sample grown on a standard (001) wafer at a temperature of 50 mK. The graph contains traces of the longitudinal resistance versus the magnetic field for current paths along the cleaved edges. In order to correct small contact differences we match the Shubnikov-de Haas-oscillations at small fields of these perpendicular directions. Only at the half filling factors 9/2,11/2 and

\[\text{Fig. 1: Anisotropic behavior of a } 13.4 \times 10^6 \text{ cm}^2/\text{Vs mobility sample grown on a normally oriented wafer. The inset picture marks the current flow and the voltage probes. The longitudinal resistance versus the magnetic field is shown for perpendicular directions. For the half filling factors 9/2 and 11/2 a minimum between two flanking peaks is visible in the easy direction (dotted), while in the hard direction (solid) a maximum exists.}\]

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13/2 do both curves differ significantly from each other. In the easy or [011]-direction a minimum appears flanked by two side peaks at half filling, while in the hard or [011]-direction a huge maximum at the same position is visible. This anisotropic effect, first observed by Eisenstein et al., shows the largest maximum-minimum-ratio for these crystal orientations and is independent of the specific sample or wafer. The effect might be attributed to the formation of a striped electron phase, which is pinned by an unknown mechanism to the crystal. Surface steps on the wafers are discussed as a candidate being responsible for the pinning of the anisotropy.

For this reason the experiments are continued with samples from several misoriented wafers. We concentrate our efforts on wafers miscut towards the (111)-plane, because as illustrated by the atomic force microscopy image in Fig. 2 surface steps are aligned along the easy direction. In this case we would expect an enhancement of the anisotropic effect if the pinning is caused by surface steps. In addition 1° miscut angle is favorable, because at 9/2 filling the grating by the steps is nearly in resonance with that of the proposed stripes.

In Fig 3. we present measurements of the anisotropic directions from a 1° to (111) misoriented sample at 5.1 mK, which possesses a mobility of $13.1 \times 10^6$ cm$^2$/Vs equal to the sample of Fig. 1. Even at base temperature the anisotropic behavior is much less pronounced in comparison to Fig. 1 as only a small minimum and a slightly higher maximum at 9/2 filling survives. We conclude that surface steps are not responsible for the observed pinning of the anisotropy. Furthermore we believe that the anisotropy found in the misoriented sample is of different origin as indicated by new Hall data.

**Fig. 2:** Atomic force microscopy image of a wafer with 1° to (111) misorientation after growth. Surface steps are apparent.

**Fig. 3:** Measurement of the longitudinal resistance of the wafer shown in Fig. 2. The mobility of $13.1 \times 10^6$ cm$^2$/Vs is equal to that from the normally oriented wafer and temperature is lowered by a factor of 10 with respect to Fig. 1. Even at base temperature the anisotropic behavior is obviously quenched, because only a small minimum and a slightly higher maximum at 9/2 filling factor survives.

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Magnetotransport of polarization induced 2DEGs in undoped AlGaN/GaN heterostructures

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The identification of scattering mechanisms which limit the low temperature mobility of two dimensional electron gases (2DEGs) in undoped AlGaN/GaN heterostructures is of fundamental importance for optimizing the interfaces of these structures. The investigation of transport properties provides information about the influence of scattering at dislocations, point defects, interface roughness, and composition fluctuations.

For the determination of quantum and transport scattering time as well as the carrier concentration, mobility, and effective electron mass we have performed Hall- and Shubnikov-de Haas (SdH-) measurements on AlGaN/GaN heterostructures with different sheet carrier concentrations and high electron mobilities (up to 3 x 10⁴ Vs/cm²). From the ratio between quantum and transport scattering time we can draw conclusions about the significance of the different scattering mechanisms. In addition, angle dependent SdH measurements were used to confirm the two-dimensional character of the polarization induced electron gases and to investigate the tilt angle dependence of transport properties.

In Fig.1 the measured 2DEG Hall-mobilities in AlGaN/GaN heterostructures are shown in comparison to values of AlGaAs/GaAs heterostructures versus sheet carrier concentration [1]. The sheet carrier concentrations of 2DEGs in the AlGaN/GaN heterostructures are increased by increasing the Al-content of the barrier. Because of the strong attraction between positive polarization induced bound interface charges and free electrons the average distance between the 2DEGs and the AlGaN/GaN interface decreases with increasing Al-concentration and increasing sheet carrier concentration, dropping below 20 Å for x > 0.25. As a consequence, the drift mobility should be much more affected by interface roughness scattering in AlGaN/GaN heterostructures than in AlGaAs/GaAs heterostructures, where polarization induced interface charges are absent.

Temperature dependent Hall-measurements and Shubnikov-de Haas experiments in tilted magnetic fields for 2DEGs with different sheet carrier concentrations are shown in Fig.2 and 3. For sheet carrier concentrations of 2.1x10¹² cm⁻², a maximum mobility of 28000 cm²/Vs is obtained below 10 K. At room temperature, 2DEG Hall mobilities between 1320 and 1610 cm²/Vs are observed, increasing as 1/T³ with decreasing temperature. For

Figure 1: Low temperature 2DEG Hall-mobility in AlGaAs/GaAs and AlGaN/GaN heterostructures versus sheet carrier concentration.

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temperatures below 100 K, a further decrease in temperature results in no or only a small enhancement of the mobility, which in AlGaAs/GaAs heterostructures is explained by significant scattering of electrons due to ionized impurities. Note that contrary to AlGaAs/GaAs heterostructures (Fig. 1), a decrease of the low temperature mobility, $\mu_{2\text{DEG}}$, with increasing sheet carrier concentration is observed ($\mu_{2\text{DEG}} \propto n_s^{(-1.1\pm0.2)}$), so the limiting scattering mechanism in AlGaN/GaN heterostructures must be different. The reduction of mobility with increasing sheet carrier concentration indicates a significant contribution of interface roughness scattering to the scattering mechanism of electrons as predicted by Oberhuber et al. [2].

In addition to the Hall effect measurements, we performed low temperature ($T = 430$ mK) Shubnikov-de Haas (SdH) experiments. The quantum scattering time, $\tau_q$, of an Al$_{0.1}$Ga$_{0.9}$N/GaN heterostructure with a sheet carrier concentration of $2.1 \times 10^{12}$ cm$^{-2}$ was measured to be 0.23 ps independent of the tilt angle between the 2DEG plane normal and the magnetic field (Fig.3). The transport scattering time is measured to be one order of magnitude higher than the quantum scattering time ($\tau_\text{t}/\tau_q = 10$). This indicates that the scattering of electrons is dominated by small angle scattering mechanisms.


Figure 2: 2DEG Hall-mobility versus temperature for AlGaN/GaN heterostructures with different sheet carrier concentrations.

Figure 3: SdH-measurements at tilted magnetic fields. The sheet carrier concentration of the 2DEG is $2.4 \times 10^{12}$ cm$^{-2}$.
Hole transport of laterally modulated Si\(_{1-x}\)Ge\(_x\) channels on vicinal Si surfaces

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Growth on substrates which are intentionally tilted for a few degrees from crystal planes like (001) or (113) (so called “vicinal” surfaces) has attracted considerable interest recently. The reason for this is mainly due to the fact that vicinal substrates show properties different from untilted surfaces, e. g. enhanced tendency for step-bunching during the growth of strained layers which can be favorably exploited for growing self-assembled highly regular steps. The work presented here concentrates on the growth and characterization of compressively strained Si\(_{1-x}\)Ge\(_x\) layers on vicinal (113)-Si substrates. Additionally, low-temperature transport and magnetotransport measurements have been performed on modulation doped p-Si\(_{1-x}\)Ge\(_x\) channels on such stepped layers. A strong anisotropy of the resistance and magnetoresistance of the holes is found.

Small irregular surface steps are always present on vicinal (113)-Si surfaces due to the miscut of the wafer. These irregular steps bunch together during epitaxial deposition of Si and subsequent high temperature annealing at T = 1100°C in ultra-high vacuum, as shown by atomic force microscopy (AFM) in Fig. 1(a). The step heights are mainly multiples of a unit step of 4 monolayer height. The varying terrace widths and a bending of step bunches contribute to surface step inhomogeneity. Growth of a strained Si/SiGe multilayer on such an annealed (113)-Si buffer at appropriate growth conditions results in the self-organized formation of very homogeneous terraces with step heights of several nanometers. This is due to stress induced step-bunching and repulsive interaction of neighboring bunches. Figure 1(b) shows an AFM image of a sample consisting of 18 double-layers of 2.5 nm Si\(_{0.55}\)Ge\(_{0.45}\) / 10 nm Si capped by a 2.5 nm thick Si\(_{0.55}\)Ge\(_{0.45}\) layer. Very regular steps with a mean terrace width of ~240 nm and a step height of ~4 nm (25 monolayers) demonstrate the self-ordering of step bunches. The orientation of the steps is given by the direction of the substrate miscut.

![Fig. 1: Atomic force microscopy images of two samples on (113)-Si substrate with a miscut angle of ~1.0° containing 100 nm Si annealed at T = 1100°C (a) and overgrown with 18 multilayers of Si\(_{0.55}\)Ge\(_{0.45}\) / Si capped by a Si\(_{0.55}\)Ge\(_{0.45}\)-layer (b).](attachment:image.png)

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In the following we discuss the influence of such step bunches on the transport properties of holes in modulation doped p-Si$_{1-x}$Ge$_x$ channels, which have been grown on annealed Si buffer layers and Si$_{1-x}$Ge$_x$/Si multilayers, as discussed in the previous section. L-shaped Hall-bars have been aligned to well-defined directions by means of standard lithography and wet chemical etching in order to study the influence of the current direction on resistivity, Hall carrier density and mobility. Thick SiGe channels with a high hole density grown on weakly stepped (113)-Si reveal only a small anisotropy in resistivity and Hall mobility with a ratio of less than 1.5 between the $[\overline{3}3\overline{2}]$ and the perpendicular $[\overline{1}0\overline{1}]$ direction. This suggests that an intrinsic anisotropy of hole transport in strained (113)-SiGe quantum wells is weak. It might originate in an anisotropic effective in-plane hole mass and in anisotropic interface roughness scattering caused by intrinsic shear strain and intrinsic interface steps.

Figure 2(a) shows the resistivity observed in different directions as a function of temperature of a 5 nm thick p-Si$_{0.65}$Ge$_{0.35}$ layer with a hole sheet density of $p \approx 8 \times 10^{11}$ cm$^{-2}$ on a substrate as shown in Fig. 1(a). At temperatures below about 100 K, the resistivity increases strongly and an anisotropy of $\rho_\perp / \rho_{||} \approx 4$ develops. The resistivity is maximum for the current flow perpendicular to the step bunches. The carrier densities as determined from Hall measurements are independent from Hall bar orientation within experimental accuracy. These results suggest that the hole gas is still two-dimensional but laterally modulated within the SiGe layer. The SiGe layer thickness is modulated by accumulation of SiGe material at the Si step edges which form wire-like structures, as shown by transmission electron microscopy (TEM) and AFM. The layer thickness modulation gives rise to a lateral modulation of the hole confinement energy whose strength depends on the thickness modulation. Decreasing the effective carrier density strongly enhances the anisotropy in resistivity as shown in Fig. 2(b). This can be understood by an increasing resistivity of depleted SiGe layer regions in between the wires for the Fermi energy getting comparable to the lateral potential barriers (see inset in Fig. 2(b)).

![Resistivity vs. Temperature](image1.png)

**Fig. 2:** (a) Temperature dependent resistivity along different directions for step bunches towards a direction which is $30^\circ$ off $[\overline{3}3\overline{2}]$ towards $[\overline{1}0\overline{1}]$. (b) Resistivity anisotropy $\rho_\perp / \rho_{||}$ as a function of the sheet density of (113)-Si$_{0.65}$Ge$_{0.35}$ p-channels.
Tunneling between quantum wells in the quantum Hall regime

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The well established epitaxial growth of GaAs/AlGaAs heterostructures relies heavily on high crystalline interface quality. The resulting high electron mobility makes this material system favorable for investigation of fundamental electron-electron interaction in quantum transport. In combination with the technique of cleaved-edge overgrowth we have fabricated a novel tunnel structure in non-planar geometry for investigation of magnetotunneling in the quantum Hall regime. Here we present first results of tunnel spectroscopy of integer quantum Hall states.

The samples consist of two separately contacted perpendicular high mobility two-dimensional electron systems (2DESs) forming a T-shaped structure. These 2DESs are realized as 200 Å thick quantum wells epitaxially grown with the method of cleaved-edge overgrowth (CEO): a (001)-quantum well (A) is cleaved along the perpendicular (110)-plane and overgrown with a modulation doped (110)-quantum well (B) in a second epitaxial growth step (Fig. 1 inset). The quantum wells are additionally separated by a 50 Å thick AlGaAs tunnel barrier. Applying bias voltages of up to several hundred mV we measure the current between the two 2DESs. In Fig. 1 we show the resulting asymmetric tunnel current with a voltage applied to quantum well (B) and with quantum well (A) grounded. This asymmetry can be explained by the different screening behavior in both quantum wells: self-consistent calculations of the electron density show significant depletion of the quantum well (A) next to the tunnel junction for negative bias. This leads to a voltage drop over the depletion length and a nearly constant electric field within the barrier resulting in an approximately constant tunnel current. For positive bias the calculation indicates noticeable accumulation of the electrons in the system (A) directly at the edge combined with the formation of bounded wire states at higher bias. At a roughly constant density in well (B) this accumulation causes an increase in current. At about 0.1 V the current exhibits significant negative differential resistance. The subband structure of the quantum wells might possibly cause such an effect. For further analysis we plan to investigate samples with various quantum well and barrier widths.

**Fig. 1:** Tunnel current between separately contacted quantum wells (A) and (B) at a bias voltage applied to the system (B) with a grounded system (A). The inset shows a schematic section of the sample structure fabricated by cleaved-edge overgrowth.

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A magnetic field perpendicular to the (110) quantum well causes Landau quantization in well (B), while the electron states in system (A) stay almost unchanged. Positive bias gives rise to tunneling of electrons from the edge of the quantum well (A) into the 2D bulk states of the system (B). For an applied magnetic field of up to 14 T the Landau quantization energy is of order 10 meV, still below the subband quantization (about 40 meV). For bias voltages sufficiently below 40 mV the electron density in system (A) changes only little. Therefore with positive bias the electron system (A) acts as a well-defined probe for the electronic states in the quantum well (B). The variation in the density of states due to magnetic field affects the tunneling current (Fig. 2 (a)). Especially for higher magnetic fields resonances in the tunnel current due to Landau levels become clearly visible. When the Fermi energy in well (A) is energetically matched to a Landau level in well (B) the tunnel current reveals a maximum. For reverse bias, i.e. for tunneling of electrons into the unchanged constant 2D density of states in the quantum well (A), no such structure can be seen. Fig. 2 (b) shows a grayscale plot of I-V-curves as a function of the magnetic field. The observed structure indicated by the dashed lines represents the well known Landau fan, the splitting of the quantized electronic states proportional to the magnetic field. The origin at zero magnetic field is related the bottom of the lowest subband compared to the Fermi energy. The value of about 12 meV corresponds to an electron density of $3.3 \times 10^{11}$ cm$^{-2}$, which is in good agreement with Shubnikov-de Haas measurements in the 2DES of quantum well (B). The Landau quantization in well (B) also causes an oscillation of the 2D ground energy, which results in deviations of the data from the ideal Landau fan (see Fig. 2 (b)), especially observable between 6T and 8T for $v=4$.

**Fig. 2:** (a) Tunneling current versus bias at a magnetic field of 0, 4 and 8 Tesla perpendicular to quantum well (B). With an applied magnetic field clear peak structures arise in the I-V curves, which can be attributed to Landau levels. (b) Contour plot of the tunneling current exhibits the Landau fan.

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Enhanced $k_\parallel$ filtering effects in ballistic electron emission experiments

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Tunneling of electrons through nonepitaxial interfaces of materials with strongly different electronic structures is presently not very well understood. An excellent method of studying properties of these interfaces with a high lateral as well as energetic resolution is Ballistic Electron Emission Microscopy (BEEM) in conjunction with a probing heterostructure buried below the interface. For this a GaAs/AlGaAs double barrier resonant tunneling diode (DBRTD) is used as a highly selective filter, which makes it possible to analyze the energy-$k_\parallel$-space distribution of electrons passing an Au/GaAs interface (see inset in Fig. 1). To obtain a deeper understanding of the new phenomena we performed a multi-band, multi-channel calculation based on the Landauer-Büttiker formalism within the semi-empirical tight-binding framework.

If the RTD is covered with a 10 nm GaAs cap between the top barrier and the Au-contact a linear increase of the BEEM current above some threshold tip-voltage is observed theoretically as well as experimentally (see Figs. 1,2). At the bias of the current onset, electrons from the Fermi-level of the STM-tip are energetically aligned with the RTD resonance level. A restriction to the propagation is imposed by the strongly differing effective masses between Au and GaAs. In consequence, the metal-semiconductor interface acts effectively as a filter: Only electrons with a small $|k_\parallel|$ can propagate in the GaAs conduction bands. With increasing bias $V_t$, higher energy electrons are injected into the conduction band. This leads to a linear increase in the BEEM current. This effect is independent of the interface morphology. The inclusion of Au atoms at interstitial positions within the first few atomic layers of the GaAs cap does not change the BEEM spectrum.

An interesting situation occurs when the protective GaAs cap layer is thinned down to approximately only 4 nm. Experiments reveal a step-like current voltage characteristic as

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it is shown by the dotted curve in Fig. 2. This characteristic shape can be found in various subsurface RTD structures although it seems to be more pronounced in conjunction with narrow energy filters. Applying the tight-binding model with an ideal Au/GaAs interface to this case one still retains the linear current increase with a slightly later onset. The linear increase is in accordance with effective mass calculations, but clearly deviates from the experimentally found sub-linear slope. Furthermore there is no trace of interferences in the cap layer, which would be a possible explanation of the observed sub-linear slope. The clear-cut Au/GaAs interface is obviously a highly idealized picture of the actual situation: BEEM studies have shown that Au quickly diffuses more than two monolayers deep into the GaAs. If Au atoms are assumed to be randomly distributed over a few interstitial sites of the first two monolayers of the GaAs cap the $k_\parallel$ conservation is relaxed due to interface scattering. Although the modification of the physical model is rather weak, the resulting effect is profound. Fig. 1 compares the calculated current voltage characteristics of an alloyed interface with those of an ideal interface. The corresponding experimental data is shown in Fig 2. In accordance with the experiments we see a slow, but nonzero further increase of the current. The sharp rise at roughly 1.25 V stems from electrons tunneling through the GaAlAs L valleys. Different distributions of the interstitials and a different shape of the super-cell have been tested, but the qualitative behavior remains unaffected. The introduction of scatterers just below the interface leads to a redistribution of the electrons into the side-valleys of GaAs. A detailed evaluation of the distribution of the current in $k_\parallel$-space reveals a characteristic dependence of the interface. In comparison with the distribution for an ideal interface the $|k_\parallel|$-values above approximately 0.17 nm$^{-1}$ are suppressed in the alloyed structure for $V_t$ larger than 1.10 V, which is roughly the bias where a deviation from the linear increase occurs. The step can be asserted to enhanced $k_\parallel$-filtering: Electrons are confined to mostly low $k_\parallel$-values and an increase in the bias does not result in a larger number of electrons that are able to tunnel resonantly. Since the step vanishes when the DBRTD is buried deeper into the GaAs, a proportion of the transmitted electrons must tunnel through quasi-localized states generated by the interstitials. When the Au/GaAs alloy is close to the DBRTD the interface states will couple to the quasi-bound state of the RTD and electrons are able tunnel resonantly via this path.

