Program Digest, 2019 IEEE International Ultrasonics Symposium (IUS)
Glasgow, Scotland, October 6-9, 2019

Growth, Properties, and Applications of $Al_{1-x}Sc_xN$ Thin Films

Paul Muralt
Electroceramic Thin Films Group, EPFL
Lausanne, Switzerland
paul.muralt@epfl.ch

Vladimir Pashchenko
Silicon Austria Labs GmbH
Villach, Austria
vladimir.pashchenko@silicon-austria.com

Fazel Parsapour
Electroceramic Thin Films Group, EPFL
Lausanne, Switzerland
Fazel.Parsapour@gmail.com

Stefan Mertin
Electroceramic Thin Films Group, EPFL
Lausanne, Switzerland
stefan.mertin@vtt.fi

Bernd Heinz
Evatec AG
Trübbach, Switzerland
bernd.heinz@evatecnet.com line

Pascal Nicolay
Carinthian Tech Research AG
Villach, Austria
p.nicolay@fh-kaernten.at

***Abstract*— The discovery of enhanced piezoelectricity in solid solutions of AlN and ScN is certainly one of the most important events in piezoelectric MEMS. As compared to pure AlN, it brought a crucial factor 2 to 3 improvement in a number of figures of merit governing the performance of MEMS devices. The aim of this contribution is to give a short overview on actual topics in processing, properties, and applications in RF filters and sensors.**

Keywords*— *piezoelectric, thin film, AlN-ScN, radio frequency

I. INTRODUCTION

The tremendous increase of piezoelectricity realized when alloying the wurtzite structure AlN with the rocksalt structure ScN ($Al_{1-x}Sc_xN$ for x<0.45) was published 10 years ago [1]. The new thin film material does not only improve existing devices produced with AlN, it may also allow for the exploitation of new resonance modes in RF components, because the coupling factor rises to a useful magnitude. In micro sensors, AlScN appears to be stronger than PZT. The AlScN system is also an interesting playground for predicting properties by modelling based on density functional theory (DFT). In the following, a disturbing growth issue, the so-called abnormally oriented grains (AOG), is addressed, a comparison of experimental results for the thin film transvers piezoelectric coefficient $e_{31,f}$ with DFT predictions is presented, and two novel structures for RF resonators and delay lines and are introduced.

II. GROWTH

The growth of AlScN thin films appears to be very close to the one of AlN. Few parameters of the magnetron sputter process need to be adjusted. One of the difficulties was (or still is) the fabrication of good compound targets when using a single target process. This approach is preferred for high rate deposition, and usually combined with a DC pulsed power supply [2]. One issue is however much different. The alloy of AlN and ScN in the wurtzite structure is a metastable material, which becomes obvious when performing the growth process at high temperature [3]. We think that the occurrence of abnormally oriented grains (AOG) [4] is related to the metastability of the material. AOGs are growing out of desired c-axis oriented, columnar grains, starting at grain boundaries [5]. They are growing to quite large diameters and reduce piezoelectric properties and quality factors. It was found that the AOGs did not nucleate at the interface with the substrate, but during growth of c-axis oriented grains at high energy grain boundaries, at which systematically higher Sc concentrations were detected [5]. It is thought that these secondary nuclei form as ScN rich phase in the rocksalt structure, before switching back to wurtzite. The AOGs grow faster, and finally protrude from the c-textured film surface, having at their end a pyramidal shape with three facets of a hexagonal wurtzite crystal: one (0001) and two (110) facets (fig. 1). Process conditions favouring less compact grain boundaries, and lower surface diffusion across grain boundaries are thought to promote nucleation of AOGs. The smoothness of the substrate (bottom electrode) and the electrical situation with respect to the plasma of the source was found to play a crucial role.

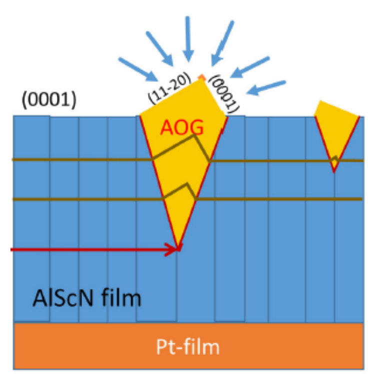


Fig. 1. Schematic cross section explaining the formation and growth of abnormally oriented grains (from [5]).

