Bandgap engineering of three-dimensional phononic crystals in a simple cubic lattice

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Bandgap engineering of three-dimensional phononic crystals in a simple cubic lattice

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In this work, we present a comprehensive theoretical and experimental study of three-dimensional phononic crystals arranged in a simple cubic lattice. The band structure is analytically modeled as a 3D mass spring system and numerically calculated within the corresponding simple cubic Brillouin zone. We report on a design yielding a record bandgap of 166% relative width, validated by simulations and measurements of longitudinal and shear wave transmission in different spatial directions. In the additively fabricated samples, gap suppression reaches −80 dB relative to a solid reference. Comparison of different unit cell geometries showcases approaches to engineer gap width and suppression, as well as transmission bands outside the gap. Published by AIP Publishing. https://doi.org/10.1063/1.5049663

Phononic crystals, acoustic analog of photonic crystals, can tailor the propagation of elastic and acoustic waves through periodic heterogeneous materials due to their unique band structure. Prediction and control of phononic bandgaps, frequency regions where wave transmission is suppressed, have been studied in the past few decades primarily for 1D and 2D lattices. Experimental demonstrations can be found for solid cylinders, or in micromachined plates, e.g., for thermal and acoustic isolation, or material defect characterization.

Lattices of spheres embedded in a matrix practically demonstrated phononic bandgaps for simple 3D arrangements. More complex geometries including hollow elements, cellular solids with cubic symmetry, or periodic bicontinuous cubic network structures proved yet unfeasible to fabricate. Only recent advances in additive manufacturing fully opened the third dimension, printing polymer, ceramic, or metal crystals for, e.g., acoustic imaging, vibration isolation, or liquid sensing. This has allowed ultra-wide phononic bandgap materials, with previously unattainable bandwidths. Most experimental works focus on one unit cell design and variations to characteristic dimensions. We present a comprehensive theoretical and experimental comparison of different unit cell geometries arranged in a simple cubic lattice to illustrate this avenue of utilizing complex 3D designs for precise engineering of desired phononic bandgap characteristics over an ultra-wide frequency range.

Here, we focus on 3D phononic crystals arranged in a simple cubic Bravais lattice. In our primary design, solid masses are predominantly concentrated as balls in each corner of the unit cell and connected by thin, elastic beams. The effect of unit cells deviating from this geometry is discussed in the experimental results. To validate our numerical models and experimental results, we can analytically calculate the elastic behavior of such an infinite lattice of interacting masses with a mass spring model. In our case, this calculation is similar to phonon dispersion in a simple cubic atomic lattice. Assuming linear springs, point masses, and no losses, the equation of motion for the displacement \( \mathbf{u} \) of a mass \( m \) considering its six nearest neighbors [Fig. 1(b), red masses] can be written as

\[
\mathbf{m} \ddot{\mathbf{u}} = C \sum_{j} \left( \mathbf{u}_{j} + \mathbf{u}_{j-} - 2 \mathbf{u} \right) \mathbf{e}_{j};
\]

where \( C \) is the spring constant, \( u_{\pm} \) denotes the displacement of nearest neighbor in the positive and negative \( x, y, \) and \( z \) directions, respectively, and \( \mathbf{e} \) is the Cartesian unit vector. A solution of the form \( e^{i(\mathbf{k} \cdot \mathbf{r}) - \omega t} \), with wave vector \( \mathbf{k} \), lattice constant \( a \), and angular frequency \( \omega \), results in

\[
\mathbf{M} \omega^{2} \mathbf{u} = \mathbf{M} \mathbf{u};
\]

where \( \mathbf{M} \) represents a \( 3 \times 3 \) Cartesian matrix containing the corresponding spring stiffness elements. To calculate the dispersion relation \( \omega = \omega(k) \), we have to solve the eigenvalue problem \( \omega = \sqrt{\lambda/m} \) of this matrix. For nearest neighbor (nn) interaction, only the diagonal elements are filled, yielding eigenvalues and eigenfrequencies

\[
M_{jj} = 4C \sin^{2} \left( \frac{ak_{j}}{2} \right), \quad \omega_{j} = \sqrt{\frac{4C}{m} \sin^{2} \left( \frac{ak_{j}}{2} \right)}.
\]