Furthermore the BEEM spectra were studied as a function of the magnetic field applied parallel to the tunneling current. Plotted as a function of the inverse magnetic field, the current exhibits an oscillatory behavior in $1/B$ from which a $k_\parallel$-filter width can be deduced which agrees well with the theoretical results.

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First principles study of spin-electronics: Zero-field spin-splitting in superlattices

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Spin electronics is a fascinating, emerging new technology that attempts to use a genuine quantum mechanical effect for switching that promises to consume much less power than present day devices: the electron’s spin. An important ingredient for the realization of spin-transistors is the so-called Rashba effect. This is a gate voltage induced spin-splitting of band edge states in the absence of externally applied magnetic fields.

Zero-field spin-splittings of electronic band edge states near III-V heterostructure interfaces are caused by the relativistic spin-orbit interaction and have been observed mostly near interfaces. It is well established by now that there are two mechanisms that give rise to splittings of band edge Kramer pair states that are linear in the Bloch wave vector, namely the Dresselhaus effect or bulk inversion asymmetry (BIA) and the Rashba effect or structure inversion asymmetry (SIA). However, the physical origin of the latter, i.e., its magnitude and the relevance and role of macroscopic electric fields and strain has remained controversial. No quantitative calculations of BIA plus SIA effects beyond semi-empirical k-p-theories have been published so far.

We have studied the spin splitting of conduction and valence bands by performing first-principles local density functional calculations of pseudomorphic AlAs/s-GaAs and InP/s-AlSb superlattices with [001] and [111] growth orientation. The latter orientation gives rise to large built-in piezoelectric fields. These allow us to study the effect of macroscopic fields on the spin-splittings.

The zero-field spin splitting of a nondegenerate (Kramers doublet) band edge state can be characterized by an effective spin Hamiltonian $H = \sigma \cdot B_{\text{eff}}(k_\parallel)$, where $\sigma$ is the Pauli matrix vector and $k_\parallel$ is the lateral wave vector perpendicular to the growth direction. The magnitude and the direction of the effective field $B_{\text{eff}}$ is determined by symmetry and depends on $k_\parallel$ and the considered band state but we omit the latter label for brevity. The spin splitting of a Kramers pair near $\Gamma$ is then given by $\Delta E_{\text{spin}}(k_\parallel) = 2|B_{\text{eff}}(k_\parallel)|$ and contains a term linearly proportional to $k_\parallel$. Generally, the effective magnetic field term can be written as $B_{\text{eff}} = B_R + B_B$, where the Rashba or SIA term equals $B_R = \alpha_R k \times n$ (n is the unit vector along the growth direction) and the bulk Dresselhaus or BIA term equals $B_B = \alpha_B (-k_x, k_y, 0)$ and $B_B = \alpha_B (k_y - k_x, k_x - k_y, -k_x - k_y)$ for the [001] and [111] growth directions, respectively. For the [111] growth direction, $B_R$ and $B_B$ are parallel to each other and one obtains $\Delta E_{\text{spin}}(k_\parallel) = 2 |k_\parallel (\alpha_R + \alpha_B)|$ independently of the direction of $k_\parallel$. Thus, $\alpha_R$ and $\alpha_B$ cannot be determined separately in an ab-initio calculation. For the [001] growth direction, on the other hand, the spin splitting is $\Delta E_{\text{spin}} = 2 |k_\parallel| [\alpha_B^2 + \alpha_R^2 - 2\alpha_B\alpha_R\sin(2\theta)]^{1/2}$ and depends on the angle $\theta$ between $k_\parallel$ and [100]. This angle dependence allows a separate determination of both $\alpha$-parameters for [001] superlattices.

We first consider strained layer short-period AlAs/s-GaAs superlattices and depict in Fig. 1 the two lowest conduction and top light hole bands very close to the $\Gamma$-point. The two lowest conduction bands in both [001] and [111] superlattices have predominantly $\Gamma$-character with some mixing of X and L states, respectively. In contrast to the [001]

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superlattice, the lower symmetry in the biaxially strained [111] superlattice induces a macroscopic field that we find to be equal to 0.5 MV/cm (see Fig. 2).

In the [001] (AlAs)$_3$(GaAs)$_3$ superlattice, our analysis of the linear-k spin splittings yields $\alpha_B = 0.034$ eV\AA for the lowest conduction band. These values change only weakly for longer superlattice periods; we find $\alpha_B = 0.029$ eV\AA and in an (AlAs)$_6$(GaAs)$_6$ superlattice. The Rashba term is zero for these superlattices with common atom (As in this case) owing to the $D_{2d}$ symmetry of the system.

In the [111] (AlAs)$_3$(GaAs)$_3$ superlattice, on the other hand, the sum $\alpha_R + \alpha_B = 0.13$ eV\AA is much larger for the lowest conduction band. This large difference is caused by pronounced band folding effects in the short-period [111] superlattice and originates in the mixed $\Gamma$ and L character of the lowest conduction band. Indeed, inbulk GaAs, we find $\alpha_R + \alpha_B = 0.20$, 0.15, and 0.135 eV\AA for $k = 1/3L$, 2/3L, and the L-point, respectively. The values in AlAs are slightly smaller. The macroscopic electric field can be altered by varying the lateral lattice constant and has only a small effect on this result, consistent with the detailed results given below.

To further investigate the role of the interface asymmetry versus macroscopic field, we have performed calculations for [001] and [111] InP/s-AlSb superlattices. Contrary to the AlAs/GaAs system, the bulk constituents share no common elements in this case which, by symmetry, leads to a macroscopic electric field even in the [001] case. Quantitatively, this macroscopic field is about 2 MV/cm for the unrelaxed (InP)$_3$(AlSb)$_3$ superlattice but becomes nearly zero once the atoms are allowed to relax so as to minimize the total crystal energy. For the lowest conduction band (which has dominantly InP-type $\Gamma$-character), we find $\alpha_R = 0.11$ and $\alpha_B = 0.015$ eV\AA for the unrelaxed case with the high electric field. In the relaxed case, where the field is almost zero, $\alpha_R = 0.10$ eV\AA becomes larger whereas $\alpha_B$ remains unchanged. This result clearly shows that the microscopic arrangement of atoms at the interface, rather than the macroscopic field, determines the magnitude of Rashba effect.

Fig. 1: Calculated dispersion relations for lowest conduction and light hole bands near the $\Gamma$ point for a [111] (AlAs)$_3$(GaAs)$_3$ superlattice as a function of the lateral wave vector.

Fig. 2: The macroscopic average of the electrostatic potential in (AlAs)$_3$(GaAs)$_3$ [001] and [111] superlattices along the superlattice axis. The thin lines guide the eye to show the macroscopic electric field.
Hyperfine studies of isotopically engineered amorphous Germanium

Tobias Graf, Estelle Bauer, Martin S. Brandt and Martin Stutzmann

In crystalline semiconductors, the anisotropy of ESR spectra directly provides information about the microscopic symmetry of an electronic wave function. This information is not available anymore in amorphous materials due to the lack of long range order. However, the nuclear hyperfine splitting still may be used to study the extent and the state of hybridization of a defect wavefunction.

In undoped amorphous germanium (a-Ge) the dominant defect is the dangling bond, which is an uncoordinated Ge \( sp^3 \) hybrid orbital, pinning the Fermi level near midgap. Its spin Hamiltonian is given by

\[
H = \mu_B H \cdot g \cdot S + \sum I_i \cdot A_i \cdot S
\]

with an electronic spin \( S=1/2 \), the gyromagnetic tensor \( g \), the nuclear spins \( I_i \) of the central atom and the nearest neighbors, and their individual hyperfine tensors \( A_i \). The size of the hyperfine splitting is to first order determined by the Fermi contact interaction, which is isotropic and directly proportional to the amplitude of the electron wave function at the position of the nucleus.

Both Si and Ge nuclei have only one stable isotope with a nuclear spin. This spin is quite large in \( ^{73}\text{Ge} \) \(( I=9/2 \), natural abundance 7.8% \) compared to that of \( ^{29}\text{Si} \) \(( I=1/2 \), natural abundance 4.7% \) which leads to a fivefold higher number of nuclear spin states per \( ^{73}\text{Ge} \) atom. To increase the number of levels even more, the weaker localization of dangling bonds in a-Ge extends the nuclear interaction over a larger number of neighboring nuclei. Therefore, no resolved hyperfine interaction is expected for a-Ge.

On the other hand, the hyperfine contribution of \( ^{73}\text{Ge} \) to the dangling bond resonance cannot be neglected in a-Ge and hydrogenated amorphous Germanium (a-Ge:H). At

\[
\text{Fig. 1: Broadening of the EDMR line with increasing } ^{73}\text{Ge content caused by hyperfine interaction between dangling bonds and the background of the nuclear spins.}
\]

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different microwave frequencies spin resonance experiments of natural a-Ge:H have been performed previously. They allowed to separate contributions to the linewidth that depend on magnetic field and therefore have to be attributed to variations in $g$-factor and not to hyperfine interaction. For samples with engineered $^{73}$Ge concentration from 0 to 100%, we now observe a change in linewidth, which definitely is caused by hyperfine interaction with $^{73}$Ge.

As shown in Fig. 1, the ESR linewidth at 9 GHz is increasing from 40 G in samples prepared only with $^{70}$Ge up to 300 G in samples with 100% $^{73}$Ge. Because of the broad ESR lines and the limited amount of isotope-engineered a-Ge, it would be extremely hard to detect resonance lines as wide as these above the background signal of a conventional ESR spectrometer. For this reason we used electrically detected magnetic resonance (EDMR) based on spin-dependent tunneling transport between neighboring defect sites.

Even without any resolved hyperfine structure, the observed isotope-broadening enables us to give an estimate for the localization radius of the dangling bond electron in amorphous germanium. It is estimated that in addition to the central atom the hyperfine interaction of at least three backbonded atoms and their next-nearest neighbors have to be taken into account to explain the observed lineshapes.

![Fig. 2](image)

**Fig. 2:** The linewidth of a-$^{70}$Ge, which does not have a nuclear spin, scales linearly with microwave frequency or magnetic field. The continuous lines are a fit based on a disorder-broadened powder pattern.

Additionally, an a-$^{70}$Ge sample without any nuclear spins allows us to extract the origin of the residual linewidth. Excluding hyperfine, dipolar and exchange interactions, the remaining mechanisms are lifetime and $g$-factor broadening. The former is expected to depend only weakly on the magnetic field, whereas the latter is directly proportional to field and microwave frequency as can be verified in the Hamiltonian given above. As shown in Fig. 2, the overall linewidths for different microwave frequencies $\nu$ are approximately the same if plotted as a function of $g = \frac{h\nu}{\mu_B^2}$, thus showing the dominant influence of $g$-anisotropy. The fits in Fig. 2 are based on a powder pattern with $g_{||}=2.013$ and $g_{\perp}=2.026$ with additional broadening due to disorder.

work performed in collaboration with T. Ishikawa and K.M. Itoh (Keio University, Japan) and E.E. Haller (UC Berkeley, California)
Spin resolved optical investigations on 2-dimensional systems

Jörg Frankenberger, Matthias Brittinger and Artur Zrenner

Optical spectroscopy is a powerful tool to investigate spin-dependent phenomena in 2-dimensional semiconductor structures. In order to obtain information about the spin of photo-created carriers we use different methods such as photoluminescence (PL) and photoluminescence excitation spectroscopy (PLE). These experiments give insight in the polarization dependence of carrier creation and recombination processes. In high magnetic fields only certain spin orientated transitions are allowed. Polarization sensitive measurements therefore give the possibility to investigate the spin states of the optical transitions.

For our experiments we use high mobility remote doped AlGaAs/GaAs single quantum well (QW) structures. The 2DEG in the 15 nm QW has an electron density of about \(2.8 \times 10^{11} \text{ cm}^{-2}\) and a mobility of \(2 \times 10^6 \text{ cm}^2/\text{Vs}\) at 4.2 K. Because of the low carrier density in the sample it is possible to tune the filling factor below \(\nu = 1\).

Our experimental setup consists of spatially resolved optics which enables us to adjust the polarization of the excitation and detection channel independently.

A typical result of a PL measurement at different magnetic fields is shown in Figure 1. It exhibits the PL response at different magnetic fields analyzed in \(\sigma^+\) and \(\sigma^-\) polarization. The Landau fan chart shows optical transitions of different occupied Landau levels. With increasing magnetic field the carriers condense in the lower Landau levels while higher levels are depleted. The depopulation of the higher levels results in the disappearance of the corresponding optical transitions. At \(B = 6T (\nu = 2)\) only the lowest Landau level, which consists of two different spin levels remains occupied. The Zeeman

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Fig. 1: PL at different magnetic fields showing a typical Landau fan chart. Polarization analysis exhibits details of the spin properties of the recombinating carriers. Detection of \(\sigma^-\)-polarized light in the upper plot and \(\sigma^+\)-polarized light in the lower plot.

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splitting of these lines is clearly resolved. The comparison between the $\sigma^+$ and $\sigma^-$-detection shows that the upper Zeeman component is predominantly $\sigma^+$-polarized and the lower line is mainly $\sigma^-$-polarized. This enables us to identify the corresponding hole levels and to draw conclusions about the valence band structure.

For further increasing magnetic field the higher spin level is expected to deplete resulting in a spin polarized 2DEG at $\nu=1$ ($B = 12 T$). In such a regime the optical response is totally polarized. In the presented measurement the depletion of the higher spin level does not lead to the disappearance of the corresponding optical transition. Instead the intensity of this line increases with respect to the other Zeeman component. Therefore the total polarization of the optical response vanishes. This features are evidences of level mixing in the valence band.

To get further information about the spin behavior we perform PLE measurements at different magnetic fields. The interband selection rules allow only transitions between certain electron and hole spin levels. This results in different absorption spectra for $\sigma^+$ and $\sigma^-$-excitation. So it is possible to assign absorption lines to corresponding spin states. Figure 2 shows PLE spectra for $\sigma^+$ and $\sigma^-$-excitation. Spin selective absorption is clearly developed for the lines A and B within the first excited Landau level.

Hence it is possible to learn about the spin conservation by analyzing the energy-relaxation from the excited state to the detected ground state. The spin of the excited carriers can be retained or lost. The associated states determine the polarization of the emitted light, they are energetically separated at high magnetic fields. Hence it is possible to distinguish between spin flip and spin conservation both on the basis of polarization and transition energy (Fig. 3).

Fig. 2: Absorption spectra of a 2DEG for differently polarized excitations.

Fig. 3: Schematic diagram of the possible spin states at high magnetic field. Relaxation with and without spinflip results in optical transitions with different energies and polarization.

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Charged excitons in single self-assembled quantum dots
Frank Findeis¹, Martin Baier, and Artur Zrenner²

Semiconductor quantum dots (QDs) occupied by neutral multi-exciton complexes are often referred to as artificial atoms. Occupancies with different numbers of electrons and holes result in charged exciton complexes. In analogy to QDs with neutral occupancies, charged exciton complexes in QDs may be considered as artificial ions. Few-particle theory predicts binding energies for charged QD excitons in the order of some meV. This allows the controlled manipulation of energetically well separated few particle states under the action of an external gate electrode. Discrete and stable numbers of extra charges are thereby possible via the Coulomb blockade mechanism.

For controlled charging of individual QDs a special electric field tunable n-i structure has been grown by molecular beam epitaxy. The In₀.₅Ga₀.₅As QDs are embedded in an i-GaAs region 40 nm above an n-doped GaAs layer 5×1₀¹⁸ cm⁻³ which acts as back contact. The growth of the QDs is followed by 270 nm i-GaAs, a 40 nm thick Al₀.₃Ga₀.₇As blocking layer, and a 10 nm i-GaAs cap layer. As a Schottky gate we use a 5 nm thick semitransparent Ti layer. The samples were processed as photodiodes combined with electron beam structured shadow masks with apertures ranging from 200 nm to 800 nm. Schematic overviews of the sample and the band diagram are shown in Figs. 1 a and b. The occupation of the QD with electrons can be controlled by an external bias voltage V_B on the Schottky gate with respect to the back contact. For increasing V_B the band flattens and the electron levels of the QD are shifted below the Fermi energy of the n-GaAs back contact, which results in successive single electron charging of the QD. In our experiments excitons are generated optically at low rate and form charged excitons together with the V_B induced extra electrons in the QD. We used a HeNe laser (632.8 nm) for optical excitation and a cooled CCD camera for detection of the PL. The sample was mounted in a confocal low-temperature, high magnetic field microscope. In Fig. 2 we present PL spectra as a function of V_B in the range of -550 mV to +400 mV. The PL intensity is displayed as gray scale plot. As a function of V_B we find a series of lines with discrete jumps in the emission energy. Those lines are assigned to radiative s-shell transitions of neutral X⁰, single charged X⁻, and double charged X²⁻ excitons, as marked in Fig. 2 and discussed in the following.

Fig. 1: (a) Photodiode combined with a near field shadow mask. (b) Schematic band diagram of the structure for zero bias.

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For large negative $V_B$ the electron levels in the QD are far above the Fermi energy of the n-GaAs back contact and the QD is electrically neutral. Optically generated excitons can relax into the QD, but before radiative recombination the carriers tunnel out of the QD due to the high applied electric field. For $V_B > -0.5$ V the QD is still uncharged, but in the smaller electric field radiative recombination gets more likely and the $X^0$ emission line appears at 1307 meV. With increasing $V_B$, the $X^0$ line shifts to higher energies due to the quantum confined Stark effect in the decreasing electric field. For $V_B = -0.35$ V a new emission line appears below the $X^0$ line at 1302.5 meV, indicating the static occupation of the QD with one electron. The $X^-$ binding energy with respect to the $X^0$ is determined to $\Delta E_{X^-} = 4.6$ meV by the measured difference in emission energies. For $-0.35 < V_B < 0$ the $X^0$ and $X^-$ line coexist, which is a consequence of the statistical nature of non-resonant optical excitation. In the presence of one extra electron, the capture and subsequent decay of an electron hole pair leads to the emission of a $X^-$ photon. If only a single hole is captured we expect a $X^0$ photon, and if a single electron is captured we expect no photon, but instead electron back transfer to the n$^+$ region. At $V_B = 0$ V the QD is charged with a second electron. This leads to the appearance of two new characteristic emission lines (marked in Fig. 2), which are assigned to the $X^{2-}$ decay. The main line of the $X^{2-}$ emission appears only 0.3 meV below the $X^-$ line, whereas a much weaker satellite peak appears 4.6 meV below the main line at 1298.1 meV. The appearance of two emission lines is characteristic for the $X^{2-}$ decay. The energy difference between the two $X^{2-}$ lines corresponds to the difference in the s-p exchange energies between the two possible final states with parallel or antiparallel spin orientation of the two remaining electrons. At $V_B > 0.19$ V only one broad emission line remains. This indicates filling of the wetting layer (WL) states with electrons. Here, weakly confined electrons are interacting with the carriers in the QD, causing a broadening of the detected s-shell decay in the QD.

In summary, we have demonstrated bias controlled charging of a single QD in PL experiments. The few-particle interaction energies determined experimentally for the $X^-$ and $X^{2-}$ states are found to be in good agreement with a theoretical model for situations where the spatial extent of the hole wave functions is smaller as compared to the electron wave functions.

