Stress and Dislocation Evolution in Silicon-doped $Al_xGa_{1-x}N$ Thin Films grown on SiC Substrates

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Silicon incorporation has been reported to both generate tensile stress in GaN and $Al_xGa_{1-x}N$ films, leading to crack formation, and to increase surface roughness. The latter effect is thought to be responsible for the former, either through a decrease in the average size of effective crystallites defined by gaps in the roughening surface [1] or a reduction in the energy barrier to threading dislocation (TD) inclination, which results in a strain gradient [2]. In this study, *in-situ* curvature measurements were used in combination with post-growth transmission electron microscopy (TEM) to directly investigate the effects of silicon doping on the evolution of stress and the behavior of threading dislocations in $Al_xGa_{1-x}N$ ($x = 0.28$–0.37) thin films grown by metalorganic vapor phase epitaxy.

A series of $Al_xGa_{1-x}N$ samples were grown on (0001) 6H SiC substrates using a ~80 nm AlN buffer layer at 1100 °C and 50 Torr using trimethylgallium, trimethylaluminum and ammonia as precursor gases and SiH_4 as the dopant source. A Multi-beam Optical Sensor System (k-Space Associates) was used to record changes in substrate curvature *in-situ*, which were converted to incremental changes in film stress via Stoney's equation. The effect of SiH_4/group III ratio on stress evolution was initially investigated. A ~200 nm thick undoped AlGaN layer was initially grown on the AlN buffer layer followed by growth of a Si-doped AlGaN layer. Stress-thickness vs. thickness plots obtained during the growth of these samples are shown in Fig. 1(a). In this type of a plot, negative and positive slopes correspond to compressive and tensile incremental growth stresses, respectively The undoped AlGaN grew under an initial epitaxial compressive stress of ~2-3 GPa, which relaxed with increasing film thickness and similar behavior was observed for Si-doped AlGaN grown at lower SiH_4/group III ratios. However, at a SiH_4/group III ratio of 1×10^{-3}, which corresponds to an electron concentration of ~ 3×10^{18} cm^{-3}, a transition from compressive to tensile incremental growth stress was found to occur shortly following the introduction of SiH_4 into the reactor. The compressive-to-tensile transition became more pronounced as the SiH_4/group III ratio was increased. Cross-sectional TEM (XTEM) micrographs (Fig. 1(b-c)) obtained on a undoped/Si-doped $Al_{0.28}Ga_{0.72}N$ sample that exhibited a compressive-to-tensile transition, indicated that the dislocations are predominantly edge-type and exhibit a change in the average projected dislocation angle from $8.1 \pm 5.7°$ in the nominally undoped region to $17.0 \pm 4.9°$ after SiH_4 introduction. These results provide direct experimental evidence that the inclination of threading dislocations, induced by the introduction of Si-doping, gives rise to a gradient in the film stress on the order of 6.6 GPa-μm^{-1} in this sample. The experimentally measured stress gradient is in close agreement with the value of 7.4 ± 2.1 GPa-μm^{-1} predicted by the "effective climb" model of dislocation inclination [2].

The inclination of threading dislocations by Si-doping might also be expected to yield reduced dislocation densities in $Al_xGa_{1-x}N$, by providing opportunities for dislocation interaction and annihilation. To investigate this further, a series of $Al_xGa_{1-x}N$ samples were grown in which SiH_4 introduced at varying thicknesses (0 to 200 nm). The stress observed to transition from compressive to tensile shortly after SiH_4 addition in all cases (Fig 2(a)). Preliminary TEM characterization (Fig. 2(b-c)) of these samples indicates a reduction in threading dislocation density from 6.6×10^{10} cm^{-2} for nominally undoped AlGaN to ~2.8×10^{10} cm^{-2} for the film in which SiH_4 added at the beginning of growth.

