Hidden translational symmetry in square–triangle-tiled dodecagonal quasicrystal

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Received 31 December 2014, revised 11 March 2015
Accepted for publication 12 March 2015
Published 21 April 2015

Abstract

We show that a two-dimensional 12-fold quasicrystal tiled with squares and triangles can be generated as a triangular periodic lattice in which the unit cell is replaced by a cluster of 19 elements defining an elementary supercell with a dodecagonal boundary. As a straightforward consequence, we obtain analytically the exact Fourier spectrum of the dodecagonal quasicrystal that can find interesting applications for modeling purposes. In perspective, since our spatially periodic assembling allows restoring Bloch-type periodic boundary conditions, photonic band gap calculations will be possible without approximating the quasicrystal geometry. We foresee extending the same basic idea to other quasiperiodic patterns.

Keywords: photonic quasicrystals, dodecagonal rotational symmetry, far-field diffraction

1. Introduction

Quasicrystals (QCs) are materials forming a more general class of crystalline structures in which atoms and molecules are arranged into ‘quasiperiodic’ lattices rather than periodic ones [1–5]. They lack the typical translational symmetry of periodic crystallographic materials but manifest self-similar point patterns, which bring in the advantage of rotational symmetries not achievable in common crystals, by folding the space into more complex configurations [6, 7]. Like periodic patterns, quasiperiodic ones are characterized by long-range correlations which makes them exactly hyperuniform in terms of order metrics [8], but they also uniquely manifest a further degree of freedom which results from the phason elastic fluctuations of the cluster aggregate substructure [9].

In the last decade, QCs have been successfully employed for fabricating the quasiperiodic counterpart of photonic crystals [10], termed photonic quasicrystals (PQCs). Advantages of PQCs rely on the onset of more isotropic band gap for light confinement [11–13], the existence of a larger number of degrees of freedom (non-equivalent sites in the pattern geometry) for controlling light in unconventional fashions [14, 15], and the possibility of using materials with lower dielectric contrast [16, 17], with consequent benefits in terms of fabrication and application versatility [18]. Among the two-dimensional PQCs more extensively studied, we find those showing 8-, 10- and 12-fold rotational symmetries in the reciprocal lattice. However, given a particular symmetry, the tiling geometry may vary, which affects dramatically the band gap properties [16, 19]. Examples of well-known geometrically-generated structures are Ammann–Beenker, Penrose, and square–triangle (Stampfli’s inflation [20]) tilings which have, respectively, octagonal (8-fold), decagonal (10-fold) and dodecagonal (12-fold) rotational symmetries [7, 16]. Recently, there has been great interest in square–triangle dodecagonal (STD) aperiodic patterns, in particular in relation to their extraordinary transmission properties [21] and potential applications in photonics [22–26]. The same 12-fold quasicrystalline structures have been found for metal alloys, chalcogenides and liquid crystals, suggesting the universal nature of dodecagonal quasicrystals with respect to structure scale [27–31]. Overall, these results suggest stimulating perspectives for engineered nanoscale materials for plasmonics and photonics. For instance, STD symmetric structures allow implementing complete photonic band gap materials relying on the spatial isotropy of the pattern even for low dielectric contrast [11]. The STD pattern is usually built by inflation
geometric rules [11, 20]. Given the lack of translational symmetry, designing the ideal geometric photonic band gap parameters require, computationally demanding large supercell approximation of finite structures, rational approximants, or extended zone schemes in the reciprocal space [32, 33]. The density of photonic states can be determined by full-wave simulations [14, 22]; however, multiple scattering effects in extended structures might affect the expected properties [12, 32]. The accuracy of calculation and extension of the pattern are thereby limited by the efficiency of the numerical approach.

