Development of piezoelectric microelectromechanical systems for multiaxial motion and sensing

Kristina Bespalova
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A doctoral thesis completed for the degree of Doctor of Science (Technology) to be defended, with the permission of the Aalto University School of Electrical Engineering, at a public examination held at the lecture hall AS1 (TUAS building, Maarintie 8, 1018) of the school on 15 March 2024 at 12:00.

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Piezoelectric materials offer several advantages for MEMS applications due to their superior direct electromechanical coupling and low voltage consumption, especially when compared to electrostatic-based MEMS. Integrating piezoelectric thin films in MEMS also allows for a significantly smaller chip footprint than devices employing other transduction techniques. Furthermore, thin piezoelectric films can be integrated into the fabrication of multifunctional devices capable of three-dimensional motion (3D motion). Such 3D piezoMEMS enable driving and sensing along the x, y, or z-axes using components of a single element. This distinguishes 3D piezoMEMS from conventional MEMS that utilize elements that often facilitate motion in only one direction.

This dissertation investigates the development of a new fabrication approach and adapting and optimizing existing fabrication techniques for 3D piezoMEMS fabrication. Pure lateral motion of a single MEMS element is implemented by placing metal organic chemical vapour deposited aluminium nitride (MOCVD AlN) thin films on the vertical surfaces of the Si cantilever. The fabrication approach demonstrated in the work unlocks the piezoelectric and electrode material deposition potential on vertical sidewall structures in the fabrication of advanced 3D piezoMEMS.
To my grandparents Anna Alekseevna Prohodova (Lozkina) and Georgii Semënovich Prohodov
This research was conducted at Aalto University in the Electronics Integration and Reliability Unit of the Department of Electrical Engineering and Automation. This work was financially supported by two ECSEL Joint Undertaking under grant number Ecsel-783132-Position-II-2017-IA and ECSEL18 Project NewControl under grant agreement No. 826653-2. Additionally, this work was supported by the School of Electrical Engineering funded doctoral position. The research for this dissertation utilized the facilities of the Aalto University OtaNano Micronova Nanofabrication Centre and Nanomicroscopy Centre.

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Espoo, September 2023

Kristina Bespalova
Acknowledgements
Abbreviations
Symbols
List of Publications
Author’s Contribution

1. Introduction 13
2. Lateral motion in MEMS 15
   2.1 Actuation mechanisms for lateral motion in MEMS 15
3. Lateral motion in piezoelectric MEMS 19
   3.1 Lateral actuation via piezoelectric effect 20
   3.2 Critical parameters for Piezoelectric MEMS 24
   3.3 Prospects and challenges for laterally actuated piezoelectric MEMS 27
4. Next-generation piezoelectric MEMS 29
   4.1 Concept of multiaxial motion in piezoelectric MEMS 29
   4.2 Next-generation materials for piezoelectric MEMS 32
5. Design and fabrication of piezoelectric MEMS 35
   5.1 FEM simulations of a device performance 36
   5.2 In-plane piezoelectric actuator fabrication 40
   5.3 Surface quality 44
   5.4 AlN crystal quality, microstructure and uniformity on the vertical sidewalls 46
   5.5 Electrical connection to the sidewalls 52
6. Characterization of piezoelectric MEMS 57
   6.1 Motion tests 57
7. Conclusion 59
References 61
Publications 73
### Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D</td>
<td>Three-dimensional</td>
</tr>
<tr>
<td>3D piezoMEMS</td>
<td>Three-dimensional piezoelectric-based MEMS</td>
</tr>
<tr>
<td>AFM</td>
<td>Atomic force microscopy</td>
</tr>
<tr>
<td>Al&lt;sub&gt;1-x&lt;/sub&gt;Sc&lt;sub&gt;x&lt;/sub&gt;N</td>
<td>Sc-doped AlN</td>
</tr>
<tr>
<td>Al&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>Aluminium oxide, sapphire</td>
</tr>
<tr>
<td>ALD</td>
<td>Atomic layer deposition</td>
</tr>
<tr>
<td>AlN</td>
<td>Aluminium nitride</td>
</tr>
<tr>
<td>BE</td>
<td>Bottom electrode</td>
</tr>
<tr>
<td>BF</td>
<td>Bright field</td>
</tr>
<tr>
<td>BHF</td>
<td>Buffered oxide etch</td>
</tr>
<tr>
<td>CTE</td>
<td>Coefficient of thermal expansion</td>
</tr>
<tr>
<td>CVD</td>
<td>Chemical vapour deposition</td>
</tr>
<tr>
<td>DRIE</td>
<td>Deep reactive ion etching</td>
</tr>
<tr>
<td>EBSD</td>
<td>Electron backscatter diffraction</td>
</tr>
<tr>
<td>EDX</td>
<td>Energy dispersive X-ray analysis</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite-element method</td>
</tr>
<tr>
<td>FIB</td>
<td>Focused ion beam</td>
</tr>
<tr>
<td>FinBAR</td>
<td>Fin bulk acoustic wave resonators</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full width at half maximum</td>
</tr>
<tr>
<td>HF</td>
<td>Hydrofluoric acid</td>
</tr>
<tr>
<td>HNO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>Nitric acid</td>
</tr>
<tr>
<td>HRXRD</td>
<td>High-resolution X-ray diffraction</td>
</tr>
<tr>
<td>ICP-RIE</td>
<td>Inductively coupled plasma reactive ion etching</td>
</tr>
<tr>
<td>KOH</td>
<td>Potassium hydroxide</td>
</tr>
<tr>
<td>LiNbO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>Lithium niobate</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>MEMS</td>
<td>Microelectromechanical systems</td>
</tr>
<tr>
<td>MOCVD</td>
<td>Metal organic chemical vapour deposition</td>
</tr>
<tr>
<td>NEMS</td>
<td>Nanoelectromechanical systems</td>
</tr>
<tr>
<td>PiezoMEMS</td>
<td>Piezoelectric-based MEMS</td>
</tr>
<tr>
<td>PMUT</td>
<td>Piezoelectric micromachined ultrasonic transducers</td>
</tr>
<tr>
<td>PolySi</td>
<td>Polysilicon</td>
</tr>
<tr>
<td>PVD</td>
<td>Physical vapour deposition</td>
</tr>
<tr>
<td>PZT</td>
<td>Lead zirconate titanate, PbZrTiO$_3$</td>
</tr>
<tr>
<td>RIE</td>
<td>Reactive ion etching</td>
</tr>
<tr>
<td>RMS</td>
<td>Root mean square</td>
</tr>
<tr>
<td>SAED</td>
<td>Selected area electron diffraction</td>
</tr>
<tr>
<td>SAW</td>
<td>Surface acoustic wave</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning electron microscopy</td>
</tr>
<tr>
<td>SiC</td>
<td>Silicon carbide</td>
</tr>
<tr>
<td>SOI</td>
<td>Silicon-on-insulator</td>
</tr>
<tr>
<td>STEM</td>
<td>Scanning transmission electron microscopy</td>
</tr>
<tr>
<td>TE</td>
<td>Top electrode</td>
</tr>
<tr>
<td>TEM</td>
<td>Transmission electron microscopy</td>
</tr>
<tr>
<td>TMAH</td>
<td>Tetramethylammonium hydroxide</td>
</tr>
<tr>
<td>XRC</td>
<td>X-ray rocking curve</td>
</tr>
<tr>
<td>ZnO</td>
<td>Zinc oxide</td>
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</table>
### Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>$A$</td>
<td>Electrode area</td>
</tr>
<tr>
<td>$C$</td>
<td>Stiffness</td>
</tr>
<tr>
<td>$d_{xx}$</td>
<td>Piezoelectric strain coefficient [mV⁻¹]</td>
</tr>
<tr>
<td>$d_{xx,f}$</td>
<td>Effective longitudinal piezoelectric coefficient</td>
</tr>
<tr>
<td>$E_{dissipated}$</td>
<td>Energy dissipated by a system</td>
</tr>
<tr>
<td>$E_{stored}$</td>
<td>Energy stored by a system</td>
</tr>
<tr>
<td>$e_{xx}$</td>
<td>Transverse piezoelectric coefficient [C m⁻²]</td>
</tr>
<tr>
<td>$e_{xx,f}$</td>
<td>Effective transverse piezoelectric coefficient</td>
</tr>
<tr>
<td>$f_0$</td>
<td>Resonance frequency</td>
</tr>
<tr>
<td>$f_p$</td>
<td>Parallel resonance frequency</td>
</tr>
<tr>
<td>$f_s$</td>
<td>Series resonance frequency</td>
</tr>
<tr>
<td>$h$</td>
<td>Height of a cantilever</td>
</tr>
<tr>
<td>$K_a$</td>
<td>Piezoelectric coupling factor</td>
</tr>
<tr>
<td>$k_{eff}^2$</td>
<td>Effective electromechanical coupling factor</td>
</tr>
<tr>
<td>$k_i^2$</td>
<td>Electromechanical coupling factor</td>
</tr>
<tr>
<td>$L$</td>
<td>Length of a cantilever</td>
</tr>
<tr>
<td>$l$</td>
<td>Displacement</td>
</tr>
<tr>
<td>$Q$</td>
<td>Quality factor</td>
</tr>
<tr>
<td>$Q_{anchor}$</td>
<td>Anchor loss</td>
</tr>
<tr>
<td>$Q_{other}$</td>
<td>Other losses in a system</td>
</tr>
<tr>
<td>$Q_{TED}$</td>
<td>Thermoelastic damping</td>
</tr>
<tr>
<td>$R_q$</td>
<td>Surface roughness</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$V$</td>
<td>Applied voltage</td>
</tr>
<tr>
<td>$V_{DC}$</td>
<td>Direct current bias voltage amplitude</td>
</tr>
<tr>
<td>$V_{pp}$</td>
<td>Peak-to-peak voltage amplitude</td>
</tr>
<tr>
<td>$w$</td>
<td>Width of a cantilever</td>
</tr>
<tr>
<td>$W_E$</td>
<td>Electrical energy</td>
</tr>
<tr>
<td>$W_M$</td>
<td>Mechanical energy</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2\theta$</td>
<td>Diffraction angle</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Relative permittivity</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>Permittivity of free space</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Resistivity</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Angle between incident beam and sample surface</td>
</tr>
</tbody>
</table>
List of Publications

This doctoral dissertation consists of a summary of the following publications, which are referred to in the text by their Roman numerals.


Author’s Contribution

**Publication I:** “Characterization of AlScN-based multilayer systems for piezoelectric micromachined ultrasound transducer (pMUT) fabrication”

The author planned the research together with the co-authors, and conducted the samples annealing in a vacuum furnace, SEM imaging, and surface roughness measurements using AFM. AlScN and top electrode material deposition were provided by the VTT Technical Research Centre of Finland. The author also prepared the lamellas for TEM in FIB and analyzed all the results of the research. TEM analysis of the samples was performed by Dr. Glenn Ross. The manuscript was written by the author with the help of the co-authors.

**Publication II:** “In-plane AlN-based actuator: Towards a new generation of piezoelectric MEMS”

The author planned the fabrication process based on discussions with the co-authors. She designed the fabrication flow of the device and made the layout of all masks for the photolithography. The author personally executed all steps for actuator fabrication, including patterning, etching and AlN depositing using MOCVD. EBSD analysis of the samples was performed by Dr. Glenn Ross. The author analyzed the results and wrote the manuscript with the help of the co-authors. The author also created all the visual materials.

**Publication III:** “Metalorganic chemical vapor deposition of AlN on high degree roughness vertical surfaces for MEMS fabrication”

The author planned the concept of the paper with the co-authors and conducted all experimental work including the preparation of the patterned substrates, MOCVD deposition of AlN, characterization and analysis of the grown AlN films – structural and morphological assessments. The author analyzed the results and wrote the manuscript with the help of the co-authors.
Publication IV: “Atomic layer deposition of AlN using atomic layer annealing—Towards high-quality AlN on vertical sidewalls”

The author conducted AFM analysis of the AlN films. Additionally, she participated in the results discussion and reviewed and commented on the manuscript. The manuscript was written by Dr. Elmeri Österlund.

Publication V: “Unlocking the potential of piezoelectric films grown on vertical surfaces for inertial MEMS”

The author participated in the definition of the concept for the paper and fabricated the samples. The author participated in the interpretation of the results with other co-authors. The original manuscript was written by MSc. Artem Gabrelian.
1. Introduction

Controlled and precise transduction at the micro- and nanoscale provides a wide range of possibilities for micro- and nanoelectromechanical systems (MEMS/NEMS). It allows the detection and measurement of physical quantities, such as acceleration [1], pressure [2] and rotation [3]. It also enables actuation in MEMS devices, where mechanical movement is utilized to perform specific tasks, such as positioning [4], switching [5] and manipulating objects [6]. Furthermore, MEMS devices convert mechanical vibrations or displacements into electrical energy for energy harvesting [7].

