

Developing production process for high performance piezoelectrics in MEMS applications

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Abstract

The technical challenges in the deposition of $Al_{1-x}Sc_xN$ films are discussed, with specific focus on the manufacturing of bulk-acoustic-wave (BAW) resonator-based filters for radio frequency (RF) communications. The advances in physical vapour deposition (PVD) techniques are introduced. Besides of enlarging the sputter target, the use of a DC+RF source allows us to achieve stress levels of less than ± 50 MPa over the whole wafer surface (up to 5mm edge exclusion). Misoriented grain density has reached satisfactory levels of $\sim 0.1 \mu m^2$ over $2.5 \times 5 \mu m^2$ area for $Al_{0.7}Sc_{0.3}N$ thin films. An example of stress engineering of free-standing cantilever is also presented.

INTRODUCTION

The huge interest in increasing the operating frequency and bandwidth of the RF filters driven by the 5G wireless technology demands new materials with enhanced electromechanical coupling coefficient. Not any more satisfied with AlN thin films for BAW RF filters, material scientists have devoted considerable efforts to improve the its properties by exploring the effects of statistical substitution of Al with other elements in the periodic table. It is in this context that Akyiama and his co-workers [1] reported a dramatic increase in the piezoelectric coefficient when Sc atoms replace Al ones up to approximately 43% in 2009.

Within the frame of $Al_{1-x}Sc_xN$ thin films, extending BAW technology to higher frequencies requires the use of thinner films and higher levels of Sc dopants to keep the coupling coefficients at the largest level dictated by bandwidth requirements. However, high Sc doping level also poses new challenges for $Al_{1-x}Sc_xN$ thin film deposition. This includes the alloyed target manufacturing, the stricter requirement for stress range and more difficult control over the textured film growth.

In this paper, we discuss the challenges for $Al_{1-x}Sc_xN$ thin film processing and our approaches to achieve highly uniform $Al_{1-x}Sc_xN$ films with stress range under 100 MPa. In the end, we demonstrate with an example how to achieve free-standing cantilevers for bimorph structures.

TECHNICAL CHALLENGES FOR $Al_{1-x}Sc_xN$ THIN FILM PROCESSING

When it comes to the production of $Al_{1-x}Sc_xN$ thin films for the industry, three challenges have to be solved:

- How to introduce Sc into AlN lattice efficiently;
- How to control the stress and thickness uniformity of the $Al_{1-x}Sc_xN$ film across the wafer;
- How to maintain the AlN Wurtzite textured lattice growth with a certain Sc doping level.

While other deposition techniques like metal-organic chemical vapor phase deposition and pulsed laser deposition start to emerge in this field of application, sputter deposition is still the mainstream technique to deposit $Al_{1-x}Sc_xN$ films.

A versatile approach to deposit $Al_{1-x}Sc_xN$ thin films is co-sputtering, where Al and Sc targets are sputtered independently and simultaneously in the same chamber. The Sc concentration can be adjusted by changing the power ratio of the two targets. Flexible and ideal for process development, this approach is not ideal for mass production, as it is very challenging to ensure adequate stress control (more about this topic later) and to achieve high levels of productivity. Therefore, this technique is mainly used for research purposes and played a very important role in the early stage of $Al_{1-x}Sc_xN$ exploration.

The preferred solution is therefore to use the same proven configuration already existing for high volume fabrication of RF filters with a single wide target. To do this, we need an $Al_{1-x}Sc_x$ alloyed target with the same dimension. Though difficult due the complexity of Al-Sc binary alloy system [2], fabrication of such a target is nevertheless feasible. The business case represented by opportunities in 5G communication has stimulated target manufacturers to make significant investments, resulting in remarkable improvements throughout a whole range of Al-Sc compositions in the recent years. It is now possible to produce high-quality, high-Sc content targets (up to 40%Sc), which enables the mass production of $Al_{1-x}Sc_xN$ throughout the whole piezoelectric range of the phase diagram.

The Sc content is not the only parameter which influences k_t^2 , as the piezoelectric response is also influenced significantly by the film stress (see Fig. 1.). Extremely accurate stress control within the wafer surface and from wafer to wafer in any production process is then essential for the successful production of RF filters of bandwidth precision dictated by the wireless communication standards. For Sc contents of about 30%, only deviations of ± 50 MPa are tolerated: an extremely small value for thin film depositions.