A film with a lot of AOGs was inspected in more in detail [6]. The c-textured growth mode was abandoned after about 20 % of film thickness, to give place to a rather chaotic mode with abnormally oriented grains. The information on grain tilts derived from nano diffraction mapping was used to simulate the structure by finite element modelling. Quite a convincing fit to the experimental impedance curves was obtained, yielding a good proposition for the involved materials constants. It also became clear that the assembly of AOGs has a net overall piezoelectric response.

III. Properties

The transverse piezoelectric coefficient $e_{31,f}$ of a thin film can be conveniently and relatively precisely measured in the direct mode by a 4-point bending method [7]. This coefficient is important for sensors, actuators, and energy harvesters based on beams and membrane structures. Fig. 2 shows a comparison of various experimental values with DFT values. There is quite a good agreement at the end points. The experiment suggests that the real values are somewhat larger than the DFT values in the Sc concentration range of x=0.06 to 0.32. This transverse coefficient is composed of two standard e-coefficients and stiffness constants:

$$e_{31,f} = e_{31} - \frac{c_{13}^E}{c_{33}^E} e_{33} \qquad (1)$$

This means that one cannot reduce the difference to one constant alone.

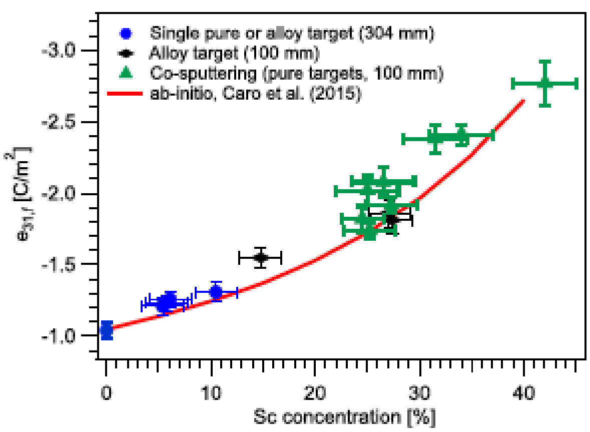


Fig. 2. Transverse piezoelectric coefficient (from [8]) from experiment and DFT modelling [9].

IV. Applications

A. Solidly mounted Lamb wave resonators

The currently dominating electroacoustic technologies for mobile phone communication are based on surface acoustic wave devices (SAW) on mainly $LiNbO_3$ single crystal surfaces, and thin film bulk acoustic wave devices (BAW) with AlN thin films vibrating in the thickness mode (TFBAR). Lamb wave resonators (LWR) attract much attention, because they enable for lower frequencies with thin film resonators. Their frequency depends less on the layer thickness, and more on the period of the interdigitated electrodes. The lowest order symmetric mode (S_0) of AlN Lamb wave resonators has been explored since 2002 [10] using AlN. However, only moderate electromechanical coupling factors (k^2) were reached, much smaller ones than with BAW resonators. In addition, the quality factor Q was also much smaller. For filters, the figure of merit is the product k^2Q. Logically, AlScN should increase the piezoelectric coupling of Lamb wave devices. However, it was not shown yet that AlScN increases as well k^2Q.

We investigated Lamb wave devices based on $Al_{0.85}Sc_{0.15}N$ thin films, a first type with free-standing membranes (FS-LWR), a second type with an acoustic Bragg reflector (solidly mounted SM-LWR). In the SM-LWR resonators, the FoM was significantly improved as compared to the FS-LWR, reaching values close to 12 for k^2Q_s, and 18 for k^2Q_p at an operation frequency of 1430 MHz. All devices showed an excellent agreement with FEM predictions, regarding resonance frequency and piezoelectric coupling. The quality factors of the SMR devices were 5 to 6 times larger than the ones of the free-standing structures. This increased performance justifies more research in this direction to increase the quality factor even more. In addition, there is an interesting discrepancy between the coupling factor of an infinite LWR, and a finite one with grating reflectors. Possibly one can still gain a lot of coupling by improving the reflectors.

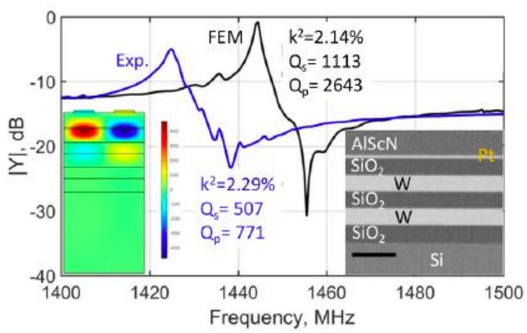
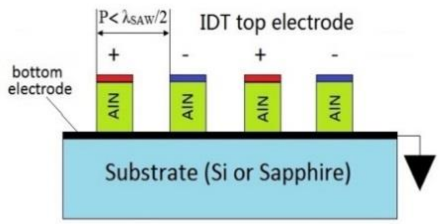


Fig. 3. Schematic cross section explaining the formation and growth of abnormally oriented grains (from [11]).

