Numerical Study on High Sensitivity Biosensing Scheme Based on Waveguide Phononic Crystal

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1. Introduction

Phononic crystals have been widely studied in the past decades for waveguides, filters, resonators, and so on. By designing different dimensions, materials and arrangements of the scattering inclusion in phononic crystals, one can control the elastic-wave propagation behavior for various applications. Recently, sensors based on phononic crystals have drawn much interest. For example, the liquid sensor based on the cavity mode [1] and the biosensor with localized resonant pillars [2] have been studied, showing the high sensitivity potential. However, these phononic crystal sensors operate only at relatively low frequencies from hundreds of kHz to tens of MHz, which restricts their sensitivity and needs a larger volume of analyte.

Meanwhile, compared to other biosensors like quartz crystal microbalance (QCM) biosensor, using picosecond ultrasonics can create the GHz range resonance and thus has the potential for ultra-sensitive sensing [3]. However, since the laser inevitably brings excess heating, biomolecules like proteins will deteriorate on the sensor surface, and accurate measurement cannot be realized. Moreover, metal materials with high thermal conductivity are usually used for the substrate layer for immobilizing biomolecules, which exacerbates this problem.

In this work, we will present a phononic-crystal design to achieve a highly sensitive biosensor, which is operated with picosecond ultrasonics. This biosensor can separate the laser heating areas for wave generation and detection from the sensing area, where biomolecules are attached, so as to prevent the biomolecule deterioration. Moreover, based on our simulation result, this biosensor has the potential for a ~fg level detection limit due to the sharp transmission change in GHz range waveguide resonance, which shows the good adaptability for biosensing.

2. Structural Design

The schematic of our biosensor is shown in Fig.1. This sensor includes two parts: the periodic strips structure and the phononic crystal structure. Two groups of periodic metal strips on the substrate are designed to generate and detect the elastic waves using the pump and probe light pulses, respectively. Between two groups of strips, the free-standing phononic-crystal layer with an artificial line defect at the center part is designed for waveguiding and sensing. The phononic crystal is comprised of disk-shape gold inclusions and silica matrix, where the gold surface is functionalized for the biomolecule immobilization. The working principle of this biosensor is as followings: Before the sensing, the pump light is irradiated on the one group of strips, and the elastic wave will be generated. It passes through the phononic-crystal waveguide and is detected by the probe light on the other side. Then, after the attachment of bioparticles (target molecules), the frequency of the waveguide mode will be shifted, and the transmission efficiency will change. Because the detection efficiency will become the maximum at the generation frequency, both the frequency and amplitude changes will significantly affect the detection amplitude, realizing the biosensing.

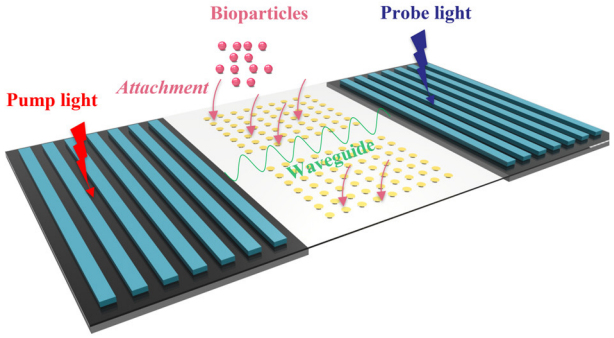

Fig. 1 Schematic of proposed biosensor based on phononic crystal using picosecond ultrasonics.

3. Dispersion Analysis

To demonstrate the above designed biosensor, the finite element method (FEM) is used to study the dispersion and transmission characteristics of phononic crystals using COMSOL Multiphysics 5.4. Meanwhile, to simplify the calculation, the phononic crystal is designed as a composite consisting of the Au cylinders embedded in the silica matrix, with the square array distribution. The three-dimensional single-cell model of phononic crystal is studied for the first step. For in-plane directions, periodic

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boundary conditions are applied to the side surface according to the Bloch-Floquet theorem:

$$u_j(x+a, y+a, z) = u_j(x, y, z)e^{i(k_x a + k_y a)} \quad (j = x, y, z)$$

where a is the lattice constant, u_j denotes the displacement component, and k_x and k_y are the Bloch-wave-vector components along the irreducible Brillouin zone (IBZ). On the top and bottom surfaces, the stress-free boundary conditions (i.e., the free boundary condition) are adopted.