In this paper, we show that a two-dimensional 12-fold pattern of pillars positioned at the vertices of a square–triangle tiling can be generated by defining a triangular periodic lattice having a suitably designed elementary supercell of 19 geometric elements. This design allows individuating a sort of ‘hidden’ translational symmetry in the STD quasicrystal. It is in fact revealed only by defining a suitable pattern’s substructure in which the key factor is the splitting of the boundary pillars into two complementary subunits, which merge again after translating the substructure along the triangular lattice vectors. We term this substructure as quasicrystal’s ‘supercell’. This translational symmetry provides an easy way to obtain an analytical closed form for the Fourier spectrum of the STD quasicrystal in terms of the supercell pattern. The knowledge of the far-field diffraction has already been shown to provide interesting information on the photonic band structure [13]. In perspective, our study will help implementing accurate photonic band gap designs and light-extraction devices based on STD quasicrystals. By restoring the Bloch-type boundary conditions (with a periodic supercell), it will be possible to determine the band diagram for an ideal infinite structure without approximating the quasicrystal geometry.

2. Results and discussion

Our simple approach for generating two-dimensional STD tiling patterns re-establishes the translational symmetry into the pattern by defining an ‘elementary supercell,’ as sketched in figure 1. The basic cell has an inner structure consisting of 7 full circles (a regular heptamer) plus 12 circular sectors on the boundary defined by a 12-sided polygon. The side of the inner hexagon is \( l \). The key feature that allows generating the 12-fold pattern of pillars (‘atoms’) is the splitting of the peripheral ‘atomic’ sites into two complementary subunits so that, by translating the cell, they will merge and share a common site, a process which eventually results in an aperiodic array of atoms. It is worth noticing that the supercell does not have a 12-fold rotational symmetry. The final pattern can be assembled as described in figure 2. It is worth noting that, this approach allows us to analytically formulate the far-field diffraction spectrum as a function of the transmittance \( g(x, y) \) of the basic unit (elementary supercell). An example of 12-fold symmetric tiling with squares and triangles of side \( a \) is shown in figure 2(a); this will be the final tiling of the structure generated starting from the elementary supercell.

The cell is again shown for clarity in the top panel (i) of figure 2(b), which describes the idea for composing the pattern. Without loss of generality for our purposes, we simply consider an amplitude binary pattern in order to define the transmittance \( g(x, y) \): the white circular area has transmittance equal to 1 whereas the black area is equal to 0. The border of the unit cell comprises 12 circular sectors of 3 sizes, 7\( \pi /6 \) and 5\( \pi /6 \) rad, respectively, which are symmetrically located with respect to the origin. As shown in figure 2(b), panels (ii) and (iii), they are oriented in such a way that a proper translation of the basic structure along the independent directions of a 3-fold periodic lattice of unit vectors \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \), with steps in the horizontal \( (x) \) and vertical \( (y) \) directions given by \( h_x = (2 + \sqrt{3}) l \) and \( h_y = \sqrt{3} h_x / 2 \), allows generating the full pattern according to the STD tiling of figure 1(a). Panel (ii) of figure 2(b) shows the composition of three repeating supercells. The circular sectors on the border of the basic units are merged to form a full bright circular area. The dodecagonal pattern of finite size can be generated by repeating the process \( N \) times along the horizontal direction and \( M \) times along the vertical one. Thereby, the final pattern can be generated as a matrix of \( N \times M \) unit cells, and an example is given in figure 2(b), panel (iii) for \( N = M = 3 \). Figure 2(c) shows a larger structure: its Fourier spectrum demonstrates the 12-fold rotational symmetry resulting in the final tiled pattern of circles (figure 2(d)). Typical two-dimensional photonic designs consist of circular pillars and voids. However, our particular choice of a circular pillar is not a restriction since the transformations required to build the basic unit and its reflection symmetries allow including arbitrary geometric entities as dielectric scatterers.

In order to calculate the Fourier spectrum of the two-dimensional dodecagonal pattern of circles of equal radius \( r \), we express the total transmittance \( t(x, y) \) as a convolution \( (\otimes) \) of the transmittance \( g(x, y) \) of the basic structure and a
replica function \( r(x, y) \) as \( t(x, y) = r(x, y) \otimes g(x, y) \). The replica function can be written as

\[
r(x, y) = \frac{1}{2h_xh_y} \left[ \text{comb} \left( \frac{x}{h_y} - \frac{1}{2} \right) \text{comb} \left( \frac{y}{2h_y} - \frac{1}{2} \right) + \text{comb} \left( \frac{x}{h_y} - \frac{1}{2} \right) \text{comb} \left( \frac{y}{2h_y} - \frac{1}{2} \right) \right],
\]

where the comb functions can be expressed as a sum of delta impulses:

\[
\text{comb} \left( \frac{x}{h_y} \right) = \sum_{n=-\infty}^{\infty} \delta \left( \frac{x}{h_y} - n \right)
\]

\[
\text{comb} \left( \frac{y}{2h_y} \right) = \sum_{m=-\infty}^{\infty} \delta \left( \frac{y}{2h_y} - m \right).
\]

