EFFECTS OF HETEROSTRUCTURE STACKING ON ACOUSTIC DISSIPATION IN COUPLED-RING RESONATORS

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ABSTRACT

We describe a systematic study on quantifying the effects of heterostructure layer stacking upon measured dissipation and quality factors (*Q*s) of AlN-on-Si coupled-ring breathing mode micromechanical resonators. For the first time, we design and fabricate resonators of the same lateral dimensions but with different stacking layers, namely, Si, AlN-on-Si, and Al-on-AlN-on-Si. With both optical and electrical readout techniques, we measure the fundamental radial-extensional mode and its *Q* values and compare the observed and simulated energy dissipation. For the same device geometry, the results show that the bare Si device has the highest *Q* (11,304). Adding an AlN layer leads to a reduction in *Q* for the AlN-on-Si device by a factor of ~1.46 compared to bare Si device. Top layer metallization further compromises the *Q* by a factor of ~1.85. Modeling of the dissipation processes suggests that neither the thermoelastic damping (TED) nor the anchor loss is the limiting loss factor. A piezoelectric-specific loss mechanism known as charge redistribution loss and interface loss are both possible limiting mechanisms.

INTRODUCTION

Microelectromechanical systems, or MEMS resonators, are promising candidates as a miniature and integrated alternative to crystal oscillators. The two most common transduction mechanisms for MEMS resonators are capacitive and piezoelectric, with piezoelectric transduction having higher electromechanical coupling efficiency resulting in lower motional impedance. To exploit the piezoelectric effect, structural stacking consisting of several layers, including an electrode layer, a piezoelectric layer, and an elastic layer is required. Stacking of layers in a mechanical vibrating system results in energy loss due to mismatch of elastic properties between each layer and interfacial strain jump between layers, diminishing quality factors (*Q*s) and limiting the performance of these devices [1, 2]. To mitigate this loss and improve the *Q*s while maintaining strong electromechanical coupling in piezoelectric MEMS devices, a systematic investigation on interface energy dissipation mechanisms, optimization of layer matching, and material choices is required.

Aluminum nitride (AlN) is an attractive candidate for piezoelectric MEMS, possessing high piezoelectric coupling coefficient [3], excellent acoustic velocity, and low dielectric loss [4]. In addition, AlN MEMS devices can be monolithically integrated with Si CMOS technology [5]. Among many piezoelectric materials (*e.g.*, zinc oxide (ZnO), lead zirconate titanate (PZT), and gallium nitride (GaN)) used in MEMS, only AlN bulk acoustic resonators (BARs) [6] have been successfully demonstrated in commercialization and adopted in many products, including in radio frequency (RF) communication and signal processing modules. Yet, loss mechanisms in AlN resonators and other piezoelectric resonant MEMS devices are not fully understood and piezoelectrically transduced resonators exhibit significantly lower *Q*s than their capacitive MEMS counterparts [7].

To study these loss mechanisms in piezoelectrically transduced resonators, we have fabricated three types of coupled-ring MEMS resonators with different stacking layers: aluminum (Al)/AlN/silicon (Si), AlN/Si and bare Si. The coupled-ring breathing mode resonator utilizes an in-plane bulk acoustic wave (BAW) resonance mode to provide high *Q* at MHz range frequencies [8]. While some preliminary studies have been conducted on dissipation mechanisms in AlN-on-silica coupled-ring resonators [9], further investigation is needed to understand the dominant underlying loss mechanism in piezoelectrically transduced resonators. In this work, in addition to conventional electrical transmission measurements, we investigate loss mechanisms within and between layers of the vibrating element using optical in-plane (lateral) displacement detection techniques based on the knife-edge effect. In contrast to an electrical transmission measurement that requires establishment of a complete circuit loop with a complete piezoelectric stack, the optical method we use is highly versatile, providing a way to measure resonance characteristics for all three types of devices. By comparing measured *Q*s of the three types of resonators and their simulated energy dissipation values from finite element modeling (FEM), we are able to quantify the energy loss at the AlN/Si and Al/AlN interfaces, elucidating detailed dissipation behaviors in such piezoelectric MEMS devices.

