Circular Patterned Test Structures for Precise Determination of Piezoelectric Thin Film Constants: Application to Sc$_x$Al$_{1-x}$N

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Abstract

Piezoelectric scandium aluminium nitride (Sc$_x$Al$_{1-x}$N) thin films are very promising candidates for applications in micro-electromechanical systems due to enhanced piezoelectric properties. To study the influence of deposition parameters on the piezoelectric response, Sc$_{27}$Al$_{73}$N with $x = 27\%$ Sc was deposited by reactive sputtering. For determination of piezoelectric constants, platinum electrodes were utilized to measure the piezoelectric deflection via Laser Doppler Vibrometry and compared to finite element simulations. A new electrode design for enhanced accuracy and reduction of computational effort is introduced. Circularly arranged ring electrodes (‘bull’s eye’) enable the precise and simultaneous determination of $d_{31}$ and $d_{33}$.

Keywords: Scandium, AlN, Sc$_x$Al$_{1-x}$N, Piezoelectric, Vibrometer, Comsol, MEMS

1. Motivation

Nowadays, piezoelectric aluminium nitride (AlN) thin films are implemented into a large variety of Si-based MEMS devices for actuation or sensing purposes.[1] AlN is a suitable material for energy harvesting systems based on MEMS resonators as well as for FBARs, core components in duplexers in handheld communication systems. Most recently, transition metal doping of AlN, foremost with Scandium (Sc) was introduced up to $x=42\%$ in Sc$_x$Al$_{1-x}$N a fivefold increase of the piezoelectric constant $d_{33}$ was reported [2]. Thus, the efficiency of AlN based MEMS devices could be enhanced as illustrated by the electromechanical coupling factor $k_e^2 = e_{33}^2 / (C_{33}\varepsilon_r)$ that acts as the key figure of merit in FBARs. Here, $e_{33}$ is the piezoelectric stress constant and $C_{33}$ is the elastic stiffness.

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Upon doping AlN with Sc, $e_{33}$ increases, accompanied by a pronounced softening of the material – decreasing $C_{33}$, while only a weak increase of $e_i$ is observed. Hence, a tremendous increase of the coupling factor could be obtained by exploiting w-Sc$_x$Al$_{1-x}$N thin films. In this study, the deposition parameters are optimized to maximize the piezoelectric constants $d_{33} \approx e_{33} / C_{33}$ and $d_{31}$ of Sc$_x$Al$_{1-x}$N thin films ($x=27\%$).

2. Thin Film Deposition

Sc$_x$Al$_{1-x}$N thin films were deposited on n-doped Si(100) substrates via DC magnetron sputtering from a 100 mm ScAl alloy target with a fixed Sc concentration of $x = 30\%$ at nominally unheated substrate temperatures. The Ar/N$_2$ ratio was varied as it already proved to be an important parameter to achieve highly c-axis oriented w-Sc$_x$Al$_{1-x}$N thin films even at lower concentrations of Sc [3]. Simultaneously, the influence of substrate bias was studied using either a grounded ($= 0$ V), floating ($= 17$ V) or biased ($= 37$ V) substrate. Other deposition parameters, such as chamber pressure $p = 2.5$ μbar, plasma power $P = 400$ W and target-substrate distance $d = 65$ mm were kept constant. In addition, the sputtering time was adapted to yield a film thickness of about 500 nm. Prior to the deposition process, the substrates were cleaned by an in-situ ion etching process. The concentration $x = (27 \pm 2)\%$ of Sc was determined by energy dispersive X-ray spectroscopy (EDX, Oxford Instruments X-Max 50). Circularly shaped platinum electrodes with a thickness of 100 nm were sputter deposited on the samples and patterned via a lift-off process.

3. Mechanical Properties

Design and simulation of piezoelectric based MEMS devices require accurate knowledge of the complete piezoelectric rigidity tensor or, alternatively of the compliance matrix. *Ab initio* density functional theory (DFT) was applied to investigate w-Sc$_x$Al$_{1-x}$N with several selected Sc concentrations. Applying the Vienna Ab initio Simulation Package (VASP) [4], the elements of the rigidity matrix for Sc$_x$Al$_{1-x}$N thin films, are obtained for 4x4x2 supercells with 64 atoms on the Al/Sc sublattice. Results for all four independent elements of the rigidity matrix are shown in Figure 1.

