Frequency-dependent acoustic energy focusing in hexagonal ceramic micro-scaffolds

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Abstract

Acoustic properties of a periodic hexagonal structure composed of thin rods are studied by finite element method (FEM) using Bloch boundary conditions. As a template for designing the computational unit cell, an additive-manufactured SiC scaffold fabricated by the robocasting method is used. The calculations show both angular and frequency dispersion of the acoustic waves with wavelengths comparable to the spacing between the rods, i.e., in a millimeter scale, indicating interesting acoustic properties in the MHz range. The dispersion character leads to focusing of the energy propagation into the directions of the rods of the hexagonal structure. This is illustrated by a modal-based calculation of the propagation of longitudinal and out-of-plane shear wave packets with a dominant wavelength.

Keywords: robocast scaffold, phononic crystal, acoustic energy focusing, Bloch analysis

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1. Introduction

Micro-architected periodic structures often exhibit phononic-crystal behavior with acoustic phenomena taking place in the frequency ranges much lower than for any crystalline matter found in nature, such as frequency band gaps in MHz range [1, 2, 3, 4, 5]. Moreover, due to their highly ordered periodical arrangement, these structures are able to focus the acoustic waves along certain principal directions given by the geometry [6, 7, 8, 9].

With the rise of additive manufacturing (AM) methods, phononic crystals with various geometries can be easily produced [10, 11, 12]. Robocasting is a direct ink writing AM method, by which periodic structures consisting of layers of thin rods are printed from colloidal gel inks based on micro-sized powders [13, 14]. Silicon carbide (SiC) is often utilized for robocast scaffolds due to its favorable thermomechanical properties. Cai et al. [15] produced robocast scaffolds based on SiC with sintering additives of Al_2O_3 and Y_2O_3 , utilizing pressure-less spark plasma sintering (SPS) for consolidation. The sintered scaffolds exhibited significant linear shrinkage when compared to green bodies, and the SPS lead to almost fully dense scaffolds with uniform microstructure while maintaining the geometric alignment of the rods. Román-Manso et al. [16] produced several SiC-based robocast scaffolds which differed in the mean size of the used SiC powders or in ratios between SiC and the sintering additives of Al_2O_3 and Y_2O_3 . These scaffolds also preserved the designed geometry very well after the sintering and exhibited low porosity values and good indentation hardness. Furthermore, SiC was chosen as a material for support structures for electrically conductive robocast scaffolds with addition of graphene fillers [17], or for Fe-doped scaffolds for catalytic purposes [18].

Kruisová et al. [19] studied elastic and acoustic properties of the SiC-based scaffolds by resonant ultrasound spectroscopy (RUS) and finite element method (FEM) modeling. From the sintered scaffold, which had a perpendicular orientation of the rods in neighboring layers, a rectangular parallelepiped sample was cut. The elastic coefficients of this sample were then obtained by measur-

ing free elastic vibrations by contactless RUS. The resonant spectrum of this sample consisted of sharp resonant peaks with high quality factor indicating low internal friction, suggesting that the rods are well-sintered and there is a good interlinking between the layers at the rods intersections. Due to the geometry, this scaffold macroscopically exhibits tetragonal symmetry. When applying FEM, it was shown that such a periodic scaffold is highly anisotropic in the tetragonal plane, which leads to the acoustic energy focusing along the ceramic rods. In the following works by Koller et al. [20, 21], acoustic properties of six types of scaffolds with three different types of material symmetry were studied. It was shown that in tetragonal scaffolds, where the rods in neighboring layers are perpendicular, focusing of the acoustic energy along the rods is observed. Much stronger focusing occurs when the in-plane spacing between the rods is increased.

In another work of Kruisová et al. [22], transmission of ultrasonic waves through four types of SiC-based scaffolds was studied. Longitudinal ultrasonic waves with frequencies varying from 2 MHz to 12 MHz were sent through the scaffolds in one of the directions of the ceramic rods, and the amplitudes of transmitted waves were measured. The wave propagation in these structures was also studied by FEM. It was shown both theoretically and experimentally that these scaffolds, which have characteristic dimensions of 0.1–1 mm, exhibit phononic-crystal behavior with frequency band gaps in MHz range. This directly showed the interesting behavior of these structures – in standard crystals, phenomena such as the frequency band gaps can be observed in hardly reachable THz range.