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Surface properties of hydrogenated diamond

Christof Sauerer, Christoph E. Nebel¹, and Martin Stutzmann

Although diamond is basically an insulating material, the control of conductivity by doping opens up the field for electronic applications. The feasibility of these applications is based not only on the bulk properties but also on the unique surface properties of diamond. In particular, two surface terminations, hydrogen and oxygen, of diamond are stable in air. The hydrogen termination of diamond is important in terms of stabilizing the surface structure and generating negative electron affinity (cold cathode applications). Hydrogen termination is easily obtained by exposing a diamond thin-film surface to a hydrogen plasma during or after plasma chemical vapor deposition (CVD). It generates p-type conductivity which is restricted to the surface region (10 nm) and hydrophobic properties of the surface.

The oxidized diamond surface is isolating and hydrophilic. Figure 1 shows the wetting angles of hydrogen (Fig. 1a) and oxygen terminated diamond (Fig. 1b) where the water drop forms a hemisphere. The wetting angle of hydrogen terminated diamond is about 95°.

The conductivity of the p-type layer generated by hydrogen termination at T = 300 K is about $10^{-4}$ 1/Ω, weakly temperature dependent towards lower temperatures but decreasing at T > 350 K several orders of magnitude. Fig. 2 shows a typical example. The conductivity is due to about $10^{12}$ to $10^{14}$ cm$^{-2}$ holes, detected by Hall experiments, propagating with mobilities of 10 to 100 cm$^2$/Vs. Up to now, the generation/recombination properties of holes in the surface conducting layer are not understood.

The fabrication and operation of field effect transistors (FETs) using this surface conductive layer have been demonstrated [1]. In our group the nano fabrication of transistor structures using an atomic force microscope is currently investigated.

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The highly conductive hydrogenated surface layer is locally oxidized by applying a voltage bias to the tip. The structuring is performed in contact mode by a n⁺-silicon cantilever. Fig. 3 shows an examples. The local oxidation with -10V tip bias and a scanning speed of 0.1 µm/s generates isolating lines of 100 nm in diameter. The lines are about 1.5 Å deep.

Fig. 3: AFM image of a locally oxidized diamond surface (square). The line is isolating, has a diameter of 100 nm and is about 1.5 Å deep.

Materials Science
Influence of growth parameters on group-V incorporation in MBE-grown antimonides

Markus Grau¹, Rüdiger Knappe, Gerhard Böhm, Ralf Meyer and Markus-Christian Amann

Lasers in the 2-3 μm range are attractive for applications in molecular spectroscopy, trace gas sensing and chemical process control. Such lasers can be fabricated from GaInAsSb/AlGaAsSb heterostructures on GaSb substrates with GaInAsSb as active region material and AlGaAsSb as cladding material. The AlGaAsSb claddings are several μm thick and therefore it is important to achieve lattice matching for these layers. Another crucial requirement for the growth of this laser structure is the tight control of composition and strain of the active GaInAsSb layers in order to adjust the emission wavelength.

From the epitaxial point of view the growth of quaternary AlGaAsSb or GaInAsSb differs strongly from materials with only one group-V element. In materials with a single group-V element like GaInAs, the lattice-matching condition can be achieved by growing the layer with a certain group-III flux-ratio (e.g. Ga/In) independent of growth temperature or V/III flux-ratio. In contrast to this behavior, the incorporation of Sb in layers with another group-V element depends on various growth parameters.

We investigate this dependence with growth series of GaAsSb and GaInAsSb layers. Especially GaAsSb is a suitable material for these investigations as it can be grown on GaAs, InP and GaSb covering the whole range of Sb concentrations. Additionally, it is a ternary material, making a definite characterization by high resolution X-ray diffractometry (HRXRD) possible.

In order to compare the incorporation of group-V elements in layers grown with different group V fluxes, the ratio \( x_{Sb}/F_{Sb} \) is considered (\( x_{Sb} \): concentration of Sb in the layer; \( F_{Sb} = \Phi_{Sb}/(\Phi_{Sb} + \Phi_{As}) \), i.e. fraction of Sb flux compared to total group-V flux). Fig. 1 depicts the \( x_{Sb}/F_{Sb} \) ratios as a function of the V/III flux-ratio for GaAsSb layers grown on three substrates with different growth temperatures. Due to the high strain of GaAsSb grown on GaSb and GaAs substrates, these growth investigations were done with superlattices, whereas on InP we used bulk layers. The Sb-incorporation shows a strong dependence on the V/III flux-ratio in the four growth series. Generally, Sb-incorporation decreases with increasing total group-V flux.

Fig. 2 shows the Sb-concentration in GaAsSb/GaSb-superlattices grown on GaSb. The growth parameters (group III and V fluxes) were the same for all layers and only the

\[ x_{Sb}/F_{Sb} = \Phi_{Sb}/(\Phi_{Sb} + \Phi_{As}) \]

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growth temperature was varied from 470 °C to 545 °C. The Sb-incorporation decreases with increasing growth temperature with $\Delta x_{\text{Sb}}/\Delta T \sim -0.0003/\text{K}$.

More interesting for the laser application than GaAsSb is GaInAsSb which is the typical quantum well material for lasers on GaSb. In order to evaluate the Sb-concentration for this quaternary material, we performed photoluminescence and HRXRD measurements with GaInAsSb/GaSb-superlattices. The growth conditions for the GaInAsSb/GaSb-superlattices were again the same for a series of growth runs with temperatures between 390 °C and 520 °C. In this case, the Sb-incorporation decreases even stronger with increasing growth temperature with $\Delta x_{\text{Sb}}/\Delta T \sim -0.0007/\text{K}$ (Fig. 2). At low temperatures the gradient $\Delta x_{\text{Sb}}/\Delta T$ decreases.

The optimization of growth temperature with respect to optical quality of GaInAsSb is shown in Fig. 3. The photoluminescence intensity varies by a factor of more than two over the considered temperature range and has a clear maximum around 430 °C. A similar result is found for the full width at half maximum (FWHM) which shows a minimum of 5 meV for growth temperatures between 430 °C and 450 °C.

Further growth investigations on AlGaAsSb are planned in order to determine dependencies of Al-, Ga- and In-concentrations on group-V incorporation. This should allow the controlled growth of GaSb-based lasers.

Fig. 2: Sb-concentration in GaAsSb/GaSb- and in GaInAsSb/GaSb-superlattices versus growth temperature. Group-III and -V fluxes were the same within each series.

Fig. 3: PL measurements at $T = 4 \text{ K}$ of GaInAsSb/GaSb-superlattices. Best results are obtained for a growth temperature of 430 °C.
Chemical beam epitaxy of Antimony-based compounds

Fabian Köhler¹, Gerhard Rösel, Gerhard Böhm, Ralf Meyer, and Markus-Christian Amann

In electronically tunable laser diodes, a large continuous wavelength shift of more than 10 nm can be obtained by the implementation of modulators based on the plasma effect. However, these devices suffer from the additional heat production caused by the tuning current. This current can be reduced using a type-II superlattice (SL) structure in the modulator (fig. 1). These heterostructures provide a spatial separation of electrons and holes from each other. Due to the reduced overlap of the wave functions, the recombination of carriers is suppressed leading to longer carrier lifetimes and thus lower current consumption and heat production. One possibility to fabricate type-II superlattices is to grow alternating layers of GaInAsP and GaAsPSb on InP substrates. Using phosphorous instead of aluminum to achieve the desired band structure opens the possibility of regrowth after structuring. This is necessary to fabricate buried heterostructures.

In this contribution, we report about preliminary investigations on the growth of Sb-containing compounds such as InPSb and GaAsSb by Chemical Beam Epitaxy using the precursors Triethyl-Gallium (TEGa), Trimethyl-Indium (TMIn), Arsine (AsH₃), Phosphine (PH₃) and Triethyl-Antimony (TESb). While TEGa and TMIn reach the substrate uncracked, AsH₃, PH₃ and TESb are cracked at 1050 °C.

We started the implementation of Sb in CBE by growing InPSb on InP substrates. As InPSb is compressively strained, we grew InPSb/InP superlattices in order not to exceed the critical layer thickness. The x-ray diffractograms of these samples demonstrate compressively strained superlattices (fig. 2). From the measured lattice mismatch the Sb concentration can be calculated easily by Vegard’s law resulting in the relation of precursor supply and crystal composition (fig. 3). Hereby, the derivation of linearity can be explained by the increase of compressive strain suppressing the incorporation of the larger Sb atoms. The results described above show, that we can use TESb as precursor for Sb in CBE. In order to grow type-II SLs, however, we need materials such as GaAsPSb or GaAsSb. The latter can be used for growing type-II SLs GaAs₀.₅₂Sb₀.₄₈/Ga₀.₄₇In₀.₅₃As, which is favor-

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able to start with, as both layers are ternary instead of quaternary.

Therefore, we investigated the growth of GaAsSb and found a very strong dependence of the growth rate on the growth temperature (fig. 4). From the drop on the low temperature side an activation energy $E_A$ can be calculated for the decomposition of TEGa, while the decrease on the high temperature side can be attributed to desorption of Ga. Since such small parameter windows are not useful, we decided to implement a solid Ga source into the CBE machine. This Ga effusion cell defines a constant growth rate of GaAsSb, as the sticking coefficient of Ga now is 1 (fig 4, dashed line).

With the results described above we were able to grow GaAsSb/GaInAs superlattices. Fig. 5 shows the photoluminescence of a SL consisting of $\frac{3}{2}$ periods. The transition energies are smaller than the band gaps of the concerning materials, but can be attributed to transitions, in which electrons recombine with the spatial shifted holes (fig. 6).

In conclusion we have established antimony based compounds in CBE using TESb, which is thermally cracked at 1050 °C. Thereby, solid Ga instead of TEGa leads to a significant improvement when growing GaAsSb. This makes it possible to fabricate GaAsSb/GaInAs superlattices. The photoluminescence exhibits signals which can be attributed to optical transitions in a type-II superlattice.

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supported by DFG
AlGaN/GaN based lateral polarity heterostructures
A. P. Lima, C. R. Miskys, O. Ambacher, M. Stutzmann

The strong internal electric fields in wurtzite AlGaN/GaN heterostructures resulting from charges fixed at surfaces or hetero-interfaces by an abrupt change of the pronounced spontaneous and piezoelectric polarization in III-nitrides have drastic effects on the band profiles, carrier distributions and electronic transport properties of these wide bandgap semiconductors. Due to bound interface charges and their screening by free carriers, it is possible to achieve two dimensional hole (2DHG) and electrons gases (2DEG) with high sheet carrier concentrations without the conventional modulation doping known from the AlGaAs/GaAs heterosystem. Furthermore, a significant reduction of the effective activation energy of deep acceptors in III-nitrides is observed in AlGaN/GaN superlattices. In these structures, the orientation of the piezoelectric and spontaneous polarization, the sign of interface bound sheet charges, and the exact location of 2DEGs and 2DHGs is determined by the respective polarity of the epitaxial film, which can be either Ga- or N-face, as schematically shown in figure 1.

It was shown recently that the polarity of GaN layers grown by Plasma Induced Molecular Beam Epitaxy (PIMBE) on (0001) sapphire substrate can be controlled to be either N- or Ga-face by use of suitable nucleation layers. GaN deposited directly on oxygen terminated sapphire substrates by PIMBE always exhibits N-face polarity. In contrast, GaN with Ga-face polarity is achieved by prior deposition of a thin (≈ 5-10 nm) AlN nucleation layer completely covering the sapphire substrate (see figure 1). This allows the realization of lateral polarity heterostructures (LPH), with potential applications in novel electronic devices.

In the present work, we describe the preparation by molecular beam epitaxy and first electronic properties of such AlGaN/GaN LPHs. The samples were grown in two steps, using a Tectra MBE equipped with conventional effusion cells and an Oxford Applied Research CARS25 plasma source for the generation of nitrogen radicals. First we grew a 10 nm thick AlN nucleation layer on a 2 inch c-plane sapphire wafer. The sample was then patterned ex-situ by wet etching with a hot (100°C) 50% KOH solution. The pattern was defined by optical lithography using the combination of a metal/photoresist mask with stripes and squares having lateral dimensions between 1 and 100 µm. The etch procedure turned out to be the crucial step of the process.

Fig. 1: Ga- and N-face polarity of GaN deposited on sapphire substrate. The AlN nucleation layer is deposited prior to GaN in order to achieve Ga-face polarity.

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Damage to the sapphire surface and its oxygen termination can lead to the formation of GaN with mixed polarity (uncontrolled growth of small domains with different polarity). In addition there are problems related with an efficient protection of the AlN layers by the mask against the etching. After optimized patterning of the nucleation layer, the substrate showed clean areas of undamaged sapphire adjacent to the non-etched AlN nucleation layers.

The patterned substrate was overgrown by PIMBE with a heterostructure consisting of a 1000 nm thick GaN buffer layer, 30 nm Al$_{0.3}$Ga$_{0.7}$N and a 30 nm GaN cap layer. The alloy composition was determined by high resolution X-ray diffraction. Figure 2 shows optical microscopy images of two different areas of the sample surface after the overgrowth. The sharp borders between the areas grown directly on sapphire and on the AlN nucleation layers demonstrate the high quality of the etch and overgrowth procedure used. The optical contrast is due to a different surface roughness and slightly different growth rates for N- and Ga-face regions, respectively.

The polarity of the overgrown GaN/AlGaN/GaN heterostructures was determined by means of C-V profiling measurements. Figure 3 shows the result of these measurements performed on the area grown directly on the sapphire surface as well as on the area overgrown on the AlN nucleation layer.

In both cases, spontaneous formation of a two dimensional electron gas with similar sheet concentration occurs at the heterointerface. The 2DEG is located at the upper GaN/AlGaN interface for the heterostructure grown on the sapphire substrate without AlN nucleation layer, as expected for N-face polarity. On the other hand, the 2DEG is located at the lower AlGaN/GaN interface for the heterostructure grown on the AlN nucleation layer, which corresponds to a Ga-face polarity.

If the AlGaN/GaN LHPs are suitable for electronic tunneling devices is a topic of ongoing research.

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Polarization induced 2D hole gas in GaN/AlGaN heterostructures

Stefan Hackenbuchner¹, Jacek Majewski, Günther Zandler, Peter Vogl

Efficient electronic and optoelectronic nitride-based devices require an equally high concentration of free electrons and holes. This is extremely difficult to achieve in nitride based materials since the ionization energy of the most commonly used Mg acceptor is very high. In fact, this limitation has severely hampered the development of nitride based heterostructure bipolar transistors or laser diodes in UV regime so far. Recently, it has been proposed that this problem may be overcome by utilizing the strong pyro- and piezoelectric character of these materials. Unstrained nitride layers exhibit a spontaneous dielectric polarization, whereas strained layers possess both a spontaneous as well as a piezoelectric polarization. The difference between the dielectric polarization in different materials or in strained and unstrained layers, respectively, generates electrostatic charges at the interface. These charges, in turn, cause strong internal electric fields that may pull the acceptor energies below the Fermi level.

We have performed quantitative calculations in order to predict the maximal hole sheet density in GaN/AlGaN heterostructures and in GaN/AlGaN superlattices. Our analysis is based on the self-consistent multiband k.p-envelope function theory for holes. The interaction of carriers with one another and with ionized acceptors has been treated within the Hartree approximation. Polarization induced surface charges at the interfaces have been included in the Poisson equation for the electrostatic potential. The system of 6x6 equations for the components of the envelope functions and the Poisson equation have been discretized on a non-uniform mesh. The dependence of the eigenstates on the lateral wave vector has been taken into account. The hole density has been calculated by summing over the discrete eigenstates, weighted by the Fermi distribution function, and by integrating over the lateral Brillouin Zone.

The parameters of the 6x6 k.p Hamiltonian matrix (including the 4 deformation potentials) for wurtzite GaN and AlN have been taken from ab-initio calculations and were linearly interpolated for AlGaN alloys. The transverse interface charge that enters the Poisson equation has been determined as the difference in the normal components of the transverse polarization in adjacent materials. The values of the spontaneous polarization and piezoelectric constants have been taken from first-principles calculations for GaN and AlN and have been linearly interpolated for alloys. The strain in the materials was calculated within elasticity theory. For this purpose, the interpolated experimental lattice and elastic constants of the constituent bulks have been used.

We predict that very high two-dimensional hole gas (2DHG) concentrations can indeed be achieved. As concrete examples, we have calculated the properties of periodic GaN/AlGaN superlattices at T=70 K with an Aluminum concentration of 30% and various well (GaN) and barrier (AlGaN) widths. The barriers have been assumed to be homogeneously p-doped with Mg-acceptors with a concentration of 5x10¹⁹ cm⁻³. The resulting hole sheet densities are shown in Fig. 1. It can be seen that the density is quite low for short well and barrier widths but increases and further saturates for thicker layers. This result can be understood from the spatial dependence of the acceptor level energies relative to the Fermi energy, which is depicted in Fig. 2. In superlattices, the polarization induced interface charges yield an intrinsic electric field of opposite sign in the GaN wells and the AlGaN barriers. This variation causes a corresponding spatial saw-tooth type.

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dependence of the valence band edge. In short period superlattices, most of the Mg-acceptor levels do not fall below the Fermi energy. Accordingly, the hole density supplied by the acceptors is nearly zero in this case. Increasing barrier and well widths result in a growing number of acceptors whose energy levels lie below the Fermi energy. Thus the number of free holes increases. The ionized acceptors are located around the interfaces with positive charge, whereas the generated holes accumulate at the negative-charged interfaces. Thus the polarization charges are screened and thereby the intrinsic electric field is diminished. Consequently, the hole densities tend to saturate with increasing layer widths. Our calculations predict a saturated hole sheet density of roughly $1.5 \times 10^{13} \text{ cm}^{-2}$ for GaN/AlGaN superlattices with 30% Al-concentration. Recent experiments by Ambacher et al. (WSI) seem to confirm the present predictions.

**Figure 1.** Calculated hole sheet density (a) and averaged hole density (b) of the GaN/AlGaN superlattice with 30% Al concentration in the barriers as a function of the barrier (b) and well (w) widths in nm. The average hole density has its maximum at a barrier and well width of 6 nm and reaches $6.2 \times 10^{18} \text{ cm}^{-3}$. The concentration of the Mg-acceptors was $5 \times 10^{19} \text{ cm}^{-3}$.

**Figure 2.** Spatial dependence of the valence band edge $E_v$ in the GaN/AlGaN superlattice (30% Al content). The GaN well and AlGaN barrier widths are equal to 2 nm. The dashed line indicates the position of the Fermi level. The energies of the neutral and ionized Mg-acceptor levels are indicated by full and open circles, respectively. The corresponding density of the 2DHG is depicted in the lower part of the figure.
**DX-centers in Si-doped AlN**

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In AlGaAs alloys, it is well established that the incorporation of donor atoms such as silicon can lead not only to shallow dopant states, but also to more complex states with deep metastable levels, so called DX-centers. These centers are of particular relevance for device applications, since they act as metastable deep traps and can seriously affect e.g. carrier densities. A detailed investigation of these defects therefore is important both for a fundamental understanding of III-V semiconductors as well as for their applications.

A DX-behavior is also found for Si donors in group-III nitride alloys, in particular AlN and AlGaN alloys with high Al content. Here, we summarize different experimental results allowing the determination of a configuration coordinate diagram of the DX state in these materials.