![Fig. 1. (a,b) Elastic rigidity tensor elements $C_{ij}$ of w-Sc$_x$Al$_{1-x}$N from density functional theory](image-url)
4. FEM based evaluation of voltage induced piezoelectric deflection

Recently, Hernando et al. introduced the FEM based evaluation of interferometrically determined deflection curves from quadratic electrodes on AlN thin films. This approach accounts for the inherent substrate bending by a complete simulation of a structure consisting of substrate/bottom-electrode/thin film/ top-electrode configuration [5]. Our work extends the above-mentioned approach and uses simple circular and bull’s eye shaped platinum electrodes deposited on ScxAl1-xN with x = 0.27, as shown in Fig. 2. Based on the rotational symmetric test structure design, the computational effort of FEM deflection simulations with Comsol is significantly reduced. Hence, the piezoelectric constants $d_{31}$ and $d_{33}$ can be simultaneously swept within a large range with a resolution of 0.1 pm/V to find the best match between simulation and measurement. For simple circular electrodes the kHz range frequency voltage is applied on the top electrode while for bulls-eye electrodes the inner disc and the outer ring exhibit a 180° phase shifted excitation, whereas the substrate acting as ground for both electrode types. The bull’s eye based simulation includes the aluminium ground plate as the deflection field extends further than the Si wafer thickness. Hence, the substrates were bonded to the ground plate by a two-component conductive epoxy glue (Polytec EC 101). Comparing an evaluation of a measurement conducted at an excitation frequency of 65 kHz for both electrode designs, as shown in Fig. 3, the advantages of the newly designed bull’s eye electrodes are visibly. The phase shifted excitation enables a more precise determination of $d_{31}$ and $d_{33}$ due to enhanced differences in the displacement curve shapes. Best fit of FEM-based deflection curve and LDV measurement is determined automatically via a least-deviation algorithm using MatLab. There, all simulation results for each pair of ($d_{33}$, $d_{31}$) are compared with those gained form the measurements and the piezoelectric constants are determined by simulation applying a least deviation fit procedure to the measurement.
5. Results

For evaluating the piezoelectric constants of the deposition series of ScₓAl₁₋ₓN thin films the displacement curves were calculated with Comsol for a range of d₃₃ = 1 pm/V up to 20 pm/V while d₃₁ was simultaneously swept for each d₃₃ such that d₃₁ > -d₃₃/2 up to d₃₁ < -d₃₃/2 + 2 pm/V. For each thin film several displacement curves were measured with an applied voltage of U = 10V at frequencies of f = 20 kHz and f = 65 kHz. The averaged results for d₃₃ and d₃₁ are depicted in Fig. 4. The observed piezoelectric response is maximized for the thin film deposited with an argon concentration of c = 25% at a substrate bias of 0 V. The maximized mean measurement values are d₃₃ = 13.2 pm/V and d₃₁ = -5.8 pm/V, thus being close to the predicted values of the ab initio calculations (d₃₃ = 14.4 pm/V and d₃₁ = -5.6 pm/V).

6. Conclusions

This work demonstrates the use of circularly shaped electrodes for single- and two-port measurements of the piezoelectric constants (d₃₃, d₃₁) of thin films. Simultaneous and precise evaluations of both piezoelectric constants are conducted by measuring the surface deflection upon application of an AC voltage to disc or bull’s eye shaped electrodes and subsequent best fit to FEM based deflection curves. The method was applied to a series of DC sputter deposited ScₓAl₁₋ₓN (x = 27%) thin films using elastic constants from ab initio based calculations. The piezoelectric response (d₃₃ = 13.2 pm/V and d₃₁ = -5.8 pm/V) was maximized for an argon concentration of 25%, grounded substrate and provides a step towards the usage of ScₓAl₁₋ₓN thin films for improved piezoelectric MEMS devices.

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References