RESNATOR DESIGN AND SIMULATION

Among various resonance modes, we focus on the in-plane breathing mode of coupled-ring resonator. For bare Si ring resonators, the first in-plane breathing mode resonance frequency (f_0) can be calculated using

$$f_0 = (1/2\pi)\sqrt{E_Y/(\rho R_1 R_2)}, \tag{1}$$

where R_1 and R_2 are the inner and outer radius of the ring, respectively, E_Y is the Young's modulus, and ρ is the mass density of Si. The calculated f_0 is ~10MHz for a Si resonator with R_1 of 75 μm and R_2 of 195 μm. Since the mode is insensitive to device thickness variation, adding additional thin layers (compared to the Si substrate) will not dramatically alter the resonance frequency of this mode.

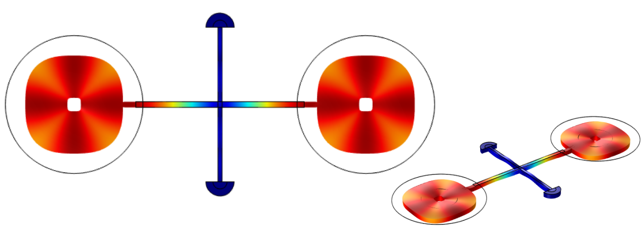
To connect the rings, we design a coupling rod to have a length extensional mode resonance frequency identical to the breathing mode resonance of the two rings. Thus, we establish a system with symmetric motion when vibrating in its lateral expansion mode [9].

For the analysis of dissipation mechanisms, anchor loss and TED are the most commonly regarded loss mechanisms in MEMS resonators operated in ideal conditions. By focusing on the in-plane breathing mode, we avoid introducing large frequency shifts from additional layers, allowing for frequency-independent comparison between variations. The in-plane breathing mode, when coupled with appropriate anchor nodal point design, provides a relatively anchor-loss and TED insensitive platform that is suited for investigating the effect of additional layers.

In addition to anchor and TED losses, there is a piezoelectric-specific loss mechanism known as charge redistribution (CR) loss. While vibrating, the strain profile in piezoelectric layer of the resonator is not uniform, causing uneven charge distribution across the electrodes. The charge tends to redistribute to resolve the gradient [7], resulting in energy loss through electromagnetic radiation by electron-to-photon conversion [10] or by kinetic loss to electrons.

Table 1: Material constants used in simulations

Parameter	Si	AlN
Young's modulus (GPa)	163	345
Mass density (kg·m^{-3})	2330	3300
Thermal expansion coefficient (K^{-1})	2.6×10^{-6}	4.2×10^{-6}
Thermal conductivity (W·m^{-1}·K^{-1})	130	60
Heat capacity (J·kg^{-1}·K^{-1})	700	600



Material	Si	AlN/Si	Al/AlN/Si
Q_{Total}	27,565,182	83,340	11,399

Figure 1: Resonance mode FEM simulations with corresponding simulated Q for each piezoelectric stack variation. Both anchor loss and TED are considered for bare Si and AlN/Si stacking, with CR loss also considered for Al/AlN/Si stacking. Without CR loss, the Q of Al/AlN/Si is nearly identical to that of the AlN/Si variation.

Through FEM simulations, we analyze the coupled-ring radial-extensional mode to isolate the effects of common loss mechanisms. The results show that the resonance frequency of this particular mode is ~10MHz for all three layer variations, which confirms the calculated value introduced above. Furthermore, by computing plausible dissipation mechanisms, including anchor loss (minimized by design), TED, and CR damping (only present in the Al/AlN/Si staking), we can estimate total Q of each device type (Fig. 1). Our simulations indicate that, as expected, adding material layers significantly reduces Qs in these resonators.

