Microsc. Microanal. 28 (Suppl 1), 2022
doi:10.1017/S1431927622002471

Strain-Engineering of Aluminum Scandium Nitride Films Grown Directly on Silicon by Utilizing a Gradient Seed Layer: Application of 4D-STEM Technique

Pariasadat Musavigharavi[1,2*], Rossiny Beaucejour[3], Roy H. Olsson III[1], and Eric A. Stach[2,4]

[1.] Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA, United States.
[2.] Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, United States.
[3.] Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA, United States.
[4.] Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, PA, United States.
* Corresponding author: pgharavi@seas.upenn.edu

Aluminum Scandium Nitride (AlScN) films grown directly on Silicon at high Sc alloying levels (20.3-36.6 atomic %) using reactive co-sputtering shows the formation of anomalous grains (AOGs). Here, a gradient seed layer and proper process gas mixture is combined to inhibit formation of AOGs in AlScN with up to 36% Sc alloying even when grown directly on Si. In this study, "Four-dimensional scanning transmission electron microscopy" (4D-STEM) technique is employed to systematically investigate the nanoscale order by measuring the average spacing between atoms within certain regions in the film and determining the strain [1]. The strain map confirms a significant decrease in the out-of-plane component of the lattice parameter at the film/silicon interface.

The cross-section TEM sample was prepared in a Plasma-focused Ion Beam (TESCAN S8000X PFIB-SEM) system using the in-situ lift-out technique. The sample was coated with electron beam and ion beam deposition of Pt protection layers to prevent charging and protect the sample surface during FIB milling. At the final cleaning stage, a low-energy Ga+ ion beam (5 keV) was used to reduce FIB-induced damage. A sample with parallel surfaces and a general thickness of ~ 50 ± 5 nm was prepared. Scanning/transmission electron microscopy (S/TEM) characterization and image acquisition were carried out on a JEOL F200 TEM operated at 200 kV accelerating voltage. 4D-STEM strain mapping was performed using STEMx (Gatan Inc., USA) on a Gatan OneView *in-situ* camera (4k × 4k resolution). A diffraction pattern acquisition time of 0.04 s was used, and drift correction was performed every two rows. All quantification results presented in this work were calculated with Digital Micrograph software (DM, Gatan Inc., USA).

To assess the effect of gradient seed layer with gradient Sc alloying level on the distributed strain through the interface, 4D-STEM technique was employed to precisely characterise the lattice parameters of the film in both in- and out-of-plane directions. Bulk acoustic wave resonators fabricated from low stress and AOG free $Al_{68}Sc_{32}N$ films grown directly on Si demonstrate high frequency operation of 3.6 and 4.8 GHz, high electromechanical coupling > 18%, and quality factors in excess of 500. In conclusion, we showed that the electrical properties of AlScN film strongly depend on the distributed strain to the substrate interface [2].

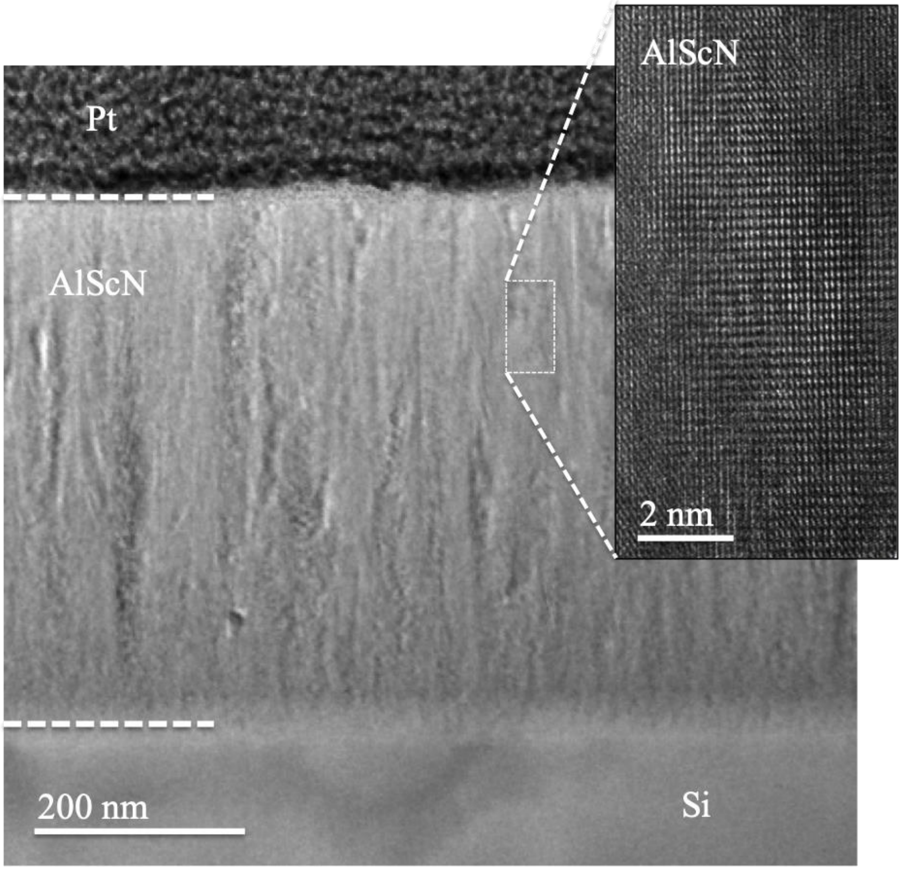

Figure 1. The cross-section TEM image of AlScN film on silicon substrate. Inset: High-resolution TEM image of the AlScN film.

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https://doi.org/10.1017/S1431927619000497.
[2] The authors acknowledge funding from the NSF CAREER Award (1944248) and in part The Defense Advanced Research Projects Agency (DARPA) Small Business Innovation Research (SBIR) under award HR0011-21-9-0004. This work was carried out in part at the Singh Center for Nanotechnology at the University of Pennsylvania, a member of the National Nanotechnology Coordinated Infrastructure (NNCI) network, which is supported by the National Science Foundation (Grant No. HR0011-21-9-0004).

https://doi.org/10.1017/S1431927622002471 Published online by Cambridge University Press