

## Strain Engineering in Aluminum Scandium Nitride Thin Film using Four-dimensional Scanning Transmission Electron Microscopy (4D-STEM) Technique

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Recently, researchers have focused on enhancing the piezoelectric properties of AlN by doping Sc atoms to different percentages and have observed ferroelectricity in AlScN, a III-V semiconductor based material, for the first time.<sup>1</sup> However, many questions remain concerning the evolution of the ferroelectric properties and the morphological changes induced by the addition of Sc in AlN thin films. Here, the ‘four-dimensional scanning transmission electron microscopy’ (4D-STEM) technique is employed to systematically investigate nanoscale order by measuring the average spacing between atoms within certain regions in a 20 nm Al<sub>0.64</sub>Sc<sub>0.36</sub>N thin film and determining the strain. This technique records a full image of the STEM probe in diffraction space using high-speed electron detectors.<sup>2</sup>

The average interplanar distance ( $d_{\text{spacing}}$ ), corresponding to the (0002) planes of the wurtzite crystal structure in the AlScN film, is calculated from the intensity-distance line profile in Figure 1. The AlScN film grown on the Pt (111)/Si (100) substrate shows a decrease in the out-of-plane lattice parameter with the film thickness, which indicates the presence of in-plane compressive strain specifically close to the film/Pt interface. Our results demonstrate how the strain varies in the regions nearest to the AlScN/Pt interface through 4D-STEM diffraction (Figure 2). The strain map confirms a significant increase in the out-of-plane component of the lattice parameter (~4%) at the interface. The lattice parameter in the Pt template decreases as a function of distance from the Pt/Si interface. The emergence of ferroelectricity in AlScN is connected to the gradual evolution from the initial wurtzite structure (space group #186, P6<sub>3</sub>mc) to the layered hexagonal structure (space group #194, P6<sub>3</sub>/mmc) that also causes the enhanced piezoelectric coefficients with increasing Sc content and tensile strain.<sup>1</sup>

These results provide an understanding of the atomic structure of AlScN/Pt heterostructures and open the way toward the applications of this material in ferroelectric memories and microelectromechanical systems (MEMS).

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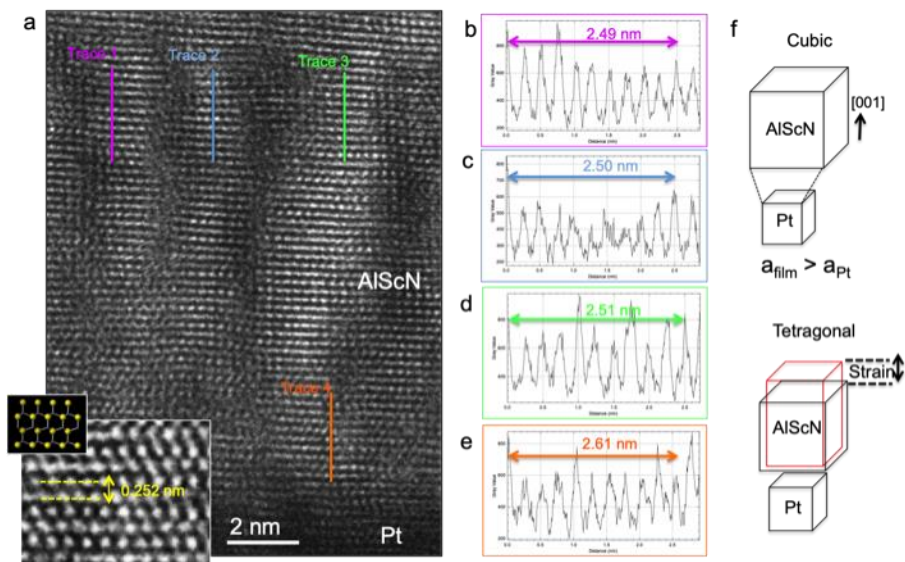


Figure 1. (a) High-resolution TEM image of the AlScN film. Inset: the atomic-resolution TEM image of the AlScN film. (b–e) The intensity–distance line profiles across the row of atomic planes indicated by the colorful lines, used to calculate the average spacing (using Digital Micrograph); from top-left to the top-right and the bottom of the film respectively. (f) The schematic illustration of increased spacing at the bottom of the film.

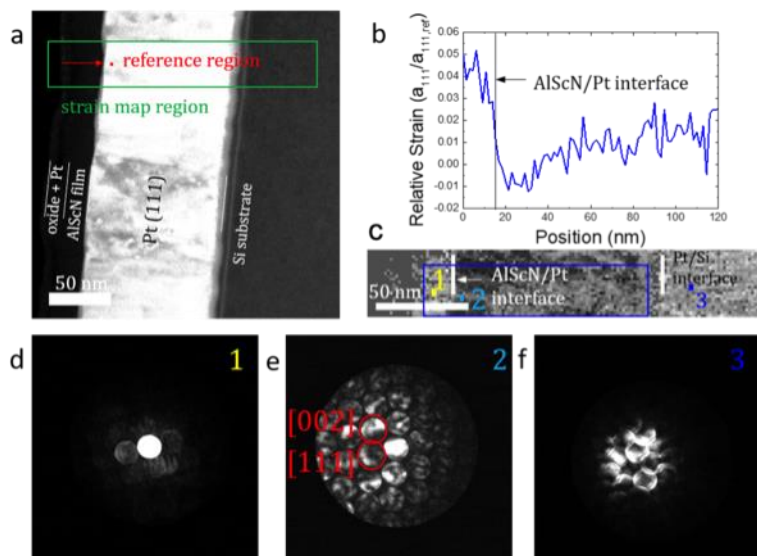


Figure 2. (a) Dark-field STEM image of the AlScN/Pt/Si. (b) Column-wise averaged relative strain line-scan from the region of interest marked by the blue rectangle in (c) Map of relative strain in AlScN film and Pt(111) template. Note that a point in the Pt is chosen as the reference where relative strain is defined to be 0. CBED patterns from (d) AlScN film, (e) Pt (111) template, and (f) Si (100) substrate.

## References

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