DX-centers are formed because a large lattice relaxation of the Si atom away from the substitutional site in combination with the capture of an extra electron is energetically favorable (Fig. 1). This is depicted in a more quantitative way in the configuration coordinate diagram of Fig. 2: the lowest parabola to the right represents the \( DX^0 \) state, which is occupied by two electrons. This state has undergone a large lattice relaxation and is the stable ground state. The parabola above it symbolizes the thermodynamically metastable \( DX^0 + e^- \) state plus one electron in the conduction band. The two parabola to the left depict the substitutional donor states of the Si atom. The lower parabola to the left corresponds to the substitutional neutral shallow donor \( d^0 \), which is also metastable, and the upper left parabola shows the ionized \( d^+ \).

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state, with one and two electrons in the conduction band, respectively.

Experimentally, the two most prominent signatures of DX-behavior are a persistent photoconductivity and a persistent electron paramagnetic resonance (EPR) signal at low temperatures. This is summarized in Fig. 3, where the lower solid line shows the temperature dependent conductivity of an AlN:Si sample upon cooling in the dark. At low temperatures, the sample has become highly resistive. Illumination with light of energy greater than approx. 1.5 eV increases the conductivity by more than eight orders of magnitude. After switching the light off, the high conductivity persists and even increases slightly with increasing temperature, before quenching above approx. 60 K. Simultaneously, a persistent EPR signal is observable only after illumination at low temperatures.

These findings can be readily explained in terms of DX-behavior. After cooling in the dark, the system is in its energetically most favorable DX− ground state. This state is diamagnetic (all valence electrons of the Si atom are paired), so no EPR is observable, and there are no delocalized electrons available for conduction. Upon illumination with light of sufficient energy, the Si can be metastably transferred to the substitutional d0-state. A relaxation back from d0 to DX− is hindered by the energy barrier between these states (Eb in Fig. 2). In the d0 state, the Si atom is paramagnetic and can thus be observed in EPR, and there are delocalized electrons available for conduction. An increase in temperature eventually allows a transition back to DX− over the energy barrier.

This picture can be tested and refined by studying the quenching of the persistent photoconductivity, as well as the electronic noise properties of Si-doped group-III nitride samples. Especially noise measurements prove to be a powerful tool allowing the determination of the energy barriers between d0 and DX−, because the fluctuations are directly linked to the dynamics of the charge carriers. Thus, noise measurements can be used to determine potential barriers or transition energies (Ea, Eb in Fig. 1) between the levels. In contrast, the net difference between two energy minima (thermal activation energy Er in Fig. 1) governs the thermal equilibrium occupation number of the levels and therefore the conductivity.

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Cubic BN films on diamond: stability and valence band offsets

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Cubic boron nitride (c-BN) has significant technological potential based on material hardness, low chemical reactivity, high thermal conductivity, and its very large band gap. Since epitaxially grown c-BN films usually contain an admixture of other crystallographic phases, a major technological challenge is to find a suitable substrate material that supports the epitaxial and pseudomorphic growth of pure c-BN films. Previous phenomenological macroscopic calculations as well as some experimental data suggest diamond to be a promising candidate.

We have performed full ab-initio calculations in order to study and predict the stability of interfaces in heteropolar (001) diamond/c-BN pseudomorphic heterostructures. Our theory is based on the first-principles total-energy pseudopotential method within the local-density-functional formalism. We have used norm-conserving separable pseudopotentials and a preconditioned conjugate gradient algorithm for minimizing the total crystal energy with respect to both the electronic and ionic degrees of freedom.

In heterovalent diamond/BN heterostructures, the "ideal" abrupt (001) interface contains tetrahedral bonds with more than 2 or less than 2 electrons per bond, leading to a macroscopically charged interface that is energetically unstable. Local charge neutrality can be restored by forming chemically intermixed interfaces. We have studied the electronic and structural properties of charge compensated, pseudomorphic (001) interfaces with one and two mixed interface layers. In these structures, diamond has been taken as the unstrained substrate. There are two abrupt diamond/BN interfaces, with C-B and C-N bonds across the interface. These interfaces can be neutralized by replacing in one layer of boron (or nitrogen) 50% of B (or N) atoms with C atoms. We have considered three lateral atomic arrangements c(2x2), 2x1, and 1x2. When there are two mixed layers in the interface, the chemically plausible reconstructions contain two types of atoms A, B with A:B = 1:3 in each mixed layer, and a 2x2 lateral arrangement. All studied interfaces have been modeled by superlattices with up to 16 monolayers.

We have calculated the formation enthalpy $\delta H$ of all heterostructures discussed above. We find the enthalpy of formation of $(C)_{2n}(BN)_n$ superlattices with abrupt interfaces to be equal to 1.3, 1.5, and 1.54 eV per interface unit-cell area for $n = 2, 3,$ and 4, respectively. For all structures with mixed interfaces, $\delta H$ decreases slightly and lies in the range between 1.0 and 1.1 eV/(unit-cell area), being nearly equal to $\delta H$ for non-polar (110) heterostructures. This clearly indicates that pseudomorphic diamond/c-BN heterostructures are thermodynamically stable towards disproportionation.

The calculated valence band offsets (VBO) of the polar heterostructures depend sensitively on microscopic details of the interface geometry. Consider, for example, the c(2x2) C/BN (001) heterostructure with one mixed layer. The two different C/N and C/B interfaces (i.e., with C/N and C/B mixed layers) can be obtained from each other by swapping cations and anions, i.e. by reversing the polarity of the interface. While we have obtained nearly the same formation enthalpy for these interfaces, the VBO’s of the C/B and the C/N interface differ from each other by 0.9 eV. Furthermore, we find that the VBO’s of the reconstructed interfaces are largely determined by the chemical composition of the interface but depend very little on the lateral atomic arrangement. Altogether, we predict the VBO’s of the diamond/BN (001) heterostructures to lie in the range of 1.0 - 1.8

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eV, with the top of the valence band to be lower in c-BN than in diamond. The calculated VBO of the non-polar diamond/BN (110) interface equals 1.35 eV, in good agreement with previously calculated values. Using the experimental indirect minimum band gaps of 5.5 eV for diamond and 6.4 eV for BN, we obtain a type-II band alignment, with conduction band offsets in the range 0.1 – 0.9 eV.

Our calculations show that the formation of cubic BN on a diamond substrate is energetically very unfavorable. To investigate the role of the substrate lattice constant on the relative stability of various crystallographic phases of BN, we have calculated total energies per atom for hexagonal, rhombohedral, cubic and wurtzite structures of laterally strained BN. The growth axis was taken along the hexagonal direction in all cases (which corresponds to the [111] axis in the cubic phase). In these calculations, the hexagonal lattice constant $a$ is kept equal to the substrate lattice constant, whereas the lattice constant $c$ and the atomic positions in the unit cell are fully relaxed to minimize the total crystal energy.

The calculated epitaxial structural energies are depicted in Fig. 1. The minimum energy of the c-BN lies 0.12 eV above the minimum of the equilibrium hexagonal phase. The plotted total energies take into account the appreciable zero-point vibrational energies. We find our predicted transition pressure from the hexagonal to the cubic phase of 10.3 GPa to be in excellent agreement with the known experimental value of 10 Gpa.

Fig. 1: Calculated epitaxial energies for hexagonal, cubic, and wurtzite crystallographic phases of BN. The zero of energy is taken at the minimum of the hexagonal phase.

The epitaxial energies for the rhombohedral phase (that are not depicted in Fig. 1) are very close to the values of the hexagonal phase. For the whole range of the lateral lattice constants shown, the wurtzite phase is not accessible by epitaxial growth. The hexagonal phase is stable for lattice constants up to 2.65 Å and transforms to the cubic phase for larger lattice constants. It suggests that substrates with hexagonal lattice constants larger than the critical value of 2.65 Å should be more favorable for the direct growth of the cubic phase of BN. Diamond, by contrast, possesses an hexagonal lattice constant of 2.52 Å which is nearly lattice matched to hexagonal BN ($a = 2.513$ Å).
N-type doping of CVD-diamond by sulfur

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Diamond is a promising semiconductor material for many electronic as well as biomedical applications. Intrinsic and p-type material (doped with boron, $E_A \approx 370$ meV) are already available with good quality. However, the question of finding a shallow n-type dopant for diamond is still open. It was well known that nitrogen is a deep donor with an activation energy of 1.7 eV. Recently it has been reported that phosphorus introduces a hydrogen-like level around 600 meV below the conduction band. However, such a level cannot be considered a shallow level donor. As in silicon, sulfur would be expected to be a double donor in diamond, but until very recently, efforts to obtain n-type doping using sulfur in diamond were not successful. In 1999, Sakaguchi et al. announced n-type doping behaviour in diamond by sulfur, but later several papers showed that in those samples, electronic properties were actually dominated by unintentional boron doping. On this work, however, we have been able to confirm the n-type behaviour in a diamond layer to which $\text{H}_2\text{S}$ was added to the $\text{CH}_4/\text{H}_2$ mixture during deposition.

In order to characterize the electronic properties of the films, Ti (200 Å)/Pt (200 Å)/Au (3000 Å) contacts in Van-der-Pauw geometry for Hall-experiments or in co-planar geometry with a gap of 0.8 mm for photoconductivity measurements have been evaporated onto the samples. Rapid thermal annealing at 500 °C for 10 minutes has been applied to generate ohmic contacts.

Hall experiments have been performed in the temperature regime 175 – 350 K at magnetic fields up to 2 Tesla. Without any pre-illumination with UV light, the layers are too resistive for Hall experiments. Hall experiments performed during or after UV-illumination clearly reveal n-type conductivity. The electron density ($n_e$) and electron mobility ($\mu_e$) as a function of inverse temperature are shown in Fig. 1. $n_e$ is activated (thermal ionization energy of the donor) with about 360 meV. $\mu_e$ decreases from about 350 cm$^2$/Vs at 222 K to 250 cm$^2$/Vs at 290 K. Switching off the UV-illumination causes a decrease of the electron density by a factor of five as carriers recombine or are trapped in deep defects. Most importantly, the sign of the Hall-coefficient is invariably n-type.

Fig. 1: Carrier concentration and mobility measured by photo-Hall experiments. The activation energy of the carrier concentration is 360 meV. The Hall sign definitely indicates n-type conduction.

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Photoconductivity spectroscopy was applied to study the electronic structure of the sulfur dopant. Without any UV-illumination, an onset of photoconductivity at 1eV is detected, rising monotonously towards higher energies. However, if spectrally resolved photocurrent is measured after UV-illumination or under UV-bias, the absorption properties of the diamond changes dramatically. As shown in figure 2, the photocurrent spectrum exhibits different maxima and minima due to phonon-assisted absorption in the excited states. From the oscillatory cascades, excited states at 228meV, 353meV, 369meV, 450meV, and 471meV are deduced above the ground level. A LO-phonon energy of 161(±1) meV was derived from the data, in good agreement with indirect optical transitions at the conduction band minimum $k_{\text{min}}=(0,0,0.76)$. Also thermo-stimulated current peaks from the ground level to the excited states at 353 meV, 369meV, and 471meV can be detected.

In figure 2, one can see two dominant ionization energies, at 374 meV and 483 meV. We attribute these ionization energies to the donor levels introduced in diamond by sulfur as a double donor. The existence of two levels was confirmed by annealing the sample at 210K after pre-illumination with UV. In this situation, all the carriers trapped in the shallower level are thermally excited to the conduction band, and no longer contribute to the photocurrent. The result of this experiment indeed showed a photocurrent spectrum with an onset absorption at 483 meV, and no detectable photocurrent at lower energies.

The Constant Photocurrent Method (CPM) was also used to determine the cross-section of both levels. In figure 2 the results of the CPM under bias-UV illumination and after annealing the sample are shown. As expected, the capture cross-section of the deeper level is larger than that of the shallower.

In this work, we have proved that sulfur introduces two donor levels in diamond, one at 374 meV and one at 483 meV. The n-type character of the sulfur was confirmed by Hall experiments.

Fig. 2: Normalized spectrally resolved photocurrent measured at 70K after UV-illumination. The photocurrent shows different maxima and minima which are due to oscillatory photoconductivity. From the spectrum, two sulfur related levels can be observed at 374 meV and 483 meV.
Interstitial clusters in Si

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Interstitials are atoms that are positioned between or sharing normal lattice sites. Native interstitials that arise from the atoms that constitute the lattice itself are called self-interstitials. They are created inadvertently during ion implantation or by irradiating the sample with, say, protons with sufficient energy. These processes can lead to the formation of point and eventually extended defects depending on energy, dose and annealing temperature. These extended and planar defects are believed to induce transient enhanced diffusion of Boron, a limiting factor in controlling dopant profiles which hampers the further reduction in size of next-generation sub-micron semiconductor devices. Therefore it is highly desirable to develop a theory that describes the microscopic processes that occur during the formation of extended defects, namely the aggregation of small compact clusters to elongated chains and then “rod-like” defects oriented in the \{311\} plane. The latter defects range in size from 1-100 nm in width and up to 1 µm in length.

The growth of interstitial clusters can be studied theoretically by recently developed molecular dynamics schemes that allow one to record microscopic processes for time periods up to 1 µs with fs resolution. A super-cell of 512 Si atoms contains \( n \) additional Si interstitials and the atoms are subject to a classical many-body potential within the modified embedded atom method that is tested against \textit{ab initio} calculations. The trajectory of all atoms and the total energy of each relaxed configuration are recorded allowing us to find stable or metastable structures. In particular, the method allows one to find candidates for the ground state structure of complex defect types such as the tri-interstitial \( \text{I}_3 \) or the tetra-interstitial \( \text{I}_4 \) consisting of an interstitial aggregate of three or four interstitials, respectively (Figs. 1 and 2).

It is important to augment these semiempirical studies by \textit{ab initio} density functional calculations in order to reliably predict the energies and transitions paths of these structures. Several properties of point defects such as point group symmetries, deep levels in the band gap, optical transition energies, localized vibrational modes or localization of the wave functions can then be correlated to experimental data obtained from electron paramagnetic resonance (EPR), deep level transient spectroscopy (DLTS), photoluminescence (PL) or localized vibrational mode spectroscopy (LVMS) measurements.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{tri_interstitial.png}
\caption{Tri-interstitial. The interstitials (arrows) are placed at three bond-centered sites. Remarkably, all atoms are four-fold coordinated. Although this defect is not the lowest energy structure for \( \text{I}_3 \), it could account for the W-line seen in photoluminescence experiments [1].}
\end{figure}

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We now briefly discuss some of the highlights obtained by the molecular dynamics and \textit{ab initio} calculations. Single interstitials $I_1$ are found to be very mobile and combine to di-interstitials $I_2$ or tri-interstitials $I_3$ that are also very mobile. Compact clusters containing up to 20 interstitials can be formed subsequently. However, compact clusters containing more than five atoms are found to be unstable with respect to the formation of elongated chains that are lower in energy. These elongated chains $I_n$ act as traps for additionally introduced interstitials by capturing them eventually at the chain ends (Fig. 3) forming an $I_{n+1}$ chain as the ground state structure.

Our studies indicate that the energetically favorable shape of interstitial clusters evolves from compact to elongated and eventually “rod-like” \{311\} defects when more and more interstitials are being injected. Steady improvements of empirical potentials for silicon in combination with new algorithms reaching up to µsec time scales offer exciting opportunities to directly probe the critical steps of interstitial cluster growth.

\textbf{Fig. 2:} Formation energy of a tetra-interstitial during a parallel-replica run at 800 K and the core structure of the ground $I_4$-$D_{2d}$ cluster. The starting configuration consists of four randomly distributed interstitials in a 512-atom cell. After 20 interstitial jumps, a metastable $I_4$ precursor is formed, releasing 5.4 eV (off the scale). Once the transition to $I_4$-$D_{2d}$ occurs (arrow), no more transitions are observed within 10 nsec. Again, all atoms are four-fold coordinated.

\textbf{Fig. 3:} Schematics for an interstitial trap by an elongated chain. 
(a) An interstitial is placed at the nearest hexagonal site. 
(b) An extra chain is formed by concerted motions of the interstitial and the atoms at the end, releasing 2 eV.

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Er$^{3+}$ luminescence in a-SiO$_x$:H

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Luminescent rare earth ions such as erbium, europium or terbium are favourable candidates for the incorporation into host materials which provide an effective excitation mechanism. Their intra-4f transitions are screened by the exterior 5s and 5p shells thus remaining energetically unchanged by the host matrix. Especially erbium shows a luminescence at 1.54 $\mu$m which corresponds to the transmission maximum of conventional silica based optical fibers. (See energy level scheme in fig. 1.)

Er$^{3+}$ has been introduced into several host materials, particularly in those compatible with conventional Si technology. Er-doping of crystalline silicon however revealed a number of problems, e. g. a limited solubility ($< 10^{19}$ cm$^{-3}$) or the strong thermal quenching of the room temperature photoluminescence. Due to a reduction of the local symmetry, codoping with oxygen or carbon makes the Er transitions more probable, thus increasing the PL efficiency. Amorphous silicon has an erbium solubility higher than $10^{20}$ cm$^{-3}$ and a greatly reduced thermal quenching of the Er-PL due to less efficient excitation energy backtransfer. A more favourable erbium environment is realised by the residual oxygen ($< 1$ at. %) always present in a-Si:H. In addition to these advantages, amorphous hydrogenated silicon suboxides (a-SiO$_x$:H) contain up to 50 at. % oxygen so that the most favourable local environment of erbium can be achieved. Furthermore the tunable optical gap of a-SiO$_x$ allows to optimise the energy transfer process from the host to the Er$^{3+}$ ions and to further reduce the temperature quenching of the luminescence.

a-SiO$_x$ samples were fabricated on Corning 7059 glass by plasma enhanced chemical vapour deposition (PECVD) and implanted with different erbium concentrations at the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Er$^{3+}$ luminescence of a-SiO$_x$:H (annealed for 1 h at 300 °C) implanted with different doses of erbium. The double peak structure of the $^4I_{13/2} \rightarrow ^4I_{15/2}$ transition at 1538 and 1550 nm results from the crystal field splitting of the host material.}
\end{figure}

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Forschungszentrum Jülich by Ch. Buchal. The oxygen content of the samples was about 30 at. % corresponding to a band gap $E_{04}$ of 2.3 eV, and the Er concentrations were $10^{18}$, $10^{19}$, $10^{20}$ and $2\cdot10^{20}$ cm$^{-3}$.

The implantation particularly of larger Er doses caused significant implantation damages greatly deteriorating the optical properties of the a-SiO$_x$ matrix. The Urbach tail width increased according to the structural disorder introduced and also an order of magnitude more dangling bonds were created at the highest implantation doses. Annealing at temperatures between 250 and 300 °C for one hour was able to reverse these unwanted effects of implantation – however only partly so for Er concentrations above $10^{20}$ cm$^{-3}$. Also the luminescence of the Er ions could only be observed after annealing.

Figure 1 displays the Er-PL peak after annealing the samples for 1 h at 300 °C. The crystal field splitting of the surrounding matrix leads to a characteristic double peak structure at $\lambda = 1550$ and 1538 nm. The Er emission can be seen for the three highest implantation doses and increases with the erbium concentration. No signal can be seen for an unimplanted sample.

In order to investigate the energy transfer mechanism from the amorphous host material to the Erbium ions the PL temperature quenching was studied. The intrinsic a-SiO$_x$ and the Er$^{3+}$ photoluminescence are shown in fig. 2 at 77 and 300 K. The intrinsic PL is a broad peak with its maximum at 1.37 eV. The Er line however is only 10 - 15 nm in width. The quenching factor $Q$ for the suboxide PL is roughly 20 for an increase from 77 K to room temperature, but is only a factor of 2 for the Er peak. This indicates that the excitation mechanisms of erbium and the intrinsic luminescence are different. A nonresonant defect related Auger effect and a resonant dipole mediated Förster transfer mechanism are two models which are currently discussed controversially.

