1D and 2D Phononic Crystal Sensors

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Abstract

Acoustic band gap materials, so-called phononic crystals, provide a new sensor platform for determination of material properties in small cavities. The sensor employs specific transmission windows within the band gap to determine properties of a component that builds the phononic crystal. The frequency where transmission takes place is correlated to material properties and permits the determination of several parameters of practical interest like concentration of an analyte. The capability of the concept will be demonstrated with a one-dimensional arrangement of solid plates and liquid filled cavities and a two-dimensional periodic arrangement of liquid filled holes in a solid matrix.

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1. Introduction and motivation

Phononic crystals are periodic composite materials. A device consists of periodically arranged scattering centres with acoustic properties different to a homogeneous matrix surrounding the scatters. The most strikingly feature of phononic crystals are frequency bands (stop bands) within which sound cannot propagate through the structure. Since the spatial modulation of the material parameters of the phononic crystal is in the same order as the acoustic wavelength in the stop band, they can be realized in a wide geometric dimension range. With frequencies in the MHz-range phononic crystals are realized with dimensions similar to those used in microfluidic devices. A favourable design of a device combining phononic crystals and microfluidics is a solid matrix with periodically arranged holes, which may become part of a microfluidic system. An important feature of phononic crystals emerges if the holes are filled with a liquid. Transmission peaks or narrow transmission bands appear within the band gap. This feature can be attributed to resonance phenomena, some of them to the confined liquid. The 'resonance' frequency (frequency of maximum transmission) is a measure similar to that applied in acoustic microsensors which depends on acoustic properties of the material confined in the holes. Therefore, phononic crystals provide a new platform for sensing liquid properties in small cavities, specifically microchannels or microreactors.
2. Background

The concept of band gaps can be explained by the multiple scattering of waves within a phononic crystal. When a set of scatters is positioned periodically in the matrix, waves are strongly scattered among the scatters. A band gap appears when having destructive interference of waves happens in a given direction.

Several methods have been developed to investigate the band structures of elastic waves propagating in phononic crystals: the plane wave expansion (PWE) method, e.g. [1], the finite difference time domain (FDTD) method [2], and the multiple-scattering theory (MST) [3]. For sensing applications the calculation of the transmission and/or reflection coefficients is required which can be done e.g. with the layer MST (LMST) [4]. We have applied this method to finite two-dimensional phononic crystal slab with a certain number of layers of cylindrical scatters. Cylinder scatters in a monolayer are arranged periodically along one direction. Identical monolayers are stacked one by one along the perpendicular one. The LMST considers the acoustic waves scattering by three steps. It starts from the displacement distribution of a central cylinder. Next scattering matrices of the monolayer and the matrices for one scattering plane are derived. The matrices for one scattering plane are used to obtain the matrices of a slab with two scattering planes. The procedure is repeated to obtain the matrices for a slab with 2n scattering planes. For details, see [4]. Computation is performed numerically and is therefore time-consuming when a high frequency resolution is required even though LMST has found to be much more effective than FDTD.

We therefore have reduced the concept to one dimension without losing general validity. Modeling has been performed by using the impedance concept in propagation problems based on a chain matrix technique. Here, geometric and material properties of the elements building the one-dimensional phononic crystal define a propagation matrix and a transfer matrix. In this concept the layer i is understood as quadrupole with an input voltage, $u_i$ as equivalence of stress and current, $i_i$ as equivalence of particle velocity, and an output voltage, $u_{i+1}$ and current $i_{i+1}$. The calculation of an overall effective impedance of the phononic crystal starts from the front port with known boundary conditions. The key issue of the concept is that each single layer has a frequency dependent effective acoustic impedance different from the characteristic impedance of the material. It considers reflection and transmission of acoustic waves at the interface of the layer as well as wave interference inside the layer. Two layers have therefore an effective impedance which is NOT just the sum of the impedances of each layer:

$$ Z = \frac{Z_i + Z_{i+1}}{1 + \frac{Z_i Z_{i+1}}{Z_{ci}^2}} $$

with

$$ Z_i = jZ_{ci} \tan \left( \frac{\omega \rho_i}{Z_{ci} h_i} \right) $$

(1, 2).

$Z_i$ is the effective impedance of the i-th layer, $Z_{ci} = \rho v_i$ the characteristic impedance of the respective material building the layer with $\rho$ being the density and $v_i$ the velocity of the acoustic wave, $h_i$ is the thickness of layer $i$. The overall effective impedance of the phononic crystal replaces the (characteristic) impedance of a semi-infinite virtual material having the same properties relative to reflection and transmission of acoustic waves. Details can be found e.g. in [5]. The transmission spectrum can easily be calculated from eq. 3 when assuming normal incidence:

$$ T = \frac{4Z_1 Z_2}{(Z_2 + Z_{eff})^2} $$

(3).

