Finite element analysis of surface elastic waveguide based on pyramidal phononic crystal

1 | INTRODUCTION

In these recent years, the phononic crystals (PnC) and the phononic waveguides (PnW) fascinate researchers and scientists. These structures are recently used for microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS). The principal role of the PnC is the control of the elastic waves propagation [1–4]. A phononic crystal is a periodic structure made of two or more mixed materials, whose mass densities and elastic coefficients are periodically changed in space. According to this periodicity, three types of PnC can be structured. The first one is the one dimensional PnC [5], the second one is two dimensional PnC [2, 6, 7] and the third one is three dimensional PnC [8]. It can be a solid-solid, solid-fluid or fluid-fluid, phononic crystals.

One of the principal properties of these periodic structures is the phononic band gaps, in which we can use the PnC for several fields of applications such as waveguide [9–11], frequency filter [11], and fluid sensors [12]. Recently, many articles are published to exhibit the dispersion properties of PnCs. A thin plate based on a periodic inclusions [13] or periodic deposition of holes [14] or periodic deposition of pillars [15, 16] are theoretically studied [15, 16], and experimentally investigated [17] to analyse the propagation of Lamb waves [18].

Furthermore, a thick slab with periodic inclusions, in particular holes [19], and periodic pillars [20–22], are theoretically studied [21], and experimentally demonstrated [17, 23], to command the surface acoustic wave (SAW) propagation. For the pillars PnC waveguide, two types of band gaps exist. The first one is due to the Bragg scattering [23, 24], which the wavelength is of the order of the lattice parameter, while the second one is due to the local resonance of the pillars at a large wavelength [15, 16, 20]. The elastic energy in the pillars PnC waveguide is restricted within the pillars and the vicinity area [9, 25, 26], that present serious challenge worth to find good structures, in which the energy is well focused in the pillars A PnC with cylindrical pillars [21] and a PnC with inverted conical pillars [25] are studied.

Many theoretical methods have been developed to study periodic structures and PnC waveguides. A PnC waveguide with periodic holes is analysed and the transmission spectra are calculated by a finite difference time domain (FDTD) method [19], while the plan wave expansion (PWE) method is developed to draw the band structures [1, 27, 28].

In recent years, the finite element method (FEM) is used to find the band structure and the frequency transmission spectrum of the PnC waveguide [29]. Especially the commercial COMSOL multiphysics code, by modifying the elastic equation to be adapted to the partial differential equation (PDE) model [9]. In this study, we theoretically explore the reality of the band gap due to the local resonance through the PnC waveguides made of periodic pyramidal pillars, using the FEM method; we analysed surface wave of pyramid pillars deposited on a thick slab based on silicon.

Indeed, the pyramid pillars have an increased mass density from the top surface to the lowest pyramid surface, whose elastic energy can be well restricted within the upper surface, in which it can be shown a good SAW waveguide. The first chapter presents the model and the method of calculation. The band structure and the corresponding transmission spectrum are calculated, in the second chapter. Finally, by changing the pyramid geometry, the localization of the band gap and the surface mode are investigated.

2 | THEORY AND PnC SURFACE WAVEGUIDE MODEL

A pyramid deposited on a thick square silicon substrate is an elementary unit cell of the phononic structure of the elastic waveguide. The periodicity of this unit cell in the \((x, y)\) plan forms our phononic crystal. These pyramids are oriented perpendicular to the \([100]\) and \([010]\) directions on the \((001)\) surface of silicon, as shown in Figure 1. The geometrical parameters of the unit cell are the lattice constant \(a\), the height of the pyramid \(h_{1}\) and the base of the pyramid \(d\), their dimensions are 200, 300, and 140 nm, respectively. The thickness of the substrate was selected almost five times more than the lattice constant, in order to separate the Lamb wave from the surface modes [21]. In this paper, we consider the anisotropy of silicon, then the elastic constants used in our model are \(C_{11} = 166.0\) GPa, \(C_{12} = 64.0\) GPa, \(C_{44} = 79.9\) GPa, and the mass density is \(\rho = 2329\) kg/m\(^3\).
The general governing elastic wave equation with no external sources can be written as:

