Band Gap Optimization for GHz Elastic Waves in Gold Phononic Crystals

Chi Zhang¹, Qiang Liu¹, ², *, Zhengbiao Ouyang¹, ², *
¹College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China
²THz Technical Research Center, Shenzhen University, Shenzhen 518060, China
*Email: qliu@szu.edu.cn; zbouyang@szu.edu.cn

Abstract. Elastic waves at GHz range have many interesting applications, such as microwave generation, hybrid-information processing and quantum routing. The phononic crystals (PhnCs) can help manipulate the propagation of elastic waves, due to their bandgap effect. In order to produce relatively broad phononic bandgap in the GHz range, here three types of PhnCs in gold are investigated. Phononic bandgaps are optimized in terms of tuning the shape and size of air holes. Results as provided by the finite element method show that the maximum of the gap ratio ~0.991 appears in the cross-shaped PhnCs. The proposed gold-based PhnCs may be useful for building optomechanical platform which can realize strong surface-plasmon-mechanical coupling.

1. Introduction

GHz elastic waves can interact with photons, electrons and defects in the solid crystals, and till now they have been extensively studied for many interesting applications such as microwave generation [1], acousto-optic modulation [2], hybrid-information processing [3] and quantum routing [4].

In analogy to photonic crystals, phononic crystals (PhnCs) belong to artificial material with periodic structures which provide phononic bandgaps to elastic wave. When the frequency of an elastic wave is within the phononic bandgap, the wave cannot propagate in the crystal. At present, most researches on PhnCs are focused on materials that can simultaneously produce phononic and photonic bandgaps (or the so called phoxonic crystals) to obtain strong interaction between photons and elastic waves, which is beneficial for increasing the optomechanical coupling strength [5, 6]. Inspired by that, the interaction between surface plasmonic polaritons (SPPs) and elastic waves confined in metallic nano-structures has also been recently studied [7, 8]. Resulting from the strong surface-plasmon-mechanical coupling, new optomechanical platforms may appear.

Due to the unique optical property, gold has wide applications in super-resolution imaging [10], biosensors [11] and solar cells [12]. Recently, SPP-based waveguides [13], resonators [14] in gold have been extensively studied. However, it is rarely to see any research on the phononic property (especially in the GHZ regime) of nano-structures in gold, which may hinder the potential application.

In aiming to achieve relatively broad phononic bandgap in GHz regime, this paper investigates three types of PhnCs in gold. The relationship between the geometrical design and the gap ratio of phononic bandgap are discussed in details. With proper optimizations, it is found that the cross-shaped structure can provide a high band gap ratio ~ 0.991, and the corresponding phononic bandgap extends from 1.70 GHz to 5.05 GHz. The proposed designs may be helpful for building the optomechanical system that requires strong surface-plasmon-mechanical coupling.
2. Basic Structures

Three types of PhnCs (with square, circular, and cross-shaped air holes) are studied in this paper, the diagram of the corresponding unit cell is shown in Figure 1(a), Figure 1(b) and Figure 1(c), respectively. Note that, the lattice constant $a$ for all three cases is assumed to be 200nm. In Figure 1(a), the side length of the square air hole is set as $L_1$; In Figure 1(b), the diameter of the circular air hole is set as $D$; In Figure 1(c), the side length of the longer (shorter) side of the cross-shaped air hole is denoted by $L_2$ ($L_3$), while the aspect ratio (AR) is defined as:

$$\text{AR} = \frac{L_2}{L_3}$$

(1)

In the following simulations, we use Young's modulus of gold $E = 79$ GPa, the density of gold $\rho = 19.3\text{g/cm}^3$, and the Poisson's ratio of gold $\nu = 0.42$ [15].

![Figure 1](image1.png)

Figure 1. Unit-cell diagram of PhnCs with (a) square air hole, (b) circular air hole, (c) cross-shaped air hole. For all three cases, the lattice constant $a$ is assumed to be 200 nm

According to the Bloch theorem, the mechanical field distribution in a periodic structure (with lattice constant $a$) can be written as follows:

$$u(r + a) = e^{i(k_x + k_y)a} u(r)$$

(2)

Where, $u$ represents the displacement field, $k_x$ and $k_y$ represent wave vectors along $x$ and $y$ directions in the PhnCs, respectively.

To calculate the dispersion diagram of PhnCs, periodic boundary conditions that covering the whole wave vector ranges (see the irreducible Brillouin zone (IBZ) in Figure 2) need to be applied. As noted, for the IBZ, the wave vectors scan along the path $\Gamma$-X-M-$\Gamma$ in a two-dimensional rectangular structure to find the eigen-frequencies.

![Figure 2](image2.png)

Figure 2. Schematic of IBZ in Figure 1
3. Results and Discussions
The phononic crystal band diagrams of holes in various sizes and shapes can be obtained by simulation with COMSOL software. According to the formula that describing the band gap width:

\[ \Delta f_i = f_{\text{upper}} - f_{\text{lower}} \]  

(3)

here \( \Delta f_i \) is the width of the \( i \)-th band gap, \( f_{\text{upper}} \) is the frequency of the upper edge of the \( i \)-th band gap, while \( f_{\text{lower}} \) is the frequency of the lower edge of the \( i \)-th band gap.

