MAGNETRON SPUTTER EPITAXY OF ALUMINUM SCANDIUM NITRIDE (AlScN) THIN FILMS

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Ever since the discovery of enhanced piezoelectric properties of aluminum scandium nitride ($Al_{1-x}Sc_xN$, later denoted as AlScN) in 2009, the interest in it as a next generation material for broadband RF-filters in 5G communications is still growing. In addition, it is also very attractive for other applications, where piezoelectric transducers and actuators are required, such as bio-sensing, energy harvesting, or acoustics. Here at Fraunhofer IAF, the focus is on bridging the gap between the material science and device design in order to understand how to best implement, or even to open new horizons for this exciting material. Typically, for piezoelectric resonator applications, e.g. RF filters, highly c-axis oriented AlScN layers are preferred. However, growth of AlScN on silicon – the most common substrate in RF-MEMS applications – leads to textured films, i.e., the grains are c-axis oriented out-of-plane, but randomly oriented in-plane. This gives rise to additional acoustic losses in the fabricated devices, decreasing the quality factor Q. If one can go from textured growth to epitaxial growth (clearly defined in-plane epitaxial relationship between the substrate and the film), the device performance can be further improved through superior material quality.

Magnetron sputter epitaxy

Magnetron sputter epitaxy (MSE) is a special type of sputtering process where – under particular conditions and provided that the substrate has a reasonably good lattice-match to the film material – it is possible to achieve epitaxial growth in a similar manner as in molecular beam epitaxy (MBE). In the case of group-III nitrides such as AlN or AlScN one of the most suitable substrates is sapphire, where a 30° rotation between the layer and substrate crystal lattices leads to the lowest possible lattice-mismatch. Recently, MSE process was successfully employed at Fraunhofer IAF on an Evatec CLUSTERLINE® RAD sputter tool system using reactive co-sputtering from Al and Sc targets to produce 1 µm-thick, epitaxial, piezoelectric, single-phase $Al_{1-x}Sc_xN/Al_2O_3$ with up to x=0.4 (40%) scandium incorporation (Figure 1). The sputtered layer still has columnar microstructure typical for sputtered thin films, but at the same time each of these columnar grains has a defined crystallographic relationship with the substrate. A comparison of XRD pole figures is shown in Figure 2, where, for textured $Al_{1-x}Sc_xN$/Si films, a continuous ring is observed, while for epitaxial $Al_{1-x}Sc_xN/Al_2O_3$ six distinct spots appear instead. Samples showed 0002 reflection rocking curve FWHM values in the range of 0.9° in low-Sc films and up to 1.6° in high-Sc films,

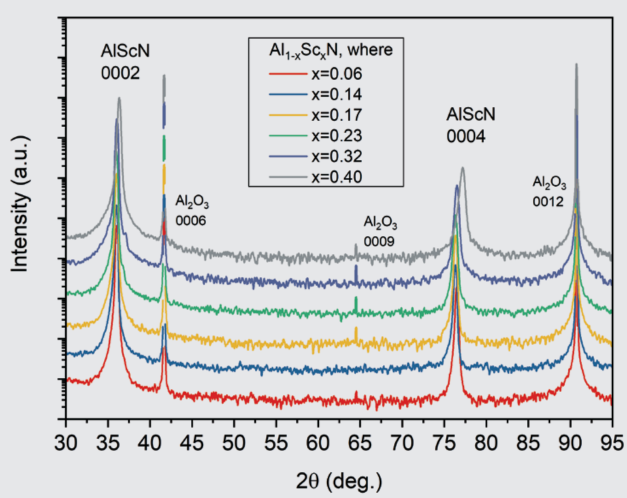

Figure 1. X-ray diffraction patterns for phase pure, c-axis oriented $Al_{1-x}Sc_xN/Al_2O_3$ thin films with different Sc concentrations denoted as x=0.06, 0.14, 0.17, 0.23, 0.32, and 0.40.