\[
\begin{align*}
-\rho \omega^2 u_x &= \frac{\partial}{\partial x} \left( c_{11} \frac{\partial u_x}{\partial x} + c_{12} \frac{\partial u_y}{\partial y} + c_{12} \frac{\partial u_z}{\partial z} \right) + \frac{\partial}{\partial y} \left( c_{44} \frac{\partial u_x}{\partial y} + c_{11} \frac{\partial u_y}{\partial y} + c_{12} \frac{\partial u_z}{\partial z} \right) + \frac{\partial}{\partial z} \left( c_{44} \frac{\partial u_x}{\partial z} + c_{11} \frac{\partial u_y}{\partial z} + c_{12} \frac{\partial u_z}{\partial z} \right) \\
-\rho \omega^2 u_y &= \frac{\partial}{\partial x} \left( c_{44} \frac{\partial u_x}{\partial y} + c_{11} \frac{\partial u_y}{\partial y} + c_{12} \frac{\partial u_z}{\partial z} \right) + \frac{\partial}{\partial y} \left( c_{12} \frac{\partial u_x}{\partial x} + c_{11} \frac{\partial u_y}{\partial y} + c_{12} \frac{\partial u_z}{\partial z} \right) + \frac{\partial}{\partial z} \left( c_{44} \frac{\partial u_x}{\partial z} + c_{11} \frac{\partial u_y}{\partial z} + c_{12} \frac{\partial u_z}{\partial z} \right) \\
-\rho \omega^2 u_z &= \frac{\partial}{\partial x} \left( c_{44} \frac{\partial u_x}{\partial z} + c_{11} \frac{\partial u_y}{\partial z} + c_{12} \frac{\partial u_z}{\partial z} \right) + \frac{\partial}{\partial y} \left( c_{12} \frac{\partial u_x}{\partial x} + c_{11} \frac{\partial u_y}{\partial y} + c_{12} \frac{\partial u_z}{\partial z} \right) + \frac{\partial}{\partial z} \left( c_{44} \frac{\partial u_x}{\partial z} + c_{11} \frac{\partial u_y}{\partial z} + c_{12} \frac{\partial u_z}{\partial z} \right)
\end{align*}
\]

(1)

where \( \rho \) and \( \omega \) are the mass density and the angular frequency, respectively. \( u_x, u_y \) and \( u_z \) are the \( x, y \) and \( z \) displacement components, respectively.

Because our phononic crystal is an infinite periodic structure, we should use the Block-Floquet theorem, in which the displacement vector can be written as the following equation:

\[
u(r + a) = \nu(r) \exp(ika)
\]

(2)

where, \( r = (x, y, z) \) is the position vector, \( k = (k_x, k_y, k_z) \) is the block wave vector. By inserting Equation (2) into Equation (1), the general governing equation can be converted into the eigenvalue problem as follows:

\[
[K - \omega^2 M] = 0
\]

(3)

In this study, we used the FEM method coded in COMSOL Multiphysics to solve this problem.

To understand the dispersion properties of elastic waves through our phononic structure, the band structure is calculated, The dispersion relation is a relationship between the angular frequency and the wave vector, while the band structure is a vibration modes of the phononic crystal in all direction of the first Brillouin zone. Then, periodic boundary conditions (PBC) according to the Block-Floquet theorem have been applied for the rectangular faces (a*h) of the unit cell for both \( x \) and \( y \) direction as follow: \( u(r + a) = u(r) \exp(ika) \), \( u(r + a) = u(r) \exp(ika) \), in order to present a periodic and infinite structure in \((x, y)\) plan. The base of the unit cell is considered as a fixed boundary, the faces of the pyramid are considered as free surfaces which mean all normal constraints to the pyramid faces are nulls, as shown in Figure 1(a).