Figure 2. (a) Two-dimensional tiling with squares and triangles of side \( a \) with 12-fold rotational symmetry (from Stampfli random recursive algorithm). (b) From top to bottom: i) elementary supercell with 19 elements: central heptamer of circles plus 12 boundary elements truncated along a dodecagonal perimeter as described in the text; ii) arrangement of 3 lattice cells; iii) two-dimensional tiling along the triangular lattice by translating the unit supercell. (c) Final pattern having 12-fold rotational symmetry and long-range aperiodic order in terms of the fundamental circular geometric elements. (d) Fourier spectrum of the pattern in (c) showing 12 sharp Bragg peaks.
By taking into account equations (1)–(3), the transmittance distribution \( t(x, y) \) can be written in terms of the basic unit function \( g \) shifted at the positions \((x_{nm}, y_{nm})\), namely as

\[
t(x, y) = \sum_{n,m=-\infty}^{\infty} g(x - x_{nm} - r/l, y - y_{nm}).
\]  

(4)

From equation (4), we obtain the corresponding reciprocal space pattern via Fourier projection as

\[
\tilde{t}(k_x, k_y) = \tilde{g}(k_x, k_y) \sum_{n,m=-\infty}^{\infty} e^{i(\frac{2\pi}{M}k_x x + \frac{2\pi}{N}k_y y)},
\]  

(5)

Figure 3. (a) Elementary supercell with \( r/l = 0.25 \). (b) Two-dimensional triangular lattice made of \( N = M = 3 \) supercells for \( r/l = 0.25 \). (c) Same as in (b) for \( r/l = 0.125 \). (d)–(f) Fourier spectra of the patterns in (a)–(c) as respectively shown on the left.
where $\tilde{g}(k_x, k_y)$ is the Fourier transform of the supercell, $k_x/2\pi$ and $k_y/2\pi$ are the spatial frequencies, and $x_m = (1 - (-1)^m) h_x/4 - mh_y$ and $y_m = mh_y$ define the periodic translations of the basic unit along the $x$- and $y$-directions according to the aforementioned procedure for generating the pattern. Finally, the spatial frequency distribution is given by

$$i(k_x, k_y) = \frac{\sin \left( N + \frac{1}{2} h_x k_x \right)}{\sin \left( \frac{h_x k_x}{2} \right)} \times \left( e^{iMk_y} + e^{i\frac{h_y}{2}k_y} \sin \left( (M + 1)h_y k_y \right) \right).$$

and it is obtained by a finite truncation of the series in equation (5), that is for $1 \leq n \leq N$ and $1 \leq m \leq M$ with odd values of $N, M$. For $N, M$ even, a similar expression holds with the sin terms interchanged in the round parentheses of equation (6).

The Fourier transform of the transmittance of the basic structure $\tilde{g}(k_x, k_y)$ can be explicitly calculated, similarly to our previous work [34], by taking into account the various single constituents (calculation is shown in the appendix). In figure 3, examples of patterns (figures 3(a)-(c)) are shown with the corresponding calculated Fourier spectra (figures 3(d)-(f)). The patterns shown on the left column are discretized into a square array of data points of pixel size $\Delta_x = \Delta_y = r/10$. The unit supercell (figure 3(a)) gives rise to a Fourier spectrum characterized by an overall hexagonal shape in which 12 Bragg peaks (figure 3(d)) can be identified on the sides of the hexagon (the zero-frequency cross arises from the finite rectangular window of transmittance). The 12-fold symmetry is already readily visible for patterns of only $N = M = 3$ supercells (figure 3(e)-(f)). The actual structure of the Bragg peaks in the spectra depends on the radius-to-pitch ratio $r/l$ and the extension of the pattern (the order of $N, M$).