MEMS development trends include miniaturization, intelligent multifunctional design, green manufacturing, and decreased power consumption [7-9]. Electrostatic and piezoelectric are common transduction mechanisms in MEMS but miniaturization is difficult to achieve in electrostatic MEMS [8]. At the same time, piezoelectric MEMS are gaining much attention recently. In addition to miniaturization capabilities, piezoelectric materials offer significant advantages for MEMS due to direct electromechanical coupling and the ability to operate at low voltages [10, 11]. Additionally, thin piezoelectric films can be used to develop multifunctional devices capable of three-dimensional motion (3D motion). MEMS that execute multiaxial motion (3D piezoMEMS) could drive and sense along the x, y or z-axes using parts of a single element. Therefore, the integration of piezoelectric thin films in MEMS adds more functionalities to the device, while enabling it to occupy a much smaller chip area than devices that use other transduction techniques. Smaller size of MEMS elements contributes to dense integration of sensors and actuators, which enables arraying for sensing with higher resolution. Another benefit of 3D piezoMEMS is the possibility of integrating elements with lithographically defined size, and, therefore, properties that are not tied to piezoelectric film thickness. This approach enables integrating large number of elements with various properties within a single chip.

The implementation of lateral motion in 3D piezoMEMS via the piezoelectric effect can be achieved through the deposition of piezoelectric films on vertical sidewalls of a Si cantilever. Modern fabrication facilities are well adapted for work with planar structures only. Therefore, the adaptation and optimization of existing fabrication techniques for 3D piezoMEMS fabrication is needed. Moreover, the deposition of piezoelectric films over complex structures with developed morphology should be studied exhaustively.
Several prerequisites need to be fulfilled to achieve high-quality piezoelectric thin films on vertical surfaces. Thus, vertical surfaces destined for piezoelectric film deposition might have high surface roughness. A high surface roughness value of the underlying substrate leads to the growth of misoriented grains of the piezoelectric film [12-14]. Misorientation in the crystal structure of a piezoelectric film deteriorates the strength of the piezoresponse generated within the film and hence the device’s performance [15]. Consequently, Si etching approaches, surface quality, and surface uniformity improvement methods should be considered before piezoelectric thin film deposition. The piezoresponse of piezoelectric thin films is also influenced by other materials within the system. The piezoelectric film has to be sandwiched between two conductive materials for its work: electrode materials. These materials can be thin metal films or highly conductive semiconductors, such as doped Si or TiN. The roughness, quality and reactivity of electrodes affect not only performance but also the robustness of the future device. Thus, both the electrode material and its interaction with the piezoelectric material and the surrounding environment are important for the operation and reliability of 3D piezoMEMS.

This dissertation studies a new concept and develops the technology of advanced MEMS devices that utilize piezoelectric thin films deposited on the vertical surfaces of Si cantilevers for pure in-plane and multiaxial motion. The aim of this dissertation is to demonstrate the integration of piezoelectric thin films grown on vertical surfaces for MEMS fabrication using standard microfabrication facilities.

The purpose of this dissertation is to answer the following research questions:

i. How to achieve pure lateral motion in piezoelectric MEMS? [II, IV–V]

ii. Is it possible to find a process flow that can be integrated into the currently existing fabrication environment for the fabrication of 3D piezoMEMS? [I–II, V]

iii. What are the capabilities and limitations of chemical vapour deposition (CVD) techniques for the growth of high-quality piezoelectric thin films on vertical surfaces? [II–III, IV]

This dissertation is organized as follows. Chapter 2 provides an overview of the techniques currently employed to achieve sensing and actuation in-plane. Both sensors and actuators are overviewed, although the main emphasis is on the actuators for ease of comparison of different actuation techniques. Chapter 3 presents the basic principles of piezoelectric materials and comprehensively examines the status of laterally actuated piezoelectric MEMS. The chapter also introduces critical parameters that can be used as a figure of merit for the evaluation of MEMS device performance. Next, Chapter 4 describes a new generation of MEMS that will utilize piezoelectric thin films deposited on vertical surfaces for the multiaxial motion – 3D piezoMEMS. In Chapter 5, the critical process steps in integrating vertical thin films in MEMS fabrication are evaluated. Chapter 6 discusses piezoMEMS characterization by motion testing in a scanning electron microscope (SEM) chamber. Conclusions and suggestions for future work are provided in Chapter 7.
2. Lateral motion in MEMS

Lateral motion in MEMS can be achieved via electromagnetic [16], electrothermal [17], electrostatic [18] and piezoelectric effects. As mentioned in the Introduction, in MEMS, motion refers to unrestricted movement of the device’s parts along different axes. Figure 2.1 illustrates a schematic MEMS device with two suspended cantilevers. The z-axis represents vertical or out-of-plane motion, while the x- and y-axes denote motion within the device’s plane, so-called in-plane or lateral motion.

Thus, a motion that occurs along the x- or y-axis only and has no additional motion components, such as tilting, twisting or rotation in other directions, denotes pure in-plane or lateral motion. The pure lateral motion in the system is desirable, as it allows actuation without energy losses on additional types of motion. In the case of sensing, pure lateral actuation eliminates parasitic crosstalk between different channels and enhances the accuracy and reliability of the sensing system [19].

2.1 Actuation mechanisms for lateral motion in MEMS

Transduction of in-plane direction can be induced by any actuation technique and used for the fabrication of accelerometers, gyroscopes, magnetometers, energy harvesters, resonators, relays and switches. One notable milestone
in the development of lateral motion in MEMS was the fabrication and prototyping of the first comb-drive structure by W.C. Tang [20] in 1989. The comb drive designed by Tang and co-authors enabled the excitation of the comb fingers parallel to the substrate’s surface. This significant advancement in MEMS technology brought capacitive accelerometers to the market and made them a mainstream product of the industry 15 years later [21]. Since then, the development of laterally actuated electrostatic MEMS has seen rapid progress with the introduction of various flexures, springs and mechanisms that enable precise and controlled lateral actuation and sensing in a wide range of devices. Electrostatic actuators use Coulomb force for actuation [22]. They can consist of two sets of interdigitated comb-like structures: a stationary comb and a moving comb. When a voltage is applied between the comb fingers, an electrostatic force acts on the surface of the electrodes, thereby contributing to the motion of the moving comb. The displacement rate depends on the applied voltage, surface area of the fingers, distance between fingers, etc. Such in-plane electrostatic actuators are used as nanoscale relays [18, 23-26], as switches [27] and for micro- and nanopositioning [22].

![Figure 2.2 SEM micrographs of different electrostatic relay designs: (a) clamped-clamped relay by R. Parsa et al. [23]; (b) Y-shaped NEM relay by W.S. Lee et al. [24]; (c) five-terminal NEM relay by D. Lee et al. [24].](image)

The capacitive MEMS can be applied for sensing. In the case of sensing, the change in capacitance between the moving and stationary fingers is measured. Comb-drive gyroscopes [28] represent the implementation of lateral electrostatic sensing in-plane. Nowadays, gyroscopes, together with accelerometers, are merged into inertial measurement units (IMUs) [29]. Electrostatic in-plane sensing has also been introduced in chemical sensors [30], mass biosensors [31] and energy harvesters [32]. In-plane sensing is quite simple to achieve in electrostatic MEMS; however, levitation (out-of-plane motion component) generates parasitic capacitance in comb drives and often leads to non-linearity of the signal [19, 33].

Electromagnetic is another example of an actuation mechanism. Electromagnetic actuation involves the interaction between electric currents and magnetic fields to induce motion. In electromagnetic MEMS, a magnetic field is generated by an electrical current flowing through a microcoil, usually made of Al or electroplated Cu. The field interacts with a permanent magnet (for example, NdFeB, permalloy or Orthonol) or another coil, thus producing a driving force [34]. The application of electromagnetic in-plane motion has been demonstrated for energy harvesting [16, 35], in addition to micro-optical switches [5], rotation mechanisms [36] and actuators [36-40]. In-plane electromagnetic sensing can be applied in multiaxial magnetometers [41].
Electrothermal MEMS uses the principle of thermal expansion to induce motion. These devices utilize the controlled heating of specific elements, often resistive heaters integrated into the MEMS platform. As the temperature of the heated element rises, it experiences thermal expansion, causing it to deform. This controlled deformation is carefully engineered to produce the desired movements within the MEMS device. Electrothermal MEMS can achieve various types of motion, such as bending, stretching or even complex multi-degree-of-freedom movements. Polysilicon (polySi) has been the dominant structural material for such MEMS [17], but some works have demonstrated actuation via Ta [17], Ni [42] and Au [43].

Table 1 summarizes examples of MEMS that enable in-plane actuation of the device’s parts via diverse driving mechanisms. As shown in Table 1, the amplitude of the lateral motion varies significantly in different MEMS from 5 nm/V to 23 μm/V. Often, large motion amplitude is a result of a compromise between miniaturization and performance strength. A detailed overview of lateral piezoelectric actuation is presented in the next chapter.
Table 1. Summary of MEMS devices enabling lateral actuation

<table>
<thead>
<tr>
<th>Actuation mechanism</th>
<th>Type of a device and material</th>
<th>Reference</th>
<th>Average size of the device*</th>
<th>Max. amplitude of in-plane motion demonstrated</th>
<th>Amplitude of out-of-plane motion*</th>
<th>Magnetic field, mT</th>
<th>Driving frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrothermal</td>
<td>Micro-optical switch, Rotation mechanism</td>
<td>Ko et al. [5]</td>
<td>1.2 x 960 μm²</td>
<td>0.1 μm/μA</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Luharuka and Hesketh [36]</td>
<td>1–2 mm</td>
<td>Rotation 0–10°</td>
<td>Observed, but minor</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cao et al. [47]</td>
<td>2000 x 10 μm³</td>
<td>0.03–0.08 μm/μA</td>
<td>Up to 10 Hz</td>
<td>ND</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ahmed et al. [36]</td>
<td>410 x 580 μm³</td>
<td>1.6 μm/μA</td>
<td>20</td>
<td>0.5, 1, 2 Hz</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Microactuator</td>
<td>Han et al. [38]</td>
<td>20 x 8.3 mm²</td>
<td>2.3–4.75 μm/μA</td>
<td>ND</td>
<td>770–790</td>
<td>1, 15 Hz</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Wang et al. [39], [40]</td>
<td>6 x 6 mm²</td>
<td>0.18 μm/μA</td>
<td>2.3–3° rotation</td>
<td>578</td>
<td>0.65, 0.78 kHz (resonance)</td>
</tr>
<tr>
<td>Electromagnetic</td>
<td>Microactuator, Ta Microactuator, polySi</td>
<td>Ni et al. [17]</td>
<td>320 x 150 μm³</td>
<td>0.1 μm/μA</td>
<td>0.01</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sinclair et al. [48]</td>
<td>120 x 450 μm³</td>
<td>1 μm/V</td>
<td>ND</td>
<td>ND</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Actuation mechanism</th>
<th>Type of in-plane motion (three types)</th>
<th>Type of a device and piezomaterial</th>
<th>Reference</th>
<th>Average size of the device*</th>
<th>Max. amplitude of in-plane motion demonstrated*</th>
<th>Amplitude of out-of-plane motion, nm/V*</th>
<th>Driving frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Out-of-plane motion of the piezoelectric film is used for in-plane motion of other parts of the structure actuated via system of springs and mechanical connections</td>
<td>Actuator, PZT</td>
<td>Y.H. Seo et al. [51]</td>
<td>300 x 600 μm²</td>
<td>245±1 nm/V</td>
<td>ND</td>
<td>1 Hz–1 kHz</td>
</tr>
<tr>
<td></td>
<td>Moonie-type resonant microactuator, PZT</td>
<td></td>
<td>Y. Fujimura et al. [52]</td>
<td>4 x 7 mm²</td>
<td>23.95 μm/V (1 axis) 67 and 10.9 μm/V (2 axis)</td>
<td>ND</td>
<td>1.5 kHz (1 axis) and 621 Hz, 288.5 kHz (2 axis) – resonance</td>
</tr>
<tr>
<td>II</td>
<td>Partially in-plane. Torsion or using non-standard piezoelectric directions</td>
<td>Actuator, PZT</td>
<td>K.R. Oldham et al. [57]</td>
<td>100 x 500 μm²</td>
<td>50 nm/V</td>
<td>Large</td>
<td>ND</td>
</tr>
<tr>
<td></td>
<td>Nanobender, LiNbO₃</td>
<td>W. Jiang et al. [58]</td>
<td>16 μm</td>
<td>5 - 20 nm/V</td>
<td>ND</td>
<td>1 MHz</td>
<td></td>
</tr>
<tr>
<td>III</td>
<td>Pure in-plane. Induced by piezoelectric films deposited on the sidewalls of the actuated structures</td>
<td>Actuator, PZT and AlN</td>
<td>N. Wang et al. [60] and S. Youshida [61]</td>
<td>500 μm</td>
<td>400 nm/V</td>
<td>~0</td>
<td>14.26 kHz (resonance)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>K. Kanda et al. [62]</td>
<td>500–1500 μm²</td>
<td>120 - 200 nm/V 140 nm/V (captured), 7 nm/V (simulated)</td>
<td>~0</td>
<td>1 kHz</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>[II]</td>
<td>20–50 x 200–1100 μm²</td>
<td></td>
<td></td>
<td>~0</td>
<td>1 Hz</td>
</tr>
</tbody>
</table>

* If the data is not mentioned in the text of the source, then it is calculated or assumed based on information provided (for example, from the figures or graphs).
Piezoelectricity is the property of certain materials to generate an electric charge in response to applied mechanical stress or pressure. The piezoelectric effect is reversible, meaning that materials exhibiting the direct piezoelectric effect also undergo the inverse piezoelectric effect. Consequently, piezoelectric materials have the unique ability to convert mechanical strain into an electrical charge and vice versa [48]. Due to these beneficial properties, piezoelectric thin films are advantageous for both driving and sensing in MEMS.

