Polarity control in hot-wall MOCVD III-Nitride epitaxy on on-axis and vicinal SiC ($000\bar{1}$) substrates

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Polarity of group-III nitrides critically impacts their properties and is a key to tuning the performance of electronic and optoelectronic devices. For instance, nitrogen(N)-polar group-III nitrides in high electron mobility transistors (HEMTs) heterostructures enables an enhanced carrier confinement in the channel with a natural back barrier, an improved device scalability, and facilitates the fabrication of low ohmic contacts.

However, growth of N-polar layers on C-face SiC substrates by MOCVD is very challenging. Previous studies reported that metal (Al)-polarity layers can occur as a result of supplying a pre-flow of metal precursors trimethylaluminum (TMAl) or by keeping a low V/III(NH3/TMAl)-ratio flow [1,2]. Thus, the initial AlN nucleation step is critical for polarity control and crystalline quality of the subsequent GaN layers [3]. Wet chemical etching using potassium hydroxide (KOH) [4] is commonly employed to determine the polarity of (Al,Ga)N thin film on a macro-scale [5] [6]. Although this method provides fast qualitative assessment, details on structural arrangements, growth mechanisms behind stabilization of specific polarity, and cause for polarity inversion remain obscured.

In this work, we report a comprehensive study of the structure of AlN nucleation layers grown by hot-wall MOCVD on on- and off-cut axis SiC(000-1) substrates. The investigations on polarity are performed in relation to growth mode (island vs 2D/step-flow) and structural properties for both types of substrates. KOH chemical wet etching combined with high-resolution X-ray diffraction measurements indicate N-polarity on a macro-scale for the AlN nucleation layers independently of the growth mode and substrate off-cut. However, aberration-corrected high-resolution transmission electron microscopy (HR-TEM) and scanning transmission microscopy (STEM) reveal a much more intricate picture. A mixed polarity is revealed for the AlN on on-axis SiC for the case of island-growth mode where V-shape inversion domains separate the underlying N-polar from the Al-polar regions. A scenario of how KOH proceeds via defects in mixed polarity AlN is outlined and it is stressed that the method may not provide conclusive polarity determination. On the other hand, for off-axis SiC pure N-polarity was inferred from the detailed TEM and STEM investigations. In this case we observe formation of Al-Al bonded layers, which are suggested to promote strain relaxation. The atomic arrangements at the interface between SiC(000-1) and the AlN nucleation layers are further discussed and growth mechanisms leading to pure N and mixed polarities on the different substrate types are proposed.

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