Prediction of band gaps in phononic quasicrystals based on single-rod resonances

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Band-gap formation in two-dimensional quasiperiodic polymer/water heterostructures (with 4- to 14-fold Patterson symmetry in this study) is governed by strong acoustic resonances of the sound-soft single scatterers. Already with an eightfold-symmetric structure the first band gap is very isotropic. For isotropy of the higher gaps higher-symmetric structures are required. However, this can also be achieved by a smart tuning of the properties of the scatterers. Their symmetry (and therewith the symmetries of the scattered fields) has to better match the symmetry of a given structure. Polygon- and star-shaped prisms on quasiperiodic structures can yield smoother and more isotropic gaps in transmission spectra.

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INTRODUCTION

The study of classical wave propagation in periodic heterostructures, i.e., photonic (PTC's) and phononic crystals (PNC's), started almost 20 years ago.[1] Since then, the promising applications such as optical computers and devices have spurred an almost exponential growth of the number of publications on PTC's.[2] Far less work has been devoted to PNC's. For these, potential applications are expected in noise control and ultrasonic technology, for instance. The similarity of PTC's and PNC's allows, to some extent, a knowledge transfer and increases the impact of discoveries in each field. The fascinating type of composite materials can be described as one-, two- (2D), or three-dimensional meta crystals built of objects which scatter electromagnetic or elastic (acoustic) waves if the wavelength is on the scale of the lattice period (for a comprehensive review, see Ref. 3).

The existence of omnidirectional band gaps, which is important for most applications, is strongly favored by high symmetries of the heterostructures. The rotational symmetry of periodic structures is limited to sixfold. For 2D quasiperiodic structures there is no upper limit and consequently quite a few publications already report the peculiarities of quasiperiodic PTC's (QPTC's) and PNC's (QPNC's) (see Refs. 4–8, and references therein). However, bands and gaps in QPNC's are well defined in particular cases only (i.e., in some systems only pseudogaps were found[9] similar to the electronic pseudogaps of real quasicrystals) and their formation and structure is not yet thoroughly understood. In the following, we present a study of the scattering properties of single rods and show how this information supports the understanding of the formation and the optimization of band gaps in QPNC's. The transmission spectra for a square lattice PNC as well as QPNC's with 8-, 10-, 12-, and 14-fold Patterson symmetry (see Fig. 1) were calculated by a finite difference approximation in the time domain (FDTD).[10] For the scattering cross-section calculations of cylindrical rods we have used a multipole-expansion method[11] and for all other rods the FDTD method.

I. SYSTEMS OF CIRCULAR CYLINDRICAL RODS

The type of scattering in PNC's has been known to be of prime importance ever since the first PNC's were created. It can be adjusted by the impedance contrast of the constituent phases as well as by the volume fraction of the scattering objects. Especially in systems with hard contrasts and sparse scatterer distributions, the mechanism for band-gap formation is based on Bragg scattering. Strong Bragg peaks in the Fourier spectrum of the underlying structures directly indicate the possible frequency ranges of the band gaps.[8,9] On the other hand, in soft-contrast systems with sufficiently high filling fraction, the resonance modes of the scattering objects can play a very dominant role in determining the frequency ranges of band gaps [the approach was used early for PNC's (Ref. 12) and recently also applied to QPTC's (Ref. 13)]. The resonance frequencies are independent of the structure, instead they scale with the speed of sound in the material of the scatterers and inversely with their size. The coupling of such resonance states in a QPNC spreads these states to form a band. The interaction of this band with the continuum band of the effective medium produces a band gap due to hybridization (for a very clear description of this mechanism see Ref. 14). The correlation of resonance frequencies and gap positions is shown in a comparison of PNC's and QPNC's of 4-, 8-, 10-, 12-, and 14-fold Patterson symmetry (Fig. 2). The heterostructures consist of polymeric rods (v_l=1800 m/s, v_s=800 m/s, ρ=1.14 kg/m^3) in water at filling fractions of 0.17. Samples of about the same thickness in direction of transmission were set up with 357, 361, 365, and 355 rods for the QPNC's with 8-, 10-, 12-, and 14-fold Patterson symmetry, respectively. Similar to what has been found by Rockstuhl *et al.*[13] for photonic systems, the band gaps occur at frequencies close to those of the resonance states in the scattering cross sections of a single rod. Nevertheless, in these (Q)PNC's the arrangement of the rods does play a crucial role. For the periodic square lattice PNC the first band gap is shifted by almost as much as its width if the direction of transmission is changed. A very bad overlap results. This overlap is clearly getting better with an increasing degree of rotational symmetry of the arrangement of the scatterers. While for the 8-fold structure mainly the first gap is absolute, for the 12-fold structure all gaps are perfectly isotropic. The increasing symmetry of the structures also leads to broadened band gaps with less sharp edges (i.e., spikes associated with localized modes appear). This effect can also be seen as due to more inhomogeneous nearest-neighbor-distance distributions of the highly symmetric structures. The shorter dis-