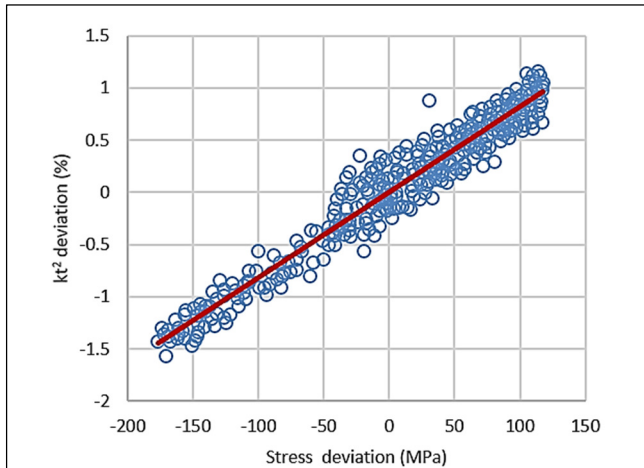


Fig. 1. Electromechanical coupling coefficient variation as a function of the stress variation for $Al_{0.7}Sc_{0.3}N$ based resonators. The two physical quantities are linked linearly. The steepness of the line increases with the Sc concentration.

For high Sc content $Al_{1-x}Sc_xN$ films, another obstacle is the tendency of these materials to show abnormally thick, misoriented crystallites or grains [3]. The introduction of Sc into the AlN Wurtzite lattice creates instabilities in the lattice and very often misorientated grains grow during the film deposition. These grains grow at a faster pace than the textured grains and appear on the film surface as pyramid shaped structures. These grains are still in the Wurtzite phase, but their (0002) axis is not perpendicular to the wafer surface. The appearance of misoriented grains causes an obvious decrease of the piezoelectric coefficient, which becomes evident only when their density exceeds a critical threshold. An excessive amount of those grains can also negatively influence the dielectric loss and cause problems in post-processing due to the very high film roughness, as these grains can be tens of nanometers taller than the film surface. Thus high Sc content $Al_{1-x}Sc_xN$ films are applicable only when the density of misoriented grains is below a certain level.

RECENT ADVANCES IN $Al_{1-x}Sc_xN$ THIN FILM PROCESSING

The efforts in the process development for $Al_{1-x}Sc_xN$ thin films are mainly dedicated to improving the thickness

uniformity, narrowing down the stress range and enhancing the textured film growth.

A simple approach to achieve better compromises between stress and thickness uniformities is to employ an enlarged target diameter. This allows us to reduce the strength of the magnetic field at the wafer edge and/or to enhance the target-to-substrate distance for a given thickness distribution. Under both circumstances, the inhomogeneity of the ion bombardment over the wafer surface is reduced, thus favoring a more uniform stress distribution. Fig. 2. shows an example of $1 \mu m$ AlN deposition using an enlarged Al target ($\Phi = 340 mm$). Excellent thickness uniformity and stress range up to 5 mm edge exclusion can be easily achieved.

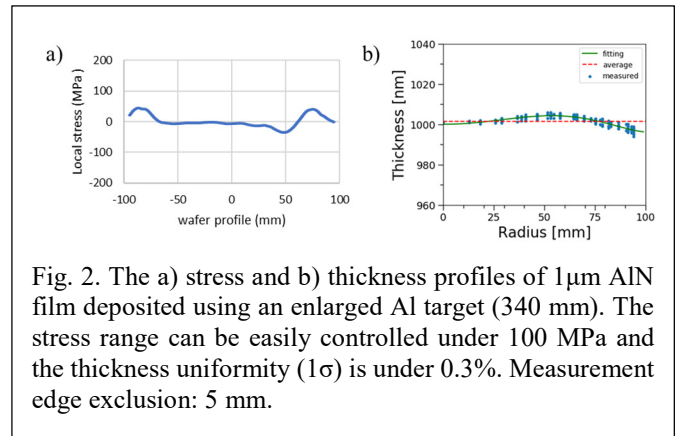


Fig. 2. The a) stress and b) thickness profiles of $1 \mu m$ AlN film deposited using an enlarged Al target (340 mm). The stress range can be easily controlled under 100 MPa and the thickness uniformity (1σ) is under 0.3%. Measurement edge exclusion: 5 mm.

On the downside however, this approach worsens the cost of ownership figure as it implies a bigger vacuum chamber, larger cleanroom footprints, and, most importantly, a much higher target cost per wafer (if it is at all possible to get manufactures able to go beyond the usual target sizes for $Al_{1-x}Sc_x$ alloyed targets). An alternative way to deal with the issue is to manipulate the stress distribution while keeping the optimized magnetron configuration and target to substrate distance for ideal thickness distribution. This is possible with DC+RF technology.

