A metasurface comprising spiral shaped local resonators for surface acoustic waves

V Kyrimi, B J Ash and G R Nash

College of Engineering, Mathematics and Physical Sciences, University of Exeter, Exeter EX4 4QF, United Kingdom

E-mail: vk247@exeter.ac.uk

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Abstract
The interaction of Rayleigh waves, propagating on lithium niobate, with a metasurface consisting of a square array of spiral-like vertical oscillators is investigated. We observe confinement of the acoustic energy throughout the height of the oscillators and note that this confinement also takes place at relatively low frequencies compared to circularly symmetric resonators of similar dimensions. A transmission study reveals that the bandgap attenuation is large (~25 dB) at both high and low frequencies, a characteristic that could be exploited in the design of new RF filters.

Keywords: surface, acoustic, waves, local, resonator, attenuation, bandgap

(Some figures may appear in colour only in the online journal)

1. Introduction

The confinement of acoustic energy has attracted much attention in recent years with a number of different confinement mechanisms used to induce this phenomenon, including the slowing down of the velocities of surface acoustic waves (SAWs) [1], or exploiting the property of inhomogeneous media to have continuously varying longitudinal and shear velocity profiles [2], the latter exhibiting localization even at the anti-resonance frequency. SAWs are characterised by displacements which decay exponentially with depth into an elastic material, and the maximum amplitude of the displacement induced by a SAW is small compared to the SAW wavelength. The interaction of SAWs with resonant structures patterned on a semi-infinite medium [3, 4] or on a slab [5], is very promising for various technological applications due to the ability to create bandgaps for SAW devices. Apart from the confinement of acoustic energy, which allows the realisation of wave-guides and cavities, SAW bandgaps can also be used in radio frequency communications [6], sensing [7] and wireless communications [8].

Bandgap formation for elastic waves in 2D systems consisting of two composite materials, the host and the periodic structure, is dependent on both the velocity ratio and the filling ratio between the constituent materials in the case of Bragg bandgaps [9]. These Bragg gaps have centre frequencies corresponding to wavelengths up to two times the spatial period of the crystal. Recently investigated locally resonant band gaps, on the other hand, are typically centred at wavelengths at least two times larger than the spatial period of the crystal, and hence can achieve much lower frequency gaps compared to Bragg gap structures. Different geometrical configurations of resonant structures have been employed to create low frequency band gaps, such as silicon cylindrical pillars [3] and annular holes [4] for SAWs, and cylinders with a split ring cross section [10] for photonic/phononic crystals. Phononic crystal plates with periodic spiral resonators [11] have also been used to create low frequency bandgaps in the 100 Hz range. This type of interesting structure is used both by nature in the process of hearing (cochlea in human ear allows a certain frequency range to pass through (200 Hz–20000 Hz)), by humans to construct a metamaterial that acts as attenuator for chiral seismic waves [12], and as a broadband acoustic skin cloak [13]. Moreover, thanks to its structural degrees of
freedom, a spiral resonator is a good candidate for allowing the tailoring of bandgap frequency and bandwidth.

In this work, we investigate the dispersion relation of a metasurface structure, designed to control SAWs, consisting of a void/lithium niobate phononic crystal atop a lithium niobate substrate. Lithium niobate is one of the most important, and common, materials used in SAW devices due to its exceptional properties, including very strong piezoelectricity [14]. The void wall is of an Archimedean spiral shape and the spiral microgrooves shown in figure 1(a) will be referred to as spiral resonators. The lattice constant used is $\alpha = 10.9 \mu m$ and we observe bandgaps at SAW wavelengths down to $\lambda_{SAW} = 26.4 \mu m$, meaning $\frac{\lambda_{SAW}}{\alpha} = 2.42$, a ratio made possible by the locally resonant bandgap. The study shows significant acoustic energy confinement in the direction perpendicular to the surface and for certain guiding modes supported by the metasurface. Dispersion relations and displacement fields are compared to the results of a previously reported annular hole structure [4]. Enhanced acoustic energy confinement is demonstrated by the resonator’s volume being reduced. Moreover, we demonstrate that the proposed structure can shift the bandgap frequency to extremely low values, implying that the corresponding operating wavelength at the band gap is much bigger than the typical scale of the medium, as was the case in the first acoustic metamaterial studied by Sheng et al [15]. Additionally, it is shown that the increased structural degrees of freedom with respect to the annular hole structure has the effects of (i) either creating an additional bandgap at higher frequencies or (ii) increasing the bandwidth of the low frequency bandgap. A comparison between the dispersion relations and displacement field profiles for the above-mentioned structures is used to explain the absence of certain modes. Finally, by changing the depth of the spiral resonator, two modes, one of low and one of high frequency, appear to intersect the sound line with negative slope and hence negative group velocity, meaning that SAWs can propagate in an unconventional way throughout the device.

