ONE-DIMENSIONAL LINEAR ACOUSTIC BANDGAP STRUCTURES FOR PERFORMANCE ENHANCEMENT OF ALN-ON-SILICON MICROMECHANICAL RESONATORS

L. Sorenson, J.L. Fu, and F. Ayazi
Georgia Institute of Technology, Atlanta, Georgia, USA

ABSTRACT
This work introduces piezo-on-silicon linear acoustic bandgap (LAB) structures, a class of compact 1D micro-scale phononic crystal (PC) which can be directly integrated with micromechanical devices. Finite element simulations with custom-derived dispersion equations predict multiple bandgaps for coupled-ring LAB structures into the GHz region. AlN-on-Si resonator supports are replaced with coupled-ring LAB tethers to reduce acoustic loss into the substrate; the existence of bandgaps is experimentally confirmed in transmission spectra of test structures as well as quality factor (Q) and insertion loss (IL) improvements of LAB-enhanced resonators. An IL of 3.8 dB at 178 MHz and Qs of greater than 11,000 at 600 MHz in air are reported.

KEYWORDS
Phononic crystal, acoustic bandgap, piezoelectric-on-silicon resonator, quality factor, support loss, one-dimensional

INTRODUCTION
Phononic crystals (PCs) exhibiting acoustic stop-bands are of increasing interest for their inherent frequency filtering characteristics. One- [1-2] and two-dimensional [3-7] PCs have been used to create frequency bandgaps, but implementation of these structures typically requires a large area or multiple stacked layers. This work introduces AlN-on-Si and Si-only coupled-ring linear acoustic bandgap (LAB) structures, which can be implemented in minimal area without repeated stacking of material layers. LAB structures are characterized by small dimensions perpendicular to the line containing the 1D PC lattice. The bandgap properties of the LAB structure are experimentally confirmed with single-device test structures. We have successfully integrated these LAB structures as support elements of high-frequency AlN-on-Si resonators and demonstrate tangible Q and IL improvements. Converged finite element models predict bandgaps in GHz frequencies wider than 10 MHz.

LINEAR ACOUSTIC BANDGAP STRUCTURE
Recently, 1D PC structures derived by slicing a strip from a 2D PC plate have been demonstrated in simulation [8]. We have extended the 1D PC concept by generalizing the basis structure beyond strips cut from 2D PCs; instead, the design space is broadened such that only 1D periodicity is required and the PC basis can assume a variety of shapes and orientations. In this paradigm, 2D and 3D PCs can be considered specialized cases of the 1D PC with increasing dimensions of periodicity. In this work, we focus on the coupled-ring LAB structures depicted in Figure 1, for which the 3D basis is repeated at each lattice point with lattice constant a. Ring inner and outer radii (r₁, r₀), coupling beam width w, and layer thicknesses dᵢ parameterize the basis dimensions.

1D PC THEORY AND BANDGAP MODELING
The periodic nature of a PC combined with the mismatch between the basis structural material and the surrounding air or vacuum create acoustic bandgaps, or frequencies of no allowed acoustic propagation. To calculate the acoustic dispersion behavior of the coupled-ring LAB structures, modified eigenvalue analysis based on the Bloch relationship [3] is performed. Wave vector contributions to the linear elastic equations are derived and implemented in COMSOL finite element software, beginning with the linear elastic force balance equation (1) in the absence of externally applied force:

\[-\rho u_{tt} + \sigma_{ij,j} = 0 \quad (1)\]

where \(\sigma_{ij,j}\) is the first derivative of the Cauchy stress tensor with respect to \(f^\text{th}\) component, \(u_{i,tt}\) is the second derivative of displacement in the \(i^\text{th}\) direction with respect to time \(t\), and \(\rho\) is the material density. Tensor quantities are expressed with Cartesian components, while a comma separates indices from derivatives, and the Einstein summation rule applies where appropriate. The Cauchy strain tensor \(\epsilon_{kl}\) is related to \(\sigma_{ij}\) through the anisotropic Hooke’s law (2)

\[\sigma_{ij} = c_{ijkl} \epsilon_{kl} \quad (2)\]

where \(c_{ijkl}\) represents the fourth-order elastic stiffness tensor and \(\epsilon_{kl}\) is defined in (3) as

\[
\begin{align*}
\sigma_{ij} &= c_{ijkl} \epsilon_{kl} \\
\epsilon_{kl} &= \frac{1}{2} (\varepsilon_{ij} \delta_{kl} + \varepsilon_{kl} \delta_{ij})
\end{align*}
\]
In a 1D PC, the acoustic displacement wave must be of the Bloch form (4) to meet periodic boundary conditions:

$$u_i(x_m, k_n, t) = \tilde{u}_i(x_m)e^{i(k_nx - \omega t)}$$  \hspace{1cm} (4)

Equations 2-4 are substituted into (1) and differentiated to establish a characteristic wave equation including the wave vector dependence (5):

$$\rho \omega^2 \delta_{kk} \tilde{u}_k + (c_{ijkl}\tilde{u}_{ik})_{,l} + (ik_{ijkl}\tilde{u}_k)_{,l} + ik_k c_{ijkl} \tilde{u}_{k,l} - k_j k_{ijkl} \tilde{u}_{l,k} = 0$$  \hspace{1cm} (5)

Equation (5) was implemented in the COMSOL model with customized code to unwrap crossing bands and automatically obtain the bandgaps. The resulting eigenfrequencies were mapped to acoustic wavenumber $k$ over the irreducible first Brillouin zone (BZ) of the 1D PC (Fig. 2). In all cases, the finite element mesh density was refined until converged results were obtained.

