Complete phononic bandgaps and bandgap maps in two-dimensional silicon phononic crystal plates

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It is shown that it is possible to obtain complete planar phononic bandgaps in square and hexagonal (honeycomb) lattice phononic crystals formed by etching a periodic array of circular holes in a thin silicon plate (or membrane). Also, better bandgap properties are obtained using the hexagonal lattice structure; and, with practical structure sizes, it is possible-to-obtain a gap-to-midgap ratio of 18–35%.

Introduction: There has been growing interest in a special type of inhomogeneous elastic materials called phononic crystals (PCs) [1], which are materials with periodic variation in their mechanical properties. PCs are especially of interest owing to the possibility of having complete phononic bandgaps (PBGs), i.e. a range of frequencies for which the propagation of any kind of mechanical (acoustic or elastic) waves in any direction is prohibited.

Similar to the case of photonic bandgap in photonic crystals, the possibility of controlling phonons within the PBG can be used to implement a variety of efficient fundamental devices such as acoustic/elastic isolators, mirrors, filters, cavities, and waveguides by adding appropriate defects to the PC [2–4]. The existence of all these functionalities on the same PC platform can provide numerous powerful integrated structures for use in several applications. Silicon (Si) based PCs with CMOS compatible fabrication processes are especially of interest since they can be realised with electronic and photonic devices on the same substrate. Most studies on PCs have been limited to two-dimensional (2D) PCs that are infinite in the third dimension. However, realising such devices requires large extensions in the third direction to emulate 2D structures which are often undesirable.

A more practical type of PC utilises a semi-infinite medium that supports surface acoustic waves (SAWs) with 2D periodic change of elastic properties [5, 6]. In such a structure the acoustic energy is confined within approximately one wavelength from the free surface of the semi-infinite medium. The main drawback of SAW PC structures for practical applications is their potentially high loss owing to the possibility of the coupling of SAW energy to the bulk as the SAW propagates through the PC. One solution to this problem is to use a thin free-standing plate (i.e. a membrane) to limit the loss of mechanical waves to non-elastic effects. Although there have been a number of studies on these so-called PC plates, all of the reported structures either have reported only directional PBGs [7] or have been limited to solid/solid PCs [8], which have CMOS compatibility, and fabrication difficulty issues. In this Letter we investigate theoretically the existence of complete PBGs in 2D PC plates with CMOS compatible realisation comprising circular void (i.e. vacuum) holes embedded in a Si membrane. We study both square and hexagonal (honeycomb) hole arrangements of the PC plate lattice, and show that complete PBGs exist for both structures for a variety of radii of the holes and plate thicknesses. We further study the effect of plate thickness on the existence and width of the PBG and show that thickness plays a very important role in opening, closure, and size of the PBG. By comparing the PBG maps for square and hexagonal lattice PCs, we find that the hexagonal lattice PC plate has several advantages over the square lattice one, and has several wide PBGs that can be used in a variety of applications. While all the derivations are based on Si as the constituting material, the main conclusions are valid for a large class of solid materials.

Band structure calculation: A schematic of a 2D phononic crystal plate with a square lattice arrangement of holes is shown in Fig. 1*a* in which crystalline axes are aligned with x-, y- and z-directions. The structure can easily be made on a Si on insulator (SOI) wafer by etching holes through the plate using standard dry etching techniques, and then removal of the underlying insulator by wet etching. As shown in Fig. 1*a*, a is the spacing between adjacent holes, d the thickness of the plate, while r is the radius of the holes. The governing wave equation for propagation of elastic waves in non-piezoelectric media (e.g. Si) is given by

$$\nabla \cdot (\mathbf{c} \cdot \nabla_s \mathbf{u}) = \rho \frac{\partial^2}{\partial t^2} \mathrm{u} \qquad (1)$$

in which $\mathbf{u}$ is the displacement vector, $\mathbf{c}$ is the stiffness tensor, and ρ the mass density. The values of the stiffness tensor for Si used in this Letter are $c_{11} = 16.7 \times 10^{10}$ N/m^2, $c_{12} = 6.39 \times 10^{10}$ N/m^2, $c_{44} = 7.956 \times 10^{10}$ N/m^2, $\rho = 2332$ kg/m^3.

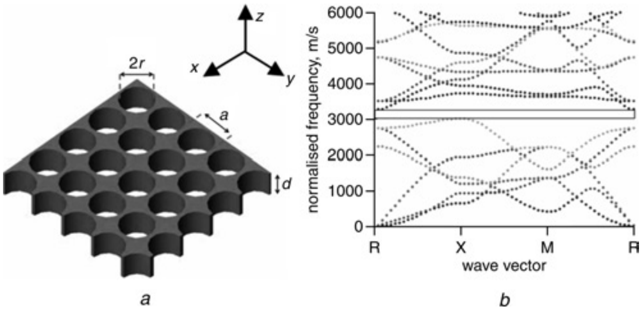

Fig. 1 *Square lattice PC plate schematic and band structure*

a Schematic of structure
b Band structure for $r/a = 0.45$ and $d/a = 0.5$

To calculate the 2D band structure of the PCs, we used a full three-dimensional (3D) plane wave expansion (PWE) technique with 441 plane wave components (found through extensive simulations to provide enough accuracy for the structures studied). To ensure the accuracy of the PWE method, we also compared the results with the band structures calculated using the finite element method (FEM), and very good agreement was achieved in all cases reported here.

A complete PBG can be found in the square lattice PC plate by carefully choosing the thickness of the plate and the radius of the holes. As seen from Fig. 1*b*, a complete PBG for the structure with $r/a = 0.45$ and $d/a = 0.5$ is obtained, and the PBG covers the normalised frequency ($f \times a$) range of $3000\ \mathrm{m/s} < f \times a < 3261\ \mathrm{m/s}$, which corresponds to a gap-to-midgap ratio of 8.3%.