2. Numerical modeling

A finite element (FE) model of the unit cell of width 10.9 $\mu m$ and depth 10.9 $\mu m$, as shown in figure 1(a), was developed in COMSOL Mutiphysics with a perfectly matched layer (PML) placed at the bottom region to avoid wave reflection. The top face of the unit cell is stress-free to allow bulk shear and longitudinal modes to couple and generate Rayleigh waves. The bottom face of the unit cell is constrained with a boundary condition imposing zero displacement. The spiral-like resonator, whose details are shown in figure 1(b), is a 6.4 $\mu m$ thickness void, atop a lithium niobate substrate. The triangular cross section with the $xz$ plane is shown in figure 1(d). Bloch–Floquet periodic boundary conditions are imposed at opposite sides of the square unit cell and a parametric sweep of wavevectors allows for the dispersion relation along the irreducible Brillouin zone shown in figure 1(c). Note that the model assumes that there is no loss within the lithium niobate.

3. Results

3.1. Dispersion analysis

Figure 2 contains the dispersion relations and displacement profiles of three different metasurfaces, previously investigated annular holes and two types of spiral resonators, Spiral-I (as shown in figure 1) and Spiral-II which has fewer spiral turns. In figure 2(a), the dispersion relation for the spiral-like structure Spiral-I, blue dots, indicates that the number of guided modes is increased compared to the guided modes supported in the previously investigated annular hole structure, red dots. Both structures are of the same height and in-plane width, as shown in the first column of figure 2(b), where the cross section of each within the $xz$ plane is shown. Although there are three high symmetry directions in the reciprocal space, note that figure 2(a) shows only the $\Gamma X$ direction, as propagation in this direction is widely used in practice for lithium niobate devices.

The increase of guided modes is associated with the number of spiral turns as confirmed by the dispersion relation of a second structure, Spiral-II, the dispersion curve for which is shown in green dots in figure 2(a). In the selected frequency region (70 Hz–130 Hz), the annular hole structure and the Spiral-II structure both exhibit three modes, whereas the Spiral-I structure, in which the number of spiral turns is increased, exhibits five modes. The rms displacement fields for the three structures at the three faces of the unit cell are shown in figures 2(b)–(d). The rms displacement field is defined as $\frac{1}{V} \sqrt{\int \left(A_x^4 + A_y^4 + A_z^4\right)}$, where $A_x, A_y, A_z$ is the amplitude of the displacement field in the $x, y, z$ directions, respectively. Displacement fields are shown at frequencies in which the third higher mode intersects the Brillouin zone boundary in the $\Gamma X$ direction (annotated in blue, red and green triangles in dispersion curves). It can be seen that surface displacement is more pronounced at the upper half of the Spiral-I resonator whereas the whole height of the annular holes resonator experiences significant displacement (figure 2(b)). In other words, large dissipation of the displacement field takes place in the Spiral-I structure, as it is shown in figure 2(c). Dissipation of the displacement field is even larger for the Spiral-II structure, as shown in figure 2(d). Note that the dissipation of displacement fields is not associated with damping of the acoustic wave into other forms of energy, but with the excitation of the resonator, and is significant for all the guided modes supported by the Spiral-II structure (results not shown here). Acoustic energy is confined to the upper half of the resonator whereas for Spiral-II, but the displacement field intensity is decreased compared to the denser spiral since the interface area between the Rayleigh wave and the resonator is decreased. Therefore, coupling is weaker and the energy needed to guide the mode 3 is higher, hence the frequency of the third higher mode at the Brillouin zone border is 126 MHz.