Piezoelectricity occurs only in materials that do not possess a centre of symmetry in the crystal structure. The absence of inversion symmetry causes the separation of oppositely charged ions in the crystal lattice under an external force, leading to the generation of an electric field, as in the wurtzite structure of aluminium nitride (AlN) shown in Figure 3.1. In a wurtzite AlN crystal lattice, the arrangement of Al and N atoms forms a tetrahedron in which each ion is encompassed by ions of the opposite polarity [49]. The charges of all ions within the non-strained crystal cell are mutually balanced, resulting in an electrically neutral structure. However, the positive and negative charges are not centralized but are slightly separated along the [0001] direction. Hence, AlN films become polarized only when the lattice is distorted along the c-axis. The crystal lattice undergoes distortion upon applied mechanical stress, leading to the spatial separation of charges within the lattice. The charge separation generates an electric field and subsequently creates an electrical potential or vice versa.

Figure 3.1 Schematic illustration of the wurtzite structure of AlN. Adopted from [II].

The strength of the piezoelectric effect depends on multiple factors, such as the material properties, crystal structure, magnitude of the applied mechanical stress, and direction of the applied stress. A suspended beam with a piezoelectric thin film positioned between the top (TE) and bottom electrode (BE) on the
upper surface of the cantilever, as shown in Figure 3.2, is a typical example of a design for out-of-plane actuation and sensing via the piezoelectric effect.

Lateral actuation of MEMS elements, such as Si cantilevers, can be achieved through various designs and geometries using piezoelectric materials. For example, piezoelectric thin films deposited on suspended Si structures can cause lateral movement of other parts of the MEMS device that are connected to the driving piezoelectric element by a system of levers and springs. However, pure in-plane motion requires the deposition of the piezoelectric materials on the vertical surfaces of the actuated structures. While the integration of planar piezoelectric thin films in MEMS has been studied extensively, the deposition of such films on patterned substrates, like vertical surfaces, can result in innovative solutions.

To fully realize the potential of piezoelectric materials deposited on non-planar or vertical surfaces, several pre-existing challenges must be addressed. First, it is necessary to understand the place such structures can take in the modern MEMS world, comparing them with existing laterally driven devices. Second, it is necessary to comprehend the difficulties behind the development of MEMS that utilize non-planar piezoelectric thin films, particularly the deposition challenges for thin films on vertical surfaces.

### 3.1 Lateral actuation via piezoelectric effect

Devices that enable in-plane motion via piezoelectric effect can be divided into three main categories, as summarized in Table 1 from Section 2.1. In the first category, structures in which piezoelectric film executes out-of-plane motion through the system of springs, interconnections and leverages cause the lateral movement of other parts of the device, as shown in Figure 3.3. For example, in a study by Y.H. Seo et al. [51], a serpentine spring, one side of which is attached to the PZT film, undergoes lateral motion due to increased vertical stiffness and reduced lateral stiffness because of deformation in the PZT layer (Figure 3.3 a–c). A similar principle was applied in the work of Y. Fujimura et al. [52], in which the suspended TE/PZT/BE structure was part of a Moonie-type bridge flexure hinge connected to the resonance spring and a moving frame (Figure 3.3 d–f). This work is remarkable, because the device was introduced in two designs: for actuation along the x-direction only and in both the x- and y-directions (Figure 3.3 f). Complex bridge-type geometry of a unimorph actuator for in-plane motion was also demonstrated in prior works [53, 54]. However,
the simulated out-of-plane displacement for these structures proved to be relatively high, only two times lower than the amplitude of in-plane motion. The fabrication of a Moonie-type piezoelectric in-plane actuator was also shown in a study by P.A. York et al. [55]. The design of this piezoelectric ceramic-based device borrows some MEMS fabrication techniques and demonstrates the potential of piezoelectric materials for in-plane motion, although the size is meant for mesorobotic applications (Figure 3.3 h). In contrast, the work of C.H. Rhee et al. [56] revealed microrobotic leg joints using a planar-deposited PZT thin film. The leg performed out-of-plane and in-plane bending in an extensive range of motion of 5–40° (Figure 3.3 i).

Figure 3.3 Illustration of the working principle of: (a) a piezoelectric laterally actuated serpentine silicon spring by Y.H. Seo et al. [51] in (b) normal state and (c) under applied voltage [51]; (d) one-axis Moonie-type bridge flexure hinge demonstrated by Y. Fujimura et al. [52]; (e) its working principle; and (f) a concept of the same device enabling two-axis motion [52]. (g) ALN-based in-plane microactuator by J. Toledo et al. [53]; (h) Moonie-type bridge flexure hinge for mesoscale robotic applications from [55]; (i) Schematic illustration of the parts of the multiaxial joint from [56].

The second category of devices that enable in-plane motion via piezoelectric effect includes devices that utilize piezoelectric thin films that are deposited on the planar surfaces and, due to specific design features, in addition to the motion within the plane, perform torsional or rotational movements of the device out-of-plane. For example, motion in-plane can be achieved by interplaying between the electric field and transverse components of the piezoelectric tensor (for example, d₃₁ for ALN) as shown in Figure 3.4.
Lateral motion in piezoelectric MEMS

Figure 3.4 Schematic illustration of a piezoelectric device that enables torsional in-plane motion of a cantilever.

Such structures can be miniature, but at the same time, the amplitude of out-of-plane motion cannot be easily ignored. In the work of K.R. Oldham et al. [57], torsion around a suspended cantilever length was considered in-plane motion, although significant out-of-plane motion was mentioned and the exact magnitude of this motion was not measured. Another example was introduced in the work of W. Jiang et al. [58], in which in-plane bending was achieved by placing two parallel electrodes on top of the beam formed in a thinned Y-cut lithium niobate layer (LiNbO$_3$) bonded to a Si substrate. The authors also demonstrated how the LiNbO$_3$ nanobenders could be zig-zag arrayed and connected to a mirror, enabling tilt along its axis, as shown in Figure 3.5 e.

Figure 3.5 (a) Schematic illustration of the of a LiNbO$_3$ nanobender showing an applied electric field, resulting in strain and displacement of the fixed beam; (b) Cross-section of a nanobender showing the strain generated by electric field generated; (c)-(e) Examples of nanobenders connected in a series in a zig-zag shape; the actuation along different directions can be achieved by varying the aspect ratio of the zig-zag pattern. Adapted from the work of W. Jiang et al. [58].

The third category of laterally moving devices includes cantilevers or other geometries that utilize piezoelectric materials deposited on the vertical surfaces of a suspended beam, as shown in Figure 3.6. When an electric field is applied between the electrodes on the sidewalls of the cantilever, the piezoelectric film deforms and empowers the in-plane motion of the structure. This type of structure provides compact size, varying deflection values and negligible out-of-
Lateral motion in piezoelectric MEMS

plane deflection, although it demands advanced fabrication methods. For example, AlN film should be oriented so that [0001] direction is perpendicular to the surface of a vertical sidewall of the cantilever. Such configuration enables achieving a greater deflection value per volt compared to the devices utilizing transverse components of the AlN piezoelectric tensor $d_{31}$, while maintaining the device’s size and thickness of the piezoelectric film unchanged. This is due to a larger value of the longitudinal component of the piezoelectric tensor $d_{33}$ compared to $d_{31}$, and larger transverse piezoelectric coefficient $e_{33}$ compared to $e_{31}$ in many piezoelectric materials, especially those crystallized in the wurtzite structure [59].

Figure 3.6 Schematic illustration of a piezoelectric device that enables in-plane motion of a microscale size cantilever.

Only a few studies have been published on the piezoelectric lateral actuation of microscale-sized cantilevers. N. Wang [60] and S. Yoshida [61] reported on the fabrication of a bimorph piezoactuator that utilizes sol-gel deposited lead zirconate titanate (PZT) for in-plane motion in 2013. The deposition of PZT was done by the filling of pre-etched cavities in Si and sequential etching of the regions around these cavities for beam formation, as shown in Figure 3.7 a–b. The motion amplitude of the 500 $\mu$m long piezocantilever was calculated as 400 nm/V from the deflection graphs available in the paper. A non-linear deflection response was registered due to the ferroelectric nature of PZT. Another PZT-based lateral piezoactuator, illustrated in Figure 3.7 c, was produced by K. Kanda et al. in 2017 [62]. PZT was sputter-deposited on the vertical surfaces of a Si cantilever formed in the device layer of the silicon-on-insulator (SOI) wafer. The device had a relatively large size of 0.5–1.5 mm, while showing a modest deflection of 120–200 nm/V value, considering the device’s size.

Figure 3.7 SEM micrographs of the fabricated PZT-based microactuators. The SEM images are from the works of: (a)–(b) S. Yoshida et al. [61] and (c) Kanda et al. [62].

In work [II], the in-plane motion of the bimorph AlN-based piezoactuator was demonstrated. AlN was deposited on the vertical surfaces of the Si cantilevers using the metalorganic chemical vapour deposition (MOCVD) method. The vertical surfaces in Si were achieved using different etching methods: cryogenic
plasma etching in sulphur hexafluoride and oxygen (SF$_6$/O$_2$) and wet etching in potassium hydroxide (KOH) aqueous solution. AlN thin films deposited on vertical surfaces achieved by wet etching revealed a strong c-axis orientation compared to the films deposited on surfaces achieved by dry etching. However, motion was captured in both types of actuators. The registered motion was $1.4 \, \mu m$ at driving voltage $V = 20 \, V$ at frequency $f = 1 \, Hz$. The simulated motion of the actuator was predicted to be $140 \, nm$ at a given driving voltage.

![Figure 3.8](image)

Figure 3.8 An example of the fabricated AlN-based piezoelectric microactuator form [II].

### 3.2 Critical parameters for Piezoelectric MEMS

The electromechanical coupling factor ($k_\varepsilon^2$) and the quality factor (Q) are two critical parameters in the evaluation of microresonator technology across various applications. $k_\varepsilon^2$ quantifies the efficiency of energy transduction between the electrical and mechanical domains, playing a significant role in determining the loss and bandwidth of an electromechanical system and can be achieved for resonators actuated by any mechanism. A higher $k_\varepsilon^2$ results in lower insertion loss, improved rejection and broader bandwidth of, for example, RF filters [62].

($k_\varepsilon^2$) can be defined as [62]:

$$k_\varepsilon^2 = \frac{\pi f_s}{2 f_p \tan(\pi f_s/2f_p)}$$

(3.1)

where $f_p$ and $f_s$ are parallel and series resonance frequencies or more commonly known in MEMS as the resonance and antiresonance frequencies, that can be obtained from impedance curves as in Figure 3.9.

At the same time, ($k_\varepsilon^2$) can be defined as [62]:

$$k_\varepsilon^2 = \frac{\sqrt{C_m C_0 \cot(\frac{\sqrt{C_m}}{2\sqrt{C_0+C_m}})}}{2\sqrt{C_0+C_m}} \approx \frac{\pi^2 C_m}{8 C_0}$$

(3.2)

$$C_m = \frac{\eta^2}{k}$$

(3.3)

$C_m$, $C_0$ are motional and static capacitance, $k$ is spring constant, and $\eta$ is electromechanical transduction factor.
In addition to $k^2$, piezoelectric coupling ($K^2$) and effective electromechanical coupling factor ($k^2_{\text{eff}}$) can be used to describe the efficiency of different piezoelectric materials in converting electrical energy to mechanical energy and energy conversion efficiency at resonance in the piezoelectric-based device, respectively. $K^2$ can be quantified as [62]:

$$
K^2 = \frac{W_M}{W_M + W_E}
$$

where $W_M$ is mechanical energy and $W_E$ is electrical energy. Or [61]:

$$
K^2 = \frac{e^2}{c^2 \varepsilon_T}
$$

where $e$ is a piezoelectric constant, $c^E$ is stiffness and $\varepsilon_T$ is material’s relative permittivity.

$k^2_{\text{eff}}$ can be quantified as [62]:

$$
k^2_{\text{eff}} = \frac{f_h^2 - f_s^2}{f_s^2}
$$

In [10], the capacitive coupling factor $k^2_{\text{cap}}$ described as the varying capacitance between two electrodes because of the displacement $l$ of one of these electrodes:

$$
k^2_{\text{cap}} = V \frac{\varepsilon_o \varepsilon_A}{l^2}
$$

where $V$ is the bias voltage, $\varepsilon_o$ is the permittivity of free space, $\varepsilon$ is the material’s relative permittivity and $A$ is the electrode area. The piezoelectric coupling factor is a result of a strain-induced variation of polarization:

$$
k^2_{\text{piezo}} = \frac{e_{xx} A}{l}
$$

where $e_{xx}$ is a transverse piezoelectric coefficient.

