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1D and 2D wide acoustic bandgap Phononic Crystal structures for performance improvement of AlN-on-Si resonators operating in GHz range

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***Abstract*—Design and simulation of Phononic Crystals (PnCs) with a wide Acoustic Band Gap (ABG) around $1\,\mathrm{GHz}$ is presented. A new PnC unit cell topology is designed, which has a very wide ABG of $138\,\mathrm{MHz}$ with center frequency around $1\,\mathrm{GHz}$ and minimum feature size of $0.6\,\mu\mathrm{m}$. Wider ABG allows better enhancement of the Quality factor (Q) by reducing the anchor loss. Effect of geometrical variation and the periodicity of PnC are discussed. ABG for 1D and 2D periodicity is simulated and geometrical dimensions to obtain similar ABG in both cases are compared.**

***Index Terms*—Phononic Crystals, AlN Piezoelectric-on-Silicon, MEMS Resonators, anchor loss, acoustic band gap.**

I. Introduction

Demand for CMOS compatible and smaller footprint devices in modern day wireless communication systems has forced a shift in focus from high-Q off chip passives like Quartz resonators and SAW filters. Quartz was quintessential for resonators due to its high Q and temperature stable properties. Thus, a paradigm shift occurred towards Micro Electo Mechanical System (MEMS) resonators [1]. Research on piezoelectric-on-silicon resonators gained consequential heed owing to its high coupling and low motional resistance, making it archetypal for low noise oscillators [2]. The main impediment was the significant anchor loss that brought down the Q of the resonator. Several techniques were discerned to prevent the loss of acoustic energy through the anchors. This included employing quarter wavelength support tethers to couple nodal locations on resonator to rest of the substrate [3], [4]. Acoustic waves were reflected back by mesa isolation in [5] and by in-plane acoustic reflectors in [6]. Using Phononic crystals (PnC) to reduce anchor loss received notable recognition [6]-[17]. PnCs are particularly devised periodic structures that does not allow acoustic waves of certain frequency range to pass through, thus creating acoustic band gaps (ABG). The existence of such absolute band gaps were predicted theoretically by [7], [8] and demonstrated experimentally by [9]. The position and width of ABG, depends on a lot of factors including the lattice constant of the unit cell, the periodic variation of density and elastic constants, the lattice symmetry, the filling fraction and so on.

PnC has been used in both one-dimensional (1D) and two-dimensional (2D) periodicity. In [10], 1D PnC ring tethers are used in Aluminum Nitride (AlN) thin-film piezoelectric-on-silicon (TPoS) micromechanical resonators to obtain two complete ABGs spanning from 73-80 MHz and from 135-148 MHz. Lin et al [11] demonstrates four ABGs with desired stop band spanning 562-624 MHz. A design of lossless anchor based on PnC strips is presented in [12] which has a band gap of $12\,\mathrm{MHz}$. An asymmetric PnC design is tried in [13]. Two complete ABGs of span $40\,\mathrm{MHz}$ and $63\,\mathrm{MHz}$ was observed around $150\,\mathrm{MHz}$ and $300\,\mathrm{MHz}$ respectively.

PnC in 2D periodicity forms a stop band for leaking longitudinal waves from 137-162 MHz in [14]. The lattice constant of the PnC was $20\,\mu\mathrm{m}$. In [15], it was shown that a wider band gap is obtained when the PnC unit cell is shaped as solid disk. This is validated in [16], wherein they obtained a band gap of $82\,\mathrm{MHz}$ at a center frequency of $142\,\mathrm{MHz}$. Siddiqi and Lee [16] compares various commonly used PnC structures around center frequency of $150\,\mathrm{MHz}$. It is noted that with center frequency around $150\,\mathrm{MHz}$, the lattice constant is considerably high and 1D and 2D periodic PnC structures could be designed to get sufficiently wider band gap. In [17], fractal shaped phononic crystals in aluminum nitride where used to obtain ultra high frequency band gaps. The fractal shaped PnC exhibit two ABGs, one from 850-950 MHz and the other from 1.05-1.15 GHz for AlN thickness of $1\,\mu\mathrm{m}$ and unit cell size of $5\,\mu\mathrm{m}$ in Γ-X direction. This work tests commonly used 1D and 2D periodic PnC structures at a center frequency of $1\,\mathrm{GHz}$, to check whether they are scalable. The lattice constant for PnC structures with band gap center frequency of $1\,\mathrm{GHz}$, is in the order of 3-4 $\mu\mathrm{m}$. This work also proposes some new PnC designs with sufficiently wide band gaps around $1\,\mathrm{GHz}$ for AlN on Si resonators.