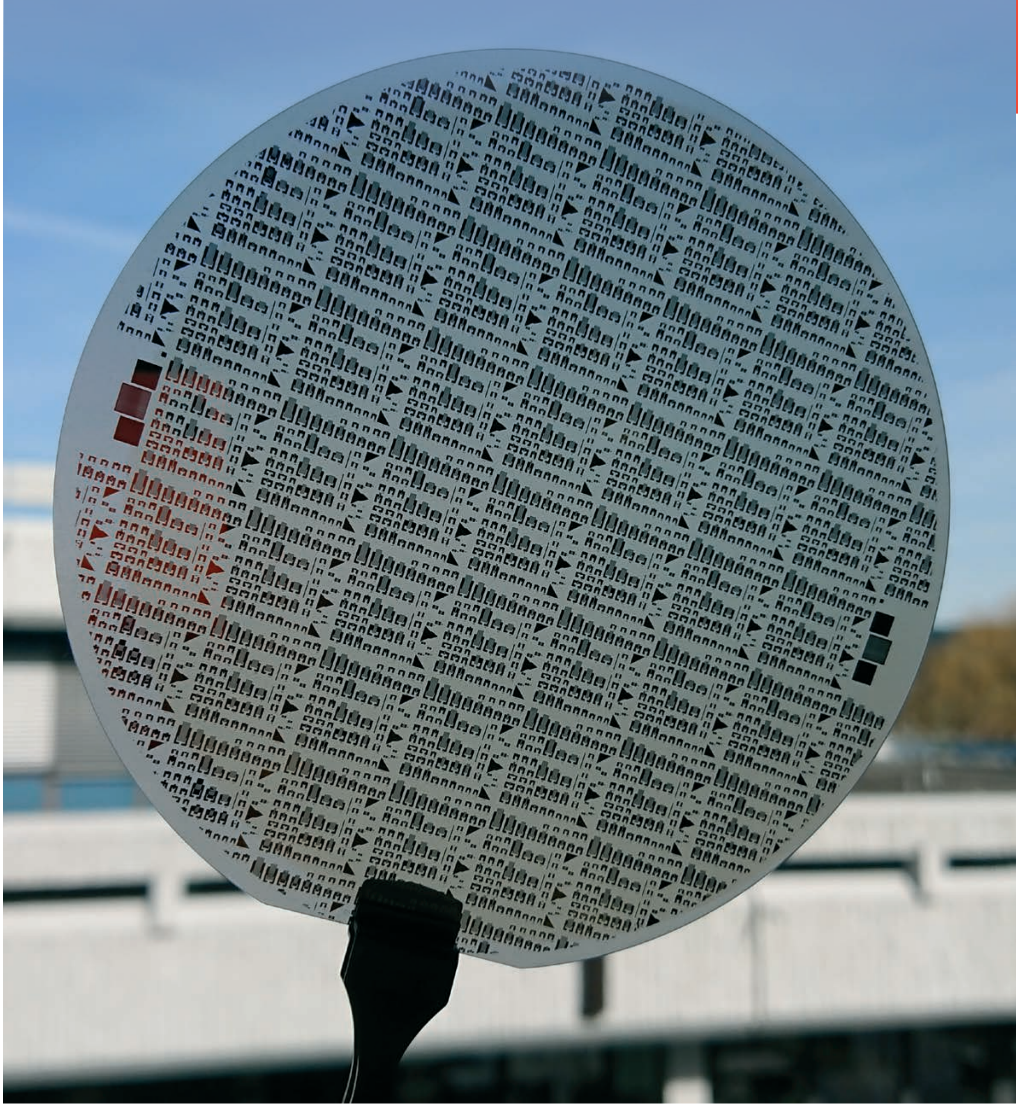

Figure 3. First surface acoustic wave (SAW) resonators fabricated based on epitaxial $Al_{1-x}Sc_xN/Al_2O_3$ layers at Fraunhofer IAF.

indicating that while highly c-axis oriented material was achieved, the material becomes more and more distorted, when enough Sc is replacing Al in the wurtzite crystal lattice.

As a first step in AlScN growth process optimization, the misoriented grains in co-sputtered AlScN/Si layers were identified and their density reduced by adjusting the target-to-substrate distance and Ar:N_2 ratio in the process gas, as is described in more detail in [1]. The same process window was used as a starting point for MSE of $Al_{1-x}Sc_xN/Al_2O_3$. However, in comparison to conventional reactive sputtering, epitaxial growth of AlScN brings additional challenges, such as higher residual stress in the films that can then lead to cracks. At Fraunhofer IAF this problem is addressed in two ways. First, by lowering the growth temperature the residual stress generated due to the thermal-expansion mismatch was partially compensated. Second, to make up for the lower temperature the total process pressure was reduced to increase the mean free path of sputtered species so that upon reaching the substrate surface they have higher kinetic energy and promote the growth of highly-crystalline material [2]. After the successful material optimization, first device performance evaluation was carried out as well. Surface acoustic wave (SAW) resonators were fabricated using AlScN with up to 32% Sc (Figure 3) and immediately showed improved electromechanical coupling as well as better overall device performance in comparison to conventional non-epitaxial layers with the same Sc concentration.

Conclusion

To conclude, while it is more challenging to find the optimum process window to achieve the MSE mode, it is already clear that epitaxially-deposited piezoelectric AlScN layers offer a huge advantage over the textured films and should be investigated further.

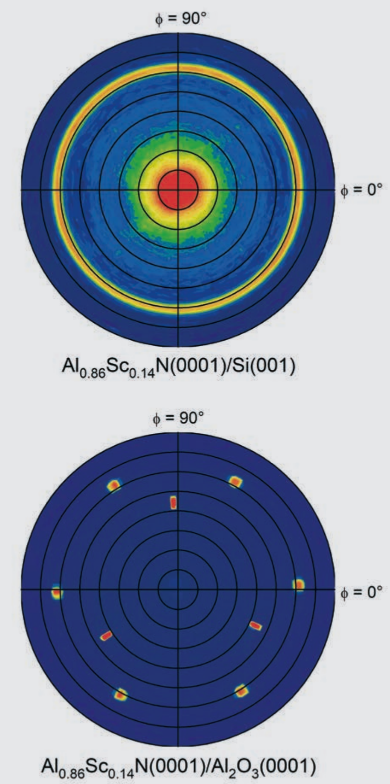

Figure 2. Comparison of x-ray diffraction pole figures for textured $Al_{0.86}Sc_{0.14}N/Si$ (top) & epitaxial $Al_{0.86}Sc_{0.14}N/Al_2O_3$ (bottom) layers.

[1]: Y. Lu, M. Reusch, N. Kurz, A. Ding, T. Christoph, L. Kirste, V. Lebedev, A. Žukauskaitė, Phys. Status Solidi (2017) 1700559.

[2]: Y. Lu, M. Reusch, N. Kurz, A. Ding, T. Christoph, M. Prescher, L. Kirste, O. Ambacher, and A. Žukauskaitė, APL Materials 6(7), 076105 (2018).

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