In this paper, we investigate a scaffold with the orientation of the rods in neighboring layers of 60° and the periodicity of 3 layers; thus, it exhibits macroscopic hexagonal symmetry. Since all directions in the hexagonal plane are macroscopically equivalent, no energy focusing was observed in the long-wavelength limit. However, when the acoustic wavelength decreases and becomes comparable to the in-plane spacing between the rods, the energy becomes focused along the rods, implying a frequency-dependent angular-dispersive character. A full FEM study of the acoustic behavior of a structure consisting of

thousands of unit cells would be computationally very demanding. This problem was addressed by Hyun et al. [23], who developed an efficient and stable basis-vector-based model reduction scheme based on adaptive quasi-static Ritz
65 vector (AQSRV), and described its use for analysis and design of acoustic meta-materials. Similarly, a continuum model for the description of high-frequency behavior was developed by Rosi et al. [24] and tested on hexagonal and hexachiral structures [25]. However, in this paper, we propose a combination of FEM study of a unit cell with special, complex phase-shift boundary conditions
70 in particular angles, followed by a simulation based on modal analysis.

2. Materials and methods

2.1. Robocast structure

The studied hexagonal scaffold structure, which is used as a template for designing the FEM unit cell, was fabricated by the robocasting technique. At
75 first, a colloidal gel ink, based on β -SiC powder with sintering additives of Al_2O_3 and Y_2O_3 , was produced by mechanical mixing of the powder mixture with ultrapure water and organic flocculants and viscosifiers. This is required because the ink needs to have highly shear-thinning rheological behavior, in order to form a thin filament when extruded through a nozzle tip following a
80 computer-aided-design (CAD) printing route, and also to provide support for the already-printed free-standing structure. In each layer, the rods are mutually parallel with constant in-plane spacing between them, and the rods in the neighboring layers are oriented in a different angle of 60° to form a hexagonal structure. The out-of-plane spacings between the layers are significantly lower
85 than the diameters of the individual rods, producing scaffolds where the rods of neighboring layers partially intersect at crossing points. After the printing, the green bodies were dried in the air, the organic additives were then burnt out, and the scaffolds were subsequently consolidated by SPS.

The studied hexagonal scaffold structure, shown in Fig. 1, consists of a
90 layered arrangement of the rods with diameter $d = 215 \mu\text{m}$, which are mutually

parallel with constant in-plane spacing $l = 576 \mu\text{m}$ in each layer. The orientation angle between the rods in neighboring layers is equal to 60° and the rods partially intersect at the crossing points with the out-of-plane spacing z between the layers. This arrangement thus leads to a periodic hexagonal structure, having
95 the out-of-plane periodicity of 3 layers, $h = 3z = 385 \mu\text{m}$.

Figure 1: Top-view of the hexagonal structure, (a) optical micrographs of the consolidated scaffold, (b) geometric arrangement of the periodic structure.

Figure 2: Computational unit cell used for FEM (a), the distance $m = (\sqrt{3}/2)l$ is given by the geometry. The right side, (b), shows an illustrative example of the calculated displacement field for the propagation of a wave with high wavenumber ($k \approx 6.54 \text{ mm}^{-1}$) in the direction corresponding to $\alpha = 20^\circ$.

2.2. FEM study

Acoustic properties of the structure were studied by finite element method (FEM) using COMSOL Multiphysics software. A representative unit cell of the periodic structure was meshed with tetrahedral Lagrangian elements, as shown in Fig. 2(a). For the calculation, material properties of SiC were utilized [19]: a density of $3.34 \text{ g}\cdot\text{cm}^{-3}$, Young's modulus of 305 GPa, and Poisson's ratio of 0.19. As the studied structure occupies a relative space of 44.4 %, the effective density is $1.483 \text{ g}\cdot\text{cm}^{-3}$. As described in [26], applying various types of periodic boundary conditions with prescribed displacement in the principal direction of the computation unit corresponds to macroscopic homogeneous straining of the structure and can be thus used for evaluation of macroscopic elastic coefficients of the hexagonal structure. The resulting constants obeying hexagonal symmetry for our structure are:

$$c_{ij} = \begin{pmatrix} 66.05 & 19.45 & 8.80 & 0 & 0 & 0 \\ 19.45 & 66.05 & 8.80 & 0 & 0 & 0 \\ 8.80 & 8.80 & 44.32 & 0 & 0 & 0 \\ 0 & 0 & 0 & 9.30 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9.30 & 0 \\ 0 & 0 & 0 & 0 & 0 & 23.30 \end{pmatrix} \text{ GPa.} \quad (1)$$