II. Theory

PnCs are elastic structures with periodic configurations of scattering inclusions. This periodicity property along with the mismatch between the structure and inclusions results in the inception of ABG. Modified eigen frequency analysis with Bloch periodicity conditions is done to obtain the band structure. From Newton's second law,

$$\rho\frac{\partial^2\mathbf{u}}{\partial^2 t} - \nabla.(\sigma(\mathbf{u}) - \mathbf{s}_0) = \mathbf{F} \quad (1)$$

where $\mathbf{u}$ is the displacement vector, σ represents density of the medium, $\mathbf{s}_0$ and $\mathbf{F}$ represents the source terms. For a time-harmonic wave,

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{u}(\mathbf{r})e^{i\omega t} \quad (2)$$

The wave equation, reduces to an inhomogeneous Helmholtz equation, assuming the same time-harmonic dependency for the source terms. (2) becomes

$$-\rho\omega^2\mathbf{u} - \nabla.(\sigma(\mathbf{u}) - \mathbf{s}_0) = \mathbf{F} \quad (3)$$

The relation between stress and strain tensor in solid materials can be written as

$$\sigma_{ij} = \mathbf{c}_{ijkl}\epsilon_{kl} \quad (4)$$

here, σ is the Cauchy's stress tensor, ϵ is the strain tensor, and $\mathbf{c}_{ijkl}$ is a fourth-order elasticity tensor. The strain tensor is defined as

$$\epsilon(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T) \quad (5)$$

$\rho(\mathbf{r})$ can be expanded into a Fourier series utilizing periodicity of the system.

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}} e^{i\mathbf{G}.\mathbf{r}} \quad (6)$$

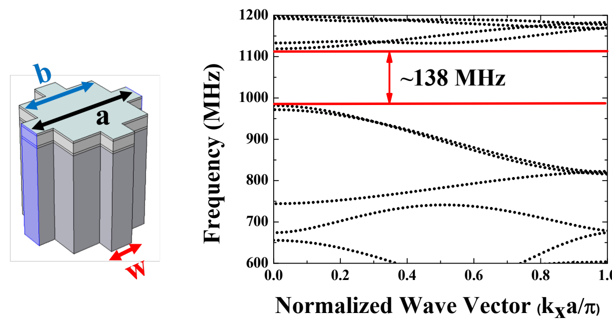
$\mathbf{G}$ corresponds to reciprocal lattice vector and its dimensionality depends on the periodic dimensionality of the medium, which can be one, two or three. Applying Bloch (or Floquet) periodicity theroem, the displacement vector can be written as

$$\mathbf{u}(\mathbf{r}, t) = e^{i(\mathbf{K}.\mathbf{r}\quad \omega t)}\sum_{\mathbf{G}}\mathbf{u}_{\mathbf{K}}(\mathbf{G})e^{i\mathbf{G}.\mathbf{r}} \quad (7)$$

$\mathbf{K}$ is the Bloch wave vector. Substituting (4), (5), (6), and (7) in (3) and assuming absence of external applied field will yield an infinite set of linear equations for eigen vector $\mathbf{u}_{\mathbf{K}}(\mathbf{G})$ [7]. This set of equations, have solutions for some eigen values $\omega_n(\mathbf{K})$, for a given value of Bloch vector. The vibrational bands one, two, three and so on corresponds to $n = 1, 2, 3..$. The band structure is obtained by sweeping $\mathbf{K}$ over the irreducible region of the Brillouin zone.