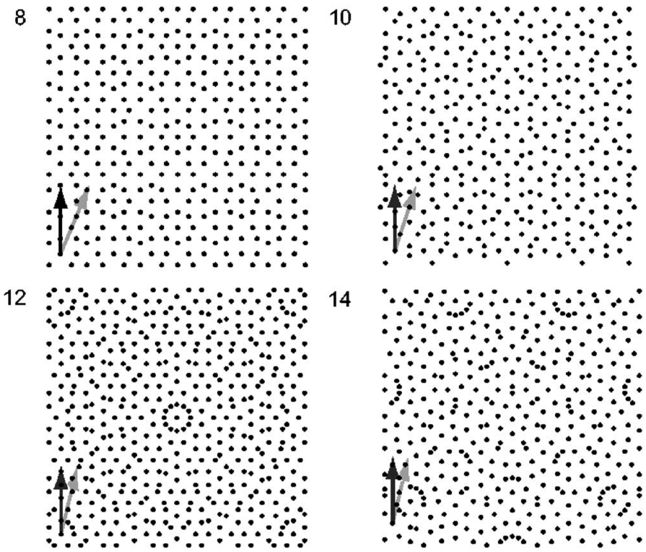

FIG. 1. Quasiperiodic structures with 8-, 10-, 12-, and 14-fold Patterson symmetry considered in this study. The arrows in each pattern designate the independent high-symmetry directions.

tances tend to broaden the gap and the wider spacings to close it. In the square structure all rods have the same coordination and thus the overlap of their scattered field lobes with those scattered from neighboring rods is equal (i.e., equal transfer parameters). Thus, for the formation of isotropic and sharply bound band gaps a structure with high Patterson symmetry and only few different vertex coordinations seems most promising (i.e., not a random arrangement). Quasiperiodic structures optimally combine this.

In order to predict the isotropy of a band gap in (Q)PNC's, the scattered wave field Ψ_s can be analyzed for the resonance, which induceds the gap

$$\Psi_s(r,\theta) = e^{i\omega t}\sum_{m=0}^{\infty} c_m(\omega)J_m(kr)\cos(m\theta), \tag{1}$$

with J_m being Bessel functions of the first kind and c_m the coefficients obtained from evaluation of the boundary condition at the cylinder surface.[11] The index m of the strongest coefficients in the spectrum of the expansion in cylindrical harmonics c_m is indicated below the resonance peaks in Fig. 2. These eigenmodes feature $2m$-fold rotational symmetry and in the case of a single-valued spectrum, the scattered field predominantly adopts the symmetry of this component.

For transmission in the two high-symmetry directions indicated in Fig. 1, the scattered waves typically encounter nearest-neighbor rods on vertices of regular n-sided polygons (with one vertex in the forward direction) for even and $2n$-sided polygons for odd n (direction of dark arrows in Fig. 1) or just between these neighbor vertices (bright arrows). Strong interaction of scattered waves (i.e., a large overlap of the scattered field lobes) occurs most likely when the field lobes point in the direction of the nearest-neighbor rods. This interaction strength spreads the bands of coupled resonance states which, by hybridization with the continuum band, produce the band gaps and determine their widths. Omnidirectional gaps can be expected from modes with lobes of the scattered fields covering rods in the directions of both the vertices of the n-sided polygons as well as those in between them; this is when n is a multiple of m (e.g., the first gap in the octagonal system). Modes of low symmetry form isotropic gaps in highly symmetric structures because the broad field lobes cannot resolve the angular fine structures of the n-sided polygons hosting the rods. This almost guarantees isotropy of the first gaps in QPNC's with large n. However, optimal performance requires a good match of structure and scatterer.