RESONATOR FABRICATION

To measure these effects, we have fabricated three types of coupled-ring piezoelectric MEMS resonators with identical lateral geometries but different stacking layers (Fig. 2). Each as-fabricated die consists of all three stack variations to minimize process variations during fabrications. The fabrication process starts with sputtering of a 1µm AlN layer onto a highly doped silicon-on-insulator (SOI) wafer. The low resistivity of the highly-doped silicon substrate allows for a conductive substrate ground layer, removing the need for a bottom electrode and reducing the number of layers and complexity of the investigation. Next, the AlN layer is etched to define the ground connections and open up the unwanted AlN layer on Si-only devices. Afterwards, 75nm of Al top metal routing and thick (500nm) gold (Au) probe pad layers are deposited, followed by the front-side etching of the resonator contours. Finally, the devices are released from the back side of the wafer using deep reactive ion etching (DRIE) followed by a short RIE oxide etch to remove the buried oxide (BOX) layer.

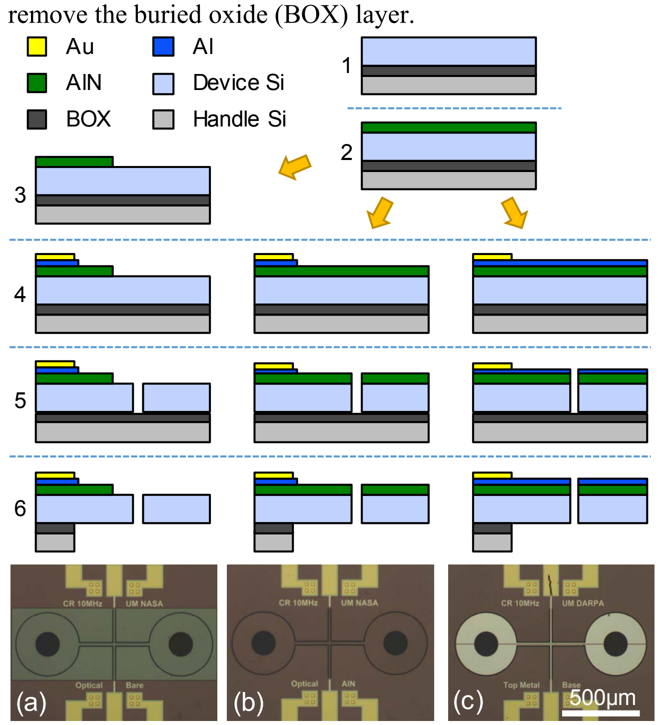


Figure 2: Device cross-section and schematic of the fabrication process. Each column shows the fabrication flow for each individual stack variation with the corresponding optical image of the device. The stacks consist of (a) bare Si, (b) AlN/Si, and (c) Al/AlN/Si. The process starts with a bare SOI wafer (1) where AlN is deposited on as the piezoelectric layer (2). The AlN is selectively etched to access the ground layer (3) and the top metal layers are deposited and patterned (4). Next, the contours of the resonators are etched from front side (5). Finally, the devices are released from back side (6).

MEASUREMENT RESULTS

In addition to theoretical modeling and FEM simulations, experimental results are critical to understanding the loss mechanisms in these devices. To investigate the effects of additional layers on these devices, we have conducted both conventional electrical transmission measurements on Al/AlN/Si devices and optical measurements on all stack variations. For the electrical measurements, we utilize two mechanically coupled piezoelectric capacitors in series for a two-port measurement configuration using a network analyzer (Fig. 3). Figure 4 shows the S_{21} parameter measurements of an Al/AlN/Si resonator at 9.899MHz with a Q of 6,084, well matching the designed frequency.

