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Approaching the intrinsic quality factor limit for micromechanical bulk acoustic resonators using phononic crystal tethers

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Abstract

We systematically demonstrate that one-dimensional phononic crystal (1-D PnC) tethers can significantly reduce tether loss in micromechanical resonators to a point where the total energy loss is dominated by intrinsic mechanisms, particularly phonon damping. Multiple silicon resonators are designed, fabricated, and tested to provide comparisons in terms of the number of periods in the PnC and the resonance frequency, as well as a comparison with conventional straight-beam tethers. The product of resonance frequency and measured quality factor ($f \times Q$) is the critical figure of merit, as it is inversely related to the total energy dissipation in a resonator. For a wide range of frequencies, devices with PnC tethers consistently demonstrate higher $f \times Q$ values than the best conventional straight-beam tether designs. The $f \times Q$ product improves with increasing number of PnC periods, and at a maximum value of 1.2×10^{13} Hz, approaches limiting values set by intrinsic material loss mechanisms.

Micromechanical resonators are critical components for sensor systems, stable timing sources, and radio frequency signal processing. There is a continual drive to improve the quality factor (Q) of resonators since high Q is necessary for high-resolution sensors, low-noise clocks, and efficient radio frequency filters. The mechanical energy that would ideally be trapped in the resonant mode of vibration is dissipated through a variety of mechanisms, leading to a reduction in Q . Intrinsic dissipation mechanisms are dependent on the resonant mode and internal structure of the resonator, and redistribute the mode energy through phonon-, electron-, or defect-mediated scattering or thermoelastic damping (TED) within the resonator body.^{1–5} Extrinsic dissipation mechanisms are classical damping mechanisms (e.g., fluidic damping, mass-loading, surface/interface loss, and tether loss), where energy is lost to the environment.^{6, 7} For bulk acoustic mode resonators operating in vacuum packages, the dominant dissipation mechanisms are phonon loss, thermoelastic damping, and tether loss. Phonon loss is a result of the anharmonicity of the material lattice, while TED is due to the irreversible heat flow across thermal gradients induced during

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SUPPLEMENTARY MATERIAL

See supplementary material for details on the seven resonator designs and the models for phonon loss and thermoelastic dissipation.

vibration.^{1, 2, 4} Tether loss^{8–11} is the energy lost through the tethers to the substrate anchors and is the subject of the experiments presented here.

In general, the goal is to design the tethers to minimize the amount of elastic energy that leaks through to the substrate. One common approach treats the tether as a transmission line, assuming that the best isolation is achieved by using quarter-wavelength tethers. For specific resonator designs, the tether dimensions can be optimized to provide improved Q .^{11, 12} Recent research into phonon-engineered structures has led to a number of designs that allow selective phonon control, from phonon cavities^{13–16}, waveguides^{17, 18}, and filters.^{19, 20} The ability to control acoustic phonon dispersion enables the design of acoustic/phononic bandgaps^{19, 20} that can be used as tethers or shields to efficiently confine energy in a phonon cavity or resonator.^{15, 21–26} In such devices, acoustic propagation is mitigated by using multiple repeating units to create a phononic crystal (PnC) that has a transmission bandgap. Several of these studies have focused on improving the Q of acoustic Fabry-Pérot resonators.^{14–16} This technique can be implemented to improve the Q of micromechanical resonators, by using PnCs as the tethers. Simple mass-link PnCs with 1-dimensional (1-D) connectivity used as the tethers have been found to be effective in recent analyses^{21–23} and preliminary experiments.^{24–26} However, the use of piezoelectric resonators with metal electrodes introduces additional dissipation within the materials and at their interfaces, thereby limiting the improvement resulting from the PnC tethers. Further, most existing experiments do not explicitly compare PnC tethers with the best straight-beam tether designs.

This letter reports on the quality factor of width-extensional mode bulk acoustic resonators (WE-BARs) with 1-D PnC tethers, including a comparison with the best performing straight-beam tethers. Unlike prior research^{24, 25} using piezoelectric resonators, this work uses monolithic resonators composed of one material, single-crystal silicon. This approach eliminates the energy losses in piezoelectric materials, metal electrodes, and at the material interfaces of composite resonators, providing tether-loss optimized resonators. By nearly eliminating extrinsic or design-dependent loss mechanisms, bulk acoustic resonators may be capable of reaching the quantum limits of mechanical motion and displacement sensitivity^{27, 28}, while operating at very high frequencies, or function as high-performance timing units that can bridge the gap between low-performance quartz clocks and chip-scale atomic clocks.²⁹ As some of the dissipation processes are frequency dependent, the metric used for comparison in this letter is the product of resonance frequency and measured quality factor ($f \times Q$), which is inversely proportional to the total energy dissipation.