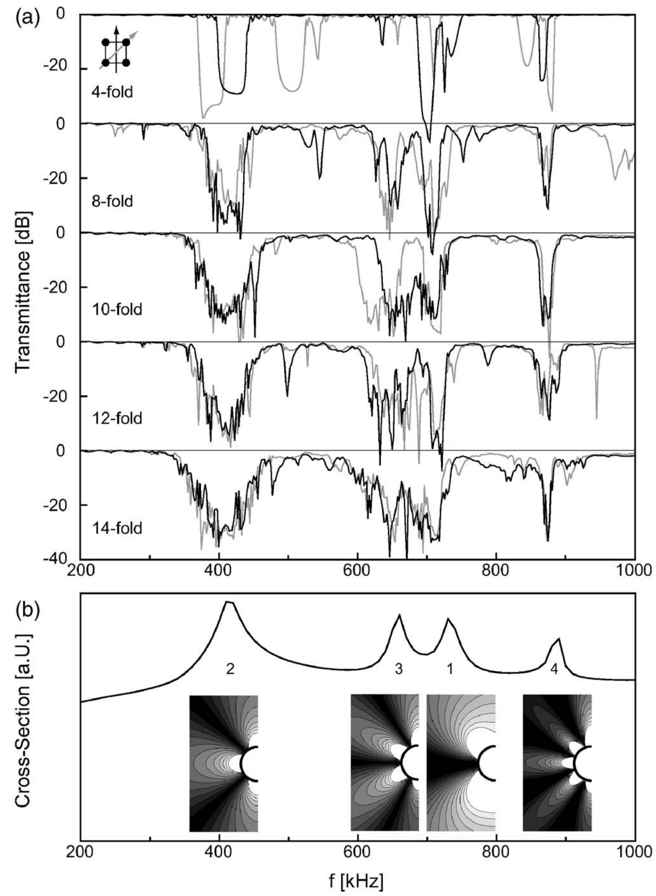

FIG. 2. Transmission spectra for square PNC and QPNC's with different Patterson symmetry (a). The two curves in each section correspond to the two directions of transmission indicated with arrows of the same line style in Fig. 1. Resonance states in the scattering cross section of a cylinder (b).

II. SYSTEMS OF POLYGONAL OR STAR-SHAPED PRISMS

Due to the dominant role the properties of single scatterers play in the band-gap formation, a more detailed examination of these seems crucial. In this section we study the influence of modified geometrical cross sections of the rods on their scattering behavior. The shapes analyzed here are regular n-sided polygons (with constant incircle) and a five-pointed star. They are interesting from many points of view. First, we have seen that the high-symmetry resonance modes

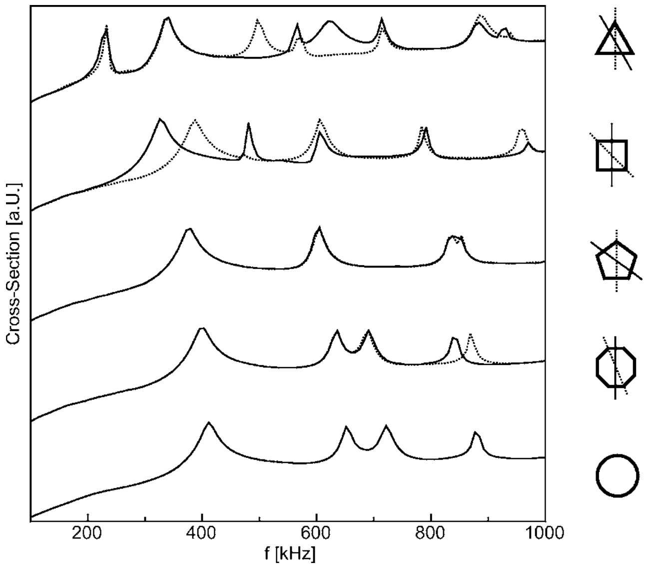

FIG. 3. Scattering cross sections for plane waves at polygonal prisms (shown on the right-hand side) in different orientations (wave incident along the lines crossing the shapes).