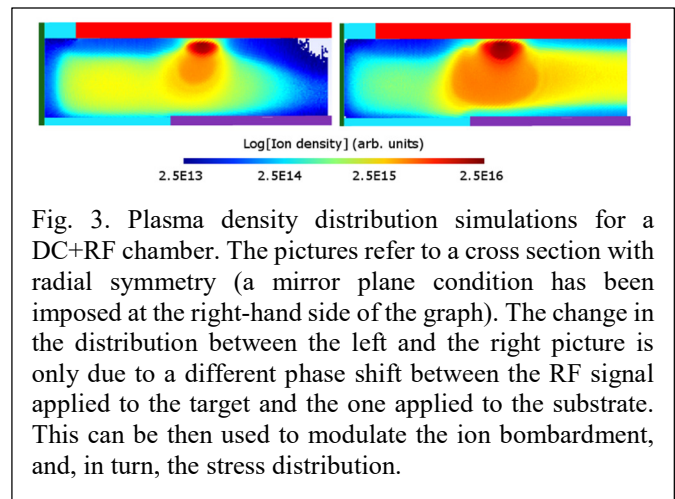


Fig. 3. Plasma density distribution simulations for a DC+RF chamber. The pictures refer to a cross section with radial symmetry (a mirror plane condition has been imposed at the right-hand side of the graph). The change in the distribution between the left and the right picture is only due to a different phase shift between the RF signal applied to the target and the one applied to the substrate. This can be then used to modulate the ion bombardment, and, in turn, the stress distribution.

The DC+RF sputtering superimposes the DC power with an RF power on the cathode. It still enables the sputtering in the DC mode, as the RF power serves mainly to discharge the target surface in a reactive process. Therefore, the good thickness uniformity from DC sputtering is preserved. Additionally, the RF power applied to the target can be synchronised to the RF power to the chuck for wafer biasing. Each time we have multiple RF signals applied to the same plasma, we can shape it if we influence the relative amplitude of the signals and the phase shift between them. As we can see from Fig. 3, the plasma intensity in a reacto can be changed locally by several orders of magnitude for different RF settings.

The combination of DC+RF is also commonly used in a variety of applications for other advantages which are offered by this technique. The transfer of this mature technology to $Al_{1-x}Sc_xN$ depositions allowed us to achieve very narrow stress distributions up to the wafer edge, and satisfy the ± 50 MPa limit requirement dictated by large amount of scandium substitution while keeping the thickness distribution easily

trimmable ($< 0.5\%$ sigma/mean) and target dimensions to the conventional ones (about 300mm diameter), as seen in Fig. 4.

The misoriented grains related to high Sc content $Al_{1-x}Sc_xN$ films have been intensively studied in the past years. As demonstrated by Sandu *et al.* [3], the presence of these abnormal grains can be associated with an excess of Sc at the grain boundaries. Target manufacturing and processing conditions can therefore significantly influence the presence of these grains. Process conditions that enhance the ion bombardment inhibit the growth of misoriented grains. Nevertheless, other requirements in terms of thickness and stress distribution give us very limited freedom in the choice of the process conditions, especially the requirement of having neutral or slightly tensile films. If we produce too compressive films, the benefit of high Sc content in the Wurtzite structure is lost by the loss of coupling coefficient given by the stress state (see again Fig. 1.). For a given target and processing condition, the number of misoriented grains can also change drastically from substrate to substrate type. On W bottom electrode it is relatively easy to grow smooth films, while the number of misoriented grains is increased if we switch to Mo electrode or bare Si. The lattice mismatch between the film and the substrate seems not to be the root cause, however, as the processing conditions of the electrodes have a big influence, as we can see in Fig. 5.

STRESS ENGINEERING FOR FREE STANDING BI-MORPH CANTILEVERS

Different from the growth of metallic films, $Al_{1-x}Sc_xN$ film is a reactive process and releases heat during the formation of $Al_{1-x}Sc_xN$ compound. As a consequence, the wafer temperature rises up during deposition to a much larger extent than metal depositions. This leads to an extensive stress gradient along the thickness of $Al_{1-x}Sc_xN$ films, which limits the introduction of $Al_{1-x}Sc_xN$ film for applications where free-standing microstructures are required. However, if there is sufficient thermal contact between the wafer and chuck, the temperature rise of the wafer during deposition will be damped and thus the stress gradient will be reduced. This can be realized with electrostatic chucking solution. The wafer is gripped by electrostatic force on the chuck, while underneath the wafer, a gas pressure is maintained between the wafer and the chuck. This gas pressure enhances the thermal transport between the wafer and chuck, thus minimizing the temperature variation on the wafer during deposition. Additionally, the deposition is still full-face, as there is no need for mechanical clamping.

