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Minimally diffracting quartz for ultra-low temperature surface acoustic wave resonators

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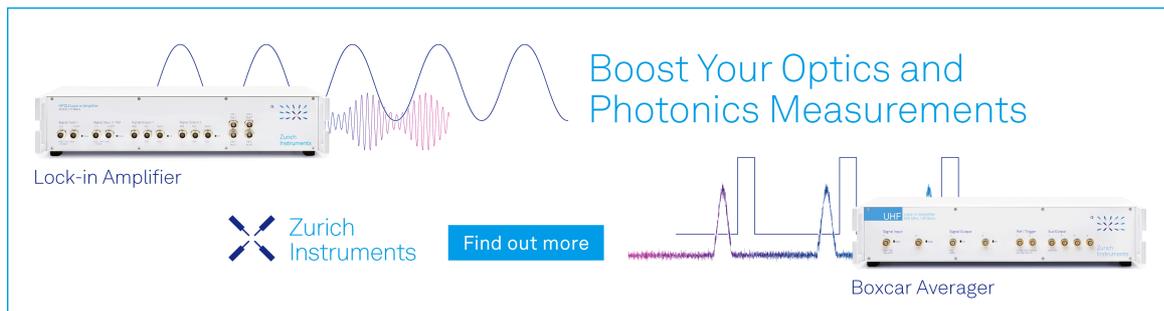
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ABSTRACT

We simulate and experimentally demonstrate the existence of an orientation of quartz, which minimizes diffraction losses in surface acoustic wave (SAW) resonators at ultra-low temperatures. The orientation is optimized for applications to quantum technologies, which benefit from high mechanical quality factors, strong electromechanical coupling, and narrow acoustic apertures. We fabricate narrow aperture SAW resonators on this substrate and measure internal quality factors greater than 100 000 at mK temperatures.

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Acoustic systems are promising resources, which offer quantum technologies a favorable combination of compact footprints,^{1,2} excellent coherence times,^{3–5} and the ability to connect disparate quantum systems.^{6–9} The emergent field of circuit quantum acoustodynamics (cQAD) has leveraged these advantages to create hybrid platforms that are capable of exploring fundamental quantum physics^{10–14} and offer the potential for quantum computation with acoustic processors.^{15–17} In particular, cQAD experiments utilizing surface acoustic wave (SAW) resonators have demonstrated increasingly sophisticated quantum control over phonons, including phonon number counting,¹² phonon-mediated qubit–qubit entanglement,¹⁸ and multipartite phonon entanglement.¹⁹

In a broad array of hybrid acoustic systems, maximizing coupling between a qubit and mechanical degrees of freedom is achieved by tightly confining mechanical strain.^{6,9,11,20–22} It can be difficult, however, to confine the strain without significantly increasing mechanical dissipation rates. In the particular example of cQAD with SAW resonators, this increase in dissipation results mainly from surface wave diffraction.¹² Consider a SAW resonator that is coupled to a nonlinear circuit element via the piezoelectric interaction of an interdigitated transducer (IDT). In such a configuration, shown in Fig. 1(a), the added IDT capacitance reduces the nonlinearity of the superconducting circuit. Thus, for many applications, the IDT capacitance must be small, corresponding to a narrow acoustic aperture W on the order of several acoustic wavelengths, λ . However, acoustic diffraction losses in SAW resonators scale quadratically with the inverse of aperture width causing resonators in this regime to suffer from high loss rates.¹² This

loss significantly limits the mechanical coherence time of hybrid systems based on SAW resonators and, thus, restricts their capabilities for quantum information processing.

Although it is possible to mitigate the deleterious effects of acoustic diffraction by appropriately curving the cavity boundaries, accomplishing this with piezoelectric media is complicated by their inherent anisotropy,^{3,23,24} anisotropy of phase velocity, electromechanical coupling, and reflectivity must all be considered. Rather than compensating for this anisotropy, it is possible to instead exploit it into naturally suppressing acoustic diffraction. At special orientations of some piezoelectric materials, as shown in Fig. 1(b), the anisotropy will induce an angle-dependent beam-steering such that waves will propagate predominantly along one axis of the substrate. The resulting wavefronts are flat and propagate with minimal diffraction spreading. Substrates that exhibit this property are known as minimally diffracting (MD) materials.¹

Our goal is to find an MD orientation of quartz, which is suitable for cQAD platforms. We choose quartz for its extremely low bulk mechanical losses at mK temperatures²⁵ and its relatively strong piezoelectricity. An MD orientation of quartz for room-temperature SAW devices was previously identified,^{26,27} however, the temperature dependence of the piezoelectric and elastic coefficients of quartz causes this cut to lose its MD property as it is cooled to ultra-low temperatures. This motivates the search for an orientation of quartz, which minimizes SAW diffraction in the low-temperature limit.