do not easily form isotropic gaps. A reduction of the symmetry of the scattering object can affect the symmetry of the modes. Second, for scatterers with lower symmetry (different extensions in different directions) the resonance frequencies should change with the direction of the incident plane wave. This variation could lead to widened gaps in QPNC's. Third, the faces of the polygons and stars form sets of broken planes, which could give rise to a stronger interaction of reflected wave intensity.

For the polygonal prisms, the scattering cross sections for plane waves are shown in Fig. 3. In the frequency range of interest they are very similar for cylindrical rods and for polygons with large n. The scattering strengths as well as the Q factors of the resonances are similar for all shapes of rods. The scattering behavior of the octagonal prism deviates from that of the cylindrical rod only in the orientation-dependent frequency of the fourth resonance. For the pentagonal rod more evenly spaced resonances appear, which are almost independent of the direction of incidence of the plane wave. The square and the triangular prisms show clearly different spectra. As anticipated, they possess more resonances at low frequencies and these depend strongly on the direction of incidence of the plane wave. Especially for the very first resonances, there are certain directions from which these modes cannot be excited at all. In oblique directions though, most modes are accessible.

Now, let us have a look at how the band gaps of a QPNC's of polygonal rods look like. Uniformly oriented pentagonal rods on the Penrose quasilattice produce the spectra shown in Fig. 4. Compared to the Penrose QPNC with cylindrical rods (Fig. 2) this QPNC clearly features more isotropic band gaps. Again, the gaps appear exactly at the resonance frequencies. Due to the unsplit second peak, there are fewer gaps but instead they agree better in their position and width for the different directions of transmission. The spectra are also smoother than those of the cylindrical rod system

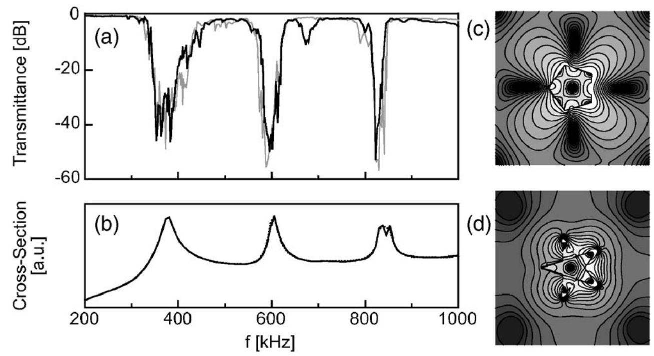

FIG. 4. Band gaps in transmission spectra of the Penrose QPNC (a) and the resonance modes of the pentagonal prisms inducing the gaps (b). The scattered fields $|\Psi_s|$ for the pentagonal (c) and the star-shaped prisms (d) at their common resonance frequency [see arrow in Fig. 5(b)].

around the second and third resonances of the cylinder, which are very close. The amplitude distribution of the scattered field $|\Psi_s|$ at the first resonance of the pentagonal prism is shown in Fig. 4(c). It features well-defined fourfold symmetry.

In Fig. 5(b) the scattering cross section of a five-pointed-star-shaped prism (incircle 0.3 mm) is shown and compared to that of the pentagonal prism. The first resonance appears at very low frequency. It reflects the larger maximal extension of the star and its intensity is weak. In the arrangement of the star-shaped rods on the Penrose structure, this mode induces only a weak attenuation peak. The second resonance frequency is almost equal to the first one of the pentagonal rod. The scattered fields at this common resonance frequency are similar as shown in Figs. 4(c) and 4(d) and can be further characterized by the radiation patterns shown in Fig. 5. These patterns show the angular distribution of scattered intensity for the far field [Fig. 5(c)] and at a distance l_e away from the scatter [Fig. 5(d)] (with l_e being the edge length of the Penrose tiling). According to these patterns, the noncylindrical scatterers produce slightly less sharp field lobes at both distances. Thus, slightly better isotropies of the gaps