When comparing two resonators of the same geometry, $k^2_{\text{piezo}}$ is much larger in magnitude than $k^2_{\text{cap}}$:

$$
\frac{k^2_{\text{piezo}}}{k^2_{\text{cap}}} = \frac{l e_{33}}{V e_0 e_r}
$$

Q factor is a measure of the energy decay rate in each cycle of oscillations, and it represents the efficiency of energy storage or damping for a resonator. A higher Q factor indicates reduced energy losses, improved energy transfer efficiency and, as a result, a narrow bandwidth around the resonant frequency. This is because a resonator with a higher Q value can retain coherent energy within the mode for a longer duration before dissipating it into the surrounding environment.

$$
Q = 2 \pi \frac{E_{\text{stored}}}{E_{\text{dissipated}}}
$$
Also, from [64]:

\[ Q = \left( \frac{1}{Q_{\text{anchor}}} + \frac{1}{Q_{\text{TED}}} + \frac{1}{Q_{\text{other}}} \right)^{-1} \]  

(3.11)

where \( Q_{\text{anchor}}, Q_{\text{TED}} \) and \( Q_{\text{other}} \) are anchor loss, thermoelastic damping (TED) and other losses, respectively. TED is caused by a mechanism related to the electrodes associated with interfacial loss [10, 64]. \( Q_{\text{anchor}} \) and \( Q_{\text{TED}} \) were found to play dominant roles in setting \( Q \) [64], and \( Q_{\text{TED}} \) made comparable contributions as \( Q_{\text{anchor}} \) in setting the \( Q \) [65]. The work of piezoelectric resonators is only possible with electrode materials, while capacitive resonators can utilize Si only. Therefore, piezoelectric resonators show a lower \( Q \) than bulk mode Si resonators, as shown in Figure 3.10.

![Figure 3.10 Overview of the reported values of the unloaded Q factor versus the resonance frequency. The predicted maximum obtainable f–Q product is represented by the dashed line for AlN (purple), quartz (black) and Si (red). Adopted from [10].](image)

The resonator figure of merit (FoM) can be defined as follows:

\[ \text{FoM} = \frac{k_{eff}^2 Q}{1 - k_{eff}^2} \]

(3.12)

Or for small \( k_{eff}^2 \) values:

\[ \text{FoM} = k_{eff}^2 Q \]

(3.13)

Currently, piezoMEMS are in the early stages of integration in MEMS. High values of the electromechanical coupling factor are among the advantages of piezoMEMS. However, \( Q \) value must be increased [66]. Thus, when designing piezoMEMS, it is essential to optimise fabrication thus to minimise losses on the electrodes and develop strategies to enhance \( Q \) [64, 66]. This dissertation does not extensively address the improvement of the \( Q \)-factor of piezoMEMS. However, in the design of devices in [II, V], Si is employed as both the BE and the structural material, which is expected to minimize losses.
3.3 Prospects and challenges for laterally actuated piezoelectric MEMS

Table 2 summarizes the strengths and weaknesses of piezoelectric actuation for both in-plane and out-of-plane motion and sensing. Piezoelectric in-plane sensing and actuation are beneficial for MEMS due to several factors. The large actuation range is desirable, as, for instance, it can improve the isolation of microswitches [67]. Power consumption for piezoMEMS can vary depending on the specific application and operating conditions and is lower for sensing applications, as it involves converting mechanical stimuli (e.g., vibration, pressure) into electrical signals. Actuation speed denotes the rate at which a device or component can respond and achieve a desired motion or displacement upon receiving an actuation signal. The response time of piezoMEMS is typically microseconds or nanoseconds, enabling fast and precise control.

Table 2. Strengths and weaknesses of piezoelectric actuation mechanism

<table>
<thead>
<tr>
<th>Strengths</th>
<th>Weaknesses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Large electromechanical coupling [10];</td>
<td>Static amplitude depends on the quality and piezocoefficient of the piezoelectric material [71];</td>
</tr>
<tr>
<td>Low voltage drive (~1V), high force [68];</td>
<td>Fabrication challenges for elements that implement pure in-plane motion [H];</td>
</tr>
<tr>
<td>Fast response [51], [69];</td>
<td>Low Q value for resonating devices [10].</td>
</tr>
<tr>
<td>Devices are smaller, but have the same sensitivity and performance as available on the market analogues [V];</td>
<td></td>
</tr>
<tr>
<td>3D motion possibility within a single MEMS element [V];</td>
<td></td>
</tr>
<tr>
<td>Large displacement is possible [68];</td>
<td></td>
</tr>
<tr>
<td>Can be used for self-powering [70].</td>
<td></td>
</tr>
</tbody>
</table>

Piezoelectric MEMS have been criticized because of their non-linear response and hysteresis due to the ferroelectric nature of many pioneering piezoelectric materials, such as perovskite-type PZT, LiNbO₃, barium titanate (BaTiO₃), and polymeric polyvinylidene fluoride (PVDF) [70, 71]. Another concern for the microfabrication of piezoelectric devices is the Curie temperature, which is very low for many ferroelectrics and is a challenge for high-temperature processes, such as bonding. With the development of wurtzite semiconductor piezoelectrics such as ZnO, AlN and Sc-doped AlN (Al₁₋ₓScₓN), this problem is no longer a concern, as the wurtzite piezoelectrics have a linear response (despite the partial ferroelectricity in Al₁₋ₓScₓN [72, 73]). Additionally, the Curie point of wurtzite piezoelectrics is much higher than that of perovskites.

In certain areas, the application of piezoMEMS is more favourable, for example, in microrobotics, due to their potential to significantly enhance appendage speed and their ability to generate high forces [68]. Moreover, piezoMEMS have moderate voltage demands [68] and the ability to recover a substantial amount of stored electrical energy through charge recovery techniques [56, 74].

At the same time, piezoMEMS are still under development, and the deposition of piezoelectric materials on the sidewalls brings several challenges to the fabrication process shown in Figure 3.11. First, the formation of structures with developed morphology requires a reliable process that provides low surface
roughness of vertical surfaces designed for piezoelectric thin film deposition. Second, the deposition of the piezoelectric thin films on the vertical surfaces itself is a complicated process. The crystal orientation and quality of the thin films play a major role, as they determine the total displacement that can be achieved in actuators, the signal's strength and the sensors' sensitivity. Finally, the electrical connection to the sidewalls should be provided over a complicated configuration – from the lateral plane to the vertical surface of the device.

### Pure laterally-actuated piezoelectric MEMS fabrication challenges

<table>
<thead>
<tr>
<th>Surface preparation</th>
<th>Materials</th>
<th>3D structures patterning</th>
<th>Electrical connection</th>
</tr>
</thead>
</table>
| - High surface roughness of non-planar surfaces | - Deposition on vertical surfaces  
- ARV needs to be axis oriented for the local performance  
- Conformal coverage of the surfaces is needed  
- Defined rear | - Use of special PRs  
- Complex removal process for PR  
- Not that quick as a standard lithography process | - Complicated electrical routing from the lateral planes to the vertical surfaces  
- Limited options for successful conductive materials deposition |

**Figure 3.11** Fabrication challenges for pure laterally actuated piezoelectric MEMS.
4. Next-generation piezoelectric MEMS

4.1 Concept of multiaxial motion in piezoelectric MEMS

Three-dimensional motion can be achieved in MEMS devices via piezoelectric thin films deposited on both vertical and lateral surfaces of the suspended structure, as shown in Figure 4.1 a. Thus, the Si cantilever achieves out-of-plane motion when voltage is applied between the top surface transducer, and in-plane motion is possible when voltage is applied between the vertical surface transducer. Such 3D piezoMEMS can be used for vibration energy harvesting in multiple directions [75], for assembly of tribology-inspired microrobots [6], scanning MEMS micromirrors [76] or stand-alone gyroscopes [V] [77].

Lateral motion is one of the components of 3D motion. As discussed in Section 3.1, pure piezoelectric in-plane motion in MEMS can be engineered by placing piezoelectric thin films and linked electrodes on the vertical surfaces of the actuated structure. Table 3 summarizes data from various studies investigating the deposition of piezoelectric materials on vertical surfaces. Currently, the deposition process of piezoelectric materials on the sidewalls has been demonstrated mostly for AlN and PZT thin films. Primarily, these materials are deposited by physical vapour deposition (PVD) [78-83] or MOCVD [84, 85], [II], [III] and less often by atomic layer deposition (ALD) [86-87], [IV]. Some works [60-61] have demonstrated PZT deposition by sol-gel.

PVD provides good compatibility with BE materials, as it requires relatively low deposition temperatures. For example, AlN with a decent c-axis orientation can be sputter-deposited with temperatures ranging from 300 to 450°C [88-91], although higher temperatures increase the quality of the films due to higher adatom mobility. Thus, Mo and Pt [78-83] have been used as BEs for sputtered sidewall AlN films, and Pt was used as a BE for PZT films [62]. PZT polarity can be manually adjusted by poling, but in the case of deposition on sidewalls, every sidewall of the device should be poled separately. Poling of one sidewall might take up to 10 minutes [62], making this process time consuming and high-yield challenging.
ALD has thus far rarely been used for piezomaterial deposition on vertical surfaces, even though it provides good conformality and can expand the number of BE materials due to low deposition temperatures. Only weak c-axis orientation has been previously confirmed for both ALD AlN deposited on the vertical Si sidewalls [IV] and for planar ALD AlN on blank Si substrates [92-93]. PZT thin films are difficult for ALD deposition in general because of the limited thermal stability of Pb-precursors [87].

Comparing piezoelectric properties, PZT has much larger piezoelectric coefficients than AlN. The transverse piezoelectric coefficient $e_{31}$ is 1.05 C/m² for AlN and 14-23 C/m² for PZT, $e_{33}$ is 1.55 C/m² for AlN and 8 C/m² for PZT, and the piezoelectric strain coefficient $d_{33}$ is 5 pC/N for AlN and 593 pC/N for PZT [59]. However, PZT contains lead, which restricts its use. Therefore, in this dissertation, AlN was chosen for integration in piezoMEMS due to its non-toxicity, CMOS compatibility and possibility of growing high-quality c-axis oriented thin films on vertical Si surfaces.
Table 3. Reported data on piezoelectric materials deposited on vertical surfaces

<table>
<thead>
<tr>
<th>Deposition method</th>
<th>Reference, year of publication</th>
<th>Height/depth of the vertical surface</th>
<th>AlN thickness on the sidewalls</th>
<th>Electrodes material/Substrate type</th>
<th>Orientation, XRC FWHM around 0002</th>
<th>Device type or content of the paper</th>
</tr>
</thead>
<tbody>
<tr>
<td>R Tabrizian et al. [78-80], 2011</td>
<td>20 μm</td>
<td>220 nm (1) 458 nm (2) 360 nm (3)</td>
<td>TE/BE: Mo</td>
<td>XRC FWHM around 0002: 1.65° (1) and 1.93° (2). Grains are tilted to the sidewall surface normal: 38° (1) and 30° (2)</td>
<td>Laterally-excited bulk acoustic resonator</td>
<td></td>
</tr>
<tr>
<td>M. Ramezani et al. [81-83], 2017 - 2020</td>
<td>20 μm</td>
<td>Vertical surfaces formed by (111) planes in Si (110) wafer</td>
<td>BE: ALD Pt and sputter deposited Mo</td>
<td>c-axis of AlN are normal to vertical Si (111) planes</td>
<td>Fin bulk acoustic wave resonators (FinBARs)</td>
<td></td>
</tr>
<tr>
<td>E. Österlund et al. [84], 2020</td>
<td>100 μm, aspect ratio 1:1</td>
<td>Vertical surfaces formed by (111) planes in Si (110) wafer</td>
<td>TE: TIN BE: Si ++</td>
<td>c-axis of AlN are normal to vertical Si (111) planes</td>
<td>Optimization of AlN deposition on vertical surfaces for MEMS application</td>
<td></td>
</tr>
<tr>
<td>K. Bespalova et al. [II], 2023</td>
<td>50 μm</td>
<td>Vertical surfaces formed by (111) planes in Si (110) wafer</td>
<td>BE: Al, Al/AIN, Pt/Cr/AIN</td>
<td>Films are crystalline but lacking c-axis orientation</td>
<td>Optimization of AlN deposition on vertical surfaces for MEMS application</td>
<td></td>
</tr>
<tr>
<td>K. Bespalova et al. [III], 2023</td>
<td>50–200 μm</td>
<td>1 μm</td>
<td>c-axis of AlN are normal to the deposition plane</td>
<td>Optimization of AlN deposition on vertical surfaces for MEMS application</td>
<td></td>
<td></td>
</tr>
<tr>
<td>E. Österlund et al. [IV], 2021</td>
<td>100 μm, 1:1</td>
<td>Varies over the vertical surface from 100 to 126 nm</td>
<td>BE: Al, Al/AIN, Pt/Cr/AIN</td>
<td>Optimization of AlN deposition on vertical surfaces for MEMS application</td>
<td></td>
<td></td>
</tr>
<tr>
<td>X. Liu et al. [86], 2004</td>
<td>5.1 μm from SEM bar, 35:1</td>
<td>Varies over the vertical surface from 16.5 to 23.2 nm</td>
<td>Si</td>
<td>Optimization of AlN deposition on vertical high AR structures</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Growth method</th>
<th>Reference, year of publication</th>
<th>Height/depth of the vertical surface</th>
<th>Thickness of the piezolayer</th>
<th>Electrodes material/Substrate type</th>
<th>Poling method</th>
<th>Device type or remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sol-gel</td>
<td>N. Wang et al. [60] and S. Youshida [61], 2013</td>
<td>18 μm, 8.1</td>
<td>2 μm</td>
<td>TE/BE: ALD Pt and Cr/Au contact pads</td>
<td>DC of 25 V for few mins</td>
<td>Laterally driven piezoelectric bimorph MEMS actuator</td>
</tr>
<tr>
<td></td>
<td>N. Wang et al. [94], 2012</td>
<td>20–50 μm</td>
<td>1–8 μm</td>
<td>TE/BE: ALD Pt</td>
<td>ND</td>
<td>Laterally driven piezo-electric switch</td>
</tr>
<tr>
<td>PVD</td>
<td>K. Kanda et al. [62], 2017</td>
<td>200 μm</td>
<td>2 and 3.4 μm</td>
<td>TE/BE: Pt</td>
<td>DC of 10 V for 10 mins</td>
<td>Piezoelectric MEMS actuator that enables motion in out-of-plane and in-plane direction depending on the shape of the beam</td>
</tr>
<tr>
<td>ALD</td>
<td>N.A. Strnad [87], 2021</td>
<td>45 μm</td>
<td>95 and 380 nm</td>
<td>Si</td>
<td>ND</td>
<td>Optimization of AlN deposition on vertical surfaces for MEMS application</td>
</tr>
</tbody>
</table>

Next-generation piezoelectric MEMS
4.2 Next-generation materials for piezoelectric MEMS

The AlN piezoresponse can be enhanced by co-doping or alloying with different elements [95]. Both terms, “doping” and “alloying”, are used in the literature to describe the incorporation of additional elements into wurtzite AlN lattice, but in this dissertation, the term “doping” is mainly used.