By sweeping the wave vector in the first Brillouin zone presented in Figure 1(b), we can solve Equation (3) to find the
FIGURE 2 (a) Band structure of PnC waveguide, the red horizontal bar represents the location of the first band gap, the blue bar represents the second band gap location, the green line represents the lowest bulk wave velocity. (b) Band structure in the FX direction. (c) The transmission spectrum of displacement field with shear polarized line source. (d) The transmission spectrum of displacement field with sagittal polarized line source.

Eigen vectors (reduced wave vector) and Eigen values (Eigen frequencies) of our system of equations.

The band structure curve exhibit the behaviour of the elastic waves through the PnC waveguide, for all direction in the first Brillion zone. To understand the band structure curve, the transmission spectrum in frequency domain of a model consists of eleven elementary cells along the x direction was calculated [20]. In this model, a perfect matched layer (PML) is applied, to absorb the reflected waves along the x direction as well as the base of the structure as Figure 1(c) shown. The periodic boundary condition (PBC) is applied for two parallel faces to x-axis along the y direction, according to the Bloque-Floquet theorem as follow: $u(r + a) = u(r) \exp(ik_y a)$, to represent an infinite structure in the y direction, as Figure 1(c) explains. To analyse the response of our structure according to the type of elastic wave excitation. The harmonic disturbance was applied as a source of excitation at the inlet edge in Figure 1(c) for two types of polarizations; the first polarization is the sagittal displacement ($u_x, u_z$), and the second polarization is the shear horizontal displacement ($u_y$) [20].

The transmission spectrum is the sum of the square of the three absolute module displacement vector components; $u_x^2 + u_y^2 + u_z^2$, calculated as a function of frequency. The output signal is integrated at the location of the outlet edge in the Figure 1(e) on the upper right surface of the waveguide, as a line parallel to the y direction, this function is an elastic energy recovering in the output of our waveguide [21].

The surface wave modes and the elastic properties (displacement field components) were analysed by a graphical representation of the displacement distribution for three modes of surface waves.

The properties of the surface modes with a defect line have been studied. A model of a finite structure is used as a waveguide. It is constituted of eleven cells along the y direction, surrounded by a PML. We represent an infinite structure in the x direction by applying a PBC boundary, as shown in Figure 1(e), to calculate the dispersion properties as well as the transmission spectrum for each defect. The sixth pyramid height has been changed and considered as a defect in the structure to form a waveguide, the height size of the sixth pyramid used in this model are; 0, 240, 300, 360 nm; the other pyramids were kept fixed at a size of 300 nm.

3 RESULTS AND DISCUSSION

3.1 Surface elastic wave analysis of PnC

If we look at the band structure presented in Figure 2, we will find that the group velocity mathematically presented as the following equation; $v_g = \frac{\partial \omega}{\partial k}$, where $\omega$ and $k$ are the angular frequency and the wave vector respectively. The dispersion relation of the phononic crystal is calculated in the first Brillion zone for all directions of the square lattice, according to the symmetry of the silicon phononic crystal and the isotropy of the materiel.

The green solid line in Figure 2(a) corresponds to the lowest bulk wave velocity, in which it can be considered as a sound cone. Similar to the photonic crystal, since the array of pillars we consider sits on top of a semi-infinite medium, the continuum of radiation states in this medium forms a sound cone [20]. In phononic crystal the sound cone is a border of the surface waves mode and the bulk waves mode, which all band inside the green line are the surface waves mode [21].

In this work, we are interested to analyse the surface elastic waves. As we can see in the band structure curve in Figure 2(a), the first sixth bands corresponds to the surface modes of our PnC waveguide, which the first band is the one that corresponds to the lowest frequency. Two band gaps exist which are located inside the green solid line (sound cone). The first band
FIGURE 3 Displacement field for the surface modes indicated in Figure 2. From the left to right are the total displacement $u$, the displacement components $u_x$, $u_y$ and $u_z$ respectively. (a) Mode 1: point A; at the frequency of 4.17 GHz, located in the second band, (b) mode 2; point B, at the frequency of 9.9 GHz, located in the fourth band, (c) mode 3; point C, at the frequency of 11.04 GHz, located in the sixth band.

gap spans from 4.2 to 4.5 GHz, in which the corresponding wavelength ($\lambda$) is about six times larger than the lattice constant $a$ ($\lambda \approx 6 \times a$). This band gap is appeared by the local resonance effect between the normal elastic band structure branches and the flat band of the PnC [20], which means that the resonant modes of the pyramids interact with surface waves of the substrate. The second band gap which is due to the Bragg scattering phenomenon, spans from 10 to 11 GHz [24], when the corresponding wavelength is about two times the lattice constant; $\lambda \approx 2 \times a$, as Figure 2(a) shown.