3. Conclusion and outlook

In summary, we show that a 12-fold rotationally symmetric, quasiperiodic pattern of pillars placed at the vertices of a square–triangle 2D tiling can actually be generated by means of a triangular periodic lattice in which the elementary cell consists of a cluster of 19 geometrical elements, 12 of them inscribed into a dodecagonal perimeter and suitably oriented. The resulting two-dimensional spatially periodic lattice allows for the simplification of challenging calculations by using periodic boundary conditions. As a straightforward consequence, we obtain the analytical formulation of the far-field diffraction spectrum confirming the 12-fold rotational symmetry. The Fourier spectrum solution may find interesting applications for modeling purposes. We are currently working on photonic band gap calculations of the STD quasicrystal. We are also investigating the possibility of extending the same basic idea to other quasiperiodic patterns. It is worth mentioning that the facile triangular assembling of the supercell might encourage the fabrication of 12-fold photonic quasicrystal fibers expanding the well-established technology of photonic crystal and band-gap fibers [35]. The knowledge of the STD quasicrystal symmetries and band structure is of potential interest for studying light propagation and confinement in complex photonic media [36–38] and photonic crystal fiber components [39].

Acknowledgments

G Zito acknowledges a postdoctoral fellowship by Ministro dell’Istruzione, dell’Università e della Ricerca of Italy, grant number FIRB 2012-RBFR12WAPY.

Appendix

Given the spatial frequencies $k_x = k \cos \theta$, $k_y = k \sin \theta$, the Fourier spectrum $\tilde{g}(k_x, k_y)$ of the unit cell can be explicitly calculated by using the complex integral

$$Q(\alpha, \beta, \theta, r) = \int_0^r x dx \int_0^\beta dx e^{ikx \sin(\theta - \varphi)} d\varphi,$$

which allows expressing the total far-field diffraction from the various scatterers present in the unit cell according to

$$\tilde{g}(k_x, k_y) = \frac{2\pi r J_1(kr)}{k} (1 + 2 \cos (kl \cos \theta)) + 4 \cos \left( \frac{1}{2} kl \cos \theta \right) \cos \left( \frac{\sqrt{3}}{2} kl \cos \theta \right) + 2 \Re \left[ Q\left( -\frac{\pi}{2}, \frac{\pi}{2}, \theta, r \right) \right] \cos \left( ks \cos \left( \frac{\pi}{12} - \theta \right) \right) + 2 \Im \left[ Q\left( -\frac{\pi}{2}, \frac{\pi}{2}, \theta, r \right) \right] \times \left( \sin \left( ks \cos \left( \frac{\pi}{12} - \theta \right) \right) + \sin \left( ks \cos \left( \frac{\pi}{12} + \theta \right) \right) \right) + 4 \cos \left( \frac{k_s}{\sqrt{2}} \right) \left( \Re \left[ Q\left( \frac{5\pi}{6}, 2\pi, \theta, r \right) \right] \right) \times \left( \cos \left( \frac{k_s}{\sqrt{2}} \right) - 2 \Im \left[ Q\left( \frac{5\pi}{6}, 2\pi, \theta, r \right) \right] \sin \left( \frac{k_s}{\sqrt{2}} \right) \right) + 4 \cos \left( \frac{k_s}{\sqrt{2}} \cos \frac{\pi}{12} \right) \Re \left[ Q\left( \frac{\pi}{6}, \frac{11\pi}{6}, \theta, r \right) \right] \times \left( \cos \left( \frac{k_s}{\sqrt{2}} \sin \frac{\pi}{12} \right) - 2 \Im \left[ Q\left( \frac{\pi}{6}, \frac{11\pi}{6}, \theta, r \right) \right] \sin \left( \frac{k_s}{\sqrt{2}} \right) \right) \times \sin \left( \frac{k_s}{\sqrt{2}} \right),$$

where $J_1(kr)$ is the (first kind) Bessel function of order one, and $s = 2l \cos \frac{\pi}{12}$.
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