The possible fabrication of IV-group-III–N nitrides was initially predicted in the work by N. Takeuchi [96] in 2002 from the first-principles calculations. Later, the doping of IV-group-III–N nitrides was studied extensively in [97-99], and the research on this topic continues. In the latest work by J. Startt et al. [95], the authors conducted an extensive literature review and used density functional theory (DFT) to calculate the change in the $d_{33}$ when AlN was doped with a wide range of transition metals. As shown in Figure 4.2, the varying colour of the element panel represents the impact of the doping element on the $d_{33}$ piezoelectric coefficient of AlN. A dark violet shade indicates an enhancement in the $d_{33}$, while a blue shade indicates a reduction in the piezoresponse. The panels coloured in grey with “n/a” indicate the absence of modelling results for certain transition metals, such as Mn, Ru, Pd, Cd, La, Re and Ir. The sensitivity of AlN to certain elements was determined by quantifying the change in $d_{33}$ in relation to the concentration $x$ of the dopant. The study showed that, according to the DFT, group IV elements such as Hf, Zr and Ti increased the $d_{33}$ of AlN to 607%, 570% and 345%, respectively. The simulation results were confirmed experimentally only for Ti by measuring the piezoelectric coefficient of the co-sputtered $\text{Ti}_x\text{Al}_{1-x}\text{N}$ thin films. The measurements also showed that after $x = 0.333$, the piezoelectric coefficient begins to decrease due to the structural changes in the wurtzite lattice at higher Ti concentrations.

![Figure 4.2](image)

**Figure 4.2** The change in the $d_{33}$ when AlN is doped with a transition metal calculated using DFT. Reprinted from [95].

AlN doping by Y, Yb and Sc improves piezoelectric response significantly, from 3.11 to 20 times [95, 97], depending on the element. Altogether, doping by Sc demonstrated the highest influence on AlN piezoresponse. The positive impact of Sc doping on the piezoresponse and electromechanical coupling of AlN was confirmed experimentally, for example, in [100-102], [I]. M. Akiyama et al. [100] demonstrated up to a 500% increase in the piezoelectric coefficient $d_{33}$ for co-sputtered $\text{Al}_{0.57}\text{Sc}_{0.43}\text{N}$ in comparison to AlN films. The enhancement of the piezoelectric properties of AlN by doping is due to the replacement of Al atoms by Sc atoms in the wurtzite structure. This leads to the softening of the lattice.
and larger charge separation because of the larger ion radius and lower electronegativity (1.61 for Al versus 1.36 for Sc [103]) of Sc atoms compared to Al [100]. Al_{1-x}Sc_{x}N can be magnetron co-sputtered from Al and Sc targets at relatively low temperatures of 300–580°C [100, 104, 105], [I] or RF-sputtered from the AlSc target [106]. Recent research has revealed the possibility of the MOCVD deposition of Al_{1-x}Sc_{x}N [107-110]. The main challenge for the MOCVD deposition of Al_{1-x}Sc_{x}N is the choice of suitable Sc precursors. Most Sc precursors have low vapour pressure or include oxygen. Oxygen incorporation might affect the quality of the deposited layer by fast oxide formation, and high vapour pressure is needed to allow a relevant amount of Sc molecules to reach a substrate and be incorporated in the thin film at a certain concentration. Sc compounds with arene ligands could result in high vapour pressure, but the process of their synthesis is complicated and requires a specialized setup, making them unfeasible for industrial-scale production [107]. Thus, the potential precursors for MOCVD Al_{1-x}Sc_{x}N are scandiocene (tris(methylcyclopentadienil)Sc) or Cp_3Sc, its analogue with MeCp instead of Cp(MeCp)_3Sc, and bis-methylcyclopentadienyl-scandiumchloride ((MCp)_2ScCl). MOCVD Al_{1-x}Sc_{x}N growth with (MeCp)_3Sc was never reported due to its difficult synthetic route, while Cp_3Sc and (MCp)_2ScCl are easier to work with and commercially available. However, these precursors require heating to 150°C and 155°C, respectively, to reach a molar flow comparable to TMAl, which is typically from 10^{-5} to 10^{-6} mol min^{-1}. For these purposes, in [107] and [109], both the Sc precursor and the gas lines that connect bubblers to the reaction chamber were heated externally using an oven (or here, “were heated by an external heating element”). All the components were checked to be compatible with a temperature of 150°C. The injection system of the reaction chamber was also heated to prevent any condensation of the precursor vapours. The reported FWHM of the omega scan around the (0002) reflection was 257 arcsec (0.016°) [107] when the GaN epitaxial layer was used on a sapphire substrate for Al_{0.7}Sc_{0.3}N. MOCVD deposition of Al_{1-x}Sc_{x}N directly on Si has not yet been reported.

Large (d_{33} = 10 – 20 pm/V [111]) piezoelectric response was recently found in the orthorhombic phase of ferroelectric hafnium oxide-based (HfO_2-based) films doped by Al, Si, Gd, Sr and Zr. Despite their attractive piezoelectric properties, HfO_2-based films currently have several factors that hinder their broad integration into MEMS. CMOS-compatible ALD HfO_2-based films are amorphous and require accurate structural engineering to be crystallized in the orthorhombic phase. The crystallization can be done via rapid thermal annealing of the films after the deposition process and formation of the internal stress via capping layers with different coefficients of thermal expansion. Moreover, due to the metastable nature of the orthorhombic phase the films should not exceed 10 nm thickness, as thicker films produce excessive stress across the film [112]. An alternative to thick HfO_2-based films could be superlattices based on thin layers of doped hafnium oxide alternating with an additional non-conductive material.
5. Design and fabrication of piezoelectric MEMS

This chapter presents the results achieved in Publications [I]–[V]. The efficiency of a MEMS device can be simulated prior to the actual device fabrication to predict its performance. Simulation is crucial not only to obtain parameters at which the device can operate most efficiently but also to ascertain whether it can be competitive compared to its counterparts. Therefore, [II] and [V] cover the finite-element method (FEM) simulation of the frequency response and deflection value of the laterally moving piezoelectric actuator and the sensitivity of the piezoelectric half-tuning fork gyroscope that utilizes AlN deposited on the vertical surfaces of the Si cantilevers. In [II], the development of 3D piezoMEMS technology is considered in more detail. To demonstrate the 3D piezoMEMS technology, the fabrication of the piezoelectric actuator was introduced in [II]. The integration of AlN in the fabrication process of a laterally driven piezoelectric actuator was implemented via MOCVD on the vertical surfaces of Si cantilevers formed in the device layer of the SOI. The most important fabrication steps of the flow are discussed in detail in this chapter.

Thus, AlN deposition on the vertical Si sidewalls for piezoMEMS fabrication requires low surface roughness of the vertical surfaces. The surface quality and crystallographic orientation of the vertical sidewalls are influential for the crystal quality and orientation of AlN thin films and the device’s subsequent performance. Achieving precise etching control and minimizing defects on Si surfaces are essential to ensure device performance and functionality. Dry etching methods provide precise etching control, but achieving smooth etching profiles is challenging without optimizing the etching parameters. Additional post-etching surface-smoothing techniques can be applied to enhance the quality of Si structures, reduce roughness, and mitigate the impact of etching-induced defects. Therefore, this chapter also compares different etching techniques used in [II]–[IV] for Si vertical sidewall formation.

Further, the deposition of AlN on the vertical surfaces in Si structures was studied in [II]–[IV]. The impact of vertical Si surface roughness on the crystal quality and crystallographic orientation of MOCVD AlN was demonstrated. The conformality of MOCVD AlN thin films over the sidewall depth was also studied. The crystal quality and film conformality of ALD AlN thin films on the vertical Si surfaces were evaluated, as well as the impact of the underlying material (Si, Al, Pt).

Fabricating an actual device is impossible without electrode material, and piezoelectric materials need to interact with other materials in a system. The
interfacial and overall stability of multilayer metal/piezoelectric systems is crucial for some high-temperature processes involved in the fabrication of piezoMEMS. For example, the MEMS hermetic encapsulation process, which is necessary for achieving mechanical rigidity and providing protection from environmental influences, is typically conducted at elevated temperatures. Al-Ge eutectic bonding applied for encapsulation is conducted above 400°C, and a novel solid-liquid interdiffusion bonding technique can be used in the temperature range of 280–340°C for a minimum of one hour [113]. At such high temperatures, AlN shows a tendency to form undesirable phases on the interface with some reactive electrode materials, for example, Mo [114], Ti [114, 116] and TiN [117]. Thus, this chapter also covers AlN and Sc-doped AlN (Al1-xScxN) interactions with electrode materials and the overall stability of electrode material during high-temperature ageing and device performance.

5.1 FEM simulations of a device performance

In [II] and [V], a finite-element method (FEM) simulation in COMSOL Multiphysics was used to explore the impact of the device’s geometry on the resonance frequency and the deflection value of the piezoelectric actuator and angular rate sensitivity of the tuning-fork piezoelectric MEMS gyroscope.

The actuator consisted of a Si cantilever with AlN films deposited on its vertical sidewalls and Al serving as a top electrode (TE). An electric field was applied between the conductive Si and TE, polarizing the AlN film and initiating the motion of the actuator. An example of the 3D plot of the AlN-based actuator and its static displacement is shown in Figure 5.1.

![3D plots of laterally moving AlN-based actuator](image)

**Figure 5.1** 3D plots of laterally moving AlN-based actuator: (a) Cantilever model; (b) Static deflection at 10 V applied [II].

The results of the resonance frequency simulation for an in-plane actuator with the parameters from Table 4 are summarized in Table 5. AlN elastic-stiffness coefficients and stress-piezoelectric constant tensors were adopted from [118] and [119], respectively.
### Table 4. Design parameters [II]

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Values</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlN thickness</td>
<td>300 nm, 1 μm</td>
<td>Thickness of the piezoelectric film on the vertical surfaces of the actuator</td>
</tr>
<tr>
<td>TE (Al) thickness</td>
<td>100 nm, 300 nm</td>
<td>Thickness of the top electrodes</td>
</tr>
<tr>
<td>L</td>
<td>200 ... 1000 nm</td>
<td>Length of the actuator. Step: 100 nm</td>
</tr>
<tr>
<td>w</td>
<td>20, 30, 40, 50 μm</td>
<td>Width of the actuator</td>
</tr>
<tr>
<td>h</td>
<td>50 μm</td>
<td>Height of the actuator, thickness of the device layer</td>
</tr>
</tbody>
</table>

The simulated resonance frequency for the piezoelectric actuators with 300 nm thick AlN films on the sidewalls is in the range of 0.024–1.694 MHz, and for 1 μm thick AlN, it is 0.028–1.800 MHz. Figure 5.2 demonstrates the simulated impedance for a 40 μm wide and 400 μm long actuator.