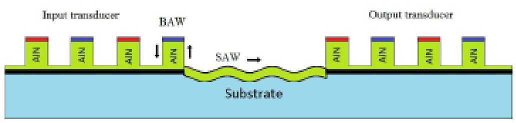
B. BAW-SAW hybrid resonators

Over the last 10 – 15 years, SAW and BAW devices turned out to be very usful also in the field of sensors. Sound velocities depend on a number of physical parameters such as temperature, strain, and pressure. In addition, loading resonators with affinity layers, at which specific molecules are attached, the application range widens up to bio-medical sensors. The SAW sensors have the possibility to employ them as passive elements with a wireless read-out. In order to study a potential improvement in coupling, a novel type of RF device was studied which couples SAW and BAW waves. We called it "Hybrid BAW/SAW device" (Fig. 4). It combines advantages of both wave types, and does not need a piezoelectric crystal for the SAW propagation. The device consists of an array of individual BAW resonators spaced at a distance of half the SAW wavelength, i.e. $\lambda_{SAW}/2$ fabricated on top of substrate carrying the SAW wave.

The BAW pillar resonators made of AlN or AlScN excite alternating tensile and compressive deformations into the substrate. A SAW is generated on the substrate having a wavelength of $\lambda_{SAW.}$ The advantages of this device are high electromechanical coupling factors (k^2) as well as high Q –factors (like in BAW). In addition, there is no need for an acoustic Bragg mirror due to the destructive interference of BAW in the substrate volume, and operational frequency is defined by the pitch. This device can be used as a SAW wireless sensor with enhanced k^2 and Q with respect to the conventional AlN/Si (Sapphire) SAW devices.



(a)



(b)

Fig. 4. (a) Schematic cross section through BAW/SAW device. (b) Schematic view of a delay line in BAW/SAW technology.

REFERENCES

[1] [1] M. Akiyama, T. Kamohara, K. Kano, A. Teshigahara, Y. Takeuchi, N. Kawahara, Adv.Mat. vol.21, pp. 593, 2009.

[2] [2] R. Matloub, A. Artieda, E. Milyutin, P. Muralt, Appl.Phys.Lett., vol 99, 092903, 2011.

[3] [3] A. Zukauskaite, et.al., J. Appl. Phys.Vol. 111, 093527, 2012.

[4] [4] S. Fichtner et al., J.Appl.Phys. vol. 122, 035301, 2017.

[5] [5] C.S. Sandu, F. Parsapour, S. Mertin, V. Pashchenko, R. Matloub, Th. LaGrange, B. Heinz, P. Muralt, Physica Status Solidi A vol. 216, pp. 1800569, 2019.

[6] [6] F. Parsapour, V. Pashchenko, N. Kurz, C. Sandu, T. LaGrange, K. Yamashita, V. Lebedev, P. Muralt, Adv. Electr. Mat. vol. 5, pp. 1800776 (1-9), 2019.

[7] [7] K. Prume, P. Muralt, F. Calame, T. Schmitz-Kempen, S. Tiedke, IEEE Trans. UFFC, vol. 54, pp. 8-14, 2007.

[8] [8] S. Mertin, B. Heinz, O. Rattunde, G. Christmann, M.-A. Dubois, S. Nicolay, P. Muralt, Surf.Coat.Techn. vol. 343, pp. 2-6, 2018.

[9] [9] M.A. Caro, S. Zhang, T. Riekkinen, M. Ylilammi, M.A. Moram, O. Lopez-Acevedo, J. Molarius, T. Laurila, J. Phys. Condens. Matter, vol. 27, p. 245901, 2015.

[10] [10] V. Yantchev and I. Katardjiev, J. Micromechanics Microengineering vol. 23, p. 043001, 2013.

[11] [11] F. Parsapour, V. Pashchenko, H. Chambon, P. Nicolay, I. Bleyl, U. Rösler, P. Muralt, Appl.Phys.Lett. 2011, vol. 114, p. 223103, 2019.