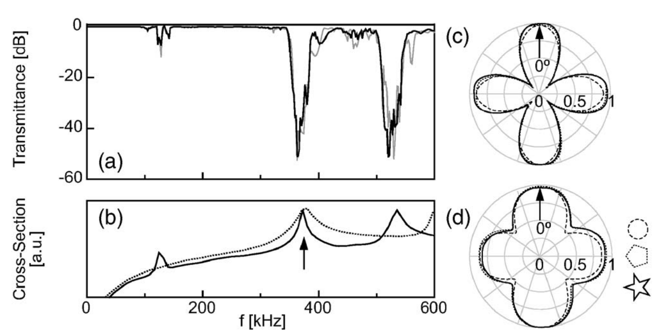

FIG. 5. (a) Band gaps in transmission spectra of the Penrose QPNC consisting of star-shaped prisms and (b) the resonance modes of single prisms inducing the gaps. Radiation patterns for resonances indicated with an arrow in (b), for the pentagonal and the star-shaped prisms as well as the first cylindrical resonance measured in the far field (c), and at a distance l_e away from the prisms (d) (with l_e being the edge length of the Penrose tiling).

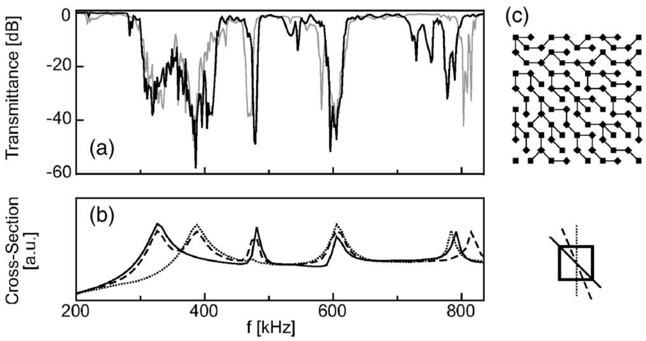

FIG. 6. All resonances of the square rods contribute to the formation of band gaps in the octagonal QPNC (a) although some of them can be excited only in certain orientations (b). The orientations of the square rods on the tiling are shown in a quarter section of the QPNC in (c).

can be expected for the Penrose QPNC with pentagonal or star-shaped prisms as compared to those of the cylindrical system. The first two star resonances produce highly isotropic transmission gaps in the QPNC. These gaps are again smoother than those induced by resonances of cylindrical rods and their width is rather small. The different widths of the coinciding gaps of the pentagonal and star systems are indicated by the different Q factors of the corresponding resonances.

To give an example for QPNC's consisting of the more anisotropic square rods, we have analyzed an octagonal QPNC. The orientations of the rods [see Fig. 6(c)] are chosen in such a way that the eightfold symmetry of the structure is preserved. Corresponding transmission spectra are compared with the different scattering cross sections of the square rod in Fig. 6. The resonances that are accessible only in certain directions all contribute to the isotropic, almost overlapping (and therewith broadened), first gap. Thus, anisotropic resonances can form isotropic band gaps at lower frequencies. At higher frequencies only the isotropic modes produce absolute band gaps. The spectra are not smoother than those of the system with cylindrical rods but despite the reduction of symmetry of the scatterers the band gaps are highly isotropic.

CONCLUSIONS

We conclude that quasiperiodic geometries are very well suited for phononic crystals consisting of soft-contrast cylindrical rods in a liquid host. The strong resonances of such rods govern the formation of band gaps and allow the high rotational symmetries of quasiperiodic structures to be fully exploited to make the band gaps isotropic (in contrast to systems without resonances[8]). In addition to the usual focus on the arrangement we have shown that simpler and more isotropic transmission spectra can be obtained alternatively by using polygonal or star-shaped rods, the scattered fields of which better match the symmetry of the structures. The high degree of isotropy seems very promising for all types of applications of such heterostructures, and may also encourage further analysis of new, interesting building blocks for phononic as well as photonic crystals other than cylindrical rods.

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