### Table 5. Simulated values of resonance frequency for actuators with varying lengths and widths [II]

<table>
<thead>
<tr>
<th>Length, nm</th>
<th>Width, μm</th>
<th>Resonance frequency fr, MHz</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AlN = 300 nm, TE = 100 nm</td>
<td>AlN = 1 μm, TE = 300 nm</td>
</tr>
<tr>
<td>200–1100</td>
<td>20</td>
<td>0.024–0.732</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>0.035–1.063</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>0.047–1.385</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.058–1.694</td>
</tr>
</tbody>
</table>

**Figure 5.2.** Simulated displacement along x-axis and impedance of the piezoelectric actuator.

The displacement in-plane direction for the actuator with varying lengths and widths is shown in Figure 5.3. The displacement out-of-plane direction was also simulated, although it is almost 70 times smaller than for in-plane direction and can be neglected. The deflection value of the actuator was simulated with a drive voltage of $V = 10$ V at the resonance frequency.
Thus, the maximum displacement value that a single actuator can achieve strongly depends on the geometry of the Si cantilever, the thickness of AlN and TE layers, and the applied voltage. Longer cantilevers result in greater displacement capability. An increase in the width of the Si cantilever leads to an increase in its stiffness. Thicker cantilevers are more resistant to bending, which results in a reduction of the maximum displacement attainable. Increasing the thickness of the AlN and TE films also contributes to an increased actuator width. Increasing the actuator’s height increases the AlN layer’s surface area, so there is more piezoelectric material to polarize, which results in a higher deflection value. Overall, the maximum deflection value in-plane direction for a 40×50×900 μm (w×h×L) actuator with 300 nm thick AlN piezoelectric layer and 100 nm thick Al electrodes on the vertical sidewalls is 7 nm/V. This value is lower than that demonstrated by PZT-based actuators [60-62]. Nevertheless, overall deflection might increase if the cantilever’s width decreases and its height increases.

In [V], FEM simulation was carried out on a gyroscope with AlN thin films deposited on the vertical sidewalls of a half-tuning fork structure, as demonstrated in Figure 5.4. The analysis includes an eigenfrequency study, sensitivity analysis and optimization. The geometry parameters of the gyroscope are listed in Table 6. The required operational frequencies for the non-optimized gyroscope parameters were 149.05 kHz and 256.74 kHz for the drive and sense modes, respectively. The initial model of the proposed gyroscope reached 0.013 mV/dps sensitivity. The surface area of a non-optimized gyroscope was 0.0846 mm².
Figure 5.4 The structure of the half-fork MEMS vibratory gyroscope [V].

Table 6. Simulated values of resonance frequency for actuators with varying lengths and widths [II]

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Value [μm], not optimized</th>
<th>Value [μm], optimized</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height of the cantilever</td>
<td>50</td>
<td>28</td>
</tr>
<tr>
<td>Width of the cantilever</td>
<td>20</td>
<td>24</td>
</tr>
<tr>
<td>Length of the cantilever</td>
<td>400</td>
<td>400</td>
</tr>
<tr>
<td>AlN thickness</td>
<td>0.3</td>
<td>0.6</td>
</tr>
<tr>
<td>Thickness of Al electrodes</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Width of the fixed end</td>
<td>35</td>
<td>35</td>
</tr>
<tr>
<td>Length between the fixed end and the fork base</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Length of the fork base</td>
<td>25</td>
<td>25</td>
</tr>
<tr>
<td>Width of the fork base</td>
<td>160</td>
<td>160</td>
</tr>
</tbody>
</table>

Angular rate sensitivity

0.013 mV/dps

1.2 mV/dps

The following parameters were selected for the optimization: AlN thickness, cantilever height and cantilever width. The optimization was done by sweeping the parameters’ values in a specific range and obtaining resonance frequency for every gyroscope’s geometry.

Figure 5.5 Comparison of the simulated angular rate sensitivity of the half-fork MEMS gyroscope before and after optimization of the gyroscope’s geometry with existing MEMS devices. The picture is adopted from [V].

39
The gyroscope’s sensitivity strongly depends on the cantilever’s geometry and might vary from 0.00125 mV/dps to 1.21 mV/dps. The computed r-Pearson coefficient suggests that the height of the gyroscope is the parameter most strongly correlated with the gyroscope’s output. As shown in Figure 5.5, the sensitivity of the proposed gyroscope after optimizing geometric parameters is comparable to the sensitivity of gyroscopes available on the market, such as ADXRS645 from Analog Devices.

5.2 In-plane piezoelectric actuator fabrication

Figure 5.6 illustrates the fabrication flow of the in-plane piezoelectric actuator that utilizes AlN thin films deposited on vertical surfaces of the Si cantilever for actuation. An SOI wafer was used as a starting substrate for the fabrication. The device layer of SOI was 50 μm thick, highly doped Si with a crystallographic orientation (110). In Si (110), the vertical surfaces are Si (111) planes that have a lower lattice mismatch with AlN than other Si planes, contributing to the higher crystal quality of AlN films. The cantilevers formed in the device layer had varying geometrical parameters 20–50 μm thick and 200–1100 μm long.

A thick 1 μm SiO₂ layer was formed on the device layer and the handle wafer of SOI by wet thermal oxidation and used as a hard mask for the subsequent Si etching. SiO₂ was patterned by standard photolithography methods and etched in buffered oxide etch (BHF), providing access to the underlying structural material. Si cantilevers and, consequently, vertical surfaces can be formed using dry or wet etching methods. Potassium hydroxide (KOH), ammonium hydroxide (NH₄OH) and tetramethylammonium hydroxide (TMAH) are commonly employed for anisotropic plane-dependent etching of Si, resulting in well-defined crystallographic planes. Dry etching involves the removal of Si material through physical or chemical processes in a gaseous or plasma environment. In reactive ion etching (RIE), the etching mechanisms involve the chemical reactions occurring on the exposed surfaces, resulting in the formation of volatile byproducts and physical ion bombardment, which enhances both the etch rate and directionality.

For the fabrication of piezoelectric in-plane actuators, a cavity-first approach was applied. The main idea of this approach was to form the body of a cantilever prior to thin film deposition, while conventional fabrication paths operate with thin films deposited on planar surfaces, followed by cavity etching and element release. The cavity-first fabrication sequence allows access to the vertical sidewalls of the cantilever and depositing the films directly on them. Two versions of the fabrication process were used. In the first, the cavities in the device layer of SOI were defined by wet etchants (KOH and TMAH). In the second fabrication process version, dry etching was applied.

Wet etching allows for atomically smooth sidewalls, while dry etching offers better control over etching parameters and enables the fast fabrication of small-size features and high-aspect-ratio structures. Figure 5.7 shows SEM micrographs of Si (110) etching profiles and the surface quality of the vertical sidewalls.
achieved using different etching methods. Deep reactive ion etching (DRIE) using the Bosch process results in straight, 90° to the cavity bottom, vertical sidewalls. However, it causes scallop formation because of the alternating etching and passivation cycles. The dry etching in cryogenic mode in inductively coupled plasma RIE (ICP-RIE), as shown in Figure 5.7 d–e, provides fast etching rates but might result in a non-ideal shape of the etching profile and defect formation on the sidewalls. Despite the low surface roughness of the vertical walls that can be achieved, one needs to consider the underetching and slanted planes forming in Si when designing a fabrication flow that incorporates wet etching methods.

The difference in surface roughness between these methods can be evaluated with the help of atomic force microscopy (AFM). In Figure 5.8, AFM scans of the vertical Si surfaces demonstrate differences in the roughness of the walls achieved with different etching methods. The roughness value of a topography is quantitatively analyzed using the root mean square (RMS) of the surface height deviation in the scanned area.
AlN deposition on the vertical sidewalls followed cantilever formation in the SOI. PVD remains the directional line-of-sight method, and the conformality of the films on the vertical sidewalls is greatly affected by the aspect ratio of the structures and substrate tilt towards the target during deposition. The tilt of the wafer during sputtering can lead to the growth of inclined grains and, subsequently, the poor performance of AlN-based devices. As previously demonstrated [78-83], PVD AlN films had a tilt from 30° to 53° to the sidewall surface, while needing to be normal to the surface for the higher device output. MOCVD provides the best crystal quality of the deposited films when compared to ALD and PVD. Therefore, MOCVD AlN was chosen for the integration into the fabrication process. However, MOCVD requires high temperatures (>1000°C) for AlN deposition. High deposition temperature limits the choice of materials that can be used in such devices as a bottom electrode (BE). Some conductive thin films have a much lower melting point than 1000°C (Al) or are prone to defect formation at this temperature (Al, AlSi, Pt) [1, 120]. Also, high temperatures can speed up the formation of undesirable phases on the electrode/piezoelectric material interface [114, 116]. Hence, the device layer of SOI was highly doped to be used as a BE and structural material simultaneously.
Top electrode material deposition (TE) follows AlN deposition. TE should provide an uninterrupted electrical connection between the vertical sidewall and a planar contact pad. ALD TiN was used as a TE for actuator fabrication, as TiN is a conductive material, and ALD provides the best uniform coverage of 3D structures compared to other deposition methods. For proper actuator functioning, the TEs located on opposite sidewalls of the Si cantilever must be isolated from each other. Therefore, the so-called Si bridge separated the two cantilevers from each other during their formation in the device layer and provided insulation between the future electrodes on the opposite sides of the actuator. The location of the so-called Si bridge area is shown in Figures 5.6 g and h. Thus, it was removed after TiN deposition, providing separation of the TEs on the left and right vertical sidewalls of the actuator.

![Figure 5.8](image1.png)

**Figure 5.8** Comparison of the roughness of surfaces achieved using different etching methods. Adapted from [III]

![Figure 5.9](image2.png)

**Figure 5.9** An example of piezoelectric actuator. The cavity formation was implemented using the dry etching method. Adopted from [II] and [IV].
Once the Si bridge was removed, the TEVs and the underlying AlN layer were patterned and etched to provide access to the Si BE. The cantilevers were released through the handle wafer DRIE from the backside of the SOI. Figure 5.10 demonstrates the final look of the devices that were fabricated using wet etching. The formation of characteristic slanted Si (111) planes in wet etchants was considered during the device design, allowing the same set of masks to be used, despite an etching method for cavity formation.

![Figure 5.10](image)

Figure 5.10: An example of piezoelectric actuator design that utilizes wet etching for cavity formation. Slanted sidewalls are visible in the corners of the cavities.

### 5.3 Surface quality

In [II], the piezoelectric cantilevers were fabricated in the device layer of SOI using KOH 40 wt% aqueous solution heated to 70°C. The etching parameters, such as temperature and solution concentration, were adopted from [84], as these parameters yielded the lowest surface roughness (2.0 nm) of vertical Si (111) planes that are formed in the Si (110) substrate during the wet etching in KOH. The subsequent MOCVD deposition of AlN on Si cantilevers resulted in a strong c-axis orientation of AlN perpendicular to the surface of the vertical sidewalls. Another set of wafers was etched in the cryogenic mode of ICP-RIE using SF$_6$/O$_2$ plasma. The vertical surfaces of the cantilevers were oriented parallel to the Si (111) planes in the Si (110) substrate. The etching recipe for ICP-RIE was optimized for an etching rate of Si equal to 1.8 μm/min. As expected, the vertical surfaces of Si achieved by ICP-RIE had a high Rq (192.5 nm). Also, the fast etching rate resulted in the bowing of the sidewall profiles, which may indicate inadequate sidewall passivation and/or ion scattering [121]. As demonstrated in [II] and [III], the rough surface of the vertical sidewalls affected the growth direction of AlN significantly. The films maintained a c-axis texture, but the growth direction of AlN and, therefore, its [0001] direction was perpendicular to the surface of the Si sidewall at every location. An applied electric field should be aligned parallel to AlN’s c-axis for the electromechanical coupling’s maximum efficiency. Thus, the films deposited on such rough vertical surfaces would likely result in the fabrication of moderate efficiency MEMS.
Si etching in KOH resulted in the formation of smooth vertical surfaces suitable for c-axis-oriented textured AlN film growth. Nevertheless, KOH cannot be considered an optimum etching solution for MEMS. KOH is not CMOS compatible due to its alkali metal potassium (K⁺) ions [122, 123]. Therefore, in [III], a CMOS-compatible 25% TMAH solution was used to form vertical sidewalls in Si. Vertical surfaces of Si achieved with TMAH etching had a low surface roughness of 4.62 nm. However, the surface had pronounced hexagonal defects – etching pits. Such defects might form in Si during wet etching because of dislocations in Si or etchant contamination by metal particles [124, 125]. AlN deposited on the vertical surfaces of Si cantilevers formed by TMAH etching was highly c-axis oriented. However, the film had pronounced defects that might be caused by etch pits. Further details regarding the growth of AlN on vertical surfaces are discussed in Section 5.3.

A few solutions were introduced to bridge the gap between the dry and wet etching and incorporate the best of both worlds. One was Si surface treatment by wet etchant after the dry etching process. Post-dry etching treatment of Si by ethylenediamine pyrocatechol water solution [126], a mixture of HNO₃:BHF:H₂O [127], or HNO₃:HF:CH₃COOH [128], HF:HNO₃:NH₄F [128], KOH/C₃H₈O [130] and TMAH [131], have been applied previously. The results of these works demonstrate that the effect depends on the combination of the pair etchant-surface morphology. Removing nanometre-scale defects of the Si surface can be achieved with TMAH treatment [131]. In [III], a combination of ICP-RIE etching followed by rapid wet etching in TMAH was tested as a smoothing method for surfaces with high surface roughness. The greatest reduction in the surface roughness value was observed for the samples treated in TMAH for 5 minutes, as shown in Table 7. The surface roughness value was reduced by 33–54% depending on the initial roughness of the sample. However, even after the treatment, the surface roughness remained high, and such a method is ineffective for smoothing high-roughness surfaces for AlN deposition.