Dissipation results from the geometric chirality which is the main structural difference between annular holes and Spiral-I/Spiral-II structures. It has been shown [12] that there is analogy between chiral electromagnetism and acoustic
Figure 1. (a) Schematic of the unit cell model. (b) Magnification in green frame shows details of the top face of the unit cell. Yellow dashed lines are parallel to the $x$-axis connecting the centres of the voids. The central void’s coordinates are $(x_c, y_c) = (5.45 \, \mu m, 5.45 \, \mu m)$. (c) Blue triangle denotes the irreducible Brillouin zone of the square lattice. $\Gamma X = XM = \frac{\pi}{\alpha}$, $XM = \sqrt{2} \frac{\alpha}{\pi}$, where $\alpha = 10.9 \, \mu m$, is the lattice constant. (d) Left panel: Spiral-I appearing in figure 4 in the manuscript. Its parametric equation is $x(t) = 0.4t \cos t \, [\mu m], y(t) = 0.4t \sin t \, [\mu m], 0 \leq t \leq 4\pi$. Middle panel: Spiral-II appearing in figures 2, 4 and 5. Its parametric equation is $x(t) = 0.4t \cos t \, [\mu m], y(t) = 0.4t \sin t \, [\mu m], \frac{7\pi}{4} \leq t \leq 4\pi$. Right panel: Spiral-I with an inversed direction sweep, appearing in figures 1, 2 and 6 in the manuscript. Its parametric equation is $x(t) = 0.4t \cos t \, [\mu m], y(t) = 0.4t \sin t \, [\mu m], x'(t) = y(t), y'(t) = x(t), 0 \leq t \leq 4\pi$. (e) Projection of $xz$-plane with the $y$-coordinate fixed at $y = 5.45 \, \mu m$ (i.e. in the middle of the unit cell), on the $xz$-plane at $y = 0 \, \mu m$. The voids are depicted in white and the lithium niobate substrate is shown in grey colour. The yellow dots mark the centre of the voids, also shown in (b).

Figure 2. (a) Dispersion relations in the $\Gamma X$ direction for the Spiral-II (green dots), annular holes (red dots) and Spiral-I (blue dots) structures. The area beyond the sound line is shaded in light grey. (b) From left to right: projection of the annular hole structures to the $xz$-plane, displacement field profiles at $X$ point and at $f = 127.8$ MHz (denoted in red triangle), in the $yz$, $xz$ and $xy$ planes. (c) From left to right: projection of the Spiral-I structure to the $xz$-plane, displacement field profiles at $X$ point and at $f = 110.6$ MHz (denoted in blue triangle), in the $yz$, $xz$ and $xy$ planes. (d) From left to right: projection of the Spiral-II structure to the $xz$-plane, displacement field profiles at $X$ point and at $f = 125.9$ MHz (denoted in green triangle), in the $yz$, $xz$ and $xy$ planes.
seismic waves introducing an imaginary component to the phase velocity of acoustic waves. Hence, the evanescent displacement field of the SAWs in the Spiral-I/Spiral-II structures is associated with the imaginary wavevector induced by chirality.

It is worth noting that the third higher mode of the annular hole structure almost coincides with the third higher mode of the Spiral-II structure for small magnitude wavevectors. However, for larger wavevector magnitudes the third higher mode for the Spiral-II structure diverges towards lower frequencies. The rms displacement fields showing the top face of the unit cell (right panels in figures 2(b)–(d)) reveal that displacement fields in the centre of the unit cell are smaller compared to the displacement field at the unit cell edges for all three structures. This third higher mode in frequency is referred to as anti-resonant mode. Except for bringing the frequency of the anti-resonant mode down, chirality also affects the group velocity of the anti-resonant modes as shown in figure 3. The group velocity of the anti-resonant modes for the annular hole, Spiral-I and Spiral-II structures is shown by the red, blue and green solid lines respectively. The group velocities of the Spiral-II and Spiral-I structures are clearly lower than the group velocity of the annular hole structure for wavevectors in the range \(2.1 \times 10^5 \text{ m}^{-1} – 2.75 \times 10^5 \text{ m}^{-1}\). At \(k = 2.1 \times 10^5 \text{ m}^{-1}\), the group velocities of the Spiral-I structure (696 m s\(^{-1}\)) and the Spiral-II structure (1085 m s\(^{-1}\)) are 50% and 23% lower than the annular hole structure group velocity (1411 m s\(^{-1}\)) respectively. At wavevectors approaching the first Brillouin zone border, the anti-resonant mode of the Spiral-I structure has a very slow group velocity (95 m s\(^{-1}\)) compared to the Spiral-II and annular hole modes (230 m s\(^{-1}\)).

