Model for the thickness dependence of electron concentration in InN films

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A model for the influence of different contributions to the high electron concentration in dependence on the film thickness of state-of-the-art InN layers grown by molecular-beam epitaxy is proposed. Surface accumulation has a crucial influence for InN layers <300 nm and superimposes the background concentration. For air-exposed InN, it can be assigned to a surface near doping by oxygen. For InN layers in the micron range the density of dislocations is the major doping mechanism. Finally, point defects such as vacancies and impurities have minor influence and would dominate the free electron concentration only for InN >10 μm. © 2006 American Institute of Physics [DOI: 10.1063/1.2364666]

Indium nitride is a low-band-gap material, which received an increasing attention over the last years due to its very prospective properties. In particular, the high electron concentration measured for In, Ga, and Al and a rf nitrogen plasma source. First, an elaborate analysis of the electron concentration in dependence on the layer thickness for MBE-grown InN films. In particular, the influence of threading dislocations (TDs) for an inhomogeneous doping will be demonstrated. The InN layers were grown in a BALZERS MBE system using conventional effusion cells for In, Ga, and Al and a rf nitrogen plasma source. First, an accurate model for the thickness dependence of electron concentration in InN films was developed. The model is based on three contributions: (i) a localized electron accumulation with specific sheet carrier concentration \( N_{\text{S,0}} \) (i.e., \( \alpha = 1 \)), (ii) a homogeneous background volume concentration \( N_{\text{b}} \) (i.e., \( \alpha = 0 \)), and (iii) an inhomogeneous carrier distribution \( n_{\text{inhom}} \) over the InN film (i.e., \( \alpha \) depends on the mechanism). Consequently, the net electron density in dependence on the InN film thickness \( th \) will be

\[
n = n_{\text{inhom}} + N_{\text{S,0}} + \frac{1}{th} \int_0^{th} n_{\text{inhom}} dz. \tag{1}
\]

The aim of this work is to model the influence of the different doping mechanisms in dependence of the layer thickness for MBE-grown InN films. In particular, the influence of threading dislocations (TDs) for an inhomogeneous doping will be demonstrated. The InN layers were grown in a BALZERS MBE system using conventional effusion cells for In, Ga, and Al and a rf nitrogen plasma source. First, an accurate model for the thickness dependence of electron concentration in InN films was developed. The model is based on three contributions: (i) a localized electron accumulation with specific sheet carrier concentration \( N_{\text{S,0}} \) (i.e., \( \alpha = 1 \)), (ii) a homogeneous background volume concentration \( N_{\text{b}} \) (i.e., \( \alpha = 0 \)), and (iii) an inhomogeneous carrier distribution \( n_{\text{inhom}} \) over the InN film (i.e., \( \alpha \) depends on the mechanism). Consequently, the net electron density in dependence on the InN film thickness \( th \) will be

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The apparent carrier concentration is decreasing with increasing film thickness similar to the most extensive studied series of InN films available in the literature, which was taken as reference. These InN films were also grown by pi-
Recently we found a very similar surface electron concentration and Fermi level position on an air-exposed InN surface by \textit{in situ} measurements of the resistance of an InN film during sputter depth profiling\textsuperscript{12} and ultraviolet photoelectron spectroscopy\textsuperscript{13}, respectively. The depth profile of the electron concentration follows in a very good agreement the oxygen concentration close to the surface estimated by Auger electron spectroscopy\textsuperscript{12,13}. Moreover, an interface charge of about \(5 \times 10^{12} \text{cm}^{-2}\), localized at the interface between InN and the GaN buffer layer, was estimated\textsuperscript{12,14} and is expected to be even higher at the interface between InN and AlN\textsuperscript{15}. The sum electron accumulation on both interfaces is superimposing the bulk concentration for InN films of up to 7.5 \(\mu\text{m}\) (Ref. 7) and explains qualitatively the observed dependence of the electron concentration on the film thickness. It is characterized by a constant sheet carrier concentration \(N_{SP}\). Consequently the dependence of the volume concentration \(n\) on the thickness \(t\) must follow a linear law \(n = N_{SP}/t\) (Fig. 2, “surface”). For \(N_{SP}\) the already mentioned values achieved by extrapolating the measured sheet carrier concentration \(N_S\) of thin InN films to zero thickness as described by Lu \textit{et al.}\textsuperscript{6} were used. Considering a surface accumulation of \(2.2 \times 10^{13} \text{cm}^{-3}\), which is independent of the buffer layer for thicker InN films, interface charges of \(0.3 \times 10^{13}\) and \(2.3 \times 10^{13} \text{cm}^{-3}\) at the interface to GaN and AlN, respectively, can be expected. The value for the GaN buffer layer is in good agreement with the sputtering experiments, which revealed an interface concentration of about \(0.5 \times 10^{13} \text{cm}^{-3}\). However, Fig. 2 clearly demonstrates that the apparent electron concentrations in this work (squares) as well as the data of Lu \textit{et al.}\textsuperscript{6} cannot be fitted with a linear law \(n = N_{SP}/t\). The smaller slope indicates the contribution of an additional, inhomogeneous doping mechanism.