With the reduced film stress gradient, it is possible to compensate the bending moment and achieve flat structures with careful stress engineering. Fig. 6. shows one example of stress gradient compensation for a freestanding bimorph structure. The in-plane stress for every 100 nm thickness is plotted against its distance to the corresponding electrodes for

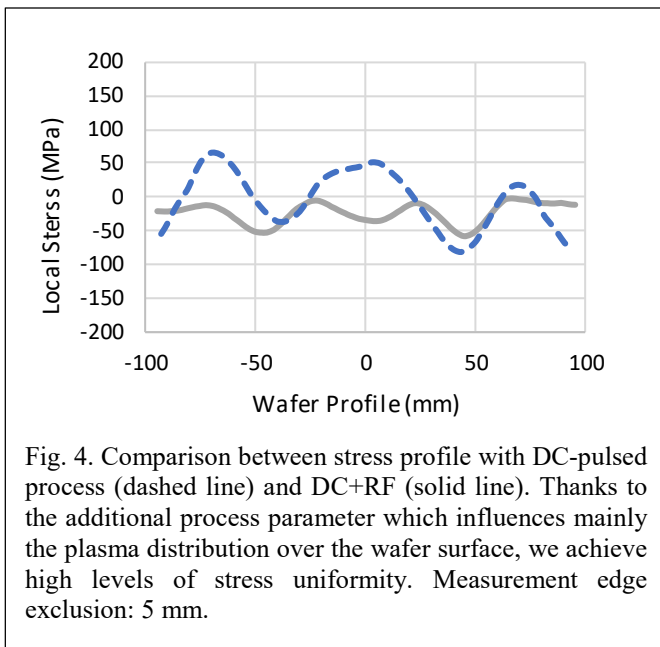


Fig. 4. Comparison between stress profile with DC-pulsed process (dashed line) and DC+RF (solid line). Thanks to the additional process parameter which influences mainly the plasma distribution over the wafer surface, we achieve high levels of stress uniformity. Measurement edge exclusion: 5 mm.

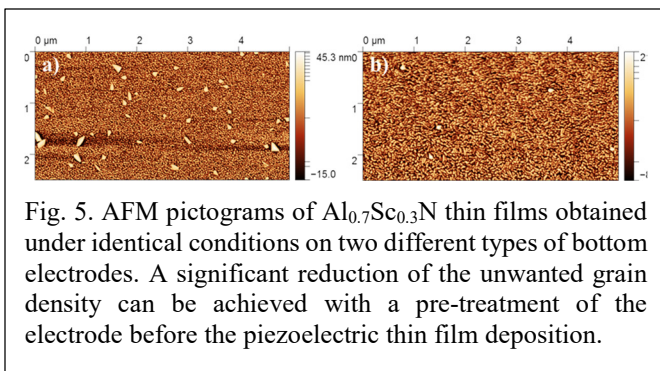


Fig. 5. AFM pictograms of $Al_{0.7}Sc_{0.3}N$ thin films obtained under identical conditions on two different types of bottom electrodes. A significant reduction of the unwanted grain density can be achieved with a pre-treatment of the electrode before the piezoelectric thin film deposition.

the first and second piezoelectric films in Fig. 6 c) and d). As one can see, there exists a large stress gradient in the first 200 nm of the as deposited film. Without any stress compensation, the stress gradient will cause a bending moment when the cantilever is released:

$$M = \int_{-t_f}^{t_f} \sigma(t) \cdot t dt = \int_{-t_f}^0 \sigma(t) \cdot t dt + \int_0^{t_f} \sigma(t) \cdot t dt$$

where M is the bending moment, $\sigma(t)$ is the in-plane stress at the distance of t to the middle electrode. Since the electrode layer is usually very thin and free from stress gradient, we can consider component from $-t_f$ to 0 as the contribution from the first piezoelectric film and 0 to t_f from the second piezoelectric film. In order to keep the freestanding cantilever flat, we have to ensure the total bending moment to be zero. Of course, the most straightforward way to achieve this is to keep $\sigma(t)$ as a constant through the whole cantilever. However, in reality, this requires extensive *in-situ* stress tuning during the deposition, which is not easily manageable. One other approach is to ensure the sum of the two bending contributions from the two films to be zero. The most convenient way is to compensate the bending moment by changing the stress of the top 100 nm layer of the second piezoelectric film, which is the finishing layer of the deposition, as indicated by the green triangle in Fig. 6. d). With this approach, we managed to bring down the deflection of cantilever dramatically after release, seen in Fig. 6. b).