In this work, we use finite element method (FEM) simulations to model diffraction and beam-steering for ultra-low temperature quartz to search for an MD orientation suitable for quantum experiments.

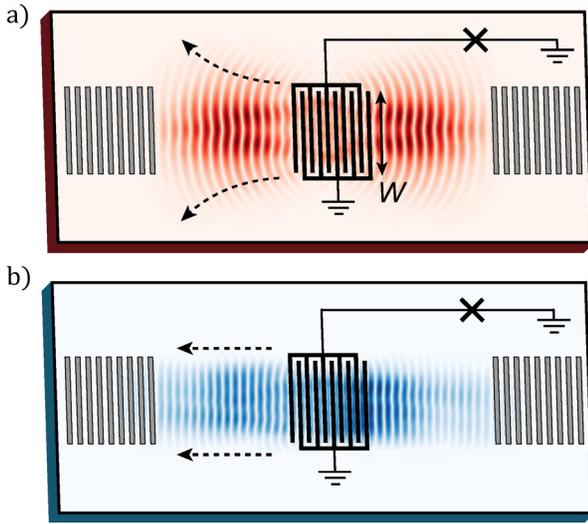


FIG. 1. Comparison of SAW diffraction on two orientations of quartz. (a) An IDT with aperture W is galvanically connected to a nonlinear circuit element (\times) on ST quartz, a common orientation of quartz for SAW devices.¹ A voltage across the IDT launches SAWs (simulated displacement amplitude shown in red), which are confined by Bragg reflectors (gray) to form a multimode acoustic cavity. The IDT, circuit elements, and Bragg reflectors are cartoons overlying SAWs shown shortly after launch in time-domain finite-element simulations. As the SAWs propagate, they diffract outwards and introduce loss in the resonator. (b) An identical geometry on a minimally diffracting (MD) orientation of quartz. SAWs (blue) on an MD orientation of quartz diffract less as they propagate, facilitating high mechanical quality factors with small IDT capacitances.

From these simulations, we identify an orientation of quartz at Euler angles²⁸ $(\psi, \phi, \theta) = (0^\circ, 40.2^\circ, 23.4^\circ)$, which minimizes SAW diffraction and beam-steering to second-order when cooled to ultra-low temperatures. We fabricate SAW resonators with two flat reflectors (see Fig. 1) on quartz at this orientation, which demonstrate high internal quality factors ($\sim 28\,000$) with very narrow (10λ) acoustic apertures. This represents a $25\times$ improvement over equivalent resonators on ST quartz, a popular orientation of quartz for SAW devices.¹ Slightly wider resonators on this substrate ($W > 25\lambda$) demonstrate extremely high internal quality factors ($Q > 110\,000$); achieving similar quality factors with narrow aperture resonators on non-MD substrates is impossible without complicated anisotropic focusing procedures. We conclude that this orientation, which we name “cryogenically optimized low diffraction” (COLD) quartz, exhibits minimal diffraction at mK temperatures.

Minimal diffraction in anisotropic materials can be understood as an effect of beam-steering, a phenomenon that causes a beam in an anisotropic medium to propagate in a direction which is not normal to the wavefront. The beam-steering angle η is the difference between the directions of the SAW wave vector \hat{k} and energy flow vector \hat{S} [Fig. 2(a)]. It can be calculated from $v(\theta)$, the SAW phase velocity as a function of planar rotation¹

$$\eta(\theta) = \tan^{-1}\left(\frac{1}{v(\theta)} \frac{dv(\theta)}{d\theta}\right). \quad (1)$$

Beam-steering vanishes at angle θ_0 for which $v(\theta)$ exhibits a stationary point. However, any finite-width IDT oriented at θ_0 will transduce SAWs at a spectrum of angles around θ_0 which, on an anisotropic substrate, necessarily exhibit beam-steering. The second-order diffractive