Obviously, the transmission spectrum curve works in with the band structure curve, where it exhibits an understandable description of the band gap. Figure 2(b) shows the band structure in the $\Gamma X$ direction. While the Figure 2(c) and (d) show the energy transmission as a function of frequency for the horizontal shear and sagittal polarized line sources in the $\Gamma X$ direction respectively. It is clear that the first attenuation corresponds to the second band in the band structure curve, while the second attenuation corresponds to the fifth band.

The guided surface wave is located in the first six bands inside the sound cone. The Eigen mode is executed and the displacement fields are calculated, to evince the nature of the dispersion relation in the surface modes. We calculate the displacement field and the corresponding displacement components in relative values, at these points; A, B and C as indicated in Figure 2(a), this points A, B and C are at the frequency of 4.17, 9.9 and 11.04 GHz, respectively.

The principal characteristic of the SAW through a periodic medium is the penetration of the elastic energy, which is confined on the small depth in order of the wavelength from the upper surface, which agree with our results as shown in Figure 3. Where the elastic energy is mostly concentrated in the
pyramid and in the vicinity area of the substrate’s surface, which agrees with references [20, 21, 29, 30].

In Figure 3, mode 1 has a shear oscillation, where the mode 2 and 3 have elongational oscillation. The displacement field of a guided mode has penetrated the surface with small deepness equals to the wavelength, which agree with references [9, 21].

In mode 1 the displacement field is localized on the pyramid, particularly $u_y$, which is the vibration directions of displacement in the pyramid are opposite with respect to the sagittal midplane ($x\z$) of the structure, it is the antisymmetric character. Which is the reason why the band gap appeared in the transmittance response in the case of the sagittal polarization.

Furthermore, the surface mode in Figure 3(a) is mostly shear polarized. In which the elastic energy is essentially confined in $u_y$ component while $u_x$ and $u_z$ is comparatively small. While in Figure 3(b), the surface mode is mostly sagittal polarized. The elastic energy is essentially distributed between $u_x$ and $u_z$, in which it agrees with the transmission spectra. In mode 3, the three displacement components all make relatively the same contribution to the displacement field.

3.2 The geometric pyramid defect on the SAW PnC

To see the influence of the geometry of the pyramid on the properties of surface modes, the band structures and the transmission spectrum, for different pyramid height sizes are calculated, all other parameters of the pyramid are the same as in Figure 1. As shown in Figure 4, the first band gap localization is shifted and the bandwidth size is changed; the centre frequency of the first band gap is higher and the size of the first band gap is larger, if the pyramid height is smaller. As shown in Figure 4, the centre frequency of the first band gap is equal to 4.33 GHz with a pyramid height of 300 nm, while the centre frequency of the band gap is equal to 6.8 GHz with a pyramid height of 220 nm.
For this latest, the bandwidth of the first band gap is larger than in the case of pyramid height of 300 nm.

Based on the results from Figure 4(a), the second band gap (Bragg band gap) is scattering from 10 to 11 GHz frequency range, when the corresponding wave length is about twice of the lattice constant. Besides, this band gap is localized at the fifth band for $h_1 = 300$ nm, once corresponding attenuations of transmission spectrum of the two polarization modes are localized in the same frequency range of Bragg band gap.

However, in Figure 4(b) the Bragg band gap is localized at the third band at 10.5 GHz for $h_1 = 280$ nm, as the first corresponding attenuation, i.e. sagittal polarization is shifted below 10.5 GHz, and the second attenuation, i.e. shear horizontally polarization is localized at 10.5 GHz.

