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Circular test structure for the determination of piezoelectric constants of $Sc_xAl_{1-x}N$ thin films applying Laser Doppler Vibrometry and FEM simulations

P.M. Mayrhofer [a], H. Euchner [b], A. Bittner [a], U. Schmid [a]

[a] Institute of Sensor and Actuator Systems, Vienna University of Technology, Floragasse 7, 1040 Vienna, Austria
[b] Institute of Materials Science and Technology, Vienna University of Technology, Karlsplatz 13, 1040 Vienna, Austria

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ABSTRACT

Piezoelectric scandium aluminium nitride ($Sc_xAl_{1-x}N$) thin films offer a large potential for the application in micro electromechanical systems, as advantageous properties of pure AlN thin films are maintained, but combined with an increased piezoelectric actuation and sensing potential. $Sc_xAl_{1-x}N$ thin films with $x = 27\%$ have been prepared by DC reactive magnetron sputtering to find optimized deposition parameters to maximize the piezoelectric constants d_{33} and d_{31}. For the accurate and simultaneous measurement of these constants Laser Doppler Vibrometry has been applied and compared to finite element (FEM) simulations. The electrode design has been optimized to rotational symmetric structures enabling a 180° phase shifted excitation, so that a straight-forward comparison of experimental displacement curves with those obtained from FEM is feasible.

1. Introduction

Micro electromechanical systems (MEMS) based on piezoelectric thin films is an emerging research area, as such devices and systems are strongly penetrating into new market applications [1]. Aluminium nitride (AlN) is increasingly used as piezoelectric material in MEMS sensors and actuators such as accelerometers [2] or to determine the viscosity and density of liquids [3,4], surface and bulk acoustic resonators [5], atomic force microscopy (AFM) cantilevers [6], or energy harvesting systems [7]. Complementary metal-oxide-semiconductor (CMOS) compatibility, high temperature and long term stability as well as low dielectric constants are beneficial properties of AlN. For the piezoelectric constants d_{33} and d_{31} values up to 6.5 pm/V and −2.9 pm/V are reported for pure AlN thin films prepared by reactive magnetron sputtering [8–10]. A significant enhancement was achieved via incorporation of scandium (Sc) into AlN, up to 27.6 pm/V for $Sc_xAl_{1-x}N$ thin films with $x = 42.5\%$ [11,12]. This increase was observed near a phase transition from a cubic to a wurtzite type crystal structure, starting at about 45%. In contrast, this work focuses on $Sc_xAl_{1-x}N$ thin films with a fixed scandium concentration of $x = 27\%$. By choosing the latter value, the formation of the cubic type crystal structure is avoided, but a strong increase of piezoelectric constants is already expected. Measurements with bulk acoustic wave (BAW) resonators based on $Sc_xAl_{1-x}N$ with $x = 35\%$ showed a piezoelectric coefficient $d_{33} = 16$ pm/V, which is below the value predicted by ab initio calculations ($d_{33} \sim 23$ pm/V) [13].

The precise knowledge of electro-mechanical constants of piezoelectric thin films is important for the design and simulation of MEMS. For example the use of finite element (FEM) software for device design requires the accurate implementation of elastic and dielectric as well as piezoelectric properties to predict precisely the performance of MEMS devices. Various measurement techniques exist for piezoelectric thin films probing either the direct piezoelectric effect, by measuring the resulting voltage upon application of mechanical stress or the inverse piezoelectric effect by measurement of the voltage induced expansion or compression. The principles of direct piezoelectric measurements were established by Lefki and Dormans for ideal cases regarding substrate clamping as well as substrate and electrode size [14]. The Berlincourt based direct measurement approach involving a reference sample with known piezoelectric properties is mentioned in this context. As this work deals with the measurement of piezoelectric constants via the indirect piezoelectric effect the discussion focuses in this direction.

Another approach, comprising the extraction of piezoelectric properties with MEMS devices, such as cantilevers, film bulk acoustic resonators (FBARs) or surface acoustic resonators (SAWs) is thoroughly covered in literature [15–18]. For an analytical

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evaluation of the piezoelectric properties some assumptions or important parameters need to be made or known, such as the quality factor, although the determination on device level is in principal beneficial, as it directly considers the intended application of the thin films. However, for studying new materials cantilever fabrication is a sophisticated and time consuming procedure and in general not feasible in an early stage of the work when process parameters are yet to be optimized. The evaluation of complete SAW devices or FBAR resonators via FEM simulation also requires input parameters such as the dielectric constant or sound velocity. They need to be included into the model and therefore induce further uncertainties.

As the typical intrinsic piezoelectric displacement of thin films is small (i.e. pm to nm range) measurement techniques are mostly based on optical interferometry, Laser Doppler Vibrometry (LDV) or piezoelectric force microscopy (PFM). Measurement of the piezoelectric displacement via single beam interferometry is not straight forward due to several reasons. First, the contribution of substrate bending is, compared to the change in film thickness not negligible, requesting an elaborated clamping. For a weakly clamped Si wafer covered with a piezoelectric layer Kholkin et al. showed that the measured piezoelectric displacement has a quadratic dependence on the electrode length. Hence, the known formula for the bending of a piezoelectric bimorph induced by the transverse piezoelectric effect is being proportional rather to d_{31} than to d_{33} [19]. Reduction of the electrode size and usage of a hard, conductive glue may be sufficient to suppress substrate bending. Moreover, a double beam interferometer for simultaneous measurement of thin film surface and substrate bottom-surface was used to minimize the impact of substrate bending [20]. However, the change in piezoelectric thin film thickness is not homogeneous below the electrode area, since the local deflection of the bottom surface of the piezoelectric thin film is also important to consider for an accurate evaluation of the displacement profile, as previously demonstrated by FEM simulations [21]. Furthermore, atomic force microscopy was used to apply the electric field via a conductive tip and measure the corresponding displacements for piezoelectric evaluation purposes [22]. However, when metallic electrodes deposited on the piezoelectric film are used the evaluation of the displacement curves is again not straight forward, but requires an in depth analysis taking the above mentioned issues into account.