Table 7. Surface roughness of the vertical sidewalls achieved with a combination of dry and wet etching in TMAH 25% at 85°C [III]

<table>
<thead>
<tr>
<th>Rq of sidewalls, nm</th>
<th>Mins in TMAH 25%, min</th>
<th>Rq after TMAH, nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>217</td>
<td>2</td>
<td>127</td>
</tr>
<tr>
<td>157</td>
<td>5</td>
<td>104</td>
</tr>
<tr>
<td>241</td>
<td>5</td>
<td>109</td>
</tr>
<tr>
<td>159</td>
<td>10</td>
<td>145</td>
</tr>
</tbody>
</table>

Another method of Si surface post-etching treatment is surface structure reordering through the increase in mobility of Si atoms at a high temperature (HT) under vacuum [132] or in a hydrogen (H₂) or argon (Ar) gas environment. However, annealing in H₂ seems to be the most attractive option. The annealing in a vacuum is known to form atomic steps in the Si surface [133], while Ar demands higher temperatures than H₂ to achieve the same smoothing effect. During thermal annealing, Si atoms migrate and smooth out the surface roughness to minimize the overall surface energy. Annealing in a gas environment proved to be efficient in surface roughness smoothing at the atomic level for Si [134] and glass [135]. The effective annealing temperature is reported to be in the range of 800–1230°C [134], but at the same time, the roughness is affected by
the gas flow and the ambient pressure. The crystal orientation of Si also seems to play a role [133, 136], however, it is not entirely clear yet in what direction Si is “easier to smooth”. The transformation of the etching profile after annealing in hydrogen has also been demonstrated previously [132, 137] after Si annealing in H₂.

In [II] and [III], prior to AlN deposition, all wafers were annealed for 5 min in H₂ at 972–986°C (300 mbar). The changes in the etching profile were not noticed, and the structure had relatively sharp edges in contrast to previous works [132, 137], as shown in Figure 5.11. Therefore, the effect of annealing on the etching profile might not be noticeable at SEM.

Figure 5.11 Top and bottom of Si cantilever formed in device layer of SOI using (a) ICP-RIE; and (b) KOH. Both annealed at 1025°C for 5 min in H₂ gas environment prior to AlN deposition.

5.4 AlN crystal quality, microstructure and uniformity on the vertical sidewalls

In [II] and [III], AlN growth was conducted in a close-coupled showerhead MOCVD reactor. The growth process in MOCVD is based on the chemical reactions of organometallic compounds in a vapour phase and gas precursors that occur inside the reaction chamber on the substrate’s surface. At the beginning of AlN growth, the substrate underwent a two-step annealing process: for 5 min in H₂ and then for 10 min in di-silane (Si₂H₆) flow at 1025°C and 300 mbar reactor pressure. The annealing in H₂ is needed to remove native oxide from the Si surface [138] and lower its roughness on the sidewalls of patterned wafers, as discussed in Section 5.3. The annealing at Si₂H₆ is used to passivate the bare Si surface and help prevent substrate roughening. A nitridation step follows the annealing. The nitridation was done under ammonia (NH₃) flow for 15 s at 100 mbar and a substrate temperature of 980°C. Trimethylaluminum (TMAI) and
ammonia (NH₃) were used as sources for aluminium and nitrogen, respectively. First, a thin low-temperature (LT) AlN layer was deposited at 980°C. HT AlN was grown at 1085°C substrate temperature with H₂ carrier gas. The growth time of HT AlN was 7000 s and corresponded to the 807–973 nm film thickness when the same recipe was used on planar Si (111). High-resolution X-ray diffraction (HRXRD) symmetrical scan shows that no reflections besides (0002) were found for AlN films deposited on planar substrates. FWHM of the XRC around (0002) reflection was 0.445° in [II], showing that films are textured and c-axis oriented. The results of the HRXRD are summarized in Table 8.

<table>
<thead>
<tr>
<th>Growth time, s</th>
<th>Thickness, nm</th>
<th>(\theta)-ω AlN (0002), (\theta) (°)</th>
<th>(\Omega) (°)</th>
<th>FWHM (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1860</td>
<td>300</td>
<td>36.1</td>
<td>18.02</td>
<td>1.320</td>
</tr>
<tr>
<td>3600</td>
<td>500</td>
<td>36.1</td>
<td>18.17</td>
<td>0.470</td>
</tr>
<tr>
<td>7000</td>
<td>1000</td>
<td>35.8</td>
<td>17.92</td>
<td>0.445</td>
</tr>
</tbody>
</table>

Figure 5.12 shows AlN film deposited on top of a Si cantilever formed in a device layer of the SOI. The crystal orientation of AlN on the sidewalls of the cantilever with respect to the crystal orientation of Si is shown in Figure 5.12 b.

![Figure 5.12](image)

With the help of SEM and energy dispersive X-ray analysis (EDX), it was shown that AlN covered Si cantilevers entirely from the top to the bottom of the cantilevers, as shown in Figure 5.13. The thickness uniformity of the films along the sidewall depth was measured using SEM. The sample was cleaved along the sidewall and ion-polished using a focused ion beam (FIB). The approximate thickness gradient was 4 nm/μm. However, the thickness gradient was non-linear in some areas on the wall, as shown in Figure 5.14. The reactor’s size likely affects the film’s thickness over the sidewall. Thus, the AlN thickness gradient along a 100 μm deep sidewall was 0.8 nm/μm [84] when the films were grown in a smaller reactor chamber. Smaller reactors provide a more controllable deposition process regarding temperature distribution and gas flow. Minor defects were also observed in AlN grown on Si cantilevers formed with the help of KOH (Figure 5.15), but their origin was not studied in this dissertation.
Figure 5.13 MOCVD AlN deposited on (a) KOH-etched surface and (b) ICP-RIE-etched surface. Adapted from [II].

Figure 5.14 AlN thickness gradient over the vertical sidewall.
The substrate surface roughness is known to affect the crystal quality and piezoelectric response of AlN films [12-14, 91]. For MOCVD AlN films, the correlation between AlN’s crystal quality and piezoresponse was demonstrated in [91]. The piezoelectric coefficient $d_{33}$ improved from 5.15 pmV$^{-1}$ to 5.40 pmV$^{-1}$ when the XRC of MOCVD AlN decreased from 10.7$^\circ$ to 2.5$^\circ$. A correlation between surface roughness and the quality of AlN was demonstrated in [15] for sputtered films. The smoothing of Si surface roughness from 4.5 nm to 0.18 resulted in a fivefold decrease in the FWHM of AlN, but the assessment of the piezoresponse was not implemented. A direct relationship between surface roughness and film quality is shown in [12] and [12]. Si cantilevers formed using ICP-RIE have an extremely high surface roughness (192 nm) of the vertical sidewalls. Therefore, AlN is expected to have lower crystal quality when deposited on vertical sidewalls than when deposited onto vertical surfaces formed by wet etching (KOH and TMAH).

HRXRD is a fast method for analyzing the crystal quality and orientation of thin films. However, it is challenging to implement for probing the films grown on a sidewall of a micron-scale cavity. The small scanning area and low signal hinder the HRXRD out-of-plane symmetrical $2\theta-\omega$ scan implementation. Therefore, the crystal orientation of AlN films on the sidewalls was tested via electron backscatter diffraction (EBSD). As shown in Figure 5.16, AlN deposited on the vertical surfaces of the Si cantilever formed via etching in KOH has a strong c-axis orientation normal to the Si (111) sidewall. A pole figure has two intense single poles related to the AlN planes that are located along the [0001] and [000$\bar{1}$] directions. As expected, AlN deposited on the vertical surfaces of a Si cantilever formed via etching in ICP-RIE has grains oriented in a broad range of directions. Nevertheless, it can be seen from the pole figure that many grains tend to grow around the [0001] direction.

![Figure 5.15](image-url) (a) Schematic illustration of the structure under study; SEM micrographs of AlN deposited on (b)-(c) ICP-RIE-etched Si surface and (d)-(e) KOH-etched Si surface [III].
Design and fabrication of piezoelectric MEMS

Figure 5.16 EBSD of MOCVD AlN deposited on (a) ICP-RIE-etched surface and (b) KOH-etched surface [II].

For a greater understanding of the crystal growth of MOCVD AlN on the sidewalls, TEM lamellas were prepared for samples etched using TMAH and ICP-RIE. The bright field scanning transmission electron microscope (BF-STEM) micrographs of AlN grown on vertical surfaces with different roughness values are shown in Figure 5.17. In both cases, the films have a grain height and size spread. For AlN deposited on vertical surfaces of Si obtained in TMAH, the grain size ranged from 0.93 to 1.13 μm. For similar films deposited on Si vertical surfaces achieved in ICP-RIE, the height of the grain was 0.61–0.93 μm. Moreover, the BF-STEM in Figure 5.17a shows that AlN grows over the voids in Si for the TMAH-etched samples. The voids are most probably the etching pits mentioned in Section 5.1.

Figure 5.17 BF-STEM micrographs of AlN films on vertical surfaces obtained using (a) TMAH and (b) ICP-RIE. The yellow arrow shows the location of pits at the AlN/Si interface [III].
AlN grains on both samples tend to grow normally to the Si surface in every location. Thus, when AlN grows on smooth vertical surfaces, for example, those formed using KOH or TMAH, most grains are perpendicular to the surface and parallel to each other, as schematically shown in Figure 5.18 a. However, when the surface has some distinguishable morphology, the AlN grains’ tilt follows the morphology of the substrate. This behaviour can be seen in a wider-area BF-STEM micrograph in Figure 5.18 c.

![Figure 5.18 Schematic illustration of MOCVD AlN growth on top of the (a) smooth Si surface that can be achieved with KOH or TMAH and (b) rough Si surface, which is usually a result of dry etching. (c) BF-STEM micrograph of AlN grown on sidewall of Si cavity achieved by etching in cryogenic mode in ICP-RIE.](image)

Figure 5.19 presents the corresponding select area electron diffraction (SAED) patterns for the films captured in Figure 5.17. The absence of round diffraction rings in SAED for the AlN (0002) reflections deposited on ICP-RIE etched Si indicates that the films are textured polycrystalline films with a tendency to maintain c-axis orientation. AlN (0002) reflections are not entirely aligned with the Si (111) reflections, indicating some tilt of the grains. At the same time, AlN grown on smooth vertical surfaces has crystallized with a preferred orientation in the [0001]-direction.

![Figure 5.19 SAED of MOCVD AlN deposited on (a) KOH-etched Si surface and (b) ICP-RIE-etched Si surface.](image)
Both ALD and MOCVD utilize chemical reactions for deposition, but ALD utilizes surface-limiting reactions. Separating the individual reactions in an ALD process allows for much higher film thickness, density and conformality control over the developed surface. Thus, in [IV], the average thickness of the AlN film was 124 nm with a deviation of 14 nm, as shown in Figure 5.20. The film thickness does not decrease significantly down to the bottom of the 100 μm deep and 2.9 μm wide cavity. Although ALD provides good conformality and recent progress has revealed the c-axis orientation of plasma-enhanced ALD (PEALD) AlN films [92, 93, 138], the piezoresponse of such films is still weaker than can be achieved for MOCVD films.

![Figure 5.20 ALD AlN film deposited on vertical sidewalls of 100 μm deep and 2.9 μm wide cavity][IV].

### 5.5 Electrical connection to the sidewalls

The requirements for the top and bottom electrodes (TE and BE) differ for piezoMEMS. Both should provide an electrical connection from a sidewall to the top contact pads, but BE also needs to be a reliable substrate for the deposition of piezoelectric thin films. Considering some high-temperature steps in the fabrication process, it is crucial to evaluate how piezoelectric materials behave when interacting with different metallization materials at high temperatures. The thermal properties of AlN are well examined and can be used to evaluate whether a particular AlN/electrode system will successfully coexist in a device. The thermal properties of AlN and diverse electrode materials can be seen in Table 9, as well as the electrical conductivity of conductive materials. Overall, a low lattice and coefficient of thermal expansion (CTE) mismatch are desired because both are sources of stress and defects for a deposited film. In [II] and [III], highly doped Si (resistivity ρ<0.005 Ω-cm) was used as a BE material for MOCVD AlN deposition, although the Si (111) surface has a more considerable lattice mismatch with AlN.
Table 9. Thermal properties and electrical conductivity of substrate materials and their lattice mismatch with AlN

<table>
<thead>
<tr>
<th>Material</th>
<th>AlN</th>
<th>Si (111) plane</th>
<th>Mo(111)</th>
<th>Pt (111)</th>
<th>Ti (111)</th>
<th>Al (111)</th>
<th>TiN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice mismatch, ~%</td>
<td>-</td>
<td>19</td>
<td>14</td>
<td>19</td>
<td>18</td>
<td>15</td>
<td>10.2</td>
</tr>
<tr>
<td>CTE, K⁻¹</td>
<td>5.27 x 10⁻⁶</td>
<td>2.6 x 10⁻⁶</td>
<td>5.1 x 10⁻⁶</td>
<td>8.8 x 10⁻⁶</td>
<td>8.6 x 10⁻⁶</td>
<td>23 x 10⁻⁶</td>
<td>9 x 10⁻⁶</td>
</tr>
<tr>
<td>Melting point</td>
<td>3000</td>
<td>1412</td>
<td>2623</td>
<td>1768</td>
<td>1668</td>
<td>660</td>
<td>2930</td>
</tr>
<tr>
<td>Electrical conductivity, S/m</td>
<td>1.6 x 10⁻³*</td>
<td>1.9 x 10⁻⁷</td>
<td>9.4 x 10⁻⁶</td>
<td>1.8 x 10⁻⁸</td>
<td>3.5 x 10⁻⁷</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

*- depends on the doping level.