As shown in the inset of fig. 2, there also appears a spectral feature at the transition $^4I_{11/2} \rightarrow ^4I_{15/2}$ ($\lambda = 980$ nm) from the second excited state of Er to its ground level. (This transition is also indicated in the energy level scheme of fig. 1.) It appears as an additional peak at 1.265 eV situated on the host PL whereas the SiO$_x$-PL at wavelengths slightly smaller than 980 nm is reduced.

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**Fig. 2:** a-SiO$_x$:H and Er$^{3+}$ photoluminescence (annealed 1 h at 300 °C) at 77 and 300 K. The resonant excitation of the erbium $^4I_{11/2} \rightarrow ^4I_{15/2}$ transition at 1.24 eV is shown in detail in the inset.
Vertical transport in silicon-based heterostructures for light emission

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As silicon is the most important semiconductor in microelectronics, it would be highly desirable to realize silicon based light emitters for integrating optical and electronic components on the same chip. With the demonstration of the quantum cascade laser (QCL), a similar device based on group IV heterostructures for wavelengths ranging from 8 to 12 µm seems possible. The design of a QC-device with Si/SiGe heterostructures has to consider several differences of this material-system compared to III-V materials. The band offset is type II with a large valence band offset. Therefore a cascading scheme for the valence band needs to be designed. This requires to take into account all types of hole subbands and their intermixing. Furthermore as the lattice constant of Germanium exceeds the lattice constant of Silicon by 4.2%, a heterostructure has a large build in strain. This limits the average Ge-content for structures thicker than about 100 nm to 18% and thus the maximum achievable intersubband spacing. Additionally, segregation of Germanium during the MBE-growth needs to be considered. The latter two points result in low growth temperatures of about 400°C.

We have designed and calculated several Si/SiGe QC-structures by employing a six band $k\cdot p$ algorithm. The structures were grown at a growth temperature of 430°C in a Riber MBE system. The samples have been processed into (400µm)$^2$ mesas and a facet, for the coupling out of light, was polished close to the mesa at a 60° angle.

Quantum-cascade structures are usually optimized for current transport in one direction. I-V-measurements (\textit{Fig 1}) on our structures show a clear asymmetry. This is due to level alignment in forward direction, which facilitates tunneling of holes through the cascade. Under reverse bias no proper level alignment can be achieved, which is reflected in the stronger blocking behaviour of the I-V-curves.

TM-polarized-light emission of the structures at 77K is detected in the integral MIR spectral range of 8 to 13µm. Measurements of spectrally resolved emission are in progress.

For shorter emission wavelengths, it would be desirable to use silicon dioxide (SiO$_2$) as barrier material because of its

\textbf{Fig 1:} I-V-curve. Inset shows the active region of the QC-structure.

\textbf{Fig 2:} TEM picture of a thin oxide layer. The arrow indicates the growth direction

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high band offsets, but its amorphous nature hampers the possibilities to overgrow these barriers with silicon of good quality.

We employ two different methods for growing thin (sub)oxide layers embedded in silicon in situ in an MBE system. For layers about two nanometers wide, the wafer surface is exposed to molecular oxygen up to a background pressure of 10⁻⁶ mbar without any silicon flux. At growth temperatures between nominally 440°C and 500°C, these layers can be overgrown with single crystalline silicon. Fig. 2 shows a TEM picture taken from such a layer. The layer is continuous and about 2 nm wide, with some lateral inhomogeneities. In the overgrown Si layer, dislocations can be seen which disappear after about 40 nm overgrowth. At about 50 nm Si layer width, the characteristic 2x1 reconstruction of a good quality silicon surface can be seen in the RHEED pattern.

To fabricate thicker SiOₓ layers, a silicon flux of 0.1Å/s is maintained while introducing oxygen into the growth chamber. These layers were grown up to 300 nm thickness. They were overgrown with polycrystalline silicon.

Both kinds of oxide layers exhibit a current blocking behavior at low temperatures, while current increases at higher temperatures with activation energies of about 50 meV as determined by temperature dependent I-V-measurements. Comparing the I-V-characteristics of a sample with one SiO₁.₆ layer of 5 nm width and a sample with two of these barrier layers 50 nm apart from each other, it is observed that a second barrier improves the current blocking behavior of the structure, rising the breakthrough voltage from about 0.5 V to about 2 V. Moreover, the activation energy derived from temperature dependent measurements is significantly higher than for a single barrier (120 meV).

Current transport across these barriers generates hot electrons, which can be used for the excitation of erbium in silicon, resulting in light emission at 1.54 µm, an important wavelength for fiber communication. Figure 3 shows the electroluminescence spectra both for unipolar n-Si/SiOₓ/Si:Er:O/n-Si and for bipolar p-Si/SiOₓ/Si:Er:O/n-Si diodes. In both samples the typical erbium-related peak is visible when injecting electrons into the Si:Er:O layer, while the peak related to the silicon at 1.08 eV is the dominant feature when electrons are injected into the polycrystalline cap layer. Compared to a conventional Er:O-doped pn diode, these diodes yield significantly higher EL intensity at low current densities (about a factor of 14). In the future it is planned to examine nin cascade structure with several SiOₓ layers followed by erbium doped layers to increase the light emission.

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TEM micrograph was provided by M. Seibt, University of Göttingen
Efficient tunable luminescence of SiGe alloy sheet polymers

Günther Vogg, Alex J-P. Meyer, Christian Miesner, Martin S. Brandt, Martin Stutzmann

Layered silicon sheet polymers based on ordered 3-fold co-ordinated sp\(^3\)-hybridized backbone Si atoms are well known mainly because of their intense luminescence and have been reported in this yearbook several times during the last years. Siloxene (SiH\(_{0.5}\)(OH)\(_{0.5}\))\(_n\) as well as the similar oxygen-free polysilyne (SiH)\(_n\) are prepared topotactically from the layered Zintl-phase CaSi\(_2\) by removing the intercalated Ca layers, leaving the \{111\} Si backbone layers intact and saturated with H- and OH-ligands, respectively. The more recent successful preparation of the Ge based counterpart polygermyne (GeH)\(_n\), which exhibits intense infrared luminescence, together with the possibility of growing layered calciumgermanosilicide Ca(Si\(_1-x\)Ge\(_x\))\(_2\) alloys, strongly suggests that alloying should also be possible in the backbone of sheet polymers leading to mixed Si\(_1-x\)Ge\(_x\) sheet polymers. Here we summarize some interesting optical properties of such polygermanosilynes (PGS). While the effect of ligand substitution on the luminescence of Si sheet polymers has been known for a long time, we have shown that the substitution of backbone atoms can similarly be used to change the optical properties of these materials. In particular, the photoluminescence can be continuously tuned from 2.4 to 1.3 eV, covering the green/yellow to near-infrared part of the optical spectrum. This tuning can be seen by the characteristic change of the colors of some PGS samples with different Ge\(_x\) content shown in Fig. 1.

For the preparation of the SiGe sheet polymers, epitaxial films of the Zintl-phases CaSi\(_2\), Ca(Si\(_1-x\)Ge\(_x\))\(_2\), with 0 < \(x\) < 1, and CaGe\(_2\) with a typical thickness of 400nm were first grown on (111)-oriented Si, Si\(_1-x\)Ge\(_x\) and Ge substrates, respectively, using reactive deposition of Ca. The topotactic, wet-chemical exchange reaction was carried out in concentrated aqueous HCl for several hours at a temperature of –30°C.

Structural studies of the PGS clearly show that these polymers are a well defined crystalline mixture of the oxygen-containing siloxene and the oxygen-free polygermyne structure depending on the Ge content \(x\).

![Fig. 1: Visual appearance under white light of some of the Si\(_1-x\)Ge\(_x\) sheet polymers studied.](image-url)
Optical characterization was performed using photoluminescence (PL) as well as diffuse reflection measurements, the latter as a measure for the absorption of the samples. In the PL spectra of the PGS at first only a slight red-shift compared to the PL maximum of 2.4eV for pure siloxene is observed with increasing Ge content $x$. For $x > 0.5$ the PL peak position shows a more pronounced shift down to the final value of 1.3eV for pure polygermyne. Fig. 2 summarizes the dependence of the PL peak position and the absorption edge of the mixed SiGe sheet polymers on the respective Ge content $x$. Both curves exhibit the same nonlinear behavior with the characteristic change at $x = 0.5$. The energy offset of 0.45eV separating the curves remains nearly constant over the whole composition range, suggesting no major qualitative change of the electronic bandstructure as a function of $x$. Since bandstructure calculations and additional experiments such as photoluminescence excitation spectroscopy show that both siloxene and polygermyne are direct semiconductors, we conclude from Fig. 2 that this also holds for the mixed SiGe sheet polymers.

Contrary to crystalline alloys, most disordered SiGe systems like amorphous alloys or mixed SiGe network polymers show a more or less linear dependence of bandgap and PL energies as a function of composition. It is therefore surprising that our sheet polymers exhibit a pronounced nonlinear behavior. Theoretical bandstructure calculations have predicted the pseudo-direct bandgap of pure polysilyne (SiH)$_n$ to be about 1eV larger compared to the direct gap of siloxene. The shift of the PL and absorption energies for $x > 0.5$ according to Fig. 2 would be compatible with a linear dependence of these energies on $x$ from pure (SiH)$_n$ to (GeH)$_n$. The deviation from this for our samples with smaller Ge content is probably caused by the well known red-shift induced by the OH groups attached to the Si atoms, missing in the samples with higher $x$. However, bandstructure calculations are needed for a detailed understanding of this point.

**Fig. 2:** Energy of the photoluminescence maximum and of the absorption edge of Si$_{1-x}$Ge$_x$ sheet polymers as a function of the Ge content $x$. 

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Self-assembly and spectroscopy of correlated Ge quantum dots in Si

Matthias Herbst, Christian Schramm, Karl Brunner, Thomas Asperger, Hubert Riedl, and Gerhard Abstreiter

The realization of opto-electronic devices based on Si and their integration in the advanced Si technology are of great interest for modern semiconductor circuits. The indirect bandgap of Si is the reason, why optical transitions in Si are inefficient. Alloying of Si with Ge has brought many advantages to Si technology. Ge islands grown in the Stranski-Krastanov-mode have a wide field of possible application. Future devices are NIR Si/Ge dot photodetectors, tunable MIR detectors with intra-valence band transitions and tunneling structures. A high volume density of Ge islands is desired for a NIR detector application based on interband transitions in the Si/Ge dot system. In this work the formation of vertically correlated small Ge islands is investigated. The emission of these Ge dots is peaked at the absorption minimum of communication fibers at 1.55 µm wavelength.

The correlation of Ge dots affects islands size, islands density, and the local strain fields which have a direct impact on band offsets and the electronic coupling of stacked dots. The Ge islands were grown at a substrate temperature of 510°C with a growth rate of 0.1 Å/s. Small islands with {105} facets in an elongated hut geometry can be obtained by depositing 8 monolayers (ML) Ge. The islands are about 2-3 nm in height, the base is 20 nm in length and 12 nm in width, determined by atomic-force-microscopy (AFM). An island density up to 1x10¹¹ cm⁻² can be achieved.

In order to investigate the vertical correlation of the Ge islands, a series of Si/Ge dot multilayers with five island layers and varied Si spacer thickness were grown with MBE and characterized by in-situ RHEED and by AFM. High strain fields appear in stacked dots which are undesirable in optical devices. Finite element simulations reveal that strain field increases strongly if the spacer thickness is reduced below a critical thickness. AFM measurements show that the density and the size of the small islands are nearly independent on the spacer thickness of more than 8 nm. If the spacer thickness is below 8 nm, big Ge cluster grow at the expense of the small Ge islands. The critical Ge

Fig. 1: The reduction of Ge coverage for the nucleation of islands (in ML) versus the Si spacer thickness. In the case of 20 nm the growth of the islands is uncorrelated. The data are determined by in-situ RHEED analysis.

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coverage for island nucleation decreases strongly with a spacer thickness of about 8 nm (Fig. 1), which fits quite well with the result obtained with simulation.

Photoluminescence (PL) measurements show a peak at about 0.8 eV. The PL peak shifts slightly to higher energies for decreasing the spacer thickness from 20 to 10 nm, due to strain relaxation and confinement. For a spacer thickness smaller than 8 nm, the band structure is modified by the high strain field and the $\Delta(2)$-electron level shifts to lower energies. This and an increased dot size may explain a small red shift of the observed PL.

In order to obtain small Ge islands without the emergence of large Ge clusters at a spacer thickness of 6 nm, the Ge coverage is reduced after the growth of the first island layer by 1 ML. The islands in the top layer are comparable in density to the single layer islands, whereas the shape of the islands is no longer elongated due to the correlated growth.

The investigated dot multilayer structures were embedded in a p-i-n structure for NIR Si/Ge dot photodetectors which are sensitive at 0.8 eV (1.54 μm). The detector structure contains 110 dot layers with 8 ML Ge and 10 nm Si spacers and was grown on a SOI substrate forming a waveguide structure (Fig. 2). The photocurrent of the sample in Fig. 3 was measured in normal-incidence geometry. A significant photocurrent at 150 K is obtained in the NIR range. The response at 1.54 μm is about 20 μA/W at 0 V bias and increases up to 4 mA/W at −5 V. This may indicate a strong influence of bias voltage on the escape probability of photoexcited holes localized in the Ge dots. The photocurrent observed is modulated by Fabry-Perot interference leading to spectrally periodic absorption maxima.

![Fig 2. Structure of a NIR Si/Ge dot photodetector. 110 dot layers separated by 10 nm thick Si spacers are embedded in the intrinsic region. The structure was grown on a SOI substrate for waveguiding measurements.](image)

![Fig 3. Photoresponse of the NIR Si/Ge dot photodetector. The oscillation in the curves is due to Fabry-Perot interference.](image)
Laser-crystallized SiGe thin films

Christopher Eisele¹, Markus Berger, Christoph E. Nebel² and Martin Stutzmann

The preparation of thin crystalline silicon germanium (SiGe) on glass is interesting for thin film solar cells. The implementation in solar cells is promising because a Si₀.₂Ge₀.₈ alloy has a direct band gap of 1.4 eV (see Fig. 1), allowing efficient absorption of the solar spectrum already in 1..2 µm.

The epitaxial growth of SiGe on amorphous substrates like glass is not possible. We therefore apply laser crystallization to grow crystalline SiGe on glass. The initial amorphous or nano-crystalline films were deposited in an UHV chamber using e-beam evaporation of Si and an effusion cell for Ge. After deposition the samples were transferred in-situ into a crystallization chamber. The laser crystallization is carried out with a pulsed frequency doubled (532 nm) Nd:YAG laser. The layer melts and crystallizes in the subsequent cooling process. Fig.2 (left) shows an atomic force microscope (AFM) image of such a laser-crystallized SiGe layer with about 20 % Si and 80 % Ge. The laser pulse energy was adjusted to about 435 mJ/cm², this results in a structure with a grain size smaller than one µm. If the homogeneous intensity distribution

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of the laser is replaced by a sinusoidal intensity distribution, lateral grain growth can be stimulated. Such an intensity profile can easily be generated by a two beam interference pattern. The intensity is adjusted to melt the layer only around the interference maxima. The crystallization starts at the solid-liquid interface and grains grow towards the center of the interference line. A typical result is shown in Fig. 2 (right), where one period of the laser interference crystallized SiGe layer is shown. The white line at the center of the interference pattern is due to material transport during the grain growth towards the center because of the higher density of the liquid compared to the solid phase of SiGe. To achieve larger grains a multi-pulse sequence can be applied. Here the interference pattern is shifted in small steps after each pulse perpendicular to the direction of the interference lines. This technique has been successfully applied already for silicon thin films.

Fig. 3 shows the absorption coefficient $\alpha$ of a laser crystallized SiGe layer measured by photothermal deflection spectroscopy (PDS). The absorption coefficient of the SiGe shown in Fig. 3 is modulated by interference oscillations of the 130 nm thick film. The data for crystalline Si and Ge plotted in Fig. 3 are taken from the literature. The absorption in the SiGe alloy is about a factor of 40 higher than in crystalline Si. As a direct consequence, the required absorber in a solar cell made out of this alloy could be much thinner than a Si absorber.

We have shown that suitable intensity profiles stimulate lateral grain growth to improve the crystalline quality. Absorption properties of SiGe alloys are promising for solar cell applications. To evaluate the potential of the laser-crystallized thin films, we currently work on improvement of the deposition and crystallization process as well as their electrical characterization.

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Semiconductor Devices
High-performance InP-based vertical-cavity surface-emitting lasers in the 1.5-1.8 µm wavelength range

Markus Ortsiefer¹, Robert Shau², Gerhard Böhm, Fabian Köhler, Jürgen Rosskopf, Matthias Zigldrum and Markus-Christian Amann

Research on long-wavelength vertical-cavity surface-emitting lasers (VCSELs) with emission wavelengths around 1.55 µm has seen numerous approaches in the past few years, but could not demonstrate a real breakthrough. The major problems for InP-based 1.55 µm VCSELs are due to poor thermal properties which can be attributed both to a low \( T_0 \) for the corresponding active regions and to an unsatisfying thermal conductivity for monolithically integrated Bragg mirrors. Furthermore, the technique of selective oxidation for strong optical and electrical confinement that lead to the well-known impressive device characteristics for GaAs-based lasers is not feasible for material systems on InP.

In contrast to the unsatisfying output characteristics of the majority of long-wavelength VCSEL structures, the device design which has been developed and successfully been demonstrated at the WSI (see Fig. 1) exhibits superior and application-suitable device performance with respect to almost any device characteristics.

The objective of this design concentrates both on the minimization of the thermal resistance and the reduction of excess heat generation. The most important design step addressing the latter one is the application of a Buried Tunnel Junction (BTJ) that enables a reduced \( p \)-side series resistance and simultaneously accomplishes self-aligned current confinement and optical index guiding. Since the spreading layer resistance for \( n \)-type material is much lower than for equally doped \( p \)-type material, our design allows lateral current injection and high-reflective dielectric mirrors with smaller thermal resistances as compared to epitaxial mirrors on InP. The front mirror on top of the upside-down mounted structure comprises an InGaALAs-DBR with pair number and composition in the high-index layers depending on the desired wavelength. Besides the thin dielectric back mirror, we use thermally advantageous InP for an efficient heat spreading and heat sinking to an integrated Au-heatsink for a reduced thermal resistance. With respect to industrial demands for low-cost fabrication, it is worthwhile to mention that all processing steps can be done on a full wafer scale.

Device characteristics for 1.5 µm and 1.8 µm VCSELs at room temperature under CW operation are given in Fig. 2 and Fig. 3.

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VCSELs emitting at 1.55 µm show output powers exceeding 2 mW for aperture sizes of 17 µm. Lasers with $D_{BTJ}=10$ µm exhibit a remarkable threshold voltage of only 0.9 V which means a difference of just 0.1 eV to the corresponding photon energy. The series resistance for these lasers is as low as 35 Ω. For VCSELs emitting at 1.8 µm, ultralow threshold currents of 190 µA for $D_{BTJ}=2.5$ µm and CW operation up to 90°C has been demonstrated. The strong index-guiding associated with the BTJ-technique enables the application of aperture diameters even far below 10 µm with excellent mode behavior as can be seen in Fig. 3. Lasers with 5 µm aperture size exhibit a side mode suppression ratio (SMSR) around 50 dB. The far-field pattern of these lasers shows a gaussian 15°-FWHM intensity distribution for the fundamental mode. With respect to single-mode VCSELs with a required 30 dB SMSR, output powers of 1 mW seem achievable. Moreover, the fabrication process of the BTJ easily allows the precise control of the aperture’s shape. This can, for example, be used to realize elliptical structures to lift the polarization degeneracy of the eigenmodes.