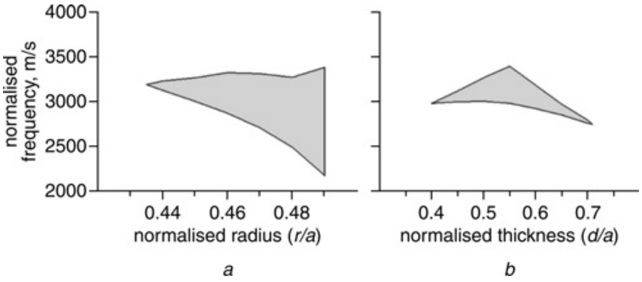

Fig. 2 *PBG extent for square lattice PC plate*

a As a function of normalised hole radius (r/a) with $d/a = 0.5$
b As a function of normalised thickness (d/a) with $r/a = 0.45$

We investigated the dependence of the PBG width on the normalised PC hole radius (r/a), and generated a gap map for a constant plate thickness ($d/a = 0.5$) as shown in Fig. 2*a*. As seen from Fig. 2*a*, the PBG opens up around $r/a = 0.43$, and its width constantly increases with increasing r/a. In Fig. 2*b*, the extent of the PBG of the square lattice PC against normalised plate thickness (d/a) for a constant normalised radius ($r/a = 0.45$) is shown. It can be seen that the PBG opens up at $d/a \simeq 0.4$, reaches its maximum width at $d/a \simeq 0.55$, and closes again at $d/a \simeq 0.7$. The results shown in Fig. 2 clearly illustrate the importance of the PC geometry on the extent of the PBG. It is also seen that a square lattice PC has limited PBG unless r/a reaches close to its maximum (i.e. $r/a = 0.5$), for which severe fabrication limitations and mechanical stability issues for the PC plate exist. As an alternative PC structure, we also investigated PCs with a hexagonal lattice as shown in Fig. 3*a*. Again, the main crystalline axes of Si are aligned with x-, y- and z-directions. The band structure of a hexagonal lattice PC with $r/a = 0.45$ and $d/a = 1$ is shown in Fig. 3*b*, and the associated phononic gap maps of the thin PC structure are shown in Fig. 4. These Figures show the advantages of the hexagonal lattice PCs over the square lattice PCs, including larger PBG size and less susceptibility to the variations in plate thickness. For example, as shown in Fig. 4, a hexagonal lattice with $r/a = 0.45$ and $d/a = 1$ has a PBG extent of $1608 < f \times a < 2298$, which corresponds to a gap-to-midgap ratio of 35%, which is large enough for all practical applications. Furthermore, the PBG for the hexagonal lattice PC opens up at $r/a \simeq 0.37$ and a reasonable PBG with gap-to-midgap ratio of 18% can be achieved with $r/a = 0.4$ and $d/a = 1$. Such PC parameters impose considerably less fabrication limitations and mechanical stability issues than those for a square lattice PC. Finally, another interesting feature of the hexagonal lattice PC is the existence of more than one PBG for a wide range of PC properties (i.e. d/a and r/a) as can be found from Fig. 4*b*.

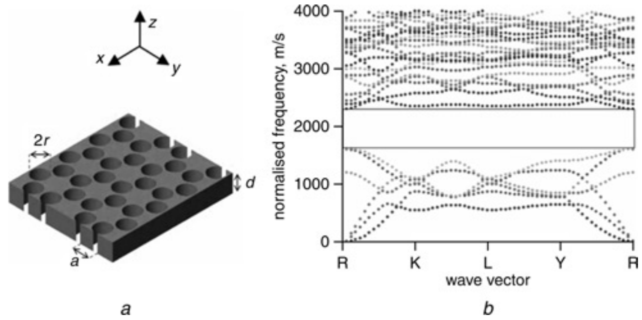

Fig. 3 *Hexagonal lattice PC plate schematic and band structure*
a Schematic of structure
b Band structure for $r/a = 0.45$ and $d/a = 1$

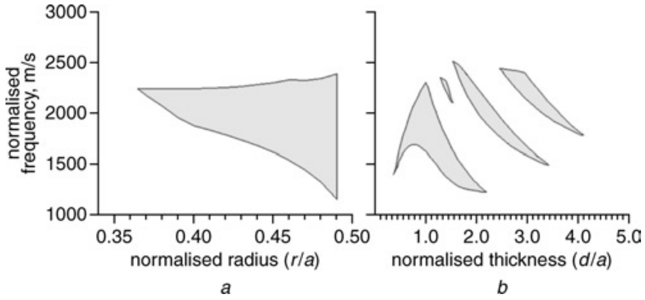

Fig. 4 *PBG extent for hexagonal lattice PC plate*
a As a function of normalised hole radius (r/a) with $d/a = 1$
b As a function of normalised thickness (d/a) with $r/a = 0.45$

Conclusion: We have shown that with appropriate choices of geometrical features complete PBGs can be obtained in PCs formed by etching square or hexagonal lattice void holes in a Si plate. Also, reasonably large PBGs (gap-to-midgap ratio $\simeq$ 18–35%) can be obtained in hexagonal lattice PC plates with practically achievable PC geometries ($r/a = 0.4$–0.45 and $d/a = 1$) that can be fabricated using a CMOS compatible fabrication process. Thus, we conclude that PCs and preferably hexagonal lattice PCs with holes etched into a Si plate provide the ability to integrate PBG functionalities with electronic and optical devices on Si.

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