Influence of scandium concentration on parameters of piezoelectric transducer based on aluminum scandium nitride

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Abstract. An analytical approach is presented that allows one to determine the influence of the scandium concentration on the input electrical impedance of piezoelectric transducer based on aluminum scandium nitride. The scandium concentration dependences of the properties aluminum scandium nitride affecting on the transducer impedance were determined by means of the approximation of the dependences obtained from their experimental values for various Sc concentration. Based on the frequency dependences of the impedance the influence of Sc concentration in Al1-xScxN piezoelectric layer on the frequencies of the serious and parallel resonance of the unloaded and loaded transducer has been established.

Keywords: piezoelectric transducer, aluminum scandium nitride, input electrical impedance, series resonance, parallel resonance

1. Introduction

Micromechanical systems are new direction in development of mechanical ones [1]. They demand new devices for forming micro displacement of micromechanical elements [2]. Ones of such devices are piezoelectric transducers. These transducers use a piezoelectric effect for forming micro displacement and often have a thin-film design. In this case, the piezoelectric layer is made of material having piezoelectric effect in thin-film design. Until now there are two materials: zinc oxide and aluminum nitride. Presently, a set of these materials are extended. In particular, the bigger prospects are connected with aluminum-scandium nitride. The thin-films of this material have several times more piezoelectric response than the films of aluminum nitride [].

The first report about of piezoelectric properties of aluminium scandium nitride thin-films has been presented in 2009 year by M. Akiama with co-authors [3, 4]. They found that for the thin films prepared by dual RF magnetron reactive co-sputtering at substrate temperature equal to 580 °C, the piezoelectric coefficient increases with increasing Sc concentration from 0 to 30 at. %. In this Sc concentration range, the piezoelectric coefficient varies from ~6 to ~16 pC/N. In [5], the authors analytically determined the elastic stiffness and piezoelectric constants of the Al1-xScxN alloys with the wurtzite structure using the density functional theory. The relative dielectric constant of Al1-xScxN thin films (x=0.1, 0.2, and 0.3) prepared by dc-magnetron reactive sputtering was investigated in [6]. In [7] the values of electromechanical coupling coefficient for Al1-xScxN (x=0.1, 0.2, and 0.3) were calculated using the data of Refs. [5, 6]. Moreira M., et al. investigated the impedance of FBAR test structures based on Al1-xScxN (x=0, 0.03, 0.06, and 0.15) piezoelectric layers [8]. Using the frequency
dependence of the impedance and the one dimensional Nowotny-Benes model they determined the
dependences of the elastic stiffness constant, relative permittivity and electromechanical coupling
coefficient on the Sc concentration in the piezoelectric layer. The dependencies of relative permittivity
and piezoelectric constant $d_{31}$ on the scandium concentration in $\text{Al}_{1-x}\text{Sc}_x\text{N}$ from 0 to 50 at. % were
determined experimentally and analytically in Ref. [9]. Umeda K. with co-authors reported the results
about the properties of $\text{Al}_{1-x}\text{Sc}_x\text{N}$ [10] obtained by experimentally investigation of aluminum scandium
nitride thin-films and BAW resonators based of them and also first-principles calculation based on
density functional theory. As a result of this study, the dependence of a number of parameters of $\text{Al}_{1-x}\text{Sc}_x\text{N}$
(piezoelectric coefficients $d_{31}$ and $d_{33}$, longitudinal wave velocity) on the concentration of
scandium was obtained. In [11], the authors experimentally found the values of piezoelectric
coefficients $d_{33}$, piezoelectric constants $e_{31}$, and relative dielectric constant for the $\text{Al}_{0.88}\text{Sc}_{0.12}\text{N}$
and $\text{Al}_{0.83}\text{Sc}_{0.17}\text{N}$ thin films. The dependences of the elastic stiffness constant, its temperature coefficient,
relative dielectric constant, longitudinal wave velocity and electromechanical coupling coefficient of
$\text{Al}_{1-x}\text{Sc}_x\text{N}$ films with $x=0 \ldots 0.7$ were experimentally investigated in [12].