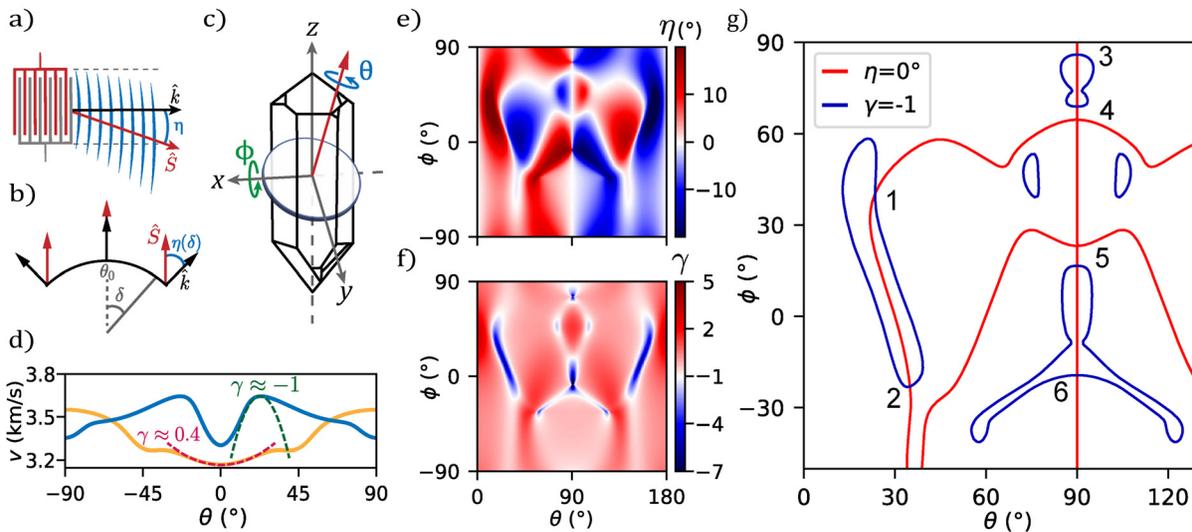


FIG. 2. Simulated SAW characteristics. (a) An IDT launches SAWs on an anisotropic substrate which exhibits beam-steering. (b) Minimal diffraction occurs when $\eta(\delta) = -\delta$ so that $\hat{S}(\delta)$ is constant and transduced SAWs propagate with minimal diffraction spreading. (c) A wafer oriented relative to quartz crystallographic axes: ϕ determines the angle at which the wafer is cut from a monocrystalline bar, and θ determines the planar rotation of a device about the wafer normal. (d) SAW velocity is shown as a function of the planar rotation for MD (blue) and ST (orange) quartz. (e) The beam-steering angle η is calculated from the simulated velocity profiles for all θ and ϕ . (f) From the simulated beam-steering, we calculate the diffraction parameter γ . (g) The contours for minimal beam-steering (blue) and diffraction (red) are overlaid. The six unique intersections of the curves represent potential MD orientations.

spread of the beam width due to this off-axis beam-steering is characterized by the diffraction parameter γ ,

$$\gamma = \frac{d\eta}{d\theta}, \quad (2)$$

which can be used to calculate the diffraction-limited quality factor Q_d of a flat SAW cavity on an anisotropic substrate²⁹

$$Q_d = \frac{5\pi}{|1 + \gamma|} (W/\lambda)^2. \quad (3)$$

Diffraction is reduced (compared to isotropic substrates) for materials where $-2 < \gamma < 0$ and otherwise increased.¹ ST quartz, for example, exhibits accelerated wave diffraction $\gamma = 0.378$, and isotropic materials exhibit $\gamma = 0$. Minimal diffraction occurs when $\gamma = -1$, a special condition such that beam-steering at small angles δ around some orientation θ_0 follows $\eta(\delta) \approx -\delta$. In this circumstance, waves transduced at angle $\theta_0 + \delta$ by a finite-width IDT will propagate in the direction θ_0 . Thus, when $\gamma = -1$, as shown in Fig. 2(b), \hat{S} points in the same direction irrespective of k , and SAWs will propagate with minimal diffraction spreading.

We, thus, search for an orientation of quartz, which (i) exhibits $\eta \approx 0^\circ$, (ii) exhibits $\gamma \approx -1$, (iii) and is tolerant to potential errors in manufacturer cutting. Due to the trigonal structure of alpha quartz, three Euler angles (ψ , ϕ , θ) are necessary to uniquely describe the orientation of a device relative to some crystallographic axes.²⁸ In this work, however, we consider only cuts where $\psi = 0^\circ$; this constraint excludes “doubly rotated” orientations, which are more difficult to cut and may result in greater variation of the final substrate orientation. The remaining angles (ϕ , θ) are illustrated in Fig. 2(c): ϕ describes the angle between the wafer-normal and the crystallographic Z-axis while θ corresponds to a planar rotation about the wafer-normal.