The electrostatic WE-BARs used in this work are shown in Fig. 1, along with simulated mode shapes of the expected fundamental mode. The fundamental resonance frequency of the WE-BAR is approximated by $f_0 = v/\lambda = v/2w$, where v is the longitudinal acoustic wave velocity, w is the resonator width, and λ is the acoustic wavelength. Three groups of WE-BARs have been studied (A, B and C), with fundamental frequencies of 167 MHz, 227 MHz and 282 MHz, respectively. Each group has seven tether designs: three PnC designs with 1, 3, and 5 unit cells each, and four conventional straight-beam tether designs with tether lengths equal to $\lambda/8$, $\lambda/4$, $3\lambda/8$ and $\lambda/2$, all with a tether width of 2 μm . The PnC unit cells (Fig. 1(c)) are simple mass-link designs with 1-D connectivity and a period, a , that is

optimized for wide bandgaps.¹⁵ Given the number of design variables, multiple solutions exist and practical constraints such as silicon layer thickness, lithographic resolution, and robustness are considered for the final PnC design. The PnC unit cell is composed of a square block of side b and two symmetric beams, each of length $(a-b)/2$ and width c . The ideal phononic bandgaps are found using finite element analysis with 1-D Floquet periodic symmetry (i.e., an infinite chain of unit cells) and a wide parametric sweep for a , b and c .^{15, 30} Design details of the resulting resonator and PnC tethers are provided in Table I. While the fabricated PnC tethers are not infinite chains, as assumed in the finite element analysis, the design procedure does result in highly reflective phononic crystals, even for 1 unit PnCs, as described shortly³⁰. The complete bandgaps shown in Fig. 2 are expected to be wider in practice due to deaf bands²³ comprised of shear or z -polarized twisting modes that do not transmit longitudinal waves across the tethers.

All resonators are fabricated on the same silicon-on-insulator (SOI) wafer, which has a $10\text{ }\mu\text{m} \pm 0.5\text{ }\mu\text{m}$ thick device layer of $\langle 100 \rangle$ silicon with a resistivity of $0.01 - 0.02\text{ }\Omega\text{-cm}$, a $2\text{ }\mu\text{m} \pm 0.5\text{ }\mu\text{m}$ thick buried oxide layer, and a $500\text{ }\mu\text{m}$ thick handle wafer. Bond pads consist of $10\text{ nm}/200\text{ nm}$ Cr/Au layers deposited using electron-beam evaporation and a liftoff process. After metallization, a 380 nm thick SiO_2 hard mask layer is deposited using plasma enhanced chemical vapor deposition and patterned using optical lithography and reactive ion etching. The Si etch uses deep reactive ion etching (DRIE) with an optimized process that yields smooth sidewalls (each etch cycle is $\approx 80\text{ nm}$ deep, with a scalloping of less than $\approx 15\text{ nm}$). The entire depth of the device layer is etched, monolithically defining the resonator, tethers and anchors. The wafer is diced and resonators are released from the substrate by etching away the SiO_2 hard-mask and buried oxide using vapor-phase hydrofluoric acid etching. Finally, resonators are mounted on a chip carrier and signal pads are wire-bonded. The use of a thick SOI device layer, and a single lithography and etch step for defining the resonator and tethers significantly reduce the possibility of asymmetry, which could potentially reduce the Q ³¹.

A schematic of the experimental setup is shown in Fig. 3, highlighting the critical optical and control elements used in the measurements. The resonators were tested at room temperature in a vacuum chamber with a pressure less than 6.67 mPa ($50\text{ }\mu\text{Torr}$). The WE-BARs are actuated electrostatically by applying a 10 mW AC input from a network analyzer to the two lateral electrodes and a 21 V DC bias voltage to the body of the resonator, V_{DC} . Instead of an electrical readout, which can suffer from high-frequency feedthrough parasitics, the photoelastic effect is used to optically measure the mechanical resonance.^{32–34} As the resonator vibrates, the body of the resonator undergoes in-plane strain. The strain modulates the refractive index of the material, and consequently the amplitude of the reflected light from a He-Ne probe laser ($\approx 100\text{ }\mu\text{W}$ incident power). The reflected light is measured using an ultra-fast Si PIN photodetector with a bandwidth of 1.4 GHz , and the output of the photodetector is measured with the network analyzer. A three-axis motion stage with a position resolution of $\approx 10\text{ nm}$ is used to precisely position the WE-BAR under test. The geometric center of each resonator is used consistently for all measurements, as maximum in-plane strain is expected there (see strain mode shape in Fig. 1(d)). Optical knife-edge displacement measurements on the free edge of the WE-BAR were used for independent confirmation of the results.³² The measured frequency and Q from

both measurements are nearly identical for each WE-BAR, indicating that these parameters are inherent to the resonator and independent of the measurement technique.