FIG. 1. (a) Simple cubic unit cell of lattice constant \( a \), with spherical masses of radius \( R \) in each corner connected by circular beams of radius \( r \); (b) linear mass spring model considering nearest neighbors (red) and next nearest neighbors (blue); (c) Brillouin zone of the simple cubic lattice in reciprocal \( k \)-space with characteristic points \( \Gamma \), \( X \), \( M \), and \( R \).
Including next nearest neighbors (nnn) into the model [Fig. 1(b), blue masses] adds a second stiffness term to the right side of Eq. (1) described by a second spring constant $C_2$. The matrix elements are given in the following symmetric form, and all elements can be obtained by substituting indices $x, y,$ and $z$ accordingly.

$$M_{xx} = 2C_1[1 - \cos(ak_x)] + 2C_2[2 - \cos(ak_x)\cos(ak_y) - \cos(ak_x)\cos(ak_z)]$$

$$M_{xy} = 2C_2\sin(ak_x)\sin(ak_y).$$

(4)

Elastic and acoustic behavior is typically visualized in a band structure diagram describing the dispersion relation. This relation is calculated in reciprocal $k$-space from the corresponding Brillouin zone of the unit cell. In our case, the simple cubic Bravais lattice is again represented by a simple cubic arrangement [Fig. 1(c)]. To describe all possible eigenmodes, the wave vector $k$ is varied along the characteristic path $\Gamma-X-M-\Gamma-R-X | M-R$, where $\Gamma$ is the cube center point, $X$ is a face center, $M$ is an edge midpoint, and $R$ is a corner point. The length of each path segment differs according to whether only one, two, or all three spatial components of $k$ are varied. In the complete band structure, we plot dimensionless frequency $f a/c$ over reduced wave vector $ka/\pi$, for optimal comparison independent of size (lattice constant $a$) and material (speed of sound $c$). For the following analytical and numerical results, the parameters of the fabricated design corresponding to Fig. 1(a) are ball diameter $2R = 0.79a$, circular beam diameter $2r = 0.05a$, elastic modulus $E = 3.2$ GPa, density $\rho = 1190$ kg/m$^3$, and longitudinal sound velocity $c = 2077.5$ m/s. We then calculate the lumped mass of a sphere and half of its connecting beams, as well as the spring constant of a solid beam with an effective length between two spheres

$$m = \rho \left[\frac{4}{3}\pi R^3 + 3(a - 2R)\pi R^2\right]$$

$$C = \frac{E\pi r^2}{a - 2R[\cos \arcsin(r/R)]}.$$  

(5)

Figure 2 depicts the results of dropping the values of Eq. (5) into (3) and (4) and solving for the eigenfrequencies considering nearest neighbors (solid red) and next nearest neighbors (dashed blue). Including next nearest neighbor interaction opens new modal bands, but nearest neighbor is sufficient to estimate the opening frequency of the first phononic bandgap. Dimensionless frequencies of 0.047 and 0.049 are calculated, respectively.

To solve for higher order modes, non-linear effects, etc., the unit cell geometry is implemented in a finite element model for a structural mechanics eigenmode simulation (COMSOL Multiphysics). Only the solid part of the geometry is considered. Including the hollow regions requires more complex simulation of acoustic-structure interaction; however, our analyses have shown the influence of air to be negligible. For a different scattering medium such as filling with liquids, this interaction needs to be included. For an infinite lattice, we impose periodic Floquet boundary conditions on all three pairs of opposite faces with parametric input of the Cartesian components of the $k$-vector, sweeping it along the characteristic path. Note that finite element mesh density has to be fine enough to adequately resolve the wavelength of higher order modes. As a rule of thumb, we employ at least 20 elements along one edge, corresponding to at least 10 elements per wavelength up to a dimensionless frequency of 2. The comparison in Fig. 2 shows the mass spring model in good agreement with the 3D FEM model (black dots). As the secondary spring constant is not directly based on the geometry, we fit it to the FEM model with a ratio of $C_1/C_2 = 28$. The analytical mass spring model is a faster alternative to calculate and validate first eigenmodes and gap opening frequency.