Moreover, in Figure 4(c), for $h_1 = 240$ nm the Bragg band gap is localized at the third band the same as both corresponding attenuations, i.e. sagittal and shear horizontally polarization modes.

For $h_1 = 220$ nm in Figure 4(d) the Bragg band gap is scattering from 11 to 11.8 GHz equivalent to both attenuations of transmission spectrum; thus, this band gap is localized at the third band in band structure curve.

Therefore, as shown in Figure 4(a) the perfect PnC waveguide is selected for $h_1 = 300$ nm because both attenuations polarizations (shear horizontally and sagittal) are parallel to the band gap in the band structures curve of Bragg band gap as well as of local resonance Band gap.

To show the effect of line defect in PnC, a model of eleven pyramids is used, for this reason the dispersion proprieties of waveguide are analysed. The phononic band structures and the corresponding transmission spectra with a sagittal polarized excitation line source and a shear horizontally polarized excitation line source are elaborated, for each line defect size as shown in Figure 5.

Figure 5(a) shows the corresponding proprieties for zero nm of the pyramid height, it is the reference point, while Figure 5(b–d) shows the corresponding properties for 300, 360 and 240 nm, of the pyramid height respectively. It is shown in Figure 5, the band structures in the finite size PnC, are still the same than that of a signal unit cell in the case of the location and widths of the band gap. There is no larger differences in the global band structures at four conditions, except some bands, which are shifted, this is worthy to be studied.

If we take Figure 5(a) as a reference, when the pyramid height is 0 nm, the 21st and 22nd band are localized at about 8 GHz frequency range, while the same bands are shifted around to 6 GHz frequency range for Figure 5(d), when the corresponding pyramid height is 240 nm PnC waveguide.
Finally, for the pyramid height of 360 nm in Figure 5(c), these bands are localized in the band gap frequency range. But for the pyramid height equal to 300 nm in Figure 4(b), this two bands are exactly localized at the band gap frequency range, it is the perfect PnC waveguide. Finally, for the pyramid height of 360 nm in Figure 5(c), these bands are localized in the band gap frequency range, when the first and the second bands are shifted below the band gap frequency range.

The transmission curve agrees well with band structures for all conditions of the height pyramid size, in which the band gap size is changed according to the bands location, this means the size of the bandwidth is being influenced by the shifted band.

The mode analysis in PnC waveguide with varied defect pyramidal height is studied in this chapter. Figure 6 displays the displacement field in the $x$–$z$ plan of different models at different Eigen frequencies in the X point, in a small pyramidal height $h_1=240$ nm (Figure 6(a)), and in a big pyramidal height $h_1=360$ nm (Figure 6(b)).

As shown in Figure 6(a) and (b), the displacement field at different frequencies is mostly confined in the pyramid or the vicinity area, the first and the second bands for the small defect and for the large defect, offer a strong localization. Those modes are mainly confined in the pyramid, for the small defect at the 5.86 GHz and for the large defect at 3.08 GHz, the elastic energy is well focused in the pyramid by the local resonance effect as we can see in Figure 6(c) and (d).

4 | CONCLUSION

Phononic (PnC) waveguides made of pyramidal pillars deposited on a thick slab of silicon is studied in this paper. The band structures and the corresponding transmission spectrum are calculated, by using the FEM method. The surface mode of SAW waves is investigated. This nanostructure can be used in nanotechnology devices at hypersonic frequency (GHz) as nano-waveguides of elastic and acoustic waves. Two band gaps are presented in pyramidal PnC waveguides, the first band gap due to the local resonance effect and the second due to the Bragg scattering.

The results showed that the first band gap is localized at 4.3 GHz. However, this band gap frequency will change if pyramid height size changes. On the other hand, the second band gap is localized at about 10.8 GHz, and it remains constant unless there is a significant variation in the pyramid height size. We numerically investigated the scheme of this variation as a function of the band gap localization, by changing the pyramid height. Thus, based on data description and analysis of the band...
gap localization and the transmission attenuation for the two bands gaps, a perfect PC is selected.

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