2. Formation of the Problem

The articles discussed above mainly considered the properties of aluminum scandium nitride and their
dependences on the Sc concentration. The results presented in the articles indicate the prospects of
using this material. However, the specific parameters of devices based on aluminum scandium nitride
have hardly been investigated. This primarily relates to piezoelectric transducers, which form the basis
of any such devices, for example, piezoelectric actuators, sensors, resonators, energy harvesting
devices, and etc. The simple structure of such a transducer consists of the piezoelectric layer on the
two sides of which the thin films electrodes are placed. One of the basic characteristics of the
piezoelectric transducer is the input impedance. Based on the frequency dependence of this impedance
one can determine the resonance and antiresonance frequencies of the piezoelectric transducer.
Concerning the transducer based on the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ piezoelectric layer the frequency dependence of
input impedance dependence has hardly been studied. In [8], the frequency dependence of impedance
for FBAR test structures based on $\text{Al}_{1-x}\text{Sc}_x\text{N}$ ($x=0$, 0.03, 0.06, and 0.15) have been presented.
However, the authors did not analyze these dependences and did not discuss the effect of Sc
concentration on their character.

Thus, to date, there is no complete information on the effect of scandium concentration on the
characteristics of piezoelectric transducers based on $\text{Al}_{1-x}\text{Sc}_x\text{N}$. In this connection, the goal of this
work is to investigate the impact of the Sc concentration on the impedance of the piezoelectric
transducer with $\text{Al}_{1-x}\text{Sc}_x\text{N}$ layer. In particular, based on the frequency dependence of the impedance, it
is important to determine the change in the resonant frequencies of the transducer as a function of the
scandium content in the piezoelectric layer.

3. Theory: Approach Used in Investigation

The input electrical impedance of piezoelectric transducers based on $\text{Al}_{1-x}\text{Sc}_x\text{N}$ is considered
analytically on the example of a bulk acoustic wave resonator with an air gap. Such a resonator has
two electrodes placed on opposite surfaces of the piezoelectric layer (Fig. 1). The air gap made by
surface micromachining separates the piezoelectric transducer from the substrate. In this case, the
acoustic load of the transducer is the electrodes contacting with air.

The input electrical impedance of the transducer under consideration can be written in the
following form [13]
Figure 1. Bulk acoustic wave resonator with an air gap: 1 – substrate; 2 – piezoelectric layer; 3 – bottom electrode; 4 – top electrode; 5 – air gap.

\[
Z_{in} = \frac{1}{j\omega C_0} \left( 1 + \frac{k_s^2}{\gamma_p d_p} \cdot \frac{j(Z_{top}^{\text{top}} + Z_{bot}^{\text{bot}})Z_p \sin(\gamma_p d_p) - 2Z_p^2 - \cos(\gamma_p d_p)}{Z_p^2 + Z_{top}^{\text{bot}} Z_{bot}^{\text{bot}} \sin(\gamma_p d_p) - j(Z_{top}^{\text{top}} + Z_{bot}^{\text{bot}})Z_p \cos(\gamma_p d_p)} \right),
\]

where \(Z_{in}\) is the input electrical impedance of the transducer; \(Z_p\) is the acoustic impedance of the piezoelectric layer; \(Z_{top}^{\text{top}}\) and \(Z_{bot}^{\text{bot}}\) are the load acoustic impedances of the piezoelectric layer on the top and bottom electrode sides, respectively; \(C_0\) is the static electrical capacitance of the transducer; \(\omega\) is the angular frequency, \(\omega = 2\pi f\); \(k_s^2\) is the electromechanical coupling coefficient; \(d_p\) is the thickness of piezoelectric layer; \(\gamma_p = \omega/v_p\); \(v_p\) is the acoustic wave velocity in the piezoelectric layer.

The load acoustic impedances of the top and bottom electrode sides take the acoustic impedances of material of the electrodes and an air into account. These impedances are (example for the top electrode)

\[
Z_{top}^{\text{top}} = Z_{top}^{\text{top}} \frac{Z_a \cos(\gamma_a d_a) + jZ_{top}^{\text{top}} \sin(\gamma_a d_a)}{Z_{top}^{\text{top}} \cos(\gamma_a d_a) + jZ_a \sin(\gamma_a d_a)},
\]

where \(Z_{top}^{\text{top}}\) and \(Z_{bot}^{\text{bot}}\) are the acoustic impedance of the top and bottom electrode, respectively; \(Z_a\) is the acoustic impedance of an air; \(d_a\) is the thickness of electrode layer; \(\gamma_a = \omega/v_a\); \(v_a\) is the acoustic wave velocity in the electrode layer.