The inhomogeneous electron distribution in InN layers was analyzed by Swartz \textit{et al.} using variable-magnetic-field Hall measurements\textsuperscript{16,17}. In addition to a part of carriers with low mobility and high density, which can be attributed to the surface accumulated layer, the values for the bulk carriers were extracted. Both bulk mobility and electron concentration are still depending on the layer thickness for InN films with a total thickness of up to about 1 \(\mu\text{m}\). For a thick film on GaN/AlN buffer (7.5 \(\mu\text{m}\)), a background carrier concentration of \(1 \times 10^{17} \text{cm}^{-3}\) was estimated. For its origin several effective donors are possible. Both oxygen\textsuperscript{13} and hydrogen\textsuperscript{18} have shown to create donor states inside the conduction band and for oxygen an effective doping efficiency of more than 50\% was observed\textsuperscript{12,13}. However, elementary analysis by secondary ion mass spectroscopy revealed a background concentration of oxygen, hydrogen, and carbon to be in the \(10^{16} \text{cm}^{-3}\) range, i.e., two to ten times smaller than the electron concentration\textsuperscript{7}. Similar to surface states\textsuperscript{19}, intrinsic defects such as point defects and dislocations are expected to create donor states inside the conduction band. As a typical point defect, vacancies were investigated by positron annihilation spectroscopy by Oila \textit{et al.}\textsuperscript{20}. N vacancies were found to be the dominating type with a concentration, which is about one order of magnitude lower than the electron concentration. All these effects can be summed up to the background concentration of \(1 \times 10^{17} \text{cm}^{-3}\) estimated by variable-magnetic-field Hall measurements on GaN/AlN buffer\textsuperscript{6,17}.

The influence of both surface accumulation and background concentration is shown in Fig. 2 by the curve “surface + background.”
On the other side, the density of dislocations in heteroepitaxial layers is typically monotonically decreasing with the layer thickness,\(^5\) and the influence of these defects explains qualitatively the dependence of the background carrier concentration on the layer thickness within the first 1 \(\mu\text{m}.\)\(^6\) For quantification, it is assumed that each dislocation creates donors with a specific distance in the growth direction. Using the concentration profile of Fig. 1, its influence is shown in Fig. 2. Similar to the TD density (Fig. 1), the concentration of the electrons from the TDs only (“TD”) starts to decrease at a thickness of about 100 nm. For the sum of all the discussed effects (“sum”), a very good agreement with the measured data is achieved if the distance in growth direction is about 1.14 nm, i.e., if in a TD only every second InN unit cell bears an effective donor or only 50% of the dislocations are active. In contrast to GaN,\(^21\) the underlying doping mechanisms of dislocations are not investigated and require further analysis. Taking the similarities of the materials into account, in particular, the dominating edge dislocations\(^5\) are creating vacancies. Previously these vacancies have been expected to be negatively charged.\(^22\) However, in contrast to GaN, the branch point energy \(E_B\) at the \(\Gamma\) point in InN is located deep inside the conduction band.\(^9\)

Intrinsic defects are charged in a way to shift the Fermi level \(E_F\) towards \(E_B\). Consequently, in \(n\)-type GaN where \(E_F > E_B\), the vacancies are negatively charged, while in InN, where \(E_F < E_B\), such defects should be positively charged, i.e., a donor-type behavior can be expected. The observed dependence of the electron concentration on the InN film thickness confirms this assumption, since for InN in the micron range the measured concentration is higher than the sum of all other possible contributions.

In conclusion, for state-of-the-art MBE-grown InN, three major mechanisms determine the apparent electron concentration on different thickness scales. First, the accumulation of electrons at the surface and the interface clearly dominates the electronic properties of InN for thin layers with \(t < 300 \text{ nm}\). For nondegenerate InN, an electron concentration below \(10^{17} \text{ cm}^{-3}\) would be necessary and already the accumulation layers would prevent to achieve this for InN films of up to \(\sim 5 \mu\text{m}\). Second, layers in the micron range are strongly affected by threading dislocations. Finally, the background concentration of InN is already well controlled and would influence the apparent carrier concentration only for films with \(t > 10 \mu\text{m}\). However, the influence of such point defects might have substantial influence on the mobility. As a consequence, for an application of InN films for electronic devices, both the reduction of the density of threading dislocations and the suppression of the electron accumulation at the interfaces are of crucial importance.

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