Acoustic dispersion curves using the dimensions given in Fig. 1 are shown from 0-500 MHz for AlN-on-Si LAB rings and Si-only rings (Fig. 3). These results indicate that the piezoelectric stack influences, but does not eliminate, the presence of bandgaps in the structure. By decreasing $d_{SO}$ of Si-only coupled-ring structures to 1 µm, several complete bandgaps up to 1.97 GHz can be obtained (Fig. 4). A bandgap of 12 MHz is predicted at 1.9 GHz, while a 22 MHz bandgap is obtained at 1.7 GHz, demonstrating the suitability of the LAB structure to ultra high RF applications.

**DEVICE DESIGN & FABRICATION**

Devices were fabricated on a silicon-on-insulator (SOI) substrate with 10-µm device layer thickness ($d_{SO}$) using a process similar to [9]. The piezoelectric stack consists of 100-nm Mo electrodes and 1-µm thick AlN. LAB structures were formed during patterning of the stack and device definition.

Specialized LAB test structures were developed to experimentally verify the bandgaps predicted in simulation. Claw-shaped AlN-on-Si transducers, which operate with a wide bandwidth up to 500 MHz, are connected through coupled-ring LAB structures (Fig. 5(a)). The transducers are designed to avoid any strong resonances over the band of operation.

LAB structures are good candidates to enhance the performance of high-frequency micromechanical resonators, which can be significantly affected by acoustic loss through support tethers. To demonstrate the effectiveness of the LAB structures, AlN-on-Si resonators were designed with six periods of coupled-ring supports. Identical devices with simple beam tethers, whose width equals $w$ of the coupled-ring basis, are fabricated side-by-side with the LAB-enhanced devices for comparison.

**EXPERIMENTAL RESULTS**

All measurements, obtained with an Agilent E8364B vector network analyzer, were taken in air at room temperature unless otherwise noted with standard SOLT calibration. Transmission measurements of a six-period, Si-only LAB ring test structure with nine rows and corresponding reference are shown in Fig. 5(b), confirming the predicted large complete bandgap from 160-205 MHz (Fig. 3(b)). Compared with the reference beams, transmission through the LAB structures is strongly suppressed below the noise floor. The experimental result is in good agreement with finite element predictions of the $S_{21}$ frequency response (Fig. 5(c)). To reduce computation time of the frequency response simulation, the finite element simulation was performed in 3D for a test structure with one row of six coupled rings. Admittance parameters were obtained by applying appropriate electrical boundary conditions to the
piezoelectric layer and converted to S-parameters assuming 50 Ohm terminations.

Several examples of quality factor improvement in high-frequency resonators with AlN-on-Si LAB supports are given (Figs. 6, 7). To eliminate the effect of material property variations across the wafer, comparisons were made between adjacent devices.

Fig. 6 shows the $S_{21}$ response of a third-order LAB-enhanced lateral-extension-mode resonator at 213 MHz, which falls in the predicted bandgap from 210 to 223 MHz (Fig. 3(a)). This device demonstrates an 82% Q improvement and 4.9 dB IL improvement over an identical resonator with simple tethers. The simulated strain patterns suggest that the LAB structures effectively block acoustic energy from coupling to the substrate.

The 11th-order resonator with AlN-on-Si LAB supports (Fig. 7(a)) exhibits a low IL of 3.8 dB at 178 MHz, which is located in the large bandgap between 159 and 192 MHz (Fig. 7(c)). The same device has a Q of 11,400 at 603 MHz compared to the equivalent simple tether device Q of 7,200, suggesting existence of a bandgap at this frequency (Fig. 7(d)). The highest measured Q improvement for this design is from 1,450 to 1,930 (32%) with corresponding IL improvement of 2.17 dB at 178 MHz.

To verify repeatable improvements due to LAB tethers, adjacent pairs of several third-order designs were measured across multiple fabrication runs and across each wafer. An average Q improvement of 2x and average IL improvement of 30% are obtained (Fig. 8).

**DISCUSSION & CONCLUSION**

Linear Acoustic Bandgap structures have been presented in this work as a compact solution for integration with high-frequency MEMS devices. Bandgaps calculated using the finite element method are experimentally confirmed by measuring the $S_{21}$ response of LAB test structures. The large complete bandgaps created by the coupled-ring LAB structure prevent additional substrate loss through the resonator supports, which is confirmed by Q and IL enhancements of several devices when compared with their reference counterparts. A comparison of 11th-order and 3rd-order devices indicates that the IL can be improved by using high-order longitudinal extensional resonators. Although these resonators suffer more interfacial loss—and therefore lower device Q—than their equal-pitch low-order counterparts, additional damping is compensated by the improvement in IL.

Converged finite element simulations predict multiple complete bandgaps into the 0-2 GHz range,
suggested by a high-frequency mode of reference resonator (right).

suggesting the utility of LAB structures at even higher frequencies where support loss will be a dominant part of the overall Q. Due to the myriad variations possible with a 3D basis in a 1D PC, engineering of the bandgap to application requirements is possible, e.g., by choosing a different thickness. With these attractive attributes, the LAB structure shows potential to become a standard component of high-Q resonant MEMS designs.

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Contact
*L. Sorenson, tel:+1(312)833-0391; logan.sorenson@gatech.edu