Equation (1) for the input electrical impedance contains the parameters that characterize the material of the piezoelectric layer and depend on the Sc concentration in it. These parameters are \(Z_p\), \(k_s^2\), \(v_p\). To find the input electrical impedance of piezoelectric transducers it is necessary to determine the dependences of these parameters on the Sc concentration.

The dependence of acoustic impedance of the piezoelectric layer, \(Z_p\), on the Sc concentration can be found using the following relation

\[
Z_p = \rho v_p,
\]

where \(\rho\) is the density of the piezoelectric material.

The density of Al_{1-x}Sc_xN alloy can be presented through the densities of AlN and ScN as follows

\[
\rho_{AS} = (1 - x)\rho_A + x\rho_S,
\]

where \(\rho_{AS}\), \(\rho_A\), and \(\rho_S\) are the densities of Al_{1-x}Sc_xN, AlN, and ScN, respectively.

The electromechanical coupling coefficient, \(k_s^2\), is a function of the parameters, characterizing the mechanical, piezoelectric, and electrical properties of Al_{1-x}Sc_xN.
\[ k_i^2 = \frac{e_i^2}{c_33 + e_{33}^3}, \tag{5} \]

where \( c_{33}, e_{33}, \) and \( \varepsilon_{33} \) are the elastic stiffness constant, piezoelectric constant, and relative dielectric constant of \( \text{Al}_{1-x}\text{Sc}_x\text{N}. \)

The analytical scandium concentration dependences of the parameters, characterizing the properties of \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) (\( c_{33}, e_{33}, v_p, \) and \( \varepsilon_{33} \)), were determined by means of the approximation of the dependences obtained from their experimental values for Sc concentration in the range of 0–0.5. These dependences were approximated by the 2-nd power polynomial. The experimental values of the above parameters for the various Sc concentrations were taken from the following references: for elastic stiffness constant – [5, 12]; for piezoelectric constant – [5]; for the acoustic wave velocity – [10, 12]; for relative dielectric constant – [6, 8,12].

The static electrical capacitance of the piezoelectric transducer including in (1) was determined as follows

\[ C_0 = \frac{e_0 e_{33} A}{d_p}, \tag{6} \]

where \( e_0 \) is the dielectric constant; \( A \) is the overlap area of the transducer electrodes. This capacitance depends on the Sc concentration due to dependence of \( \varepsilon_{33} \).

4. Results and their discussion

The above proposed analytical approach was used to study the effect of the Sc concentration on the impedance of the piezoelectric transducer with \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) layer. The transducer under investigation (Fig. 1) had the Al electrodes with thickness of 0.15 \( \mu \text{m} \). The overlap area of the transducer electrodes (square shape) was chosen to be 0.04 mm. The effect of the Sc concentration on the impedance of the piezoelectric transducer was investigated for the following variants:

1. The thickness of piezoelectric layer was constant and equal to 1.094 \( \mu \text{m} \). This value corresponded to parallel resonance frequency at 5 GHz for the Sc concentration equal to 0 (pure AlN). Two types of the piezoelectric transducer were considered: unloaded and loaded (account of load acoustic impedance in according to (2)).

2. The parallel resonance frequency was constant and corresponded to 5 GHz in the range of the Sc concentration from 0 to 0.5. To implement this condition the thickness of piezoelectric layer was varied. In this case also, two types of the piezoelectric transducer were considered: unloaded and loaded.

Frequency dependences of the input electrical impedance of the unloaded piezoelectric transducers based on AlN and \( \text{Al}_{0.8}\text{Sc}_{0.2}\text{N} \) is presented on Fig. 2. As one can see from these dependences, the transducer based on \( \text{Al}_{0.8}\text{Sc}_{0.2}\text{N} \) with the same thickness of the piezoelectric layer has lower frequencies of series and parallel resonance compared to the AlN transducer. The amplitude of the impedance module of parallel resonance for the \( \text{Al}_{0.8}\text{Sc}_{0.2}\text{N} \) transducer is less by several orders than amplitude of that for the AlN transducer.