III. Design and Simulation

Figure 1a depicts a unit cell of the designed PnC structure, with lattice constant, $a = 3\,\mu\mathrm{m}$. The structure is essentially, a cuboid along with a cross shaped link. The minimum feature size corresponds to the width of the link, $w = 0.6\,\mu\mathrm{m}$. Side of the square on top of cuboid, b is $2.1\,\mu\mathrm{m}$. COMSOL Multiphysics [18] was used to compute the acoustic band structure of the designed cell. Bloch periodicity conditions were set, to the two faces of the cell corresponding to the X coordinate for 1D simulation and to four faces corresponding to the X and Y coordinates for 2D simulation. Parameters k_x and k_y were defined, which denotes the wave vector along the x- and y-axis respectively. A parametric sweep was done in the wave vector along the boundary of the irreducible Brillouin zone. The variables a, b, and w were varied in order to optimize the band gap. The aim was to obtain a complete band gap as wide as possible around $1\,\mathrm{GHz}$, which is the center frequency of the resonator to which these structures are stowed, in tethers for 1D and on the substrate for 2D. The primary advantage of having a very wide band gap is that, the enhancement of Q is feasible over a sizable frequency range. Also, a larger band gap ensures that, the resonant frequency of the resonator falls well within the band gap despite variations that could occur while fabrication. The stack used is Mo-AlN-Mo-Si. Molybdenum is used as both top and bottom electrode for the resonator. Aluminum Nitride is the piezoelectric material used. Thickness of Silicon, Aluminum Nitride and Molybdenum are $5\,\mu\mathrm{m}$, $0.5\,\mu\mathrm{m}$ and $0.1\,\mu\mathrm{m}$ respectively. Figure 1b shows the band structure of the designed unit cell. It can be seen that a band gap of $138\,\mathrm{MHz}$ was obtained with minimum feature size limited to $0.6\,\mu\mathrm{m}$. Various other commonly used PnC structures were also tested with the same minimum feature size of $0.6\,\mu\mathrm{m}$. All these structures were optimized by varying the geometrical dimensions, so as to obtain maximum band gap around $1\,\mathrm{GHz}$.



(a) (b)

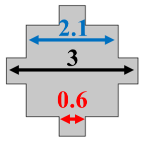
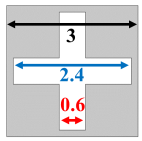
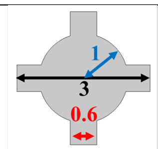
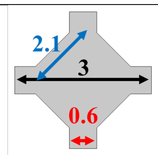
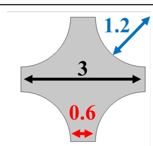
Fig. 1: (a) Unit cell of the PnC; (b) Band structure of the first irreducible Brillouin zone obtained by Finite Element (FE) analysis for PnC in 1D periodicity.

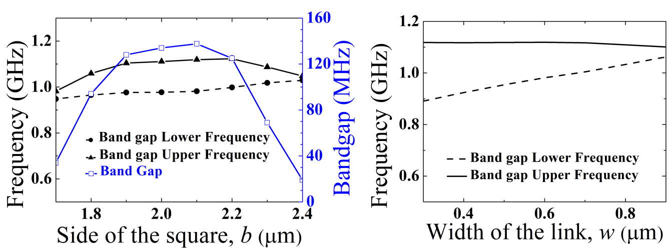
IV. Results and Discussion

Figure 2a shows variation of the band gap with the side of the square on top of cuboid, b at $w = 0.7\,\mu\mathrm{m}$. It can be seen that the maximum band gap occurs at, $b = 2.1\,\mu\mathrm{m}$. Now, by setting $b = 2.1\,\mu\mathrm{m}$, w is varied so as to find the optimum value of w. Figure 2b shows the variation of band gap with width of the link. As the width reduces, band gap can be seen increasing. Width of the link is the minimum feature size which, is set by lithography constraints. So, the minimum feature size is set at $0.6\,\mu\mathrm{m}$ considering fabrication process. All the structures were designed with minimum feature size of $0.6\,\mu\mathrm{m}$. This method, of varying one parameter while others were kept constant, was used to obtain the maximum band gap in all structures.