In addition, the gap ratio (GR) is employed to define the relative width of the phononic bandgap:

\[ GR = \frac{\Delta f_i}{f_{\text{mid}}} \]  

(4)

where, \( f_{\text{mid}} \) is the intermediate frequency of the \( i \)-th band gap as expressed by:

\[ f_{\text{mid}} = \frac{f_{\text{upper}} + f_{\text{lower}}}{2} \]  

(5)

In the following, we will show how the geometry of the air holes in the unit cell could affect the GR.

3.1. PhnCs with Square Air Holes
For PhnCs with square air holes inside (see Figure 1(a)), it is found that even we extend the \( L_1 \) from 10 to 190 nm, there is no phononic band gap. Figure 3 shows the phononic band diagram for \( L_1 = 190 \) nm.

As found, band gaps along X-M and M-\( \Gamma \) exist, however no absolute band gap appears; similar results could be found in Wang’s work [16]. This phenomenon may be involved with the small coupling between the resultant forces along \( x \) and \( y \) directions in the unit primitive cell. Since the single bond along \( x \) (or \( y \)) direction could be considered as a resonator, the mechanical energy is reflecting back and forth in the \( x \) (or \( y \)) direction (notice the 90 degree sharp turn between the nearest bond), as a result, the flow of mechanical energy from \( x \) to \( y \) (or vice versa) in this PhnCs is relatively limited [17].

![Figure 3. Phononic band diagram of PhnCs with square air-holes for \( L_1 = 190 \)nm](image)

3.2. PhnCs with Circular Air Holes
For PhnCs with circular air holes inside (see Figure 1(b)), the relationship between GR and \( D/a \) is shown in Figure 4(a). As noticed, there is a cut-off point which appears at \( D/a = 0.74 \), when \( 0.74 < D/a \), the GR of band gap appears to increase linearly with \( D/a \). For example when \( D/a=0.95 \), the GR gets a relatively large value \( \sim 0.45 \) and the corresponding band gap width reaches 1.52 GHz (from 2.65 to 4.16 GHz, and the intermediate frequency is 3.40 GHz). Figure 4(b) shows the band diagram when \( D/a=0.95 \).
For PhnCs with cross-shaped air holes, we divide the discussion into two parts. Firstly we explore the relationship between $L_2/a$ and GR by fixing $AR = 0.1$. As shown in Figure 5(a), there also appears a cut-off point as $L_2/a = 0.75$; and when $L_2/a$ is above 0.75, GR of PhnCs increases monotonically with $L_2/a$. Notice that, when $L_2/a = 0.95$, the corresponding band gap width reaches 2.24 GHz (from 1.93 to 4.17 GHz) and the intermediate frequency of band gap is 3.05 GHz, the corresponding band diagram is shown in Figure 5(b).

![Figure 5](image)

**Figure 5.** (a) The relationship between GR and $L_2/a$ of the PhnCs with cross-shaped air-holes when the AR is fixed as 0.1. (b) The phononic band diagram of the PhnCs with cross-shaped air-holes, here $AR=0.1$ and $L_2=190$nm.

In the following, we explore the relationship between GR and AR by fixing $L_2 = 190$nm, as shown in Figure 6(a). It turns out that the GR of the first band gap begins to appear at AR = 0.05 and becomes maximum at AR = 0.28; when AR increases to 0.56, the first band gap becomes a complete cut-off. Similarly, for the second and third bandgaps, the cut-off frequency and the corresponding maximal point can be also found.

It is noted that the maximum value of GR for the first, second and third band gaps are found to be 0.991, 0.756 and 0.556, respectively. For the first case, the maximum of GR appears when AR = 0.28, and the corresponding band gap width is 3.35 GHz (from 1.70 and 5.05GHz), noting that the intermediate frequency of the band gap is 3.37 GHz. The phononic band diagrams for observing the maximum of GR in the first, second and third band gap regimes are respectively shown in Figure 6(b), Figure 6(c) and Figure 6(d).
Figure 6. (a) The relationship between the GR and AR of the PhnCs with cross-shaped holes when the $L_2/a$ was fixed as 0.95. (b, c, d) The phononic band diagrams of the PhnCs with cross-shaped air-holes with different AR. In (b) for the first bandgap, the maximum of GR is 0.991, here AR=0.28 and $L_2=190$nm. In (c) for the second bandgap, the maximum of GR is 0.556, here AR=0.44 and $L_2=190$nm. In (d) for the third bandgap, the maximum of GR is 0.556, here AR=0.64 and $L_2=190$nm.

4. Conclusions

In this paper, we have examined three types of 2D-PhnCs in gold, including square, circular and cross-shaped air holes. Simulations based on finite-element method illustrates that the shape and size of the air holes play important role in deciding the GR of the PhnCs. It is found that, the PhnCs with cross-shaped holes produce a relatively broad phononic band gap than the other two holes. Optimization results show that the GR gets a maximal value of about 0.991, while the bandgap width is 3.35GHz (from 1.70 to 5.05 GHz). Combined with the unique property of gold which can support surface plasmon polaritons, the proposed designs may provide options for building hybrid-plasmonic-mechanical system that works in the GHz regime.

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6. References

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