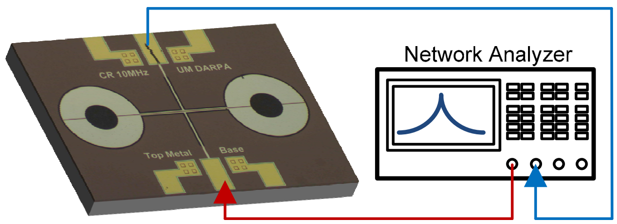


Figure 3: Schematic illustration of the measured electrical transmission coefficient (insertion loss) of Al/AlN/Si devices.

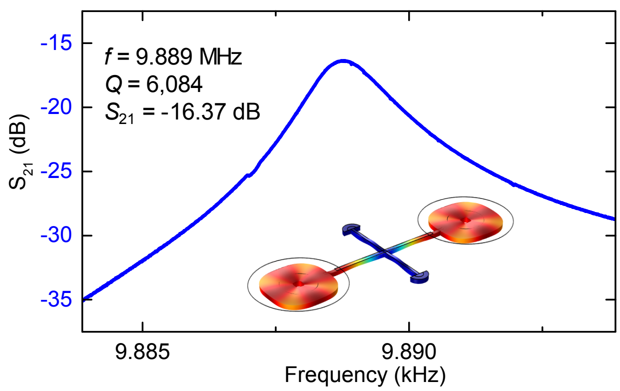


Figure 4: S-parameter measurement of an Al/AlN/Si device.

In addition to a purely electrical measurement, we also investigate the loss mechanisms within and between layers using a custom-built optical in-plane (lateral) displacement detection system based on the knife-edge effect (Fig. 5). We use an amplitude modulated 405nm (blue) laser to photothermally excite the coupled-ring resonator by parking the laser spot at the joint of the coupling rod and the ring. The radial extension motion of the ring is transduced by a 633nm (red) laser – the expansion and contraction of the ring while vibrating in the breathing mode alter the reflected red laser power due to the knife-edge effect [11] and this power variation is detected by a photodetector (PD). A network analyzer can resolve the frequency response of the resonator through this transduction scheme. In contrast to electrical transmission measurements that require electrical circuit loops with the complete Al/AlN/Si stack, the optical method here is versatile, providing a way to measure resonance behaviors of all three stack variations. This allows us to not only compare a full piezoelectric stack, but investigate the effect of individual layers on device performance.

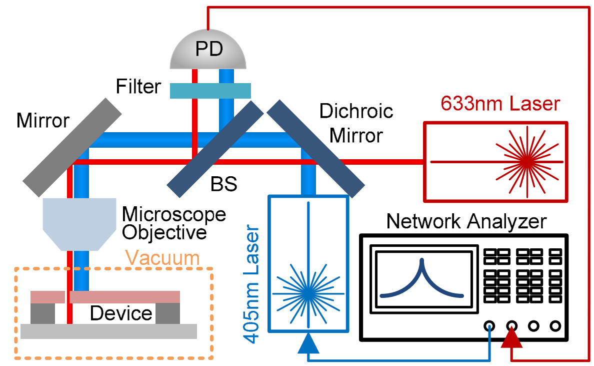


Figure 5: Dual-laser measurement system for the optical excitation and detection of mechanical resonances. A 405nm amplitude modulated laser is focused on the rod-and-ring intersection for photothermal excitation, while a 633nm laser is focused on the edge of the ring and a PD is used to detect the transduced power variation of the 633nm laser.

From the optical interferometric measurement results, we find that the measured Qs clearly decrease as the numbers of additional layer increase (see Fig. 6 and Table 2). Even adding a thin (75 nm) Al layer induces considerable damping, which is predicted in simulation through the CR damping limit (a Q drop from ~83,300 to ~11,400 due to CR loss is predicted by COMSOL). Measured Qs are, however, much lower than the simulated results for all three types of devices, which may be attributed to either slight ring asymmetry or small structure defects unintentionally induced during fabrication. Another important source of loss could be interface loss, which is not easily predicted and not included in the simulated performance. Neither TED or anchor loss alone can explain the low Q measured for bare Si devices ($Q_{\mathrm{measured}} \approx 11{,}300$ and $Q_{\mathrm{total,simulated}} \approx 27{,}565{,}000$).