Fig. 2:  Light-current characteristics for 1.5 µm (left diagram) and 1.8 µm (right diagram) BTJ-VCSELs. The dashed line on the left side is the current-voltage curve for $D_{BTJ}=10$ µm.

Fig. 3:  Emission spectrum and far-field pattern of 5 µm BTJ-VCSEL at 1.55 µm.

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High-performance InGaAs-InGaAlAs-InP long-wavelength lasers

Guokui Kuang, Gerhard Böhm, Nikolaus Graf, Ralf Meyer and Markus-Christian Amann

As many gas molecules show absorption lines in the wavelength region 1.7-2.3 μm, lasers in this wavelength-range are attractive for applications in molecular spectroscopy, remote sensing of atmospheric gases as well as laser radar exploiting atmospheric transmission windows. Since the technology for InP-based lasers has been well developed during the research on 1.55 μm lasers for optical fiber communication, a lot of efforts have been made to apply this material system to lasers above 1.55 μm. Most of these lasers were reported to be grown by MOVPE or by CBE using compressively strained InGaAs-InGaAsP QWs as active region. However, very few long-wavelength lasers were grown by MBE on InP substrate. This is because it is difficult to grow phosphorus-containing materials in solid-source MBE. In order to overcome this difficulty, we have grown InGaAs-InGaAlAs-InP QW lasers by MBE, and realized high laser-performance such as low threshold, high operation temperature above 100 °C, high characteristic temperature T₀ and long emission-wavelength above 2.2 μm. The advantage of the InGaAlAs system stems from its larger conduction band offset (ΔE_c/ΔE_g) of about 0.7 compared to a value of about 0.4 for InGaAsP system. This larger conduction band offset can lead to a better electron confinement in QW and therefore, a higher temperature stability.

From this material system, ridge waveguide lasers with cleaved facets were fabricated. Fig. 1 shows typical CW output power–current characteristics of lasers operating at a temperature as high as 100 °C. It can be seen that the maximum CW output power of the 7-μm-wide laser is above 7 mW, and the power of the 10-μm laser at 500 mA is more than 6.5 mW per facet. To our best knowledge, this is the first report about CW operation at temperature as high as 100 °C for InP-based lasers above 1.7 μm. It should be mentioned that 100°C is the limit of our measurement apparatus, the lasers are likely to work at even higher temperature.

Fig.1: Typical CW output power–current characteristics of lasers emitting at 1.79μm at 100 °C. The length and width values are shown beneath the respective curves.

Fig.2: Temperature dependence of threshold current density J_th and external differential quantum efficiency η_d for a 1.98 mm long and 10 μm wide laser.

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Fig. 2 shows the temperature dependence of threshold current density $J_{th}$ and external differential quantum efficiency $\eta_d$ for the 1.98-mm-long and 10-µm-wide laser in Fig.1. All the measurements are carried out in continuous-wave (CW) mode. It can be seen that the characteristic temperature is as high as 72 K in the temperature range 10 °C to 50 °C. The external differential quantum efficiency $\eta_d$ decreases slowly with the increase of temperature, its value at 100 °C still amounts to half of that at 10 °C. This weak temperature dependence can be attributed to the strong confinement of electrons in the QWs due to the high InGaAlAs barriers.

Lasers with wavelength above 2.2 µm have also been fabricated in our laboratory. Fig. 3a shows the spectrum of a 1.02-mm-long and 10-µm-wide laser. It can be seen that the peak wavelength is located at 2208 nm. To our best knowledge, this is the longest wavelength that has ever been reported for InP-based lasers. Typical room-temperature CW output-current characteristics of two 2.6-mm-long lasers are shown in Fig. 3b. As can be seen, the threshold current for the 10-µm-wide laser is about 95 mA, which corresponds to a threshold current density of only 370 A/cm².

In conclusion, we have fabricated high-quality InGaAs-InGaAlAs-InP long-wavelength lasers grown in solid source MBE. For 1.79 µm lasers, characteristic temperature as high as 72K and maximum CW operation temperature as high as 100°C have been obtained. In addition to this, lasers operating in CW mode at room temperature with wavelength as long as 2.208 µm, and lasers operating in pulsed mode with wavelength as long as 2.27 µm have also been realized on InP substrates.

**Fig.3:** a) Spectrum of a 1.02-mm-long and 10-µm-wide laser. The maximum peak is located at 2208 nm. b) Typical CW output power-current characteristics for 2.6-mm-long lasers with 10-µm and 30-µm width. The measurement is carried out at 20°C. The threshold current for the 10-µm-wide laser is about 95 mA.

In conclusion, we have fabricated high-quality InGaAs-InGaAlAs-InP long-wavelength lasers grown in solid source MBE. For 1.79 µm lasers, characteristic temperature as high as 72K and maximum CW operation temperature as high as 100°C have been obtained. In addition to this, lasers operating in CW mode at room temperature with wavelength as long as 2.208 µm, and lasers operating in pulsed mode with wavelength as long as 2.27 µm have also been realized on InP substrates.

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Fabrication of distributed feedback laser diodes with $\lambda > 1.5 \, \mu m$

Jörg Adler, Gerhard Rösel\textsuperscript{1}, Fabian Köhler, Nikolaus Graf, Guokoi Kuang, Gerhard Böhm, Markus-Christian Amann

There is a huge demand for long wavelength laser diodes with $\lambda > 1.5 \, \mu m$ in low-cost remote sensing of atmospheric gases. However, the lasers are required to operate with single-mode emission over a broad range of temperature and drive current. This can be achieved by replacing the reflecting edges of a Fabry Perot laser diode with a Bragg grating whose reflection is wavelength dependent.

For the targeted emission wavelengths of about 1.8 \, \mu m, the grating period is approx. 270 nm and the width of a single line is 100 nm. This is beyond the possibilities of mask-based lithography, so electron-beam lithography was used to define the gratings. The total length of the grating and of a single laser is limited to 589 \, \mu m because of the limited writefield size of the SEM used for lithography.

As short DFB lasers need more gain per cavity length to reach the lasing threshold, a high gain laser structure had to be developed.\textsuperscript{[1]} (Fig. 1) The active region of this laser consists of several compressively strained 8-nm InGaAs quantum wells separated by 10-nm InGaAlAs barriers. DFB lasers with 3 and 4 quantum wells were produced, 2 QWs did not yield sufficient gain. The bottom of the laser structure (up to the InGaAs grating layer) was grown by solid source molecular beam epitaxy. The grating was etched into this layer using a CH\textsubscript{4}/H\textsubscript{2} dry etching process. The following layers were grown with chemical beam epitaxy (CBE); unlike MBE, this growth process tends to fill up the grating, smoothen the layers and reduces defects. The combination of e-beam lithography and dry etching proved to be quite successful as it enables precise control of the grating period $\Lambda$, the grating depth and the trench width.

As shown in Fig. 2 the grating is sine-like. The gap in the center is a $\lambda/4$-shift, inserted to enable single-mode emission and $\kappa L$ is 3.5.

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After fabrication of metal-clad ridge waveguide (MCRW) lasers, the wafer was cleaved into bars with 580 µm long cavity. Both facets were coated with a λ/4-layer Al₂O₃. This reduces facet reflectivity from approx. 30% to 1%, suppressing FP modes.

Fig. 3 shows the continuous-wave light output versus current (P-I) characteristic for a 5 µm wide DFB laser at a heat sink temperature of 20 °C. The threshold current was 30 mA. The CW output-power at 25 °C was approx. 3 mW at a drive current of 140 mA.

Fig. 4 shows the spectra of this DFB laser taken under an injection current of 90 mA with increasing temperature. At 20 °C the emission wavelength of the DFB mode is as long as 1.8265 µm with a sidemode suppression ratio larger than 30 dB. A tuning range of 6 nm is obtained by increasing the temperature from 20 to 60 °C. Up to 55 °C the side mode suppression is higher than 25 dB. The wavelength shift with increasing temperature is +0.14 nm/K and is caused by the change of the refractive index.

The further challenge is to expand the fabrication technology to meet the requirements for wavelengths over 2 µm.


supported by: DFG (SFB 348),
Quantum cascade lasers have shown tremendous performance improvements and technological progress since their first demonstration almost seven years ago. Lasing was restricted to a single material system, InGaAs/InAlAs lattice matched to InP until 1998. The use of (Al)GaAs heterostructures as unipolar lasers has been successfully demonstrated about three years ago. Despite significant improvements for both material systems, however, room-temperature continuous wave operation still represents the major challenge for further developments.

We have grown quantum cascade lasers based both on the GaAs/AlGaAs and the InGaAs/InAlAs materials systems in order to exploit the limiting factors for high temperature continuous wave operation.

Figure 1 shows a typical emission spectrum of a $\lambda=4.9\ \mu$m quantum cascade laser as obtained with a 640 mm grating spectrometer. The device is based on InGaAs/InAlAs heterostructures grown lattice matched on an InP substrate. The active region consists of 25 periods of a three quantum well active section and a modulation doped superlattice acting as a funnel injector. Lasing action is based on a vertical transition ($\Delta E=250\ \text{meV}$) in the three quantum well active section. The 25 period active region is sandwiched between an optical cladding employing InP, which has a thermal resistance 15-20 times smaller than e.g. the ternary AlInAs alloy and thus improves the high temperature performance of this laser. Devices have been processed into stripes of 22 $\mu$m, 26 $\mu$m and 30 $\mu$m width by optical contact lithography and deep wet chemical etching. After plasma deposition of 200 nm SiO$_2$ as electrical insulator and reactive ion etching of electrical windows on top of the ridges, Ti/Pt/Au metallic contacts have been evaporated on top of the devices. The waveguides were subsequently cleaved into bars of various length from 1-4 mm with the facets left uncoated.

Lasing action in pulsed mode for a device 22 $\mu$m wide and 3.55 mm long was observed at 4.0 A injection current corresponding to a threshold current density of 6.1 kA cm$^{-2}$ at 77 K. Lasing was observed up to 190 K. The lasing wavelength corresponds to a transition energy $\Delta E=251.6\ \text{meV}$, which is in good agreement with our subband calculations. We have also realized quantum cascade lasers based on interminiband transitions in intrinsic superlattices grown lattice matched on InP emitting at $\lambda=7.7\ \mu$m. Here the waveguide contains InAlAs as cladding material, which has a larger thermal resistance than InP and consequently lasing action is achieved only up to 109 K. In the obtained wavelength regions several gases such as CO (4.61 $\mu$m), N$_2$O (4.47 $\mu$m) or OCS (4.87 $\mu$m) as well as SO$_2$ (7.29 $\mu$m), H$_2$S (7.33 $\mu$m) and H$_2$O$_2$ (7.79 $\mu$m) have characteristic absorption lines allowing e.g. gas sensing for pollution monitoring or chemical process control.

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In GaAs based quantum cascade lasers we use two GaAs layers with appropriate doping profile as optical waveguide material which allows optical confinement with relatively low waveguide losses and optimal heat dissipation (see figure 2). The active region is based on a three quantum well active section followed by a doped injection superlattice ($\Delta E=112$ meV). The measured emission wavelength ($\lambda=10.8$ $\mu$m) of such a laser is in good agreement with our calculations (11.1 $\mu$m). Lasing was observed up to 240 K. We believe the waveguide losses $\alpha_w$ to be still one of the strongest limiting factors on the performance of GaAs based intersubband lasers, with $\alpha_w$ being predominantly controlled by free-carrier absorption. Therefore we have grown several samples with an optimized ratio $\Gamma_{AR}/\alpha_w$ both the mode confinement in the active region $\Gamma_{AR}$ and the losses $\alpha_w$ in the doped cladding layers. In our reference structure, which is based on published values, the low loss 3.8 $\mu$m thick waveguide core is silicon doped with $n_{Si}=8\times10^{16}$ cm$^{-3}$ and the optical confinement is achieved by highly doped ($n_{Si}=8\times10^{18}$ cm$^{-3}$) 1.2 $\mu$m thick cladding layers. Figure 3 shows a plot of the threshold current densities versus reciprocal cavity length for four different lasers with the same active region but different waveguide designs. A good optical confinement with low threshold current densities could be achieved in the sample with a 3.8 $\mu$m thick core with a doping concentration of $n_{Si}=4\times10^{16}$ cm$^{-3}$ and a 1.2 $\mu$m, $n_{Si}=8\times10^{18}$ cm$^{-3}$ cladding reducing the waveguide losses in the core while maintaining the same confinement factor $\Gamma_{AR}$. We have achieved a reduction of the threshold current density $J_{th}(inf)=3.79$ kA/cm$^2$ compared to our reference sample (4.84 kA/cm$^2$). The other 2 samples with a lower doping of the cladding layers ($n_{Si}=6\times10^{18}$) show higher current densities than the reference laser which we believe is due to a larger penetration of the optical mode into the metallic contacts.

In conclusion we have grown several quantum cascade laser devices applicable for gas sensing in the mid-IR wavelength region. Our newly optimized large optical cavity design for GaAs based quantum cascade lasers yields promising results for further optimization of the performance of GaAs based unipolar injection devices especially also for operation at higher temperatures.
Quantum dot infrared photodetectors with lateral carrier transport

Liwen Chu 1, Artur Zrenner, Max Bichler, and Gerhard Abstreiter

The intersubband bound-to-continuum transitions in InGaAs/GaAs quantum dots are nearly independent of the polarization of incident radiation. This reflects the three-dimensional carrier confinement, leading to a different behavior as compared to intersubband transitions in quantum wells, where the transitions are only allowed for polarization perpendicular to the quantum well layers. Thus, an infrared photo-detector can be easily realized in the normal-incident geometry by using charged quantum dots.

We report on a quantum dot infrared photodetector in the lateral geometry, based on intra-conduction band transitions between the first excited states and the wetting layer subband in the InGaAs quantum dots. This transition turns out to exhibit a strong oscillator strength. The excited electrons can be transferred into an InGaAs channel located nearby the quantum dot layers, in which the lateral carrier transport can take place. The quantum dots are doped with Si such that the ground state and the first excited state in the conduction band are occupied. An interdigital top contact is annealed through the InGaAs channel and the quantum dot layers.

The photoresponse spectra of the detector structure at different temperatures are depicted in Fig. 1. The bias voltage is 0.6 V. Photoresponse of the order of A/W can be obtained for temperatures up to T=60 K. The spectra are peaked at E=186 meV (λ=6.5 µm) with a small shoulder on the high energy side. The response maximum is attributed to the transition between the first excited states and the wetting layer subband. The shoulder arises from the transition between the quantum dot ground states and the wetting layer subband. The photoresponse increases slightly with increasing temperature for T<33 K. This is probably due to the thermally activated electron transfer between the wetting layer subband and the parallel InGaAs channel. For higher temperatures, the electrons are thermally excited out of the quantum dots, which reduces the intersubband absorption in the quantum dots and results in a decrease of the detector signal. The observed photo-response is about 60 mA/W at T=77 K.

The photo-conductance gain is strongly affected by the modulation frequency. The

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dynamics of the detector structure has been investigated by frequency dependent studies of the detector signals. The photo-response spectra at different chopper frequencies \(f\) with a fixed bias voltage \(V_B = 0.6\ V\) at \(T = 30\ K\) are shown in Fig. 2. The detector signal decreases strongly with the increasing chopper frequency. The frequency dependence of the detector response is believed to be due to the back-transfer of electrons from the InGaAs channel to the quantum dots, which is expected to be rather slow due to the real space transfer of the carriers. The detector response signal can be directly observed with an oscilloscope. The detector signal is shown on the right side of Fig. 2 for \(f = 11\ Hz\) and \(f = 215\ Hz\), respectively. The upper part is the detector response signal, the lower part shows the TTL-signal of the chopper. For a typical low frequency case, the detector signal increases nearly linearly and saturates. The signal rise time is determined by the rise time of the incident light intensity, because of the finite excitation beam diameter. When the chopper frequency is increased, the detector response shows a typical photo-conductance signal. In this case, the rise time of the chopped light is shorter compared to the detector response time, and the signal rise time of the detector can be determined to be about 800 \(\mu s\) for \(f = 215\ Hz\). It gradually saturates for higher chopper frequencies. The intersubband transition time is expected to be on a much faster time scale. Recapture of electrons in the quantum dots is therefore believed to be the significant slow mechanism observed in the detector response.

An optimization of the photo-response of such detectors is expected by an enhancement of the electron mobility in the conducting channel as well as a further blocking of the electron back transfer to the dots. This requires a detailed band-structure engineering. The spectrally narrow photo-response may be of interest for sensitive spectroscopy in combination with selective gas detection.

Fig. 2: The photoresponse decreases strongly with increasing modulation frequency \(f\). The time resolved detector signal can be observed with an oscilloscope, which is shown on the right side for \(f = 11\ Hz\) and \(f = 215\ Hz\), respectively.

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Mid infrared photodetectors based on Si/Ge quantum dot structures

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Quantum dots are intrinsically suited for normal incidence operation in detector devices since their confinement potential for carriers is 3-dimensional. Furthermore, quantum dot infrared detectors (QDIP) based on the Si/Ge materials system could be an interesting solution for the needs of efficient mid-infrared devices in the range 3-5µm, due to larger valence band offsets compared to quantum wells, and of better integration with Si-technology.

QDIP devices have been studied in the mid-infrared domain using intra-valence band transitions in different types of self-assembled Ge dots in Si. The structures were grown by molecular beam epitaxy (MBE) on n-Si (100) wafers, the Ge dots form in the Stranski-Krastanov mode. Ge dots with an average diameter of 20nm, a height of 1.5 nm and an area density of 9x10¹⁰ cm⁻² form at a substrate temperature of T_G=510°C. This kind of structure with boron doped dots was used in a vertical photodetector configuration. The obtained normal incidence photocurrent spectrum is shown in Fig. 1. For a bias voltage of 0.5V at T=20K the spectrum shows a broad peak with a maximum at about 324meV (3.8µm) and a high energy tail reaching 600 meV (2µm). The peak can be attributed to transitions from states bound in the ensemble of Ge dots into quasibound states at the Si valence band edge, whereas the high energy tail results from transitions between bound dot states and the valence band continuum. The observed photoresponse is about 4.5mA/W.

A second device with similar but modulation doped Ge dots was processed in a lateral photodetector configuration, i.e. with AlAu top contacts in an interdigital transducer geometry that was alloyed through the Ge dot layers. In Fig. 1 the obtained photoresponse

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spectrum is compared to the detector in vertical configuration. The lineshapes of both spectra are very similar which is consistent with the fact that the attribution of the spectra to transitions between bound states in the dots and quasibound states or the valence band continuum should hold in the lateral case. For 0.5V bias at T=20K the spectrum shows a maximum at 284meV (4.4µm) with a photoresponsivity of 9.5mA/W, i.e. the responsivity has been doubled compared to the device in vertical configuration. No temperature dependency of the photoresponse spectra has been observed up to 100K. The maximum is redshifted by 40meV for the device in lateral configuration, because lateral transport is possible in the wetting layer or the modulation doping layers in this case. As illustrated in the inset of Fig. 1 appearance of photocurrent is therefore possible at lower excitation energies than in the vertical configuration where the carriers must get excited to the Si valence band edge to contribute to the photoresponse.