The differences between ideal mass-spring model and real geometry are illustrated in Fig. 3 showing the deformation of the unit cell for modes one, two, four, and five (discounting symmetrical modes) at wave vector $X$ corresponding to band diagrams in Figs. 2 and 4. Only the translational motion of modes one and four can be described by the mass-spring model due to the assumption of point masses and massless, linear springs. Modes based on, e.g., rotation of the masses and bending or torsion of the beams only appear in the actual geometry, with the upper bandgap limit determined by the latter. Further higher frequency modes are based on superposition and higher harmonics of the basic vibrations.

The complete simulated band structure of an infinite lattice using our primary unit cell design of Fig. 1(a) is given in Fig. 4 on the left. The first bandgap opens between the dimensionless frequencies of 0.0437 and 0.4702, yielding a relative gap to mid-gap width $\Delta f / f_e = 166.0\%$, which is the largest phononic bandgap reported in the literature. With the acrylic plastic material used in our work and lattice constants on the millimeter-scale, this corresponds to frequency ranges between roughly 10 and 100 kHz for $a = 10 \text{ mm}$ or 0.1 and...
For varying beam diameters, masses adjusted for maximum bandwidth, validation of simple beam spring theory.

The gap width is primarily dependent on stiffness and, thus, radius $r$ of the connecting beams. Its evolution is plotted in Fig. 5, with mass radius $R$ optimized for maximum bandwidth. The mass spring model offers very good agreement for the lower opening frequency of the gap up to $2r = 0.25a$, where increasing masses $2R \rightarrow a$ and thus decreasing beam lengths are needed to maximize bandwidth, invalidating simple beam spring theory.

Samples are fabricated in acrylic plastic using high-resolution microstereolithography with lattice constants between $a = 1$ and 10 mm. Details on fabrication and design challenges can be found in previous work. Density and elasticity of the printed material determine its speed of sound (measured $c \approx 2220$ m/s) and, thus, the absolute frequency, here typically 0.1–1 MHz. Photography samples of the design with $2R = 0.79a$ and $2r = 0.05a$ are shown in Fig. 6 for orientations $\Gamma X$, $\Gamma M$, and $\Gamma R$. Measurement samples consist of larger lattices with typically at minimum $6 \times 6$ lattice points in perpendicular directions. To demonstrate bandgap efficiency and reduce the influence of material losses, we choose two to four lattice points in the propagation direction to achieve comparable transmission lengths for the different orientations.

The transmission measurement setup consists of two ultrasonic contact transducers clamped on opposite sides of the fabricated sample. They are connected as the transmitter and receiver to a high-precision lock-in amplifier (HF2LI, Zurich Instruments AG, Switzerland). We employ two sets of transducers for longitudinal wave ($V103-RM$, Olympus, Germany) and shear wave propagation ($V153-RM$, Olympus, Germany). The bandgap width is measured between lower and upper $-3$ dB cutoff frequencies in the different characteristic directions for both polarizations (Table I). Experimental transmission results relative to a fully solid reference of similar length demonstrate strong transmission suppression in the first omnidirectional bandgap (indicated by shaded area) and unique transmission bands outside the gap for the different directions (Fig. 7). The measurement results are in good agreement with the semi-infinite transmission model for both primary bandgap and transmission bands when using the isotropic loss factor as a frequency-dependent fit parameter to account for damping effects. Note that in Fig. 7 longitudinal and shear wave velocity are used for the $x$-axes, respectively. Also note that the longitudinal transmission peaks are much closer to the noise floor than for shear waves, i.e., the amplitude is more zoomed in on the left. Transmitted waves are suppressed by 70–94 dB relative to a solid reference already with the low number of repetitions in the propagation direction. This corresponds to the noise floor of our experimental setup. However, due to the small beam diameter and high filling fraction of scattering volume, transmission outside the gap is also reduced.

To engineer different phononic characteristics, we utilize other simple cubic unit cell geometries (see supplementary material). This design approach is illustrated in Table I comparing variations of the ball and beam design (ball) with...
TABLE I. Comparison of simulated relative bandgap widths for different unit cells with experimental results for longitudinal and shear wave transmission in ΓX, ΓM, and ΓR, with reference results from other 3D-printed phononic crystals; bold values correspond to our primary design (Fig. 1(a)) and to Figs. 4, 7.