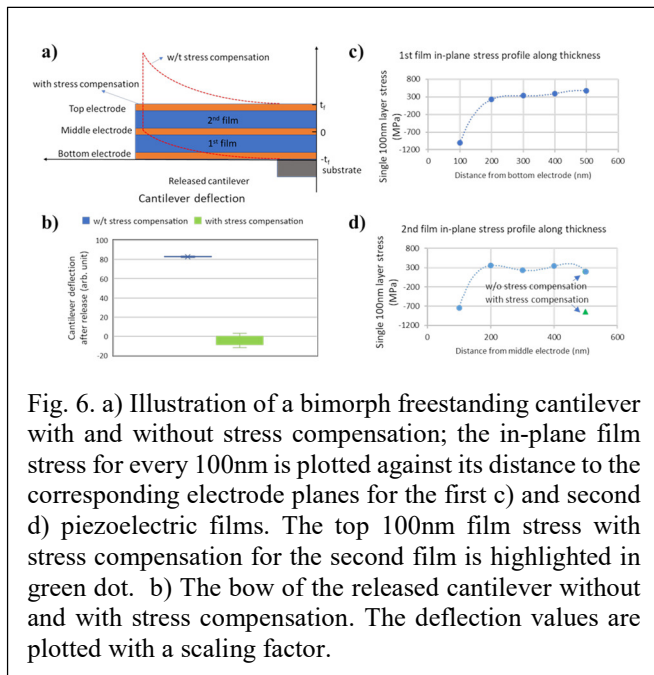


Fig. 6. a) Illustration of a bimorph freestanding cantilever with and without stress compensation; the in-plane film stress for every 100nm is plotted against its distance to the corresponding electrode planes for the first c) and second d) piezoelectric films. The top 100nm film stress with stress compensation for the second film is highlighted in green dot. b) The bow of the released cantilever without and with stress compensation. The deflection values are plotted with a scaling factor.

CONCLUSIONS

The introduction of $Al_{1-x}Sc_xN$ technology represents a leap forward in the piezo-MEMS industry. The limits of pure AlN with its relatively small piezoelectric activity can be

overcome. This allows significant improvement in the performance of devices such as piezoelectric microphones and pMUTs which can still be integrated in a CMOS chip or production line. The enhancement of the electromechanical coupling coefficient allows extended application range of BAW-based RF filters to broadband communication, which would not have been accessible with pure AlN only.

The integration of $Al_{1-x}Sc_xN$ films poses however several challenges. The historic difficulties in target manufacturing represented a significant hurdle in the productization of such a technology for a long time and limited users to cosputtering setups for relatively high Sc concentrations. However targets of 12 inches in diameter are now available for almost all the Sc concentration range of interest. The stress dependency of the electromechanical coupling coefficient is enhanced as Sc content gets higher. As a consequence, in order to achieve high yield figures on each wafer, advanced plasma shaping techniques are necessary. At Evatec we employ a DC+RF technology to finely adjust the plasma distribution over the wafer surface. This technique allows us to reach stress distribution over the wafer surface less than ± 50 MPa up to 5mm edge exclusion and well within the range required for application in high performance RF applications. The existence of misoriented grains for high Sc content $Al_{1-x}Sc_xN$ films may currently put some refrains for the industry to increase the Sc content to the limit. But with improving techniques of target manufacturing, proper wafer substrate choice and treatment, and optimization of process hardwares and conditions, $Al_{1-x}Sc_xN$ continues to be the dominating material in the field of piezo-MEMS and 5G wireless communication applications.

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REFERENCES

- [1] M. Akiyama, K. Kano, and A. Teshigahara, *Appl. Phys. Lett.* **95**, 162107 (2009).
- [2] M. O. Shevchenko *et al.*, *Powder Metall Met Ceram* **53**, 243 (2014).
- [3] C. S. Sandu *et al.*, *Phys. Status Solidi A* **216**, 1800569 (2019).

ACRONYMS

- BAW: Bulk Acoustic Wave
- MEMS: Microelectromechanical System
- RF: Radio Frequency
- PVD: Physical Vapor Phase Deposition
- DC: Direct Current