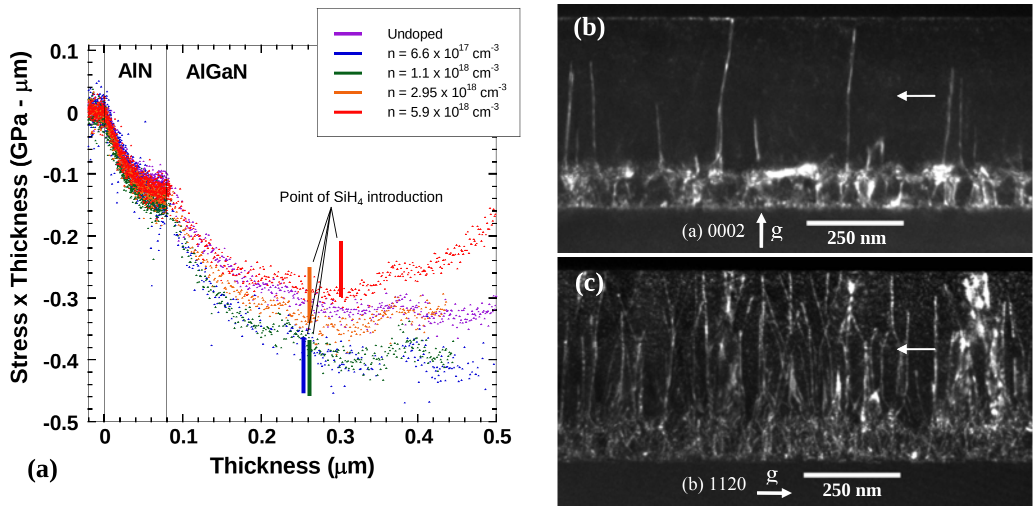

Figure 1. (a) Stress-thickness vs. thickness plots for undoped $Al_xGa_{1-x}N$ and undoped/Si-doped $Al_xGa_{1-x}N$ layers grown with increasing SiH_4/group III ratios. The thickness at which SiH_4 was added during growth is indicated for each sample. Weak beam dark-field cross-section TEM images of an undoped/Si-doped $Al_{0.28}Ga_{0.72}N$ sample obtained using (b) 0002 and (c) 112-0 diffraction conditions. The thickness at which SiH_4 was added during growth is indicated by an arrow.

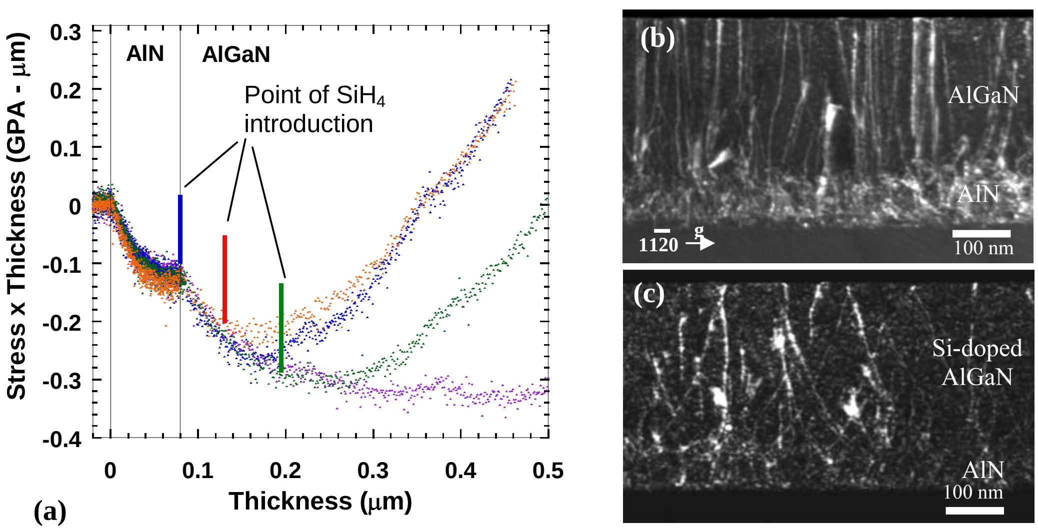

Figure 2. (a) Stress-thickness vs. thickness plots for Si-doped $Al_xGa_{1-x}N$ layers grown with SiH_4 introduced at different layer thicknesses as indicated in the figure. Weak beam dark-field cross-section TEM images obtained using 112-0 diffraction conditions for (b) undoped $Al_xGa_{1-x}N$ and (c) Si-doped $Al_xGa_{1-x}N$ in which SiH_4 was added at the beginning of growth.

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[2] A.E. Romanov, G.E. Beltz, P. Cantu, F. Wu, S. Keller, S.P. DenBaars and J.S. Speck, "Cracking of III-nitride layers with strain gradients," Appl. Phys. Lett. 89 (2006) p. 161922.