Following the Bloch theorem [27], the wave propagation in the studied periodic structure can be sought in the form of planar waves with the displacement vector of

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{U}(\mathbf{x}, \mathbf{k}) \exp[i(\mathbf{k} \cdot \mathbf{x} - \omega t)], \quad (2)$$

where $\mathbf{k}$ is the wave vector. $\mathbf{U}(\mathbf{x}, \mathbf{k})$ is the Bloch waveform with the same spatial periodicity as the printed structure. Due to that, the computation domain can be limited to a single unit cell and the solution for different $\mathbf{k}$ is found by solution of eigenvalue problem with complex phase-shift boundary conditions, known as Bloch boundary conditions. In particular, to obtain wave dispersion of acoustic

waves propagating in hexagonal plane, we applied the boundary conditions for rectangular supercell formed from 2 unit cells (see Fig 2) in the form

$$\begin{aligned}\mathbf{u}(x_1 = 0, x_2, x_3) &= \mathbf{u}(x_1 = 2l, x_2, x_3) \exp(i2lk_x), \\ \mathbf{u}(x_1, x_2 = 0, x_3) &= \mathbf{u}(x_1, x_2 = 2m, x_3) \exp(i2mk_y),\end{aligned}\tag{3}$$

and periodic boundary conditions in the direction of x_3 axis.

The wave solutions were determined for angles α (measured from the x_1 direction and following the notation given in Fig. 1) from 0° to 30° with 5° steps. The direction of the ceramic rods is therefore equal to $\alpha = 30^\circ$.

In each direction, the magnitude of $\mathbf{k}$ vector was increased from 0 to 4 mm^{-1} in 30 regular steps mapping approximately the inner two-thirds of the 1st Brillouin zone, which can be estimated as a circle with the radius π/l in the hexagonal plane. The resulting dispersion curves for the longitudinal and slow shear wave, which has the polarization in the out-of-plane (x_3) direction, are given in Fig. 3.

2.3. Modal analysis

Figure 3 shows the results of the FEM simulation illustrating that with the increasing wavenumber, i.e., with the wavelength closer to the dimensions of the hexagonal structure, the wave propagation becomes gradually both angular- and frequency-dispersive.

To provide a simulation of wave propagation through a larger sample of the structure by a time-domain-type simulation, a very large model would be necessary, implicating high computational demands and time. Therefore, in order to calculate and visualize the propagation of wave-packets with different dominant wavenumber propagating through such a structure, we utilize a method based on modal characteristics with the following principle:

1. The dispersion curves obtained by FEM are fitted with a polynomial function in frequency and interpolated into the whole range of α angles applying the hexagonal symmetry.

Figure 3: The dispersion data for the propagation of (a) longitudinal and (b) out-of-plane shear acoustic waves in the direction of the angle α with respect to x_1 -axis, i.e., $\alpha = 30^\circ$ corresponds to the direction of the rods. The curves are obtained via polynomial fit of the FEM data. The vertical lines correspond to wavenumbers chosen for the modal-simulations.

2. The excitation is then modeled, given as an initial displacement field in the form of a centered radial cosine function superimposed by a Gaussian pulse, creating a spatial wave packet. Varying the wavelength of the cosine function, the dominant excited wavelength changes, while the long-wavelength part stays constant (given by the size of the Gaussian envelope).
3. The Fourier-transformed excitation, i.e., its modal characteristics, is multiplied by the factor of $\exp[i\omega(\mathbf{k})t]$, where $\omega(\mathbf{k})$ is the frequency for each wavenumber and direction of propagation given by the fitted and interpolated dispersion data. Thus, the modal response in time t for each direction and each wavenumber is obtained.