<table>
<thead>
<tr>
<th>Design</th>
<th>Filling ratio</th>
<th>Complete gap</th>
<th>Longitudinal waves</th>
<th>Shear waves</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>ΓX (%)</td>
<td>ΓM (%)</td>
</tr>
<tr>
<td>Ball 0.79, 0.05</td>
<td>0.736</td>
<td>166.0%</td>
<td>166</td>
<td>173</td>
</tr>
<tr>
<td>Ball 0.78, 0.1</td>
<td>0.728</td>
<td>137.4%</td>
<td>140</td>
<td>157</td>
</tr>
<tr>
<td>Ball 0.6, 0.2</td>
<td>0.793</td>
<td>46.2%</td>
<td>96</td>
<td>72</td>
</tr>
<tr>
<td>Cube 0.7, 0.1</td>
<td>0.648</td>
<td>125.3%</td>
<td>139</td>
<td>169</td>
</tr>
<tr>
<td>Sphere 0.9</td>
<td>0.929</td>
<td>81.7%</td>
<td>130</td>
<td>116</td>
</tr>
<tr>
<td>Holes 0.8</td>
<td>0.784</td>
<td>24.2%</td>
<td>89</td>
<td>76</td>
</tr>
<tr>
<td>Scaffold 0.8</td>
<td>0.896</td>
<td>none</td>
<td>55</td>
<td>19</td>
</tr>
<tr>
<td>Tetragonal LS</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cuboid A = 2.0 mm</td>
<td>≈0.85</td>
<td>88.9%</td>
<td>≈79</td>
<td></td>
</tr>
<tr>
<td>Midball A 0.66, 0.05</td>
<td>0.544</td>
<td>132.2%</td>
<td>≈131</td>
<td></td>
</tr>
<tr>
<td>Midball B 0.66, 0.04</td>
<td>≈0.54</td>
<td>159.2</td>
<td>≈157</td>
<td></td>
</tr>
</tbody>
</table>

For comparison, Table I also lists selected results from other 3D-printed phononic crystals further deviating from the simple cubic atomic lattice. In the case of a woodpile structure, the largest bandgap of 33% was observed for a tetragonal arrangement with a large spacing. A lattice of simple cubic cube masses connected to a smaller simple cubic lattice of sinusoidal struts yields a theoretical complete bandgap of 89%. The highest similarity to our primary design can be found in a superposition of sphere masses placed in each midpoint of the cube edges with different shapes of connecting beams. With a beam thickness similar to our design, gap widths reach values as high as 132% and 159%. These results confirm the approach of optimized spheres connected by thin beams to converge to the theoretical maximum gap to mid-gap ratio of 200%.

For optimal designs, transmission inside the primary bandgap is suppressed by more than 80 dB relative to the solid reference. Note that wider and stronger bandgaps typically coincide with decreased transmission outside the gap. This trend is especially pronounced for rotated ΓM and ΓR lattices, which feature only angled and no straight solid connections in the wave propagation direction. The corresponding eigenmodes are not conducive especially for longitudinal wave transmission. For the primary design, relative losses reach values as high as 64 dB for longitudinal waves in the ΓR direction, with only 22 dB loss for shear transmission in ΓX. Thicker connections between the solid masses improve transmission efficiency. Conversely, angled, thinner connections and more lattice points in the propagation direction lead to a general low-pass behavior above the lower frequency limit calculated by the analytical mass-spring model with strong damping also beyond the upper bandgap limit. Details on gap suppression and transmission losses can be found in the supplementary material.

In summary, we have presented a comprehensive study of 3D phononic crystals arranged in a simple cubic lattice. A 3D mass spring model allows calculation of the first eigenmodes and phononic bandgap opening frequency. This analytical model is a fast alternative and validation tool for numerical analysis of the complete band structure. We optimized a unit cell design consisting of spherical ball masses in each cube corner connected by thin cylindrical beams to maximize the bandgap. For ball diameter 0.79a and beam diameter 0.05a, we have reported a record bandgap width of 166% relative gap to mid-gap ratio. We demonstrated the necessity to experimentally validate this theoretical bandgap for different spatial directions and wave polarizations, both simulating and measuring longitudinal and shear wave transmission with gap suppression up to 80 dB relative to a solid reference. Variations in unit cell geometry are the primary influence in resulting bandwidth, gap suppression, and transmission losses. This comprehensive methodology outlines how to design 3D phononic crystals fitting desired transmission characteristics for different applications.
See supplementary material for detailed design of the other simple cubic unit cells and for more detailed bandgap and transmission characteristics.

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