Figure 4(a) shows a typical response from the photoelastic measurement with reflected signal magnitude and phase showing a clear mechanical resonance with narrow linewidth (high Q) and large signal-to-noise ratio (SNR). See Supplementary Information for data from all three groups. Figures 4(b–e) show the evolution of the mechanical resonance as a function of V_{DC} . The resonance frequency increases slightly as V_{DC} increases up to 21 V due to a weak mechanical nonlinearity (Fig. 4(b)). The measured Q at low V_{DC} values varies significantly, as seen in Fig. 4(c). These variations in Q are not physical and are due to the low SNR, demonstrating the need for high SNR when quantitative Q measurements are required. Figure 4(d) shows that the resonator amplitude is linearly related to V_{DC} , as expected for an electrostatic resonator, since the resonator strain is linearly proportional to the voltage measured by the network analyzer, where the highest SNR is at 21 V (Fig. 4(e)). To maximize SNR and minimize measurement uncertainty in Q , all further measurements are consistently reported at $V_{DC} = 21$ V and 10 mW AC power.

Measured values of the $f \times Q$ product for all three groups are presented in Fig. 5 as a function of the tether design. In every group of identical resonators, devices with 1-unit PnC tethers have a higher $f \times Q$ product than any of the straight-beam tether devices. As the number of PnC cells increases to 3 and 5 units, the $f \times Q$ product continues to increase. For the straight-beam tethers, transmission line theory indicates that the $\lambda/4$ tethers should provide the best isolation and the $\lambda/2$ tethers the worst isolation. This is found to only be partially true. While the $\lambda/2$ tethers consistently demonstrate the worst performance, the $\lambda/4$ tethers do not achieve the best results. The shorter $\lambda/8$ tethers outperform the $\lambda/4$ tethers on average. This is supported by other evidence that favors shorter tethers¹¹, showing that the simple transmission line model breaks down for finite tether dimensions, and suggests that the tether loss has a more nuanced dependence on the relation between the wavelength, dimensions, and aspect ratios for the straight-beam tethers. The measured $f \times Q$ products for Group B (227 MHz) follow the expected trend, but have a lower observed intragroup variation for straight-beam tethers. This anomaly is not easily explained and will be studied in future work.

The measured $f \times Q$ data for all devices are plotted across the frequency spectrum (Fig. 6), along with measured values for the best silicon WE-BARs in the literature within the targeted frequency range.^{2, 35, 36} The WE-BARs measured in this study are some of the highest frequency WE-BARs operating in their fundamental mode. While definitive comparisons are not possible between these and prior experiments due to subtle differences in material properties, the $f \times Q$ values are greater than or equal to the highest previously reported values for silicon WE-BARs and at higher frequencies. The maximum $f \times Q$ product measured in this study is 1.2×10^{13} Hz at 282 MHz (Group C, 5-period PnC tethers).

The total $f \times Q$ product can be written as $(f \times Q_{total})^{-1} = \sum (f \times Q_i)^{-1}$ for i contributing loss mechanisms. For the WE-BARs presented here, total dissipation is largely dominated by tether loss and phonon loss, with a smaller contribution from TED, based on analytical models for the two latter mechanisms,² as discussed below. For phonon loss in the Akhiezer

damping regime ($2\pi f_0\tau \ll 1$, where τ is the phonon lifetime), the $f \times Q$ product can be expressed as $f \times Q_{\text{phonon}} = (\rho v^2) / (2\pi C_v T \gamma^2 \tau)$, where ρ , v , C_v , T , and γ represent the mass density, longitudinal acoustic velocity, the volumetric heat capacity, the temperature and the Grüneisen parameter, respectively.¹⁻³ Most of these parameters have been well characterized for silicon with low uncertainty. The exception is the Grüneisen parameter which has a wide range of reported values.^{2, 3, 37} Details of the models for phonon and TED loss, and the material properties for the following analysis are included in the Supplementary Information. Fitting the highest measured $f \times Q$ value to $f \times Q_{\text{phonon}}(\gamma)$, and assuming accepted material properties, yields $\gamma = 0.815$. This is a reasonable value based on prior experiments using Raman spectroscopy, which ranged from 0.91 to 1.08.³⁷ The implicit assumption in this calculation is that the highest measured $f \times Q$ is limited only by phonon loss. To provide a point of comparison, γ can also be calculated assuming the measured $f \times Q$ is comprised of equal parts tether and phonon loss, or equal parts TED, phonon, and tether loss. These two cases recover unrealistically low values of γ , 0.577 and 0.471, respectively (see Fig. 6). This comparison indicates that the first calculation ($\gamma = 0.815$) is closest to the real situation. However, it is not intended to assign values to γ or to exactly apportion total loss amongst the various mechanisms. From this analysis, it is reasonable to conclude that the optimized 1-D PnC tethers play a large role in eliminating tether loss and that the best measured designs presented in this work have $f \times Q$ values approaching the fundamental phonon loss limits. In contrast to the PnC tethers, the measured $f \times Q$ values for straight-beam tether devices fabricated on the same substrate and with the same material properties are well below the most conservative values of the phonon loss and TED limits, leading to the conclusion that they are tether limited.

