Stabilization of cubic AlN in epitaxial TiN/AlN superlattices

Ilwon Kim, Anita Madan, Scott Barnett, Shang-Cong Cheung, and Vinayak Dravid
Department of Materials Science and Engineering
Northwestern University.

There have been predictions of a high-pressure cubic(NaCl/B1 structure) phase(a_{AlN} ~ 0.405 nm) of AlN, which at ambient pressures crystallizes in a hexagonal (wurtzite) phase with a=0.3108 nm and c/a=1.601. Epitaxial TiN/B1 AlN superlattices with the modulation wavelengths 1.8 nm to 8 nm were grown on MgO(001) by D.C. reactive magnetron sputtering. AlN grew in the B1 structure at layer thicknesses ≤ 2.0 nm. For larger layer thicknesses, the AlN grows in the wurtzite structure and epitaxy is lost. Satellite reflections (up to 6) were observed in high angle XRD patterns. Dynamical theory (Paratt's formalism) was used to simulate the low angle XRD patterns and to estimate the layer thickness ratio and the modulation wavelength. These parameters were then input in a simulation program (based on a kinematical model and a trapezoidal composition modulation) used to fit the high angle XRD pattern. The lattice spacing of B1 AlN was determined to be 0.40±0.002 nm. Random lattice spacing fluctuations(Gaussian width ~ 0.002 nm) and layer thickness variations (~ 0.1 nm) were incorporated to match the observed broadening of the superlattice peaks. The interface widths were estimated to be ~ 0.1 nm. XRD simulations also ruled out the possibility that other Ti-Al-N phases e.g. $Ti_{(1-x)}Al_xN$, $TiAl_3N$ or zinc-blende AlN formed during growth. Cross-sectional transmission electron microscopy showed that the layers were well-defined and planar. Selected area electron diffraction patterns and HREM confirmed that the AlN was in a cubic phase.