Figure 3a shows the variation of center frequency with the lattice constant, a of test structure 1. It is evident that

TABLE I: Simulated Acoustic Band Gap of various PnC structures in 1D periodicity

PnC Structure	Unit Cell Dimensions (μm)	ABG Range (MHz)	Band Gap (MHz)
Test structure 1		981-1119	138
Cross Inclusion		965-1079	114
Circular disk with links		993-1093	100
Test structure 2		1004-1092	88
Test structure 3		1017-1086	69

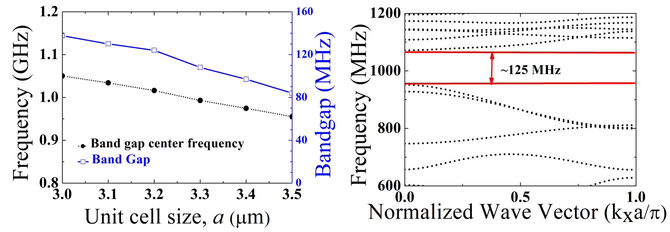


(a) (b)

Fig. 2: Variation of band gap with (a) side of the square; (b) width of the link.

the center frequency increases as we scale down the lattice constant. For each value of lattice constant, other parameters were varied to get the maximum band gap. Center frequency is inversely proportional to the lattice constant. For the required center frequency of 1 GHz, the lattice constant is found to be, $a = 3.2\,\mu\text{m}$. An ABG of 125 MHz was obtained with $a = 3.2\,\mu\text{m}$ and $b = 2.2\,\mu\text{m}$, with center frequency of 1 GHz. The band structure with $a = 3.2\,\mu\text{m}$ and $b = 2.2\,\mu\text{m}$ is shown in Figure 3b.

Table I shows the various commonly used PnC structures and their band gaps, with lattice constant 3 µm and minimum

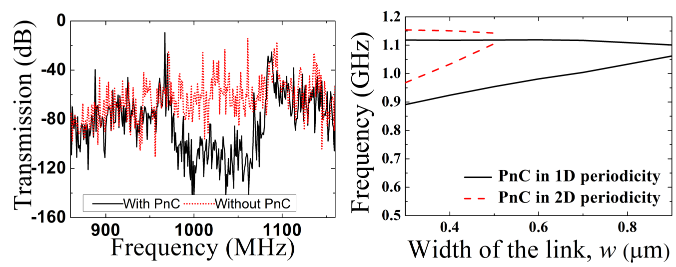


(a) (b)

Fig. 3: (a) Variation of the center frequency and band gap with lattice constant of the unit cell; (b) The band structure with center frequency 1 GHz.

feature size of 0.6 µm. Each structure was optimized for the maximum band gap keeping the center frequencies in the same range. The evaluated structures include circular disk with links, cross inclusion, and two other newly designed test structures. The fractal shaped PnC shown in [17], did not give any ABG for our stack. Since lattice constant dictates the location of the center frequency, almost all the structures have similar center frequency.

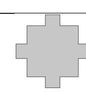
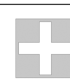
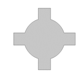
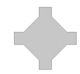
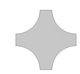
Figure 4a shows the transmission characteristics with 3 array of PnC structure, unit cell of which is shown in Figure 1a, introduced as delay lines to the resonator. It can be seen that there is ABG occurring around 1 GHz. The difference between, 1D and 2D FE analysis and the simulated transmission characteristics is that, the former assumes infinite lattice while the latter has finite array of PnC cells.

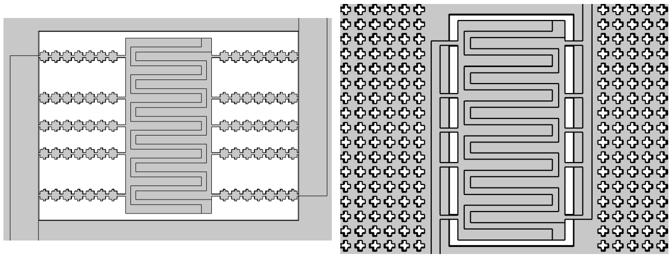


(a) (b)

Fig. 4: (a) Simulated transmission characteristics with 3 array of PnC introduced. (b) Variation of the band gap with width of the link. Dashed line represents PnC in 2D periodicity and straight line represents PnC in 1D periodicity.