The experiments also reveal a trend that has not yet been explained. As seen in Fig. 6, the maximum measured $f \times Q$ product increases with frequency (from Group A – Group C). As the $f \times Q$ limits for the Akhieser regime of phonon loss and TED are independent of frequency, the best tether designs in each group are either: *i*) not yet fully optimized (i.e., the PnC reflectivity can be improved further), or *ii*) are limited by the residual, frequency dependent effects of some other loss mechanisms. Further separation and isolation of tether loss, phonon loss, and TED can be accomplished by testing these devices under varying temperature since the temperature dependence of tether loss is expected to be small relative to other mechanisms.

In summary, this letter presents a systematic investigation of PnC tether designs and their effect on tether loss and the $f \times Q$ product for micromechanical bulk acoustic resonators. For identical resonators, PnC tethers have a better $f \times Q$ product than the best values measured for conventional straight-beam tethers. The best $f \times Q$ values are comparable to, or better than the best reported values in the literature and have been demonstrated at higher frequencies than before. These experiments strongly support the use of PnC tethers to achieve the lowest possible tether loss, without modification to the design of the actual resonator, to attain Q values approaching the fundamental loss limits.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Acknowledgments

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FIG. 1. Scanning electron micrographs of two representative electrostatic WE-BARs. (a) 3-period PnC tethers, (b) $\lambda/2$ length straight-beam tethers, (c) magnified, tilted view of a PnC unit cell, and (d) expected mode shapes at resonance for displacement and in-plane strain, computed using finite element analysis.

FIG. 2.

Phononic dispersion curves and complete bandgaps for the three PnC unit cell designs, calculated using finite element analysis of the unit cells with 1-D Floquet periodic symmetry. The WE-BARs are designed so that the fundamental resonance frequency is within the bandgap, thus confining energy efficiently in the body of the resonator to reduce tether loss.

FIG. 3.

A schematic of the experimental setup for photoelastic strain measurements of a WE-BAR at high vibration frequencies. An intensity stabilized He-Ne laser is used as a probe, with free-space optics components (mirrors, collimators, long working distance microscope objective) to focus the laser beam on the surface of the WE-BAR. The WE-BAR is placed in a vacuum chamber with signal feed-through for RF and DC input signals. The reflected, strain-modulated laser signal is detected by a fast photodetector with a bandwidth of 1.4 GHz.

FIG. 4.

Resonance measurements. (a) Amplitude and phase response using photoelastic measurement for a representative WE-BAR (Group A, 3-unit PnC tethers). Inset: Measurement graphed over a wider span clearly shows the large SNR. (b)-(e) show the resonance frequency, quality factor, maximum signal amplitude, and the SNR respectively as functions of V_{DC} .

FIG. 5.

The measured $f \times Q$ products for each WE-BAR group as a function of their tether design. The PnC tethers have between 1 and 5 unit cells for each tether while the straight-beam tethers have varying lengths that are fractions of the acoustic wavelength. Between 2 and 4 devices are measured for each design. Error bars denote the standard deviation for the measured values.

FIG. 6.

The measured $f \times Q$ product for all PnC tether WE-BARs (red circles), and all straight-beam tether WE-BARs (green triangles) in this study compared to previously reported values (blue squares)^{1, 21, 22}, as a function of frequency. A maximum $f \times Q$ of 1.2×10^{13} Hz is measured at 282 MHz. Modeled values of $f \times Q_{\text{phonon}}(\gamma)$ indicate three hypothetical combinations of tether, phonon and TED loss (blue lines). The small residual frequency dependence in measured data indicates that $f \times Q$ can be improved further, and that while close, the Akhieser phonon loss and TED limits have not been fully reached since $(f \times Q)^{\text{max}}$ is independent of frequency in both limiting cases.

Table I**Resonator and Phononic Tether Specifications**

WE-BAR Specifications				
Group	w (μm)	l (μm)	Expected Frequency (MHz)	Measured Frequency (MHz)
A	25.5	80	162	167.06 ± 0.09
B	18.5	75	224	227.61 ± 0.17
C	14.5	65	286	281.86 ± 0.40

PnC Tether Specifications				
Group	a (μm)	b (μm)	$(a - b)/2$ (μm)	c (μm)
A	20	10	5	2
B	10	9	0.5	1
C	10	9	0.5	2