Using FEM simulations,³⁰ we generate velocity curves $v(\phi, \theta)$ in the space $(\psi, \phi, \theta) = (0^\circ, -90^\circ : 90^\circ, 0^\circ : 180^\circ)$ and apply Eqs. (1) and (2) to calculate η and γ . The basis of the simulations is a 3D unit cell with two pairs of periodic mechanical and electric boundary conditions in the longitudinal and transverse dimensions. An eigenfrequency study reveals surface wave modes for a particular orientation, and the velocity of the lowest frequency mode is traced to produce $v(\phi, \theta)$. From the simulation, we also determine the SAW polarization supported by a given orientation. In particular, we search for Rayleigh-polarized (R) SAWs, which exhibit less propagation attenuation than shear-horizontal (SH) or other non-Rayleigh polarizations.¹ The crystallographic orientation is specified by rotating the piezoelectric and elastic tensors relative to the unit cell axes. To model low temperature quartz, we use piezoelectric and elastic coefficients for right-handed alpha quartz measured at 5 K.³¹ Simulated velocity curves for MD ($\phi = 40.2^\circ$) and ST ($\phi = -47.25^\circ$) quartz are shown in Fig. 2(d).

In Figs. 2(e) and 2(f), we plot the values of η and γ calculated from the simulated velocities. The contours, along which beam-steering and diffraction are minimized, are plotted in Fig. 2(g). Although the six unique intersections of these curves represent potentially desirable cuts, we find that only one is suitable for further study; the relevant properties for each cut are listed in Table I. To verify that a small error in the wafer cutting will not destroy the MD behavior, we also calculate the sensitivity parameters $|d\eta/d\phi|$ and $|d\gamma/d\phi|$. We find that orientation 1 is Rayleigh-polarized, demonstrates high

TABLE I. $\psi = 0^\circ$ 5 K quartz cuts.

	ϕ, θ ($^\circ$)	$ d\eta/d\phi $	$ d\gamma/d\phi $ ($^\circ$)	v (m/s)	Type	k^2 (%)
1	40.2, 23.4	0.41	0.003	3643	R	0.16
2	-23.1, 34.9	0.09	0.08	3374	SH	0.15
3	86.0, 90.0	~ 0	0.07	3890	R	~ 0
4	68.9, 90.0	~ 0	0.37	3778	SH	0.03
5	16.5, 90.0	~ 0	0.17	3379	SH	0.10
6	-19.3, 90.0	~ 0	0.2	3765	R	~ 0

tolerance to cut errors, exhibits a large electromechanical coupling k^2 , and minimizes diffraction. We name this orientation “COLD” quartz.

We procured COLD quartz wafers from a vendor with quoted tolerance ($\pm 0.1^\circ$, $\pm 0.03^\circ$, $\pm 0.1^\circ$). To test the performance of the substrate, we first fabricate a series of one-port resonators and vary the angle θ at which each device is oriented relative to the crystallographic axes. Double-finger IDTs^{1,29} are patterned from a 25 nm aluminum film, and SAWs are confined by etched Bragg mirror gratings with 250 elements and a reflectivity of 1 – 2% per element. The resonators are designed with wavelength $\lambda = 7.28 \mu\text{m}$ and a mirror-to-mirror cavity length of 150λ . These resonators are designed with a narrow (10λ) aperture so that losses are dominated by diffraction. In Fig. 3(a), we show the spectrum from a microwave reflection measurement of a single $\theta = 23.4^\circ$ device mounted on the baseplate of a dilution refrigerator, which is at a temperature of 20 mK. The central mode occurs at 500.24 MHz, corresponding to a 3641.7 m/s speed of sound which is 0.02% lower than the predicted value of 3642.6 m/s. This mode exhibits an internal linewidth²⁹ $\kappa_i/2\pi = 18.1$ kHz. Using Eq. (3), this represents a factor of 25 decrease in linewidth compared to an equivalent resonator on ST quartz.