### 3.2. Transmission analysis

Transmission spectrums were obtained using the COMSOL Multiphysics frequency domain model, as shown schematically in figure 4(a). An interdigital transducer (IDT) defined on the surface of the lithium niobate substrate is used to excite SAWs. The displacement field profile of the IDT source is minimal in the light blue regions. The substrate is surrounded by PMLs. Zoomed insets of the three different metasurface structures investigated in separate computational models are highlighted in dashed boxes. The substrate length, \(L\), is scaled so that the distances between the metasurface and the other domain features are always the same integer values of \(\lambda_{\text{SAW}}\). This was done to maximise computational resources for any given frequency.

In figure 4(b), the calculated transmission spectrum of the Spiral-I and Spiral-II structures is shown by blue and green solid lines respectively. Note that the Spiral-I and annular-hole structures used to calculate the results shown in figure 4 are different to those used to calculate the results shown in figure 2, but were chosen to allow a better comparison with previously reported annular hole results. For comparison, the transmission spectrum of the previously reported annular hole structure of width 2 \(\mu\text{m}\) is also shown by the red solid line.

**Figure 3.** Group velocity versus wavevector for the anti-resonant mode of (i) the Spiral-II structure (green solid line), (ii) the annular holes structure (red solid line) and (iii) the Spiral-I structure (blue solid line).

The structural parameter width is denoted in black arrows in figure 1(b). The 0.4 \(\mu\text{m}\) wide Spiral-I structure exhibits a transmission minimum at about 80 MHz, whereas the annular hole structure exhibits a transmission minimum at 90 MHz. This demonstrates that the bandgap can be shifted to lower frequencies without the need to increase the size of the unit cell, making the realisation of RF based PhC filters and other components, easier and more cost-effective. The corresponding acoustic wavelength at the transmission minimum is 4.5\(\alpha\) for the Spiral-I, and 4\(\alpha\) for the annular hole, where \(\alpha = 10.9 \mu\text{m}\) is the lattice constant, meaning that the Spiral-I structure is deeply subwavelength at the bandgap frequency region. Moreover, a second transmission minimum is shown at a frequency of 130 MHz for the Spiral-I structure which corresponds to a wavelength of 2.7\(\alpha\). This is of interest in the realisation of stop band filters. The maximum bandgap attenuation for the Spiral-II structures occurs at 83 MHz, and the bandgap attenuation in this case is significant for a wider frequency range compared to the other structures. The attenuation bandwidth can be tuned by controlling the eigenmode coupling to the Rayleigh wave (see section 3.3).

### 3.3. Dispersion/Transmission comparison

It is well known that acoustic waves incident on PhCs cannot excite all the modes predicted in theory or in computational models due to the modes’ field profiles [16]. In order to understand which of the modes can be excited using the IDT SAW source shown in section 3.2, band diagrams are plotted alongside calculated transmission on a common frequency axis in figure 5. It is clear that for the annular hole structure, mode B is highly attenuated since at that frequency the bandgap attenuation is \(-20\) dB whereas for the spiral-II structure, mode A is highly attenuated, with the bandgap attenuation reaching the value of \(-25\) dB. Observation of the above-mentioned modes displacement fields, shown in the middle panel of figure 5, and comparison to the source’s displacement field, shown in
Figure 4. (a) Frequency domain geometry schematic showing the SAW excitation source and the metasurface on top of lithium niobate substrate surrounded by PMLs. Bottom inset shows the displacement profile field in the area of the IDT transducer. Dashed boxes zoom in the area occupied by the local resonators. (b) Transmission spectrum for annular holes (red), Spiral-I (blue) and Spiral-II (green) structures.

Figure 5. From left to right: dispersion curve, bandgap attenuation and rms displacement fields for the Spiral-II structure. Rms displacement fields, dispersion curve and bandgap attenuation for the annular holes structure. A, B, and C annotate the frequency for which displacement rms fields are plotted. The magnitude of momentum in the ΓX direction at A, B and C points equals $2.88 \times 10^5 \text{ m}^{-1}$.

