Strain accommodation in InGaN epilayers and interlayers with high alloy content towards efficient photovoltaics

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High alloy content InGaN thin films are promising for high efficiency photovoltaics. To this end, it is required to elucidate the mechanisms of strain relaxation through defect introduction in conjunction to the indium content and phase separation phenomena. A systematic study was performed using samples deposited by plasma-assisted molecular beam epitaxy (PAMBE) which is a technique that can take advantage of metastability due to the lower growth temperatures. The change of growth temperature was employed in order to vary the indium content and observe the pertinent chemical and structural phenomena by transmission electron microscopy (TEM) techniques. We considered (0001) interlayers and epilayers of thicknesses starting from 1 nm and up to \sim 500 nm, and a 10-60% alloy content. The films were characterized using TEM, quantitative high resolution TEM (qHRTEM), scanning TEM (STEM) and energy dispersive x-ray spectroscopy (EDXS). In thin films, we observed that with decreasing growth temperature, distinct mechanisms of strain relaxation become dominant with a concurrent increase of the indium content. At high growth temperature, strain relaxation is accommodated by the opening up of V-defects connected to screw or mixed-type threading dislocations that continue from the GaN template. This mechanism is superseded by the so-called sequestration mechanism that comprised the self-formation of a strained buffer-like InGaN layer between the GaN template and the main film. Such a region is gradually suppressed with further lowering the growth temperature. In addition to epilayers, InGaN interlayers of increasing thickness were deposited in order to assess early stage phenomena such as material interdiffusion, interfacial roughening and introduction of extended defects (Fig. 1). Indium incorporation efficiency was found to increase with interlayer thickness up to a critical thickness of ~5 nm and a ~40% content, whereby the onset of gradual plastic relaxation was determined. On the other hand, the elastic thinner layers exhibited strain fluctuations attributed to alloy inhomogenities.

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Figure 1: HRTEM images of InGaN interlayers with superimposed strain maps depicting the relative variation of the *d*-spacing of (0002) planes. (a) A nominally 1 nm thick layer with strain fluctuations. (b) A partially relaxed layer of nominally 5 nm thickness with strain grading at the InGaN/GaN interface.