Figs. 3 and 4 show the frequencies of series and parallel resonances of the unloaded and loaded piezoelectric transducers and the spacing between these frequencies as functions of the Sc content (\( x \)) in Al1-xScxN for the thickness of piezoelectric layer is equal to 1.094 \( \mu \text{m} \). From the analysis of these dependences, it follows that with increasing the Sc concentration in the \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) piezoelectric layer with the constant thickness, the frequencies of series and parallel resonance of the piezoelectric transducer decrease monotonously and closely to linear dependence. The decrease of the resonance frequencies for the piezoelectric transducer with a scandium content of 50% (\( x = 0.5 \)) is approximately 27-30% of the values for the one based on pure aluminum nitride. The spacing between the resonance frequencies increases with increasing the Sc concentration exactly according to the quadratic law. This pattern is observed for both unloaded and loaded transducers.
Figure 2. Frequency dependence of the input electrical impedance of the piezoelectric transducer based on AlN and Al$_{0.8}$Sc$_{0.2}$N: $d_p$=1.094 µm.

Figs. 5 and 6 show the frequencies of series resonance of the unloaded and loaded piezoelectric transducers and the spacing between frequencies of parallel and series resonance as functions of the Sc content in Al$_{1-x}$Sc$_x$N for the variant when the frequency of parallel resonance is constant and equal to 5 GHz. In this case, the thickness of the piezoelectric layer was varied and its dependences on the Sc content in Al$_{1-x}$Sc$_x$N for the unloaded and loaded piezoelectric transducer are shown on Fig. 7. As one can see from Figs., 5 and 6 the frequency of series resonance of the piezoelectric transducer decreases with increasing the Sc concentration in the Al$_{1-x}$Sc$_x$N piezoelectric layer. However, if the frequency of the parallel resonance is constant, the frequency decrease of the series resonance is only 4-5% for the range of the Sc concentration in the piezoelectric layer from 0 to 0.5.

Figure 3. Frequency of series ($f_s$) and parallel ($f_p$) resonance of the unloaded piezoelectric transducer and the spacing between them ($\Delta f$) as functions of the Sc content (x) in Al$_{1-x}$Sc$_x$N: $d_p$=1.094 µm.
5. Conclusion
In this paper, we have presented the approach allowing us to analytically investigate the impact of the Sc concentration on the input electrical impedance of the piezoelectric transducer with \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) layer. The analytical dependences of the parameters characterizing the properties of \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) on the Sc concentration were determined by analytical approximation of experimental data. Based on the frequency dependences of the impedance the influence of Sc concentration in \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) piezoelectric layer on the frequencies of the serious and parallel resonance of the unloaded and loaded transducer has been established.

The proposed approach can be used to study the impact of the Sc concentration on the other characteristics of the piezoelectric transducer with \( \text{Al}_{1-x}\text{Sc}_x\text{N} \) layer and to design devices based on this transducer.

Figure 4. Frequency of series (\( f_s \)) and parallel (\( f_p \)) resonance of the loaded piezoelectric transducer and the spacing between them (\( \Delta f \)) as functions of the Sc content (x) in \( \text{Al}_{1-x}\text{Sc}_x\text{N} \): \( d_p=1.094 \text{ µm} \).

Figure 5. Frequency of series (\( f_s \)) resonance of the unloaded piezoelectric transducer and the spacing between frequencies of parallel and series resonance (\( \Delta f \)) as functions of the Sc content (x) in \( \text{Al}_{1-x}\text{Sc}_x\text{N} \): \( f_p=5 \text{ GHz} \).
Figure 6. Frequency of series ($f_s$) resonance of the loaded piezoelectric transducer and the spacing between frequencies of parallel and series resonance ($\Delta f$) as functions of the Sc content ($x$) in Al$_{1-x}$Sc$_x$N: $f_p$ = 5 GHz.

Figure 7. Thickness of the piezoelectric layer as a function of the Sc content ($x$) in Al$_{1-x}$Sc$_x$N for the piezoelectric transducer with a parallel resonance frequency of 5 GHz: 1 - unloaded transducer; 2 - loaded transducer.

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