It has been demonstrated that AlN is prone to new phase formation on the interface with Ti [114, 116] and TiN [117, 140]. AlN forms Al₃Ti and Ti₂N on the interface with Ti after one hour of annealing at 600°C [114]. Ti was used as a BE for sputter-deposited AlN in [141]. The authors reported a strong impact of the Ti underlayer on the degree of c-axis orientation for AlN film and its piezoresponse. Thus, a smooth (RMS <10 nm) surface is a requirement for high piezoelectric coefficients of AlN. The piezoelectric coefficient d₃₃ of AlN decreases from 2.55 to 1.7 pmV⁻¹ when increasing the Ti sputter pressure and thus increasing the RMS of Ti from 0.2 to 9 nm.

ALD-deposited TiN was used as a TE in [II]. The average sheet resistance over the wafer was equal to 68 Ω·☐⁻¹. ALD TiN demonstrated great conformity when deposited over a 50 µm deep cantilever with AlN on top of the cantilever. The contact pad to the sidewall electrical connection was tested by measuring the I–V curve of the material. No new phase formation on the interface with AlN has been verified via HRXRD or during observation in SEM. The motion test conducted to evaluate the performance of the piezoactuator demonstrated the unexpected behaviour of the device. The registered motion of the actuator was much larger than the simulated motion. Thus, the ALD TiN-AlN interaction was suspected to be one of the possible reasons for unpredictable motion of the device. Consequently, ALD TiN might not be the best option for piezoMEMS applications, and other BE materials should be considered.

In [I], Al, Mo, AlSi (Si concentration was 1%) and Mo/Al were tested as TE material in a multilayer system containing Al₀.₈Sc₀.₂N and AlN. All films were sputter-deposited. An example of the multilayer system under study with Al TE is shown in Figure 5.17. The structure underwent thermal ageing at 100–1000°C under a vacuum atmosphere from 30 min to 100 h.
Mo demonstrated good stability and perfect electrical connection for piezo-driving applications, as neither TE nor BE formed any phases on the interface with Al$_{0.8}$Sc$_{0.2}$N or underlying AlN thin films, even after 100 h of annealing at 1000°C. It is noteworthy that other materials tested as TE did not reveal any phase formation on the interface with Al$_{0.8}$Sc$_{0.2}$N either. However, Al, AlSi and Mo/Al formed hillocks on the surface. Hillock formation is a common phenomenon observed in thin films because of stress relaxation when a film and a substrate have different CTE [142, 143]. Al and AlSi are more prone to hillock formation on their surfaces even after annealing for 30 min at the lowest temperatures (100°C). The growth of hillocks drastically increased the $R_q$ of Al and AlSi films. Al was also found to form microfractures and voids after annealing. The depth of the microfractures in some locations was equal to the Al film thickness. This indicates that in certain areas, microfractures extended through the entire thickness of Al, exposing the underlying piezoelectric material. Al capping by Mo suppressed hillock growth until the annealing temperature was equal to 450°C.

No hillock or void formation was noticed for Mo TE up to 1000°C. It was possible to measure the transverse piezoelectric coefficient $e_{31,f}$ of Al$_{0.8}$Sc$_{0.2}$N using Mo electrodes annealed at 800°C for 300 h. Only after 100 h annealing at 1000°C, Mo surface covered by hillocks and piezoresponse measurements were no longer implemented. Mo as a BE was also utilized in previous works [144-146] for AlN and Al$_{1-x}$Sc$_x$N driving applications. However, in most of these works, PVD deposition was employed at relatively low temperatures or 300–450°C, and electrode stability was not tested. Mo was successfully used as a BE for MOCVD AlN deposition in [114, 147, 148]. In [148], a high deposition temperature of AlN affected the resistivity of Mo films. Thus, the growth temperature of AlN decreased from 1050°C to 950°C, resulting in Mo resistivity from $8 \times 10^{-5}$ Ωcm to $4 \times 10^{-5}$ Ωcm while compromising AlN crystal quality. In [114], the increase in Mo resistivity from 12.3 μΩcm to 26.4 μΩcm was explained by molybdenum nitride formation during the nitridation step prior to AlN deposition in the MOCVD reactor. The authors claimed that Mo resistivity was improved by reducing NH$_3$ flow. However, the improved resistivity value of Mo
was not specified. In [149], Mo was sputter deposited on top of the AlN seed layer following MOCVD AlN deposition. Mo delaminated during AlN growth when the reactor temperature reached 400°C. Among possible reasons for the delamination were the poor adhesion of Mo to the AlN seed layer and the quality of the Mo film itself. Mo is a good candidate for electrode materials.

Figure 5.18 (a) SEM micrographs of Al, AlSi, Mo and Mo/Al surface after annealing for 30 min at different temperatures; (b) Surface roughness of the electrode films after annealing for 30 min at different temperatures; (c) Mo surface after annealing at 1000°C for 100 h [I].

In [IV], the influence of underlying Al, Al/AlN, Pt/Cr/AlN and Si on the quality of ALD AlN was studied. It was found that the films deposited on top of the Al layer with (111) texture demonstrated the best crystal quality. The AlN layers on Si or Al/AlN and Pt/Cr/AlN without preferential orientation had no mosaic structure and were only weakly (0002) oriented. The measured piezoelectric coefficient of ALD AlN on Al was $e_{31, \tau} = -0.38^\circ\text{C/m}^2$, which is likely not efficient enough for piezoMEMS applications. However, the influence of the underlying metal films on the quality of ALD AlN holds potential significance for the future development of 3D piezoMEMS technology. Metal films are a more favourable BE material than highly doped Si, as they have greater conductivity. The deposition of metallic films using ALD has been demonstrated previously, although most are polycrystalline with a nearly random texture [150].

Nevertheless, ALD is an attractive method for the conformal deposition of thin films over structures with developed morphology, such as Si cantilevers. Theoretically, all the thin films required for 3D piezoMEMS fabrication (piezoelectric material, conductive materials for TE and BE) could be deposited within a single ALD reactor. Such an “all-in-one” approach would be convenient and might facilitate the development of 3D piezoNEMS. Therefore, the crystallinity of ALD films should be improved further.
6. Characterization of piezoelectric MEMS

The assessment of in-plane motion in MEMS poses a challenge for currently existing measurement approaches, primarily because of the small size of the moving parts of a device and the low motion amplitude. However, up to nanoscale motion can be captured in SEM and measured in micrographs via post-processing algorithms.

6.1 Motion tests

The motion of a device can be captured and quantified using several methods. The measurement of out-of-plane motion is a relatively straightforward procedure. It can be done by capturing the motion of the tip of the moving part of a device using a photonic sensor, as demonstrated in [1]. The fibre optic sensor detects the amplitude of non-coherent light reflected from the sample surface to determine the distance from the sensor to the sample surface. As a device moves, this distance increases or decreases. However, this method can be applied only to relatively large devices, as photonic sensors generally have spot diameters from 0.3 to 3 mm and cannot probe smaller devices. Smaller devices can be probed using laser Doppler vibrometry (LDV) [151] or various interferometric methods [152, 153]. However, these methods are difficult to apply for laterally moving devices, since the probing surface must move towards the direction of the laser beam.

Lateral motion capturing is possible with SEM. Motion measurement in SEM provides in-situ insights into both the dynamic and static behaviour of a device with nanoscale precision. Also, in SEM, the device is not subjected to environmental dampening, since the measurements are carried out in a vacuum. This makes the measurement results more comparable to those that could be obtained when a device is being hermetically encapsulated. In [II], the lateral motion test was conducted in an SEM chamber with the help of a nanopробing station. The actuator A2 in Figure 6.1 was set in motion by applying a 1 Hz sine wave with a 0 V$_{DC}$ bias and a 20 V$_{pp}$ amplitude on the electrodes. The lateral motion was captured, and the motion amplitude was calculated using the method described in [154].
Figure 6.1 SEM micrographs of two piezoelectric actuators during deflection measurements: (a) Top view of the piezoactuators; (b) No voltage applied; (c) Voltage applied only on A2 (20 V, 1 Hz); (d) Selectively combined image formed from the set of 50 microphotographs [II].

The observed displacement for the piezoactuator 1.4 μm differs from the simulated deflection amplitude of 70 nm (Section 5.1). Only A2 was set in motion during the motion test, while A1 remained stationary. This indicates that actuator A2 was not mechanically actuated due to unintended motion in the chamber. Also, no movement of the damaged actuators was observed (e.g., those with fractured TE on the sidewall or other defects). Therefore, the movement of the actuators most likely is caused by the deformation of AlN under the applied voltage, but the measurements also include a source of errors that have not yet been reliably investigated.

As potential factors that might affect the measurement procedure and be the reasons for the discrepancy between the simulated and observed deflection, the following influences can be considered:

1. Electrical probing in SEM was found to add sources of error in the measurement, for example, via surface charging.

2. The literature does not sufficiently cover ALD TiN as an electrode material for piezoelectric MEMS actuation. Even though TiN showed sufficient sheet resistance of 68 Ω·sq⁻¹ and revealed no phase formation on the interface with AlN, an alternative for TE material can be considered. Another conventional conductive material should be considered for application, e.g., Al or Mo.
7. Conclusion

Piezoelectric thin films are not yet widely integrated in the fabrication of laterally moving MEMS devices. This is mainly because of the difficulties related to the deposition of high-quality piezoelectric thin films on vertical surfaces. Despite the demanding fabrication process, integrating environmentally friendly piezoelectric materials in MEMS is beneficial for emerging 3D piezoMEMS that would implement multiaxial motion and sensing within a single MEMS element.

Pure lateral motion in MEMS can be achieved using piezoelectric thin films placed on the vertical sidewalls of the actuated structure. This work investigated the development of a new process technology as well as the adaptation and optimization of existing fabrication techniques for 3D piezoMEMS fabrication. The process technology exhibited in the work demonstrates the potential of the piezoelectric and electrode material deposition on vertical sidewall structures in the fabrication of advanced 3D piezoMEMS. FEM simulation of a half-fork piezoelectric MEMS vibratory gyroscope that utilizes AlN deposited on the vertical surfaces of the fork’s cantilevers indicates that its angular rate sensitivity is comparable with commercial gyroscopes while maintaining a lower surface area on a chip.

The integration of AlN in the fabrication process of a laterally driven piezoelectric actuator was implemented via MOCVD on the vertical surfaces of Si cantilevers formed in the device layer of an SOI. The crystallographic orientation of MOCVD AlN films on the vertical sidewalls was affected by the surface roughness of the underlying Si surface. High crystal quality MOCVD AlN on the vertical surfaces was achieved when wet etchants (KOH and TMAH) were implemented to form vertical surfaces in Si. Fabrication of Si cantilevers via the dry etching process in the cryogenic mode of ICP-RIE resulted in sidewalls having high surface roughness. AlN grains pursued growth perpendicular to the surface in every location of the Si sidewall. Therefore, the orientation of AlN film cannot be considered parallel to the [0001]-direction, although films are polycrystalline and textured. Such films are expected to have worse piezoelectric properties and, as a result, downgrade device performance. The limitations of the high vertical sidewall roughness can be overcome by optimization of the dry etching process or via post-etching smoothing of the Si surface, such as annealing at hydrogen atmosphere or surface oxidation, and subsequent etching in BHF. Piezoelectric actuation by ALD AlN might possibly be achieved in the future. The low deposition temperature of the ALD process allows the application of a wide range of thin metallic films as a BE deposited on the vertical surfaces prior to
AlN deposition. However, the underlying material should have a high preferential orientation and a matching in-plane lattice constant for high-quality ALD AlN deposition.

Al_{1-x}Sc_xN is a perspective material that can replace AlN and enhance the performance of piezoMEMS in the future due to its higher piezoresponse. However, integration of Al_{1-x}Sc_xN in 3D piezoMEMS would demand market available MOCVD reactors that are compatible with rare-earth precursors and stable growth on Si substrates.

Ultimately, the specific highlighted contributions of the work are as follows:

i) High-quality c-axis oriented MOCVD AlN can be deposited on vertical Si surfaces prepared with wet etching in KOH or TMAH. Dry etching methods for vertical sidewall formation might be applied, but post-etching treatment or optimization of the etching parameters is required for highly oriented AlN growth.

ii) AlN grown on vertical surfaces was integrated into piezoMEMS fabrication using existing fabrication techniques. The potential of its application for 3D piezoMEMS was demonstrated via FEM simulation of the mechanical or angular rate sensitivity of a tuning-fork piezoelectric MEMS gyroscope. The proposed gyroscope’s design retains a lower surface area on a chip while maintaining sensitivity (1.21 mV/dps) comparable to commercial gyroscopes.
References


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