TABLE II: Simulated Acoustic Band Gap of various PnC structures in 2D periodicity

Unit cell topology										
Minimum feature size (μm)	0.4	0.5	0.4	0.5	0.3	0.4	0.3	0.4	0.1	0.2
Band gap (MHz)	118	38	76	16	81	–	22	–	25	–



(a) (b)

Fig. 5: Schematic of resonator with PnC structures (a) attached in tethers in 1D periodicity; (b) placed in 2D periodicity.

In the studies conducted, k was swept from Γ point to X point of the reciprocal lattice for 1D and from Γ to X, from X to M and from M to Γ point for 2D. It was deemed enough to obtain a good model of the acoustic band structure. The minimum feature size had to be very small in order to have sufficiently large band gap for 2D periodicity. The minimum feature size in these designs is the width of the link. As can be seen from figure 4b, the band gap closes near $w = 0.6\,\mu\text{m}$ for 2D periodicity. Figure 4b indicates the variation of band gap as width of the link is reduced, for 1D and 2D test structure. The Band gap was seen closing around $w = 1\,\mu\text{m}$ for 1D periodicity and $w = 0.6\,\mu\text{m}$ for 2D periodicity with center frequency around $1\,\text{GHz}$.

Table II shows the band gap obtained for PnC in 2D periodicity and the minimum feature size required to achieve that. It can be observed that, in order to have sufficient band gap, the minimum feature size becomes very small in case of PnC with 2D periodicity. The band gap can be seen closing around $w = 0.4\,\mu\text{m}$ for circular disk shaped PnC structure. For test structures 2 and 3, the band gap can be seen closing around minimum feature size of $0.4\,\mu\text{m}$ and $0.2\,\mu\text{m}$ respectively. For cross inclusion shaped PnC structure, the minimum feature size required to have a band gap is $0.5\,\mu\text{m}$. Figure 5a shows the schematic of a resonator with PnC placed in tethers. Here, the PnC is used in 1D periodicity. Figure 5b shows the schematic of resonator, where the same PnC structure is used in 2D periodicity. From literature, it can be seen that both 1D and 2D periodicity has been used to improve Q of the resonator. However with frequency around $1\,\text{GHz}$, the lattice dimensions becomes so small that the minimum feature size required in 2D periodicity to have adequate band gap becomes very small, thus making the fabrication process challenging.

CONCLUSION

In this work, a new PnC structure is designed which gives wider ABG than any other reported PnC structure around $1\,\text{GHz}$, with minimum feature size of $0.6\,\mu\text{m}$, for AlN piezoelectric on silicon MEMS resonator. An ABG of $138\,\text{MHz}$ was obtained with center frequency around $1\,\text{GHz}$. Also, various PnC structures were tested in 1D and 2D periodicity. At smaller frequency range, that is, in the order of a few hundreds of MHz, PnC in both 1D and 2D periodicity can be maneuvered to obtain the required band gap. However, with center frequency in GHz range, the lattice constant becomes very small. In order to have adequate ABG, the minimum feature size becomes a hindrance. For 2D periodicity, the ABG is seen vanishing around minimum feature size of $0.6\,\mu\text{m}$ which is very small compared to the case of 1D periodicity. Thus at higher frequency range it is safe to assume that in order to have sufficient ABG it is better to employ PnC in 1D periodicity, that is, placing the PnC in tethers.