Note, that this overall acoustic impedance is complex; hence the transmission coefficient is also of complex nature. It considers changes in intensity of the acoustic wave when passing the interface and a phase shift.

3. Results

Only a very few studies dealing with material property determination have been published so far [6-8]. Here we demonstrate the validity of the phononic crystal sensor concept in two steps. We first analyze a reduced one-dimensional structure. Modeling has been performed on the basis of analytical solutions using a specific geometry and material properties from literature. The results with regard to the appearance of specific modes, their bandwidth and their shift when changing properties of the liquid component building the one-dimensional phononic crystal...
demonstrate the general aspects to be considered. In the second step we report on results with a two-dimensional structure with holes periodically drilled into a solid matrix. We especially concentrate on transmission features similar to those of the 1D analysis when all holes are filled with the liquid of interest.

Fig. 1 shows the impedance spectrum of the layers building the phononic crystal. The metal plates are made of aluminum ($\rho_{Al} = 2720 \text{ kg m}^{-3}$, $v_{Al} = 6170 \text{ m s}^{-1}$, $h_{Al} = 3 \text{ mm}$). This plate has its first resonance at 515 kHz, characterized by a sharp rises of the impedance to a maximum, immediately followed by a minimum (grey). 900 µm thick layers of DI-water and propanol (for data see Table 1) show similar features at 400 kHz and 340 kHz as well as 1200 kHz and 1020 kHz, respectively. None of these characteristic frequencies coincides with the frequency of maximum transmission through the whole phononic crystal as shown in Figure 2. This peak frequency has been found at 775 kHz for water and 622/628 kHz (model/experiment) for propanol. This deviation is less than that calculated from different literature data. We furthermore have tested mixtures of water and propanol and could recover the characteristic maximum at a molar ratio of 0.056 as a result of a maximum in speed of sound (see Table 1). For a concentration range between $x_2 = 0 \ldots 0.035$ of 2-propanol (0 \ldots 10%) one can estimate a limit of detection of about 0.1% [8]. When introducing a chemically sensitive coating inside the cavity, gap size as well as frequency must be adjusted to the coating thickness to be able to monitor changes in the coating. For example, having a 1 µm coating and a 100 µm gap, a promising peak could be found at about 7.5 MHz.

Both, appearance of transmission peaks within the stop band and the dependence of the peak frequency on material properties have been found for 2D phononic crystals as well. Fig. 4 shows the transmission spectrum for

<table>
<thead>
<tr>
<th>$x_2$ (water)</th>
<th>density $\rho$ (kgm$^{-3}$)</th>
<th>speed of sound $c$ (ms$^{-1}$)</th>
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<tbody>
<tr>
<td>0</td>
<td>998</td>
<td>1483</td>
</tr>
<tr>
<td>0.021</td>
<td>990</td>
<td>1545</td>
</tr>
<tr>
<td>0.035</td>
<td>982</td>
<td>1578</td>
</tr>
<tr>
<td>0.056</td>
<td>974</td>
<td>1588</td>
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<tr>
<td>0.102</td>
<td>956</td>
<td>1531</td>
</tr>
<tr>
<td>0.158</td>
<td>933</td>
<td>1472</td>
</tr>
<tr>
<td>0.230</td>
<td>908</td>
<td>1421</td>
</tr>
<tr>
<td>1 (1-propanol)</td>
<td>804</td>
<td>1220</td>
</tr>
<tr>
<td>1 (2-propanol)</td>
<td>777</td>
<td>1126</td>
</tr>
</tbody>
</table>
empty and water filled holes for a crystal having a lattice parameter of the square array of holes of 1.0 mm and the filling ratio of 0.6. The transmission spectrum of longitudinal waves through such a phononic crystal in the \textit{X} direction for the incidence of a longitudinal plane wave depicts a band gap between 1.4 MHz and 2.36 MHz when the holes are empty (a). When filling water (b) or propanol in all holes the band moves to slightly lower frequencies between 1.26 MHz/1.18 MHz and 1.9 MHz/1.7 MHz (water/propanol). The newly appearing transmission peaks move downwards with decreasing speed of sound, e.g. about 260 kHz when replacing water by propanol [8]. Optimization especially regarding separation of the transmission peak by reducing lattice symmetry will be reported in [9].

4. Conclusions

Phononic crystals provide a new platform for the determination of properties of liquids in small cavities. Transmission windows which appear when the cavities are filled with a liquid display resonance features; therefore the respective peak 'resonance' frequency can be used to determine the properties of a liquid. Both theoretical predictions based on a one-dimensional transmission line model as well as admittance spectrum analysis and transmission experiments have shown the feasibility of the phononic crystal sensor concept. The feasibility of a two-dimensional phononic crystal, where holes drilled in a solid matrix act as liquid containers, could be demonstrated theoretically. Since acoustic wave propagation is more complicated, the transmission spectrum is more involved and needs to be further optimized for sensor purposes especially relative to number and shape of the transmission peaks.

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