Ge dots with an average diameter of 35nm, a height of about 4nm and an area density of 6x10¹⁰ cm⁻² are obtained with a growth temperature of T_G=525°C. After integration of this structure in a lateral detector of the same type than the one described above we obtained very similar photoresponse spectra, but with a maximum at 374meV (3.3µm) and a responsivity of 3mA/W. This can be explained with a decreasing quantum confinement energy when increasing the dot size, leading to an increasing energy for bound-to-quasibound or bound-to-continuum transitions to the valence band edge. The lower responsivity is attributed to the lower area density of Ge dots and a slightly reduced level of modulation doping for the device with larger dots.

Dark currents measured between 10K and 77K for the latter device are shown in Fig. 2. Up to T=30K the dark current curves show a kink at a certain bias voltage. For smaller voltages the dark current is small and increases slowly with bias voltage. For higher voltages the dark current increases rapidly. In the lateral configuration the dark current is driven by the conductivity of the Ge wetting layers or the bulk Si between the interdigital contacts. At a certain voltage the barrier for hole localization within dots breaks down and leads to a rapidly increasing current. With increasing temperature the barrier is decreased and the breakdown takes place at decreasing limiting voltages. In spite of a rather low responsivity, the low dark current for small bias voltages (up to ±1V) leads to high detectivities of 1x10¹¹ cmHz⁻½/W of this lateral photocurrent detector structures.

QDIPs based on lateral carrier transport thus seem very promising for realization of large area photodetectors as the performance has been enhanced compared to the vertical configuration and QWIPs. Furthermore the processing is easy since there is only need of one metalization step for the interdigital top contact. An optimization of the devices should be achieved by growing one or more high-mobility SiGe-channels next to the Ge dot layers. The holes trapped in the dots could be transferred into this channel and enhance the lateral transport.

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Optically induced charge storage and de-charging in InAs quantum dots

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In this project, we investigate the optically induced charging and de-charging of InAs quantum dots (QD). The QD storage condition is detected through resistance changes of the adjacent 2D electron or hole channel. QD charging is achieved by resonant absorption of narrow band NIR light. The stored charge can be ejected out of the dots by wavelength selective MIR illumination.

The investigated devices are designed either for electron or for hole storage in the QDs. They consist of a modulation doped 2D detection channel which was grown on top of a layer of InAs QDs, separated by a barrier. This layer sequence is incorporated into the intrinsic region of a vertical p-i-n junction. In the case of hole storage, the optically gated transistor structures investigated in this work consist of an n-type substrate with a back contact followed by an undoped 240 nm GaAs spacer, an InAs QD layer deposited at 530°C and a 30 nm AlGaAs barrier as well as an AlAs/GaAs SL barrier. On top of this a GaAs QW with 2D hole channel was grown. The holes are provided by two p-delta-doping layers in an AlGaAs barrier. The structure is completed by a thin GaAs cap layer. Under illumination, the photo-excited electrons escape from the InAs QDs as a consequence of the vertical built-in field in the p-i-n junction (Fig. 1a). They drift to the back contact while the holes remain stored in the QDs (Fig. 1b). Typical storage times are several hours at T=145K. When the sample is illuminated in the MIR range, the stored holes can be excited out of the dot potential wells leading to an increased carrier concentration in the 2d-channel (Fig. 1c). The charging and de-charging of the dots can be monitored sensitively by the resistance changes of the 2d-hole channel. The ejection of stored charges was observed both for stored electrons and holes for a certain MIR wavelength range. A reference sample without QD

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layer showed no effect when illuminated in the NIR or MIR range. The storage effect is observable up to temperatures of about 200K. In order to investigate the wavelength dependence of the charging and de-charging process, the wavelength of the incident light was varied. Changing the NIR charging wavelength allows to address different subsets of QDs in ground and excited states. By accumulatively charging the QDs, a consecutive rise in resistance shows that selective QD charging can be performed in the wavelength domain. Persistent storage is observed only for the QD ground states where up to two charges can be stored.

By varying the MIR de-charging wavelength, information on the effective barrier height of the stored charges can be extracted. In Fig. 2, typical charging/ storage/ de-charging cycles are plotted for 2 different MIR wavelengths. Illumination in the NIR leads to an increase of the resistance due to charging of the dots. The excitation energy was chosen to be $E_{ex}=1.036\text{eV}$ ($\lambda\approx1.2\text{µm}$), leading to resonant excitation of the QD ground states. This charging is persistent in the dark for many hours at the measurement temperature of 145K. Illumination with MIR at $\lambda=3\text{µm}$, shown in the second cycle of Fig.2, causes a decrease in resistance. This indicates that stored charges are ejected out of the QDs at this wavelength resulting in an increasing carrier concentration in the 2d-channel. For MIR illumination at $\lambda=7\text{µm}$, no resistance reset is observed. At this wavelength, the photon energy seems to be too small for carrier ejection out of the QDs. The onset of the de-charging process should be related to the effective barrier height of the confining potential well. Preliminary results show a clear difference between the MIR wavelength dependence of stored holes and stored electrons. Holes can be erased at longer wavelength compared to electrons, which may be expected from the differences in barrier heights. Excitation of carriers into the continuum above the AlGaAs barrier leads to an increase in de-charging efficiency as compared to carrier excitation just out of the dots into the surrounding GaAs. A detailed study of the MIR de-charging wavelength dependence is in progress.

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In recent years, self assembled quantum dots (QDs) have been studied intensively leading to a rapid improvement in understanding the principal properties of semiconductor nanostructures. As ideal zero-dimensional systems QDs are expected to exhibit a discrete density of states, leading to sharp spectral lines in optical experiments. However, an ensemble of self assembled QDs includes dots with different sizes and shapes resulting in inhomogeneous broadening of the optical spectra. Because ensemble fluctuations obscure the intrinsic properties of individual objects one has to select single QDs to learn about their principal characteristics. From an experimental point of view single QD spectroscopy is the technique of choice to overcome this difficulty.

Due to the typically high surface density of self assembled QDs ($>1 \times 10^{10} \text{ cm}^{-2}$) a spatial resolution in the range of 100 nm is needed to isolate a single QD. Therefore we fabricated near field shadow masks with apertures ranging from 150 nm to 500 nm that allow optical access to single quantum dots. For photocurrent experiments and for controlled tuning of the electric field the QDs are embedded in the intrinsic region of a \textit{n-i-Schottky diode}. The band profile under negative bias condition is shown schematically in Fig. 1. By varying the bias voltage we are able to investigate one and the same quantum dot in the two complementary regimes of photocurrent (PC) and photoluminescence (PL). Experimentally either PC or PL can be studied according to the external bias voltage $V_b$ applied to the sample. For negative bias ($V_b<-1 \text{ V}$), corresponding to high electric field, the tunneling time $\tau_t$ of the photo excited carriers out of the QD is shorter than the radiative life time $\tau_r$. In this regime most of the carriers contribute to the PC. With increasing $V_b$ the electric field is reduced, which results in an increase of $\tau_t$. Since $\tau_r$ is in first order independent on electric field we get a transition from the regime of PC to the regime of PL.

In Fig. 2 we present PL and PC spectra as a function of $V_b$ taken from the same aperture of the shadow mask. In both cases we observe well separated sharp peaks attributed to absorption (PC) and emission (PL) of a single QD. As a function of $V_b$ a spectral red shift is observed due to the quantum confined Stark effect. In PL (Fig. 2 (a)) two lines at 1302.8 meV and 1307.4 meV ($V_b=0 \text{ V}$) marked as $X^{-}_\text{PL}$ and $X^{0}_\text{PL}$ dominate the spectra. In the PC spectra (Fig. 2 (b)) a single line, marked as $X^{0}_\text{PC}$, appears at 1303.6 meV ($V_b=-1.5 \text{ V}$). These lines arise from one and the same QD as discussed further on.

The two main emission lines $X^{-}_\text{PL}$ and $X^{0}_\text{PL}$ can be attributed to the charged ($X^{-}_\text{PL}$) and neutral ($X^{0}_\text{PL}$) exciton state of the QD as more detailed investigations have shown. In this sample at $V_b>-0.35 \text{ V}$ the QD is already charged with one electron. The charging of the QD is accompanied by discrete jumps in the emission energy due to few particle
interaction of the exciton with an increasing number of electrons. Additionally the twofold charged exciton $X_{PL}^{2}$ leads to new PL lines for $V_b > 0$V.

In the PC regime the electron states of the QD always lie far above the Fermi level of the n-GaAs back contact and the QD remains uncharged. The PC signal can be observed in the voltage range from -1 V to -2.8 V. We observe an increasing linewidth of our PC line with increasing electric field. Assuming the tunneling of excitons out of our QD as the main broadening mechanism we can deduce the tunneling lifetime $\tau_t$ due to the uncertainty relation $\Gamma \cdot \tau = \hbar / 2 \pi$. In the limit of high electric fields $\tau_t$ can be estimated to 0.3 ps from the PC line width of about 1 meV at $V_b = -2.5$V. At low fields ($V_b \approx -1$V), the PC amplitude quenches abruptly. Here the linewidth of 250 µeV is certainly not lifetime limited, but restricted by different interactions. In the transition region between PC and PL the condition $\tau_t \approx \tau_r \approx 1$ns is valid. The observed strong variation of the exciton lifetime from typical 1 ns at zero electric field to below 1 ps at 83 kV/cm can be used to tune the exciton lifetime in a QD.

To further compare the $X_0$ line position in PL and PC the quantum-confined Stark effect (QCSE) has to be taken into account. The QCSE causes a red shift of the QD ground state with increasing electric field. In Fig. 3 we show the $X_0$ line position as a function of electric field extracted from the PL and PC spectra in Fig. 2 by fitting the PC peaks with a Lorentzian line shape. The Stark shift continues monotonically over both regimes confirming that in fact one and the same QD is observed. The $X_0$ transition energy $E_{X_0}$ depends approximately parabolically on the electric field. This analysis allows to infer the static dipole moment under the condition of zero electric field. We find a positive dipole moment of $p = 8 \times 10^{-29}$ Cm, which can be interpreted in terms of a localization of the electron in the QD’s base below the hole.

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**Fig. 2:** Photoluminescence (a) and photocurrent (b) spectra of our single QD photodiode as a function of bias voltage $V_b$.  

**Fig. 3:** Spectral QCSE-shift of the ground state exciton PL and PC line with varying electric field illustrating the transition between PL and PC regime.

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Erbium in silicon is an interesting system to realize silicon-based optoelectronics at 1.54µm. Efficient excitation of erbium can be carried out by impact processes with hot carriers. The goal of this study is to figure out, whether hot holes or hot electrons are more efficient in impact exciting erbium ions.

All samples were grown by molecular beam epitaxy (MBE) and analyzed in their as-grown state. Two series of samples were grown on higly boron doped ([B]=10^{19} \text{cm}^{-3}) (100) oriented p^+ -Si substrate. In series A erbium was codoped with carbon at substitutional lattice sites, which causes optical activation of erbium comparable to codoping with oxygen. A 400nm Si_{1-y}C_y:Er layer ([Er]=5\times10^{19} \text{cm}^{-3}, [C]=5\times10^{19} \text{cm}^{-3} corresponding to y=0.1\%) was sandwiched between a Si:B buffer layer ([B]=10^{16} \text{cm}^{-3}) deposited on the substrate and a highly phosphoros doped 120nm n^+ cap-layer ([P]=10^{19} \text{cm}^{-3}). In series B oxygen codoped erbium diodes were fabricated: The 400nm thick Si:Er:O layer ([Er]=5\times10^{19} \text{cm}^{-3}, [O]=2\times10^{20} \text{cm}^{-3}) was embedded between the substrate and the 120nm n^+ cap-layer without a p^+ buffer. Van der Pauw measurements reveal a p-type behaviour with p=2\times10^{17} \text{cm}^{-3} for series A whereas series B shows strong n-doping with n=3\times10^{18} \text{cm}^{-3} at 300K. Counterdoping with boron (series B) or phosphoros (series A) allows to investigate the luminescence properties with erbium centers in either the n or the p-region of the diode as well as at different doping levels.

The diode structures of series A and B allow to figure out, whether electrons or holes are more efficient in impact excitation of the erbium ions. The erbium was incorporated either in the p-region of a diode, where there are only hot holes for excitation, or in the n-region with only hot electrons for both series. By varying the boron concentration in the Si:Er:O layer (series B) or the phosphoros amount in the Si_{1-y}C_y:Er film (series A) at fixed erbium and oxygen or carbon concentrations the width of the space-charge regions are varied.

**Fig. 1:** Integrated EL intensity at 1.54µm (T=10K) at fixed current density 88Acm^{-2} vs. space-charge region width for oxygen (series B) and carbon (series A) codoped Si:Er pn diodes.
region width of pn-diodes with the erbium incorporated either in the n- or the p-region of series A and B. For both series the EL efficiency is maximum when the erbium is incorporated in the n-region of the diode shown on the left hand side of Fig.1. Series B yields about 3300 times more EL output at 1.54µm than series A. Comparing the impact excitation process by holes and electrons, a 5000 times lower EL intensity is achieved by hot hole excitation at an equal space-charge region width of 123nm. Exciting the erbium codoped with oxygen (series B) with electrons results in an approximately linear increase of the light output vs. the effective space-charge region width. Er:O in the p-region of the diode (series B) reveals a saturation like behaviour of the EL, whereas no EL output at 1.54µm is detected for hole excitation in series A (right hand side of Fig.1). The hot carriers responsible for an impact excitation process need a minimum energy of 0.81eV, which equals the energy difference between the ground level (\(^{4}I_{15/2}\)) and the first excited state (\(^{4}I_{13/2}\)) in the 4f shell of the erbium ion. After a tunneling process through the bandgap, the carriers are accelerated by the electric field in the depletion layer of a pn diode. They need a certain distance to reach the minimum energy for impact processes. This distance is called the dark region of the diode. For electron impact excitation of erbium ions of series B no EL output at 1.54µm is observed up to a space-charge region width of 45nm. A similar behaviour is observed for holes, but holes need a larger distance (about 70nm) to collect enough energy after the tunneling process. We attribute the larger dark region to the higher scattering rate of holes compared to electrons.

Fig. 2 shows the EL-intensity vs. the current density for reverse biased diodes of both series with the erbium incorporated in the n-region. The EL-intensity of the carbon-codoped erbium diode belonging to series A was scaled by 3300. From the saturation behaviour of the EL intensity at 1.54µm about the same \(\sigma\tau=1.6x10^{-20}\text{cm}^{2}\text{s}\) for impact excitation of erbium ions by electrons is inferred for both series. The drastically lower saturation output in Si\(_{1-y}\)C\(_y\):Er diodes (series A) compared to Si:Er:O diodes (series B), however, is remarkable and indicates that either much fewer erbium ions are optically active or a comparable amount of ions is optical active, but only a small part of them can be excited efficiently by an impact process. The first explanation can be excluded as there is about the same EL output in forward biased Si\(_{1-y}\)C\(_y\):Er and Si:Er:O diodes and also the PL output is comparable for both oxygen and carbon codoping. For both, the excitation is transferred via an impurity level to the erbium valence electron on the timescale of 100µs, which is enough time for coupling between the erbium valence electron and the 4f-shell. In contrast, for impact excitation this coupling has to occur instantaneously with the impact process of the valence electron. Most erbium centers in Si\(_{1-y}\)C\(_y\) seem to exhibit a weak electronic coupling with the 4f-shell explaining the low EL output in RB.

Fig. 2: EL-Intensity vs. current density in reverse bias for erbium incorporated in the n-region of a Si:Er:O (B) and Si\(_{1-y}\)C\(_y\):Er (A) diode.

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Laser lift-off for free standing GaN LEDs

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As a result of the high melting point and the high equilibrium vapor pressure of N₂ at the growth temperature necessary to synthesize III-V nitrides, large bulk single crystals for homoepitaxy are not available. The introduction of a thin nucleation layer before the actual film growth allowed the successful use of heterosubstrates for high quality epitaxial growth and a rapid progress of the nitride technology for the development of GaN-based light emitting diodes (LEDs) and laser diodes (LDs). Besides SiC, sapphire is the most commonly used substrate, but it still imposes constraints on the GaN film quality due to the lattice and thermal expansion coefficient mismatch. Sapphire also does not permit electrical contacts to be made from the backside. This complicates contact and packaging schemes, resulting in spreading resistance disadvantage and higher voltages for device operation. Furthermore, the performance of GaN-based high current devices such as LDs and high power transistors is limited by the poor thermal conductivity of sapphire in comparison with Si or SiC, preventing an efficient heat dissipation. High brightness blue nitride LEDs and LDs based on sapphire have become commercially available but the problems mentioned above hinder further improvements of the functionality of epitaxial group-III nitrides to fully explore their large application potential for opto- and electronic devices.

To eliminate this constraint a thin-film laser induced lift-off technique can be used in conjunction with wafer bonding processes to integrate GaN with other dissimilar materials by delaminating the device from the original sapphire substrate. Laser lift-off techniques have been demonstrated to successfully separate thick GaN films from sapphire to be used as pseudosubstrates in nitride homoepitaxy experiments. The lift-off process is realized by illuminating the sapphire/GaN interface with a sequence of intense ultraviolet laser pulses of a Nd:YAG laser system, which leads to a localized heating at the GaN/Al₂O₃ interface to above 800°C. This causes thermal decomposition of about 50 nm of the GaN film and consequent delamination from the substrate. The relative hardness and chemical stability of Al₂O₃ makes the pulsed laser processing viable and very attractive in comparison with chemo-mechanical removal of the substrate or wet chemical etching of a sacrificial layer grown between the sapphire and GaN. Furthermore, the short irradiation time and absorption length of the pulsed UV-laser method permits localized laser thin film interaction preserving the microstructure and properties of the original layer.

Fig. 1: Freestanding LED membranes 250x250 µm large and 4 µm thickness fixed on epoxy. On the left a frontside view. The right image shows a contacted blue LED in operation as seen from the former sapphire side.
Using the lift-off technique we successfully and reproducibly could delaminate membranes of blue InGaN MQW LEDs from their sapphire substrate. On the left and on the right side in Fig. 1 an operating LED membrane is shown from the top surface and from the delaminated sapphire interface. No dark line features are observed over the entire LED active area showing the complete absence of microcracks. The LEDs were provided by the Fraunhofer Institut für angewandte Festkörperphysik-Freiburg and were grown on a standard one side polished 2”sapphire wafer. For this experiment, wafer stripes of 0.5x25 mm² were cut containing a series of mesa etched LEDs with an active area of 250x250 µm² and a thickness of 4 µm.

The 3rd harmonic (λ = 355 nm) of the Nd:YAG laser was used with a pulse period of 10 ns and energy of 0.3 J/cm² for the lift-off process. After delamination the residual Ga on the exposed backside was removed with HCl vapor. Electroluminescence and Current-Voltage measurements were performed to compare the characteristics of the LEDs before and after separation from the sapphire. No discernible change was seen after the lift-off process in comparison with the original device (Fig. 2). These results proved that no device degradation is caused by the laser lift-off. As the free LED membranes were still fixed on an epoxy adhesive with bad heat dissipation, a reduction in quantum efficiency was consequently observed at higher currents.

The next step to explore this interesting approach for the technology of highly efficient nitride based devices is the utilization of a flip-chip mounting procedure illustrated in Fig. 3. In this way the devices can be fixed to a receptor wafer like Si, GaAs or Cu. To increase the efficiency of light emission of LEDs and LDs, an anti-reflection coating can be deposited on the free side. In the case of Si receptor wafers, the laser induced lift-off technique allows the integration of high-quality nitride based devices with the Si integrated-circuit technology for industrial scale production.