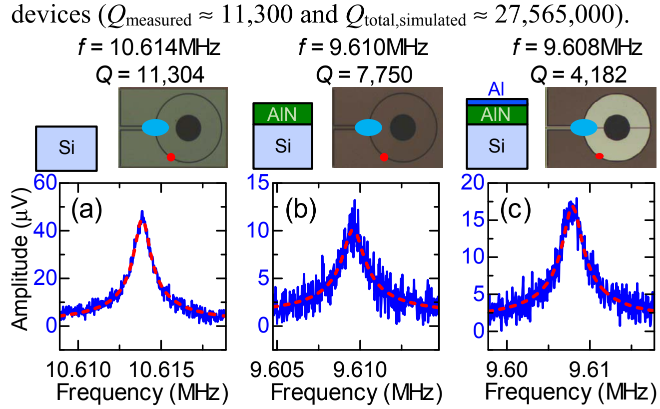


Figure 6: Optical measurement results of target resonance mode for (a) bare Si, (b) AlN/Si, and (c) Al/AlN/Si stacks. The upper panels show extracted resonance frequencies and Qs, the specific stack variation, and the positions of the laser spots for the corresponding spectra.

To interpret the effects of adding additional layers to the Si resonator, we use the measured Q of the bare Si device as the performance baseline and compare the dissipation from each additional layer directly against it. This way, we can compare the experimental results and the simulations by examining only the dissipations introduced by additional layers. We obtain a new set of Qs that closely match the measured results (Table 2) indicating the extent by which the Q drops by adding new layers to the resonator.

Compared with the pure electrical measurement scheme, the optical measurements show slightly lower Q, which might be related to asymmetric photothermal excitation on only the end of one ring (Fig. 6 *insets*). The asymmetric driving is due to the limited field of view for an ideal red laser spot size. Since the coupled breathing mode system is designed for perfect resonance frequency match among the lateral extensional mode of the coupling rod and the two rings, the asymmetric optical drive causes a lag in the response on one side of the device, introducing additional loss. This asymmetry could also help explain the large discrepancy between simulated and measured performance of the bare Si variations.

To account for the additional losses seen in the optical measurements, we have adjusted the simulated Q against the measured bare Si device performance. Table 2 compares the results, showing adding the AlN layer clearly leads to reduction in Q by a factor of ~1.46. An additional metallization layer further compromises the Q by a factor of ~1.85. The Q drops in AlN/Si and Al/AlN/Si devices could potentially be explained by the charge redistribution loss, as a factor of 2 drop is expected between AlN/Si to Al/AlN/Si variations. It is important to note that interface loss is not factored here, and may have a noticeable contribution towards these results that warrants further investigation.

Table 2: Summary of resonator quality factors (Qs)

	Si	AlN/Si	Al/AlN/Si
Simulated	27,565,182 (TED limited)	22,800 (CR loss limited)	11,399 (CR loss limited)
Electrical	-	-	6,084
Optical	11,304	7,750	4,182
Simulated (*with added measured loss in Si device considered*)	11,304	7,557	5,675

CONCLUSIONS

We have performed quantitative analysis of energy dissipation as a result of additional layers in piezoelectrically transduced MEMS resonators. We have fabricated and utilized coupled-ring resonators with bare Si, AlN/Si, and Al/AlN/Si stacks as test vehicles to explore this effect. Both FEM simulations and experimental examination show substantial drops in Qs after adding additional layers, which suggests that the charge redistribution (CR) loss may be playing a significant role in energy dissipation of piezoelectric heterostructure MEMS devices.

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