In Fig. 3(b), we observe a strong dependence of the central mode internal linewidth on θ as the resonators are rotated in 0.1° increments about the wafer surface normal. At room temperature, internal loss is minimized at $\theta = 22.5^\circ$, which is in strong agreement with our simulations. As the resonators are cooled, the central angle of minimal loss shifts to 23.7° . This is higher than the predicted angle of minimal diffraction (23.4°), but this discrepancy can be understood as a result of the velocity profile asymmetry. As the aperture width is reduced, higher angle wave vectors with non-symmetric beam-steering increasingly contribute to the transduced wavefront. This produces an additional width-dependent *effective* beam-steering η_{eff} , which is not described in Eq. (1). This phenomenon shifts the angle of minimal loss from 23.4° to 23.7° , an effect discussed in detail in the [supplementary material](#). For wider aperture devices, we expect the angle of minimal loss to shift back to 23.4° as η_{eff} approaches 0° .

To measure γ , we next fabricate a series of SAW resonators at $\theta = 23.4^\circ$, which sweep aperture width from 5λ to 40λ . In Fig. 4, we observe at both room temperature and 20 mK a monotonic decrease in internal loss as the acoustic aperture of these devices is increased. We fit the data to Eq. (3) and find that the substrate exhibits $\gamma = -0.73 \pm 0.01$ and $\gamma = -0.95 \pm 0.01$ at room temperature and 20 mK, respectively. At 20 mK, the apparent decrease in loss with increasing aperture width saturates at $W = 30\lambda$, for which the device demonstrates $\kappa_i/2\pi = 4.5$ kHz. This corresponds to an internal quality factor of 110 000, which is on the order of state-of-the-art SAW resonators.³²

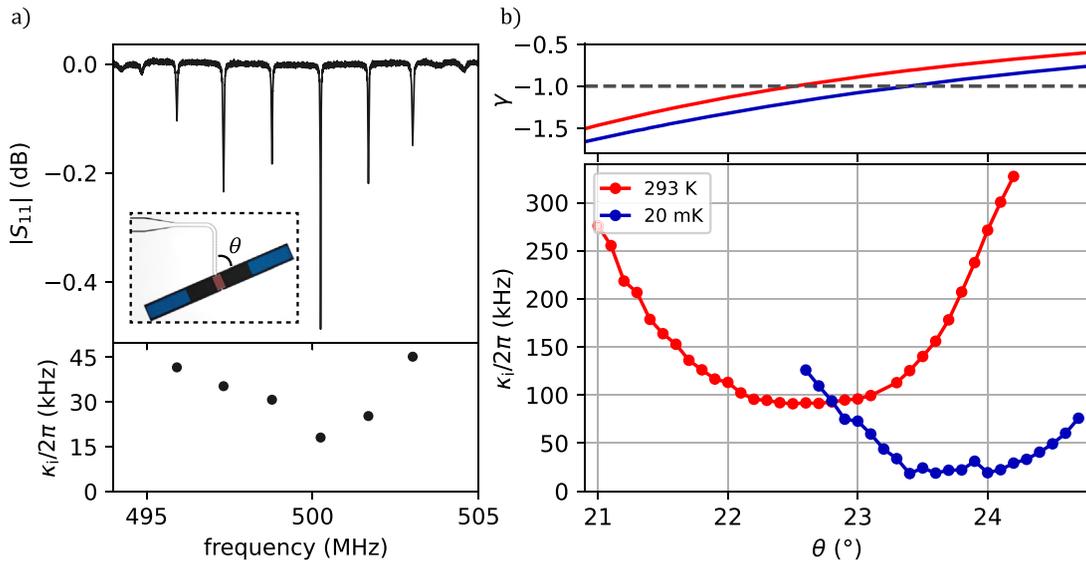


FIG. 3. Resonator loss and planar rotation. (a) A reflection measurement from a one-port SAW resonator fabricated at $\phi, \theta = (40.2^\circ, 23.4^\circ)$ and mounted on the baseplate of a dilution refrigerator cooled to 20 mK. The resonator (false-colored optical image in the inset) consists of a double-finger IDT (red) and Bragg mirror gratings (blue), which are designed with a narrow acoustic aperture (10λ). Aluminum (white) is etched away (black) to define the coplanar waveguide, IDT, and SAW cavity. Internal linewidth for each mode is plotted below. (b) Top: simulated γ for SAWs on $\phi = 40.2^\circ$ quartz at 293 K (red) and 5 K (blue). Minimal diffraction is predicted at $\theta = 22.5^\circ$ (23.4°) for warm (cold) devices. Bottom: the measured internal linewidth of the central resonator mode of each device as θ is incremented across many devices. Fit errorbars for all data points are smaller than the marker size.