**Fig. 3:** Process flow for bonding and transfer a nitride based LED from sapphire onto a receptor wafer.
III-Nitride FETs

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III-Nitrides are a promising material class for high-power high-frequency microelectronic applications at elevated temperatures. They possess large band gaps, small effective masses in the conduction band minimum and large offsets to the conduction band satellite valleys as well as high polar optical phonon frequencies. InN has the smallest effective mass of the three binaries GaN, AlN and InN, so that InGaN channel FETs are considered as a candidate for very high frequency applications. To exploit the potential of the InGaN alloy, we performed ensemble Monte Carlo calculations of this material family. It turns out, in contrary to the alloys AlₓGa₁₋ₓN and InₓAl₁₋ₓN, that the favorable influence of the decreasing effective mass of the alloy is overcompensated by the increasing influence of alloy scattering in the case of InₓGaN, resulting in a decrease of the low field mobility as well as the peak drift velocity by increasing the In content up to 50%. A favorable influence onto the drift velocity can be found in the InₓGa₁₋ₓN system only for x>50%. Therefore, in terms of high transit time frequencies, InₓGa₁₋ₓN channels might be advantageous only if very high In contents can be realized.

Fig. 1 Drift velocity of electrons in AlₓGa₁₋ₓN, InₓGa₁₋ₓN, and InₓAl₁₋ₓN as a function of electric field strength E for various alloy compositions x.

A key property of the nitrides is the fact that they possess large spontaneous and piezoelectric polarization fields, which allows to induce high channel densities in HFETs without doping. We included these polarization fields in our self-consistent Monte-Carlo simulations to investigate the ideal intrinsic DC-characteristics and transit time frequencies for undoped Ga-faced single heterostructure AlₓGa₁₋ₓN/GaN as a function of various geometry parameters. The layer structures consist of a GaN substrate and a 25 nm thick AlₓGa₁₋ₓN barrier layer with x=30%. The source gate spacing is chosen to be 275 nm while the gate drain spacing is on the order of 500 nm. The channel density, which is induced due to the divergence between the polarization in the adjacent layers is calculated to be 1.5 \times 10^{13} \text{ cm}^{-2}. For an ideal interface, the low field channel mobility was found to be 1700 \text{ cm}^2/\text{Vs}. The drain current characteristics for three gate lengths of this device is shown in figure 2. As a consequence of the high channel densities and high drift velocities in this material class, we find very high drain currents for these undoped structures. Short channel

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effects become clearly important for gate length below 200 nm, resulting in an increasingly poor off-characteristics.

**Fig. 2** As$_{30}$Ga$_{70}$N/GaN HFET drain current characteristics for gate lengths of 300 nm, 200 nm, and 150 nm, at various gate voltages in steps of 1V.

For these single heterostructure FETs, we find maximum transconductances ranging from 800 s/m to 900 S/m by varying the gate length from 300 nm to 150 nm. Thereby, the transit time frequency, calculated from the average channel velocity and the effective gate length, increases from 150 GHz up to 260 GHz at 7V drain voltage, which scales almost with the inverse gate length of the devices. This shows, that velocity overshoot effects play only a minor role in these HFETs.

**Fig. 3:** Calculated transit time frequencies for various AlGaN/GaN HFETs as described in the text.

We investigated the sensitivity of the transit time frequency onto other layout quantities of the device. The results are depicted in figure 3) for devices with a constant gate length of 300 nm. The curve labeled by 1 shows the transit time frequency for the original layout as described above. By increasing the source gate spacing from 275 nm to 600 nm we find a drop of the transit time frequency from 140 GHz to 130 GHz (see curve 2 in figure 3). Such a moderate decrease of the transit time frequency is a consequence of the high density and high mobility of the electrons in the source-gate part of the channel. A further decrease of the transit time frequency is found by increasing additionally the gate-drain spacing from 500 nm to 1200 nm. This results in lower effective channel fields and consequently to a reduction of the drift velocity in the channel, causing the observed decrease of the transit time frequency (curve 3 in figure 3). These effects become clearly more pronounced for a less ideal device with a lower channel mobility of 1000 cm$^2$/Vs and a lower channel density of 10$^{13}$ cm$^{-2}$ (curve 4 in figure 3).
Free standing Pt/GaN Schottky diodes

Uwe Karrer, Claudio R. Miskys, Oliver Ambacher and Martin Stutzmann

Large GaN substrates with good structural properties are not commercial available up to date, so device quality films are grown by heteroepitaxy on substrate materials like Al₂O₃ and SiC. An alternative to GaN single crystals are thick bulk like GaN films grown by hydride vapor phase epitaxy (HVPE) on sapphire substrates. These structures provide stress and bowing due to different lattice constants and different thermal expansion coefficients of GaN and sapphire, respectively. Sapphire also does not permit electrical contacts to be made from the backside. These restrictions can be overcome by free standing GaN layers delaminated from Al₂O₃ substrate by the laser lift-off technique. The lift-off process is realized by illuminating of the sapphire/GaN interface with a sequence of intense ultraviolet laser pulses, which leads to a localized heating of GaN above 850°C. This causes thermal decomposition of about 50 nm of the GaN film, followed by nitrogen effusion and finally the delamination from the substrate. Large free-standing and relaxed GaN films and substrates can be fabricated by this method, suitable for the realization of GaN Schottky diodes. Free-standing GaN offers the possibility to process devices on either side, which have opposite crystal polarity (Ga-face [0001] or N-face [0001]). Schottky diodes with semitransparent Pt-contacts surrounded by an Ti/Al ohmic contact were processed. The Schottky contacts were evaporated on both sides of the cleaned and electrochemically polished, atomically flat sides of free-standing HVPE GaN. Fig. 1 exhibits different IV-characteristics for Schottky diodes on GaN with different polarity. From these measurements Schottky barrier heights can be inferred by extrapolation of the exponential current increase in forward direction to zero bias. Our measurements show a higher Schottky barrier on Ga-face in comparison to N-face material.

![IV-characteristics of Pt/GaN Schottky diodes with Ga- or N-face polarity.](image)

The large spontaneous polarization of the pyroelectric GaN causes a negative and positive bound sheet charge located at the Ga- and N-face surface, respectively. For n-type GaN free electrons tend to compensate the positive surface charge, whereas the negative charge is only partly compensated by ionized donors. Fig. 2 shows the resulting band bend-

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ing and the electron concentration profile. The band bending at the Ga-face surface causes an increase in barrier height, whereas the Schottky barrier height on the N-face side of GaN is not effected by spontaneous polarization.

Fig. 2: Conduction, valence and electron concentration profiles for n-type GaN. Free electrons are accumulated at the N-face surface in order to screen the polarization induced positive surface charge, +\( \sigma \).

A current application for Pt/GaN Schottky diodes is the detection of UV-light at high temperatures. Therefore, temperature dependent current voltage measurements were carried out on semitransparent Pt-Schottky contacts evaporated on the Ga-face side. The results for temperatures up to 410 K are shown in Fig. 3.

Fig. 3: IV-characteristics of a Ga-face Pt/GaN Schottky diode measured at temperatures between 300 and 410 K.

From this set of measurements an increase of the ideality factor from 1.3 to 1.6 and a decrease of the barrier height by 200 meV is determined, if the temperature is increased from 300 to 410 K. One of the important features for UV-detectors is the behavior of the reverse current, which increases from \( 10^{-5} \) to \( 10^{-3} \) A/cm\(^2\) at 410 K. Although a significant increase of reverse current is measured, the diodes should still be suitable for UV-light detection, because the rectification ratio is more than six orders of magnitude (at \( U = \pm 1.5 \) V) over the whole range of temperatures investigated here.

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Frequency tripler with anti-serial Schottky diodes

Markus Krach¹, Jürgen Freyer, and Manfred Claassen

All-solid-state power sources are needed for a wide range of millimeter-wave and Terahertz applications, e.g. radio astronomy, atmospheric radiometry or plasma physics. For frequencies above about 200 GHz, multipliers are used since fundamental oscillators cannot deliver sufficient power. Among the applied semiconductor devices for multipliers, the Schottky diode is mostly used though its application in higher order multipliers, for example triplers, is more complex as compared to devices with symmetric capacitance-voltage characteristics. We have designed a new type of varactor structure with two inhomogeneously doped anti-serial Schottky diodes which combines the advantages of a varactor with symmetrical capacitance-voltage behaviour and the low leakage current of Schottky diodes. These devices can be preferably applied in tripler structures since no idler- and bias-circuits are needed, which makes the circuit design simpler. Anti-serial Schottky diodes with constant doping concentrations cannot be used as varactors because an applied rf-voltage leads only to a displacement of the space-charge region, i.e. the width of the space-charge of the reverse biased diode increases by the same amount by which the width of the forward diode is reduced. Thus, no non-linear total CV-characteristic appears. However, this is not valid if the doping concentration in the depletion layer is non-uniform. Then the space-charge region variations of the forward and reverse diode respectively differ from each other leading to a variable total capacitance with respect to the voltage. The shape of the resulting CV-characteristic depends on the doping profile as well as on the amplitude of the rf-voltage. The current-voltage curve of this type of varactor is characterized by the low leakage current of the Schottky-junction.

The layer sequence of the applied Schottky diodes is schematically shown in Fig. 1. A relatively large barrier height is realized by the use of an undoped AlGaAs layer below the Schottky contact. The remaining depletion zone is split up into two layers with stepwise constant doping concentration followed by a highly n-doped zone for ohmic contact. The symmetric varactor is realized by an anti-series connection of two diodes with a common Schottky contact.

To determine the device properties, a simulation programme is used which considers space-charge fields, thermionic field emission, tunnelling and impact ionisation. Energy-band diagrams of the structure are calculated by solving Poisson’s equation self-consistently for different applied voltages. These band-edge diagrams then are used to compute the I-V characteristics of the Schottky diodes. Thermionic emission of electrons over

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the barrier and tunnelling through the barrier are determined by the model of Tsu and Esaki in combination with WKB approximation. For high voltages also impact ionisation is taken into account. The capacitance versus voltage behaviour of the Schottky diode is calculated from the change of electric field with applied voltage. In Fig. 2 the I-V and C-V characteristics for a single Schottky diode are depicted showing good agreement of measured and simulated data.

The dynamic CV-characteristic of the two anti-series connected diodes, which determines the efficiency of the tripler, is calculated from the CV- resp. charge-voltage characteristic of a single Schottky diode. With this charge-voltage characteristic and the charge displacement due to the self-biasing, which is rf-voltage amplitude dependent, the total charge-voltage characteristic of the anti-series connection of two diodes can be computed. The differentiation of the total charge-voltage characteristic provides the rf-CV characteristic of the multiplier device. As an example, the resulting total rf-CV characteristic of two anti-serial Schottky diodes is depicted in Fig. 3. The inhomogeneous doping profile in the depletion zone obviously results in a strong non-linearity of the CV-characteristic which enables application in frequency multipliers.

First experimental results are achieved by a quasi-monolithical integration of two anti-serial Schottky diodes in a microstrip circuit on quartz substrate. For this purpose, the initial GaAs epitaxial material is bonded on the quartz substrate, the GaAs substrate is removed and the entire rf-circuit including the two diodes is fabricated by standard photoresist technology. The two Schottky diodes are connected in series via air-bridges between input and output circuit. Fig. 4 shows schematically the quartz chip which is placed into a split waveguide mount with two symmetrical halves. Tuning of the tripler is obtained by backshorts at both input and output waveguide. The design of the whole circuit was carried out by the help of microwave analysis programmes (ADS, HFSS). The IV-characteristic of the investigated Schottky diodes indicates relatively low leakage currents for reverse voltages up to 13 V. The diodes have a diameter of 10 µm and a series resistance of about 6 Ω. Tripler performance was tested at a fundamental frequency of 70 GHz. The experimental results show an rf-output power of 2 mW at 210 GHz with a flange to flange conversion efficiency of over 3 %. Up to this output level, saturation neither of efficiency nor of power has been observed. Since the structure of the diodes and the circuit are not yet optimized further work will focus on this field to increase the performance of the tripler.

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**Fig. 3:** Rf-CV characteristic of two anti-serial Schottky diodes

**Fig. 4:** Schematical view of the waveguide mount and quartz chip

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Vertical transistors with ultra-short channel lengths

Frank Ertl, Thomas Asperger, Rainer A. Deutschmann, Max Bichler and Gerhard Abstreiter

In our group we explore the physics of novel semiconductor nano-structures fabricated by means of the cleaved-edge overgrowth (CEO) method. The efforts spread from basic research to device related topics. Here we report on our recent results achieved in the fabrication of vertical transistors with ultra-short channel lengths.

Vertical transistor substrates are grown by GaAs/AlGaAs molecular beam epitaxy (MBE) on semi-insulating (001)-GaAs wafers. The substrates have a barrier sandwiched between 1 µm thick n⁺-GaAs source/drain contacts and differ only in the type of the barrier, as shown in Fig. 1. All MBE layers can be deposited with atomic precision to define the geometric channel length \( L \) of the transistor by the barrier thickness. We evaluate different concepts to minimize leakage currents from source to drain: barriers with p⁺-δ-doping (Fig. 1(a)) and simple or embedded hetero barriers (Fig. 1(b)+1(c)) are used. Thinned pieces of the substrates are cleaved under ultra-high vacuum conditions and a QW thick GaAs electron channel, the AlAs gate barrier and the n⁺-GaAs gate contact are deposited on the freshly exposed cleavage plane. Finally a mesa is etched on the specimen, ohmic contacts are attached and connected by silver glued gold wires.

All samples are characterized by measuring the I-V curves under gate voltage bias. In our setup the topmost contact is grounded and the source-drain voltage is applied to the bottom contact. The source-drain current is measured while simultaneously the voltage drop across the channel is recorded in 4-point-probe configuration.

Measurements of vertical transistors with a 6×10¹² 1/cm² p⁺-δ-doped barrier are presented in Fig. 2. In these devices an effective channel length \( L_{\text{Eff}} \) results from electrostatic depletion in the contact regions flanking the p⁺-δ-spike. The length of \( L_{\text{Eff}}=70 \) nm was obtained from capacitance measurements and confirmed by self-consistent calculations. I-V traces at 4.2 K (Fig. 2(a)) or at 300 K (Fig. 2(b)) from a sample with \( QW=40 \) nm channel thickness show typical subthreshold transistor behavior. For gate

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Fig. 1: Sample structure of vertical transistors fabricated by the cleaved-edge overgrowth method. Samples consist of a (001)-substrate overgrown with source/drain contacts separated by an insulating layer kind of (a) GaAs with p⁺-δ-doping, (b) AlGaAs barrier or (c) GaAs embedded AlGaAs barrier. The electron channel, gate barrier and gate contact are deposited on the (110)-plane.
voltages below 0.7 V the transistor stays in the turned-off regime, above gate leakage becomes dominant. At low temperatures the device behavior is governed by punch-through of electrons: at positive drain voltage the effective barrier height in the channel is reduced and electrons are tunneling from source to drain. At high temperatures an additional thermally activated current appears across the channel barrier. Fig. 2 exhibits both contributions as the diodic curves shift either with gate voltage or temperature.

Furthermore we study devices equipped with an Al$_{0.45}$Ga$_{0.55}$As hetero barrier, of which measurements at 4.2 K are plotted in Fig. 3. In this case the geometrical channel length is $L=50$ nm and results are shown for $QW=20$ nm (Fig. 3(a)) and $QW=40$ nm (Fig. 3(b)). Above a small positive gate voltage this device type shows turned-on transistor operation with an quasi-saturated region. The loss of the complete saturation is a typical short channel effect. Closer examination of the data reveals that the onset of the quasi-saturation shifts linearly to higher values with increasing gate voltage. When the channel thickness is raised, even though the channel cross section is increased, we observe an unexpected decrease in the average source–drain current. This behavior might be explained by additional series resistances stemming from the contact-channel coupling as the electron gas is located further away from the contacts at larger channel thicknesses.

**Fig. 2:** Typical device characteristics of a vertical transistor with $6 \times 10^{12} \text{cm}^{-2}$ $p^+\delta$-doped barrier. The channel is $L_{\text{eff}}=70$ nm long and $QW=40$ nm thick. Within the applied gate voltage range the transistor operates in the subthreshold region and punch-through behavior is visible. The barrier isolation is very good at (a) 4.2 K and is acceptable even at (b) 300 K.

**Fig. 3:** Current-voltage relation of devices equipped with Al$_{0.45}$Ga$_{0.55}$As hetero barriers and $L=50$ nm long electron channels at 4.2 K. The thickness of the channel is (a) $QW=20$ nm and (b) $QW=40$ nm. Commonly this type of device shows a quasi-saturated region. As the thickness is increased the average source-drain current decreases, although the cross section of the channel is enlarged.
5. Publications

_Electrochemical passivation of gallium arsenide surface with organic self-assembled monolayers in aqueous electrolytes_

_Two dimensional electron gases induced by spontaneous and piezoelectric polarization in undoped AlGaN/GaN HEMTs_
O. Ambacher, R. Dimitrov, M. Stutzmann, B. Foutz, M. Murphy, J. Smart, J. R. Shealy, N. G. Weimann, and L. F. Eastman

_Two dimensional electron gases induced by spontaneous and piezoelectric polarization in undoped and doped AlGaN/GaN heterostructures_

_Homogeneous line broadening in individual semiconductor quantum dots by temperature fluctuations_
M. Arzberger, and M.-C. Amann

_Low-resistivity p-side contacts for InP-based devices using buried InGaAs tunnel junction_
M. Arzberger, M. Lohner, G. Böhm, and M.-C. Amann

_Admittance spectroscopy of Ge quantum dots in Si_
T. Asperger, C. Miesner, K. Brunner, and G. Abstreiter

_Magnetic resonance investigations of defects in Ga^{14}N and Ga^{15}N_
M. W. Bayerl, N. M. Reinacher, H. Angerer, O. Ambacher, M. S. Brandt, and M. Stutzmann

_STM-photocurrent-spectroscopy on single self-assembled InGaAs quantum dots_
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_Spin-dependent capacitance of silicon field-effect transistors_
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A. Cremades, L. Görgens, O. Ambacher, M. Stutzmann, and F. Scholz

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New Schottky diode tripler for 210 GHz
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**Photoelectric properties of the 0.44 eV deep level-to-band transition in gallium nitride investigated by optical admittance spectroscopy**

**Long wavelength InGaAs-InGaAlAs-InP diode lasers grown in solid-source molecular-beam epitaxy**
G. K. Kuang, G. Böhm, N. Graf, M. Grau, G. Rösel, R. Meyer, and M.-C. Amann

**High-performance InGaAs-InGaAlAs 1.83µm lasers**
G. K. Kuang, G. Böhm, M. Grau, G. Rösel, and M.-C. Amann

**2.12 µm InGaAs-InGaAlAs-InP diode lasers grown in solid-source molecular-beam epitaxy**
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**Growth of quaternary AlInGaN/GaN heterostructures by plasma-induced molecular beam epitaxy**

**Dynamics of amplified spontaneous emission in InAs/GaAs quantum dots**

**Optical characterization of Mg-doped GaN films grown by metalorganic chemical vapor deposition**
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Low-resistance InGa(Al)As tunnel junctions for long wavelength vertical-cavity surface-emitting lasers
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M. Ortsiefer, R. Shau, G. Böhm, F. Köhler, and M.-C. Amann

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90 °C continuous-wave operation of 1.83 µm vertical-cavity surface-emitting lasers
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InP-based vertical-cavity surface-emitting lasers for 1.5-1.8 µm wavelength range
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