The resulting modal response can be calculated for any chosen time t . The corresponding displacement field can be obtained by an inverse Fourier transformation.

3. Results and discussion

Using the simulations based on modal analysis, the propagation characteristics of different wave packets through the described structure is studied.

Figure 4 shows the resulting displacement and intensity fields of longitudinal-polarized wave packets at time $t = 10 \mu\text{s}$. The chosen dominant wavenumbers correspond to the lines in Fig. 3(a), i.e., to the low-, middle- and high-wavenumber region of the dispersion relation. It is illustrated that, whereas in the low-wavenumber, i.e., the long-wavelength region, the propagation shows no angular dispersion (see Fig. 4(a)), the influence of the structure increases with the shortening wavelength. In the middle region, the displacement field is still close to radial, but the intensity field shows obvious focusing of the energy propagation in the directions of the rods. In the high-wavenumber situation, the displacement is clearly hexagonal, Fig. 4(c). This is even more pronounced in the intensity, shown on the right side of Fig. 4(c), which indicates that the energy is in such a case transmitted almost exclusively through the rods. The

150 wavelength corresponding to $k = 2 \text{ mm}^{-1}$ is $\lambda = \pi \text{ mm}$, thus about 5 times
larger than the in-plane rod spacing l .

In Fig. 5, a similar study for the case of out-of-plane shear waves at time
 $t = 25 \text{ } \mu\text{s}$ is illustrated. Due to the larger dispersion (see Fig. 3(b)), the effect
of focusing is even stronger. The lowest corresponding wavelength is about 3.5
155 larger than the rod spacing l .

Similarly to the case of band gaps at MHz range studied described in [22], in
this case, the energy focusing corresponds to the frequencies around 1 MHz, as
opposed to the frequencies in the range of THz needed for studying such effects
in standard crystalline materials. This indicates not only interesting properties
160 of the 3D printed structures but also offers a much easier way of studying the
phenomena such as energy focusing in the far more easily-reachable frequency
regions.

4. Conclusion

The precise 3D-printing technique of robocasting for creating structures of
165 ceramic scaffolds offers a fast and simple way of constructing phononic crystals
with interesting acoustic properties in the MHz range. In this paper, we studied
the case of the scaffold with hexagonal symmetry.

With the model of the unit cell designed to mimic the printed structure, we
obtained the dispersion curves of the acoustic modes in several directions by
170 FEM calculations with Bloch boundary conditions (using the idea of complex
phase shift at the boundaries). The resulting dispersion curves show increasing
angular dispersion with higher frequency, i.e., with the corresponding wave-
lengths comparable to the in-plane rod spacing of the structure. As the spacing
is equal to $576 \text{ } \mu\text{m}$, the dispersion is observable already at wavelengths of few
175 millimeters (equivalent to frequencies around 1 MHz in this case).

We studied this effect using the modal-based simulation of propagation of
wave packets through a larger area of the hexagonal structure consisting of
hundreds of cells. It can be seen that with a higher dominant frequency of the

Figure 4: The displacement field (left) and the corresponding intensity (right) of longitudinal wave at $t = 10 \mu\text{s}$ for 3 different dominant wavenumbers: (a) $k = 0.3 \text{ mm}^{-1}$, (b) $k = 1 \text{ mm}^{-1}$, (c) and $k = 2 \text{ mm}^{-1}$. The light gray lines serve as the eye-guides of the angles under which the rods are oriented.

Figure 5: The displacement field (left) and the corresponding intensity (right) of out-of-plane shear wave at $t = 25 \mu\text{s}$ for 3 different dominant wavenumbers: (a) $k = 0.3 \text{ mm}^{-1}$, (b) $k = 2 \text{ mm}^{-1}$, (c) and $k = 3 \text{ mm}^{-1}$. The light gray lines serve as the eye-guides of the angles under which the rods are oriented.

180 wave packet, the energy propagation is focused more into the direction of the rods. Already at frequencies around 1 or 2 MHz (for shear or longitudinal waves, respectively), the energy propagates entirely through the rods. Corresponding to the previous study by Kruisová et al. [22], for higher frequencies, the group velocity is close to zero; hence, there is no energy propagation above a certain point, creating an acoustic band gap.

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