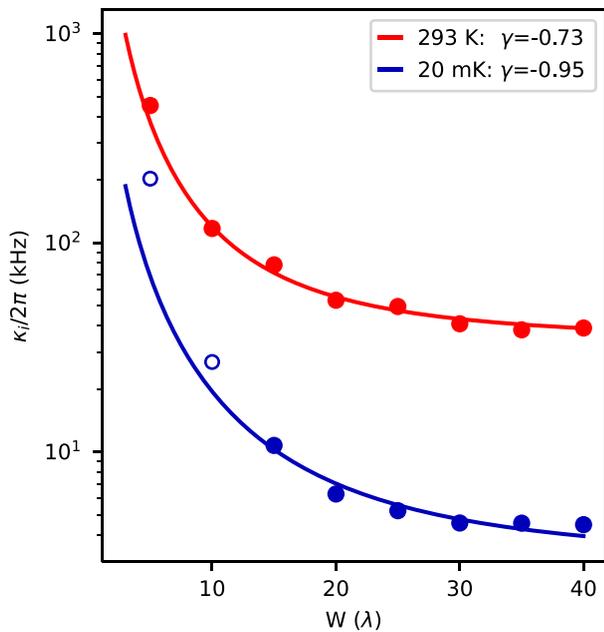


FIG. 4. Measurement of diffraction parameter. Internal linewidth of SAW resonators measured at room temperature (red) and 20 mK (blue), which sweep the acoustic aperture width. Solid lines show fits to Eq. (3), for which we find $\gamma = -0.73$ at room temperature and $\gamma = -0.95$ at 20 mK. Open circles show widths for which asymmetric diffraction becomes comparable to the residual second-order diffraction, and Eq. (3) becomes incapable of accounting for the loss. Fit errorbars are smaller than the marker size.

Notably, the fit diverges for the narrowest resonators with $W \lesssim 10\lambda$ measured at 20 mK. At these widths, odd-order contributions to diffraction loss from the asymmetric surface velocity begin to dominate, and Eq. (3) becomes inadequate for describing the losses.

There are two approaches to reduce these residual beam-steering losses: compensate for η_{eff} with device geometry or choose an orientation for which all odd-order derivatives of $v(\theta)$ vanish. Preliminary experiments suggest that it is possible to mitigate η_{eff} loss by fabricating resonators, which have a mirror aperture slightly wider than the IDT aperture to capture the misaligned portion of the beam; however, further study on this subject is required. Alternatively, the phenomenon of narrow-aperture-induced effective beam-steering can be eliminated entirely by choosing an orientation, which lies along a crystalline symmetry axis so that the velocity profile is fully symmetric about the propagation axis. Unfortunately, of the two symmetry-axis R-polarized SAW orientations identified in Table I, both exhibit extremely low k^2 . Future work may explore doubly rotated cuts where $\psi \neq 0^\circ$ to search for an MD orientation of quartz, which exhibits both greater symmetry in $v(\theta)$ and nonzero k^2 .

Improving the lifetimes of mechanical resonators coupled to superconducting circuits is critical for maximizing the capabilities of cQAD systems. By discovering a substrate which naturally suppresses SAW diffraction losses, we have provided a solution to the dominant loss source observed in previous SAW-qubit devices.¹² This will allow this class of devices to be pushed further into the strong-dispersive regime^{12,33,34} to facilitate the exploration of multimodal quantum information processing. COLD quartz may also be useful in the creation of low-loss cryogenic delay lines,^{35,36} phononic waveguides,^{37,38} and electro-acoustic phase modulators.³⁹ Crystallographic optimization has

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become less common in recent decades as standard crystal orientations for acoustic devices have emerged. In studying a nonstandard orientation of quartz, we highlight the remaining utility of crystallographic engineering for quantum applications.

See the [supplementary material](#) for more information on FEM simulations, effective beam-steering, and fabrication methods.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Alec L. Emser: Conceptualization (lead); Data curation (lead); Formal analysis (lead); Investigation (lead); Methodology (equal); Visualization (lead); Writing – original draft (lead); Writing – review & editing (lead). **Brendon C. Rose:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Writing – review & editing (equal). **Lucas R. Sletten:** Conceptualization (equal); Data curation (equal); Investigation (equal); Writing – review & editing (supporting). **Pablo Aramburu Sanchez:** Formal analysis (supporting); Writing – review & editing (supporting). **Konrad Lehnert:** Conceptualization (equal); Formal analysis (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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