The following sections discuss the deposition of highly *c*-axis oriented $Sc_xAl_{1-x}N$ with $x = 27\%$ via DC reactive magnetron sputtering together with a full evaluation of both piezoelectric coefficients d_{33} and d_{31}. For the measurement of piezoelectric displacement profiles via LDV new circular electrodes were designed and evaluated in comparison to COMSOL based FEM simulations. In addition, elastic properties for various concentrations x of $Sc_xAl_{1-x}N$ were obtained from ab initio density functional theory (DFT) calculations.

2. Thin film preparation

In order to maximize the piezoelectric response of $Sc_xAl_{1-x}N$ thin films a deposition series has been prepared via DC reactive ion sputtering. Subsequently, circular shaped platinum electrodes have been sputter-deposited and lithographically structured on top of the piezoelectric material. The thin films were deposited in a production-type sputtering system (Von Ardenne LS730S). Prior to the $Sc_xAl_{1-x}N$ deposition, the Si(100) substrates have been cleaned by an in situ ion etching process (ISE), thus resulting in the complete removal of the native silicon surface oxide and an amorphization of the surface-near crystal structure [23]. Subsequently, thin films with a thickness of 500 nm were prepared by DC reactive magnetron sputtering from a 100 mm AlSc alloy target with a fixed ratio of 30 at.% Sc at nominally unheated substrate conditions. The base pressure prior to the deposition was kept below 4×10^{-7} mbar, while the other fixed process parameters are depicted in Table 1.

During the deposition series the argon ratio in the process gas (Ar/N_2 ratio: 0%, 25%, 50%) as well as the substrate bias conditions were varied. For the latter parameter, the sputter system allows three different configurations: grounded (DC: 0 V), floating (DC: 17 V) and biased (DC: 37 V), where the depicted value for each setting is corresponding to the effective substrate self-bias. Without the exception of grounded substrate, the measured self-biase was fluctuating throughout the deposition by approximately 1 V. The deposition time was set such that the expected thin film thickness remained approximately constant at 500 nm. The scandium concentration x was measured by a scanning electron microscopy based energy dispersive X-ray system (EDX, Oxford Instruments X-Max 50). The determined value was $x = (27 \pm 2)\%$ and throughout the deposition series no significant variation of x was observed. For the purpose of an additional calibration standard pure AlN thin films with the same equipment and sputter parameters have been deposited as described by Schneider et al., including an ion etching process prior to the deposition [23]. The circularly shaped electrode design, as illustrated in Fig. 2(a) and (c), was achieved by image reversal lithography followed by a lift-off process of platinum thin films ($t = 100$ nm). For the determination of piezoelectric constants all samples were bonded to an aluminium plate using a conductive Ag epoxy glue (Polytec EC 101).

3. Elastic properties of $Sc_xAl_{1-x}N$

FEM based simulations of piezoelectric structures require the complete knowledge of the anisotropic compliance tensor of $Sc_xAl_{1-x}N$. This work utilizes elastic constants obtained from ab initio DFT (density functional theory) calculations, as shown in Fig. 1.

The simulations were conducted using the Vienna Ab initio Simulation Package (VASP) [24], applying the projector augmented wave method and the generalized gradient approximation (PAW-GGA) [25]. To obtain representative structures, $4 \times 4 \times 2$ supercells with altogether 128 atoms were constructed. $Sc_xAl_{1-x}N$ was assumed to be a solid solution, in which the Sc atoms are randomly distributed on the metal sublattice. The desired Sc content was then obtained by making use of the special quasi-random structure (SQS) approach [26]. Supercells with a Sc content of 6.25%, 12.5%, 15.625%, 18.75% and 37.5% were optimized by relaxing both, lattice constant and atomic positions, using a $2 \times 2 \times 3$ Γ-centred k-point mesh and an energy cut-off of 600 eV. The structure optimization was only stopped when residual forces and stresses were less than 0.005 eV/Å and 0.05 GPa, respectively. Next, the ground state structures were strained, using the universal independent coupling strain approach [27]. The strained configurations were again relaxed, however, with fixed lattice constants, such that only

Table 1
Process parameters for the ISE process and the $Sc_xAl_{1-x}N$ thin film synthetization (process pressure in the deposition chamber p, plasma power density P, process time t, argon gas flow υ_{Ar} and electrode distance d).

ISE					Deposition			
p/Pa	P/W cm^{-2}	t/s	d/mm	υ_{Ar}/sccm	p/Pa	P/W cm^{-2}	t/s	d/mm
0.6	6.4	60	65	60	0.25	5.1	800–1300	65

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