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Report:

Recently the fabrication and characterization of n-AlN/p- diamond UV light emitting diodes has been reported [Miskys]. Electroluminescence measurements revealed a surprisingly efficient light emission in the spectral range from *2.7* to *4.8 eV* under forward bias of the heterobipolar diode, which shows good rectifying properties. However, voltages up to more than *100 V* have to be applied due to the huge serial resistances of both the diamond and the AlN layer. To solve this problem, i.e. to reduce the serial resistance we have investigated the influence of the growth conditions and dopant concentration on the electrical properties of Si-doped n-AlN layers.

Whereas Si forms a shallow donor state in GaN and $Al_xGa_{1-x}N$ for $x < 40\%$ the state becomes deeper with increasing Al concentration, resulting in a low concentration of ionized donors at room temperature and hence a high specific resistance. In addition, for higher Si-concentrations self compensation due to simultaneous incorporation of Si impurities on Al-sites (donor-like) and N-sites (acceptor-like) occurs. In these donor-acceptor-complexes the redundant electron of the donor-like Si impurity is transferred to the acceptor-like Si and does not contribute to the electrical transport.

To overcome these restrictions and to significantly increase the charge carrier density tremendously, the Si concentration in AlN can be increased above the Mott transition, where donor orbitals overlap and an impurity band is formed. Assuming a donor state at E_D = *320 meV* a Si density of more than $10^{21}\ cm^{-3}$ is necessary, corresponding to approximately *1 %* of the overall atomic density. Currently it is not clear if it is possible to incorporate this huge amount into AlN using molecular beam epitaxy or if segregation effects occur.

To investigate this we have grown a series of AlN:Si samples under both metal- and N-rich conditions using plasma assisted molecular beam epitaxy, where we varied the Si flux between 10^{11} $cm^{-2}s^{-1}$ and 6×10^{13} $cm^{-2}s^{-1}$ resulting in a Si concentration of up to 5×10^{21} cm^{-3} as determined by elastic recoil detection analysis (ERDA) for the N-rich grown samples. Primarily in the metal-rich grown samples we observed accumulation of Si at the surface followed by a linear decrease into the AlN film. In both series of samples we found segregated crystalline Si using Raman spectroscopy and high-resolution X-ray diffraction, suggesting that a sizeable fraction of the Si impurities is not incorporated into the AlN crystallites. Atomic force microscopy revealed lateral crystal sizes of up to *500 nm* and a screw dislocation density of 2×10^{8} cm^{-2}, i.e. *2* dislocations per μm^2.

To identify a possible lateral Si accumulation we performed chemical mapping experiments using a 2.5 keV X-ray beam with a spot size of *300 nm × 700 nm* for excitation. From the recorded fluorescence spectra we investigated the lateral distribution of the integrated intensity of the Si Kα line.

For all samples we were not able to identify variations of the Si concentration on a small scale, i.e. less than *0.5 μm*. However, Si droplets with diameters in the range of *5 – 10 μm* were observed for N-rich grown samples and especially in the case of metal-rich grown samples we observed ring-like structures with a diameter of about *5 μm* (c.f. Fig 1).

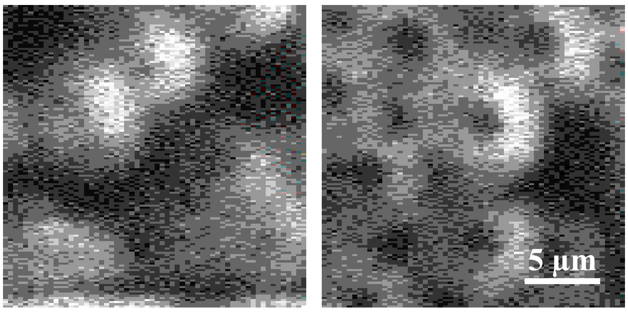

Fig. 1: Lateral distribution of Si for a) metal-rich and b) N-rich growth conditions using the integrated intensity of the Si Kα line of the fluorescence spectra.

In combination with the ERDA results we are able to relate the spatial distribution of Si, enabling us to compose a model for the incorporation of Si.

In the N-rich grown samples most of the Si is incorporated into the AlN layer. However, in the metal-rich grown saples, a metallic Al film is present on the surface during the growth process and most of the impinging Si is dissolved in this film, hindering its incorporation. Therefore, elemental Si is detected on the surface and its ring-like structures supports a simple model for solution of Si in Al. The ring-like structures are created during the cooling-down process after finishing the growth. The film starts to form Al:Si droplets when the substrate temperature is reduced. Further cooling down leads to the segregation of the Si at the edge of the droplets, which can be seen in the chemical mappings as ring-like shapes. In addition to that, below those droplets pits can be observed.

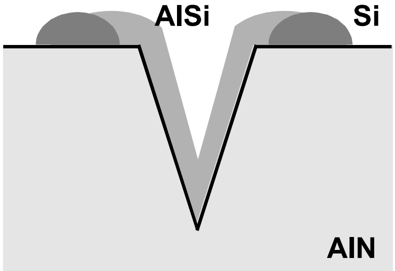

Fig. 2: Schematic model for the Si distribution on the AlN layer

Combining all results leads to the model of the Si distribution on the AlN layer after removing residual Al as depicted in Fig. 2. The accumulation of Si at the surface can be attributed to the segregated Si and the linear decrease can be explained by the coverage of the pit walls with an AlSi compound.

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