REFERENCES

[1] H. C. Nathanson, R. A. Wickstrom, "A resonant-gate silicon surface transistor with high-Q bandpass properties," Appl. Phys. Lett., vol. 7, pp. 84–88, 1965.
[2] R. Abdolvand, H. M. Lavasani, G. K. Ho, F. Ayazi, "Thin-film piezoelectric-on-silicon resonators for high frequency reference oscillator applications," IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 2008, vol. 55, pp. 2596–2606.
[3] J. S. Pulskamp, S. S. Bedair, R. G. Polcawich, D. Judy, and S. A. Bhave, "Ferroelectric PZT RF MEMS resonators," Frequency Control and the European Frequency and Time Forum (FCS), 2011 Joint Conference of the IEEE International, May 2011, pp. 1–6.
[4] J. Brotz, "Damping in CMOS-MEMS Resonators," Ph.D. dissertation, Carnegie Mellon University, June 2004.
[5] M. Pandey, R. B. Reichenbach, A. T. Zehnder, A. Lal, and H. G. Craighead, "Reducing anchor loss in MEMS resonators using mesa isolation," Journal of Microelectromechanical Systems, vol. 18, no. 4, Aug 2009, pp. 836–844.
[6] B. P. Harrington and R. Abdolvand, "In-plane acoustic reflectors for reducing effective anchor loss in lateral-extensional MEMS resonators," Journal of Micromechanics and Microengineering, vol. 21, no. 8, p. 085021, 2011.
[7] M. S. Kushwaha, P. Halevi, L. Dobrzynski, B. Djafari-Rouhani, "Theory of acoustic band structure of periodic elastic composites," Phys. Rev. B 49, 2313 (1994).
[8] M. M. Sigalas, E. N. Economou, "Elastic and acoustic wave band structure," J. Sound Vib. 158, (1992).
[9] J. O. Vasseur, P. A. Deymier, G. Frantziskonis, G. Hong, B. Djafari Rouhani, L. Dobrzynski, "Experimental evidence for the existence of absolute acoustic band gaps in two-dimensional periodic composite media," J. Phys.: Condens. Matter 10, 6051 (1998).
[10] H. Zhu, J. E. -Y. Lee, "Design of phononic crystal tethers for frequency-selective quality factor enhancement in AlN piezoelectric-on-silicon resonators," Procedia Eng, 2015, 120, pp. 516–519.
[11] C. -M. Lin, J. -C. Hsu, D. G. Senesky, A. P. Pisano, "Anchor loss reduction in AlN Lamb wave resonators using phononic crystal strip tethers," In Proceedings of the 2014 IEEE International Frequency Control Symposium (FCS), Taipei, Taiwan, May 2014; pp. 371–375.
[12] F. -C. Hsu, J. -C. Hsu, T. -C. Huang, C. -H. Wang, and P. Chang, "Design of lossless anchors for microacoustic-wave resonators utilizing phononic crystal strips," Applied Physics Letters, vol. 98, no. 14, 2011.
[13] U. Rawat, D. R. Nair, A. DasGupta, "Piezoelectric-on-Silicon array resonators with asymmetric phononic crystal tethering," J. Microelectromech. Syst, 2017, 26, pp. 773–781.
[14] H. Zhu, J. E. -Y. Lee, "AlN piezoelectric on silicon MEMS resonator with boosted Q using planar patterned phononic crystals on anchors," In Proceedings of the 28th IEEE International Conference on Micro ElectroMechanical Systems (MEMS), Estoril, Portugal, January 2015; pp. 797–800.
[15] R. Ardito, M. Cremonesi, L. DAlessandro, A. Frangi, "Application of optimally-shaped phononic crystals to reduce anchor losses of MEMS resonators," In Proceedings of the 2016 IEEE International Ultrasonics Symposium (IUS), Tours, France, September 2016; pp. 1–3.
[16] M. W. U. Siddiqi, J. E. -Y. Lee, "Wide Acoustic Bandgap Solid Disk-Shaped Phononic Crystal Anchoring Boundaries for Enhancing Quality Factor in AlN-on-Si MEMS Resonators," Micromachines 2018, 9, 413.
[17] N. -K. Kuo and G. Piazza, "Fractal phononic crystals in aluminum nitride: An approach to ultra high frequency bandgaps," Appl. Phys. Lett. 99, 163501 (2011).
[18] COMSOL Multiphysics v. 5.4. www.comsol.com. COMSOL AB, Stockholm, Sweden.