Towards GaN integration on Si: Microstructural study of ScN grown on Si(111) by plasma-assisted MBE for applications as a buffer layer

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GaN is a promising semiconductor material which has attracted significant attention last decades due to its interesting properties for future device applications. In that regard, the integration of high quality GaN on Si is currently an important research area. The growth of GaN directly on Si is very difficult due to the high lattice mismatch (-17%), thermal mismatch (56%) and the reactive interface. To reduce these effects and suppress chemical reactions, ScN has been proposed as a buffer layer, since it exhibits only 0.1% lattice mismatch with GaN [1].

ScN is a transition metal nitride semiconductor. Its rock-salt structure featuring a compatible atomic arrangement in the [111] surface orientation as the wurtzite GaN structure in the [0001] orientation [2].

The huge lattice mismatch between ScN and Si (-17%) makes their epitaxial integration difficult. In previous studies, ScN has been integrated on Si using a step-graded buffer layer composed of two different oxides, Sc_2O_3 and Y_2O_3 [3]. Moram *et al*. have demonstrated the possibility to obtain epitaxial type-B oriented ScN directly on Si by NH_3-plasma assisted MBE [4]. However, the presence of twins might be a limiting feature for subsequent growth of high quality GaN films.

In this study, thin ScN films were grown by plasma-assisted molecular beam epitaxy with a thickness ranging from 8 to 19 nm on Si (111) oriented substrates. The structural quality of the epi-layers has been investigated as a function of the thickness by XRD (X-ray diffraction), TEM (Transmission electron microscopy) and AFM (Atomic force microscopy). XRD in specular configuration confirms that the ScN epi-layers are (111) oriented and ϕ-scans show true single-crystallinity for the samples with thicknesses in the range from 8 to 17 nm. Cross-sectional TEM studies confirm the type-A oriented ScN films with respect to the substrate (Figure 1). Despite the single-crystalline nature and the lack of twin inclusions, ω rocking curves and ϕ-scans reveal tilt and twist, respectively. The morphology of the surface has been visualized by AFM showing a flat and smooth ScN surface up to 19nm thickness.

First attempts to grow GaN by PA-MBE on ScN(111)/Si(111) resulted in a single-crystalline epitaxial film which is confirmed by specular ω-2θ and azimuthal ϕ-scans determining the epitaxial relationship: GaN(0001)/ScN(111)/Si(111) and GaN[10-10] ǁScN[1-10]ǁSi[1-10] .

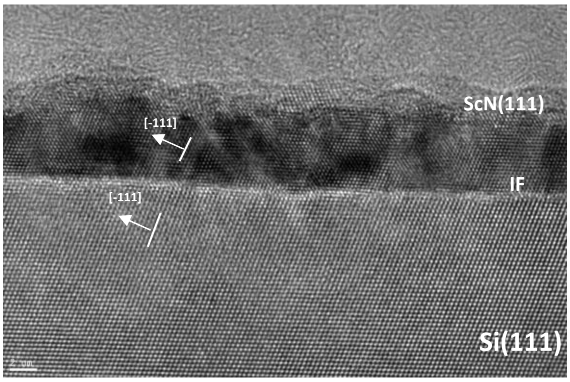

Figure 1: HRTEM image of ScN 8nm thick. The normal directions to the (-111) planes are indicated by white arrows.

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