A comprehensive study of AlN nucleation layers grown onto on-axis and 4° off-axis SiC (000$\bar{1}$) substrates and its influence on GaN growth

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Group-III nitrides have been intensively investigated and widely employed in optoelectronic and electronic devices. Recently, nitrogen(N)-polar group-III nitrides have drawn much attention due to their unique characteristics compared with gallium(Ga)-polar nitrides in the application of high electron mobility transistors (HEMTs), such as the feasibility to fabricate low ohmic contacts, an enhanced carrier confinement with a natural back barrier, as well as high device scalability.

Growth of N-polar group-III nitrides layers are expected on C-face SiC substrates. However, according to previous studies, the initial AlN nucleation step is critical to the polarity control of AlN and GaN layers on SiC substrates. The presence of hexagonal hillocks onto the surface of N-polar GaN epilayers was identified as a common problem for the growth on on-axis substrates. The formation of hexagonal hillocks can be suppressed or eliminated by employing vicinal GaN, sapphire or SiC substrates with different misorientation angles. Much work has been focused on the experimental development of N-polar III-Nitride materials. Despite intense investigations, device-grade high-quality N-polar GaN epitaxial layers remain challenging.

In this work, we study in a comparative manner epitaxial GaN layers grown onto on-axis and 4° off-axis SiC (000 $\bar{1}$) substrates by hot-wall MOCVD. GaN epilayers are grown simultaneously on both substrates employing N-polar AlN nucleation layers (AlN-NLs). We investigate the difference in surface morphology and crystal quality of the GaN epilayers on the two substrates. Growth mechanisms leading to different polarities on the two types of substrates are discussed based on transition electron microscopy (TEM) findings. 'V' shape inversion domain boundaries are observed between N-polar and Al-polar at AlN-NLs at on-axis substrate while metal rich Al-Al bonding layers are observed on off-axis substrates. The nature of AlN-NLs and its interfaces with the substrates and GaN epilayer is discussed. Atomic arrangement at the interface and possible bonding configurations are also analysed. Furthermore, the stain and free charge carriers of GaN layers are investigated by infrared spectroscopic ellipsometry.