Figure 4, reveals that there is no correlation between the displacement field patterns of the source and the eigenmodes of the resonators. However, modes B and C in the Spiral-II structure and modes A and C in the annular holes structure show one common feature in their rms displacement fields; small rms displacement fields in the centre of the unit cell and in the area outside the resonator, and large displacement fields at the unit cell edges. The smaller bandgap attenuation values for these modes can be explained by considering again the stripe-like displacement field pattern of the source, the larger the area of the unit cell that the eigenmode’s displacement field matches the source’s displacement field, the larger the coupling of the eigenmode to the incident Rayleigh wave, and hence the smaller the bandgap attenuation. This is confirmed by observing that bandgap attenuation for anti-resonant modes (C modes) is around 0 dB, whereas for mode B in the Spiral-II structure, the attenuation is significantly larger, around $-15 \text{ dB}$. Comparison of the C eigenmodes’ fields to the source indicates higher spatial correlation compared to that between the displacement field of Spiral-II B mode and the source. Moreover, comparison of the displacement fields for mode A in the Spiral-II and annular holes structure indicate that the wider bandgap shown in the transmission spectrum for Spiral-II structure results from chirality. There are multiple phase changes due to multiple reflections of the incident wave at the spiral resonator and the emergent displacement field decouples from the source, which results in increased bandgap attenuation at that frequency.
3.4. Negative group velocity

Figure 6(a) shows the calculated dispersion curve for the Spiral-I structure, where the height of the spiral has been increased from 6.4 µm to 7.8 µm, with all remaining structural characteristics unchanged. Apart from one additional mode appearing in the frequency range (0–140 MHz) compared to the shallower Spiral-I structure, two modes, with negative group velocity emerge as shown in the left panel of figure 6. The metasurface can therefore convey Rayleigh waves with group velocity anti-parallel to phase advancement. To our knowledge this phenomenon has not been reported for square arrays of chiral metasurfaces supporting SAWs, although the existence of negative group velocity SAW modes in thin film structures has been reported in [17]. The points at which the negative group velocity modes intersect the first Brillouin zone at the ΓX direction are denoted by letters A and B. The calculated rms displacement for these modes is shown in figure 6(b). As discussed previously, increased coupling of the source’s displacement field profiles to the eigenmodes’s fields profiles results in small bandgap attenuation and hence large transmission. It follows that in order to increase transmission of the predicted negative group velocity SAWs, the incident Rayleigh wave displacement field should match the fields shown in figure 6(b). This may be achievable using a more sophisticated design for the IDT. Modes A and B have also comparable displacement field profiles, meaning that by appropriate mode matching, negative group velocity modes around 118 MHz and 153 MHz, could be excited. Mode B is significantly slower compared to mode A at wavevector range \(2.5 \times 10^5 \text{ m}^{-1} – 2.88 \times 10^5 \text{ m}^{-1}\) along the ΓX direction, as shown in figure 6(c), indicating that a slow negative group velocity SAW mode could be realized at excitation frequency around 150 MHz.

4. Conclusions

In conclusion, the interaction of Rayleigh waves with novel spiral resonators has been investigated computationally. The dispersion relationships for arrays of such resonators were calculated and showed that they can used to produce band-gaps for Rayleigh waves, but at lower frequencies than those can be achieved for other phononic crystals with the same unit cell size. The value of the attenuation at the bandgap frequency was extracted from simulations of the transmission through the resonators and was found to be extremely large (−25 dB), even for a relatively small number of elements. The low-frequency bandgap was also to even lower frequency by changing the spiral density, suggesting that optimization of the structural parameters can lead to the design and fabrication of low-frequency stop band filters. Decoupling of the predicted eigenmodes of the resonator from the source has been shown to allow the creation of higher bandwidth gaps, hence a step towards controlling both bandgap central frequency and bandwidth has been made. In addition, negative slopes in the dispersion curve of the spiral structure indicate that a square array of spiral resonators, supports negative group velocity SAW modes. The use of spiral structures therefore opens an exciting new pathway for the control and manipulations of SAWs.

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ORCID iDs

V Kyrimi https://orcid.org/0000-0001-9540-4750
G R Nash https://orcid.org/0000-0002-5321-4163

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