By sweeping the Bloch wave vector along the irreducible Brillouin zone, the phonon dispersion relationship can be obtained. Here, we have simulated different dispersion curves with different filling fractions $(f = \pi r^2/a^2)$ and cell thicknesses. Unlike the phononic crystal with air hole inclusion, which is widely studied before, the Au-SiO_2 phononic crystal structure shows the largest bandgap when the filling fraction is close to 12.5% and the thickness close to lattice constant. Also, considering the fabrication limitations and the high frequency requirement for biosensing, the radius of inclusions is designed as 50 nm and the thickness with 250 nm. The simulated dispersion curve with the above parameters of a perfect phononic crystal is shown in Fig.2(a) with the absolute bandgap between 6.05-6.4 GHz.

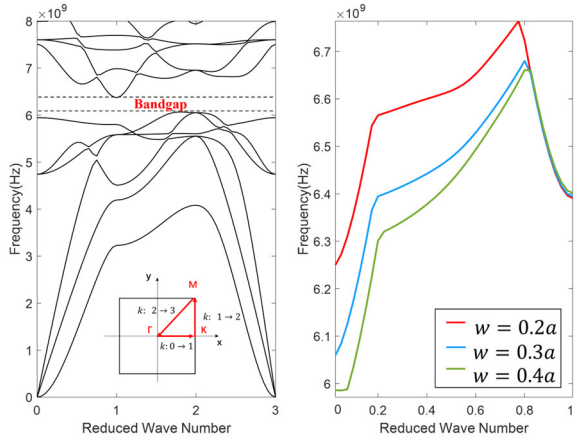

Fig. 2 (a) Dispersion curve of perfect phononic crystal; (b) Dispersion curve of waveguide modes with different line defect width.

Then, to create the waveguide mode of phononic crystal, the artificial defect is designed by "stretching" the phononic crystal in the y direction. The different waveguide modes can be obtained by changing the defect width w. It is shown that, with the increase of the defect width, dispersion curves are "dragged down" from the upper edge mode and distorted, as shown in Fig.2 (b), which has never been indicated before. Here, for biosensing, it is expected to get the isolated waveguide mode also the urgent change of transmission efficiency between the bandgap area and waveguide mode, so it is expected to keep the waveguide mode and bandgap simultaneously and the defect with of $w = 0.2a$ is designed.

4. Transmission Analysis

The transmission coefficient is simulated with the perfectly matched layer (PML) by sweeping the excitation frequency on one side of phononic crystal area and detected on the other side. For the perfect phononic crystal, the transmission spectrum can be obtained, showing the same bandgap with the dispersion curve. Then, the transmission spectrum of the waveguide phononic crystal is also calculated, showing the waveguide mode inside the bandgap. To simulate the bioparticle attachment, the mass is added to the top surface of inclusions of phononic crystals with the different total mass values. The influence on the transmission coefficient by the mass-loading effect is shown in Fig.3. It is shown that the transmission efficiency is significantly affected by the mass adding at the fixed frequency, which can realize the biosensing. To illustrate the reason of transmission coefficient change, the dispersion curve with different added mass is also simulated. It is shown that with more mass added, unlike the defect width influence, the waveguide dispersion curve evenly moves down without any twist in shape, which is unexpected and enables the linear change in transmission efficiency.

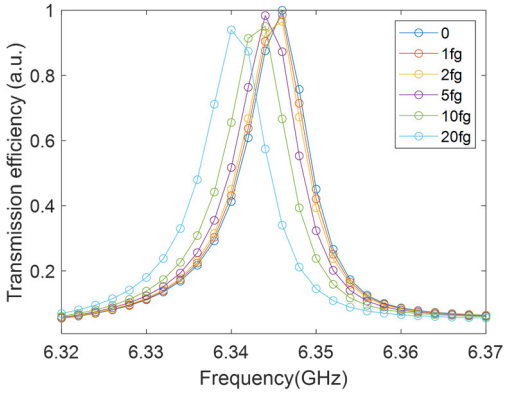

Fig. 3 Influence of mass adding to the transmission efficiency of waveguide phononic crystal

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