



Periodic diffraction from an aperiodic monohedral tiling – the Spectre tiling. Addendum

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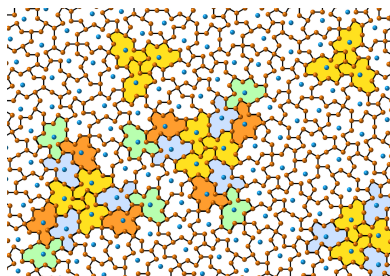
This article describes the diffraction pattern (2-periodic Fourier transform) from the vertices of a large patch of the recently discovered ‘Spectre’ tiling – a strictly chiral aperiodic monotile. It was reported recently that the diffraction pattern of the related weakly chiral aperiodic ‘Hat’ monotile was 2-periodic with chiral plane-group symmetry $p6$ [Kaplan *et al.* (2024). *Acta Cryst.* **A80**, 72–78]. The diffraction periodicity arises because the Hat tiling is a systematic aperiodic deletion of vertices from the 2-periodic hexagonal **mta** tiling. Despite the similarity of the Hat and Spectre tilings, the Spectre tiling is not aligned with a 2-periodic lattice, and its diffraction pattern is non-periodic with chiral point symmetry 6 about the origin.

1. Introduction

We reported recently (Kaplan *et al.*, 2024) that the diffraction pattern from the *aperiodic* ‘Hat’ monohedral tiling (Smith *et al.*, 2024a) was *periodic*. Periodicity arises because the set of tile vertices is equivalent to a systematic aperiodic deletion of vertices from the 2-periodic hexagonal **mta** tiling (O’Keeffe *et al.*, 2008). The underlying lattice imposes the diffraction periodicity when vertices are treated as point scatterers.

The subsequent discovery of a new aperiodic ‘Spectre’ monotile (Smith *et al.*, 2024b) invites a comparison between the diffraction patterns of its tilings and tilings by the Hat. The Hat monotile has a handedness, and every tiling by Hats is *heterochiral*: it must use both left- and right-handed tiles. In contrast, the superficially similar 14-sided polygon known as Tile(1,1) is equilateral with edge length v , allowing it to form additional tilings that are not equivalent to Hat tilings. In particular, Tile(1,1) also admits *homochiral* tilings like the one shown in Fig. 1, in which all tiles have the same handedness. Furthermore, Smith *et al.* (2024b) prove that all such tilings must be non-periodic, marking Tile(1,1) as a *weakly chiral aperiodic monotile*.

Smith *et al.* go on to show that by replacing the straight edges of the Tile(1,1) polygon with identical curves, they can produce a new family of shapes called Spectres, whose tilings are restricted precisely to be equivalent to homochiral tilings by Tile(1,1). Every Spectre is, therefore, a *strictly chiral aperiodic monotile*: a shape that admits only homochiral non-periodic tilings of the plane. Because curving the edges of Tile(1,1) does not affect the locations of its vertices, homochiral tilings by Tile(1,1) and all tilings by Spectres will have the same vertex-diffraction patterns. This invariance would not hold for diffraction studies of scattering from tile boundaries.



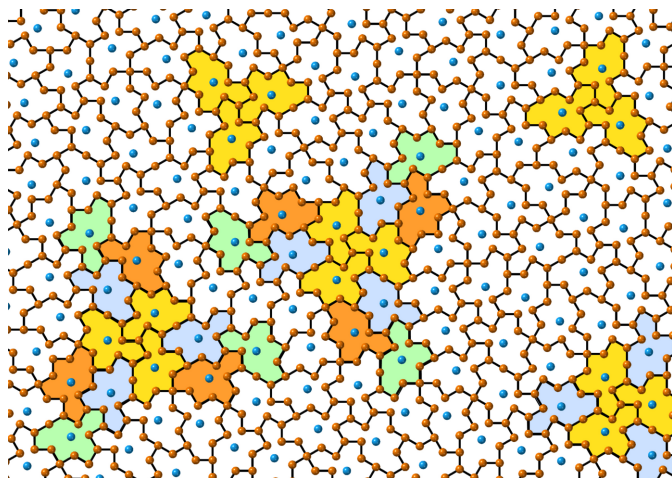


Figure 1

A homochiral tiling by Tile(1,1) – ‘the Spectre’ tiling. Orange balls indicate the tile vertices and the black lines are the straight tile edges of length v , which play no direct role in the diffraction. Blue balls locate the areal centroids of the tiles. Many patches of local threefold symmetry are present. The yellow tiles enclose the local threefold axes. Regions with larger radial extent of the threefold symmetry arise but are increasingly rare. At least 12 local threefold centres are in this view, of which we indicate five.

Importantly, unlike the Hat tiling, the Spectre tiling (Fig. 1) is a homochiral tiling by variants of Tile(1,1) that does not align with a 2-periodic lattice (Smith *et al.*, 2024b). Thus, unlike the Hat tiling, we do not expect the Spectre diffraction pattern to be periodic.

In this addendum, we confirm that the Fourier transform of the Spectre tiling is indeed non-periodic with chiral sixfold point symmetry about the diffraction origin.

2. Results and discussion

The computational methods used are the same as in our previous report (Kaplan *et al.*, 2024). We compute the Fourier transforms of sets of point scatterers representing the tiling pattern, and the intensity is the square of the scattered wave amplitude. Fourier transform intensities are equivalent to diffraction patterns when the illumination is incident normal to the plane of the tiling, in the limit of illumination wavelength $\lambda \rightarrow 0$. In this limit, the 3D Ewald sphere, which conserves the energy (wavelength) of the scattered waves, is flat and lies in the 2D tiling plane.

We computed diffraction patterns from two different representations of the tiling: from the tile vertices (as for the Hat tiling) and from the areal centroids. The orange dots in Fig. 1 indicate the Spectre tile vertices and the blue dots are the tile centroids. In a large model, the ratio of centroids to vertices is 1/6, offering a significant speed-up in the computations, although the diffraction details differ. In the previous report on the Hat tiling (Kaplan *et al.*, 2024), we used a scale u that equals the hexagonal edge length of the underlying hexagonal tiling, so the two different Hat-tile, Tile(1, $\sqrt{3}$), edge lengths were $u/2$ and $\sqrt{3}u/2$. We have adopted a different scale for the Spectre tiles, assigning v as the straight-

edge length between connected vertices. In our calculations, the scales relate with $v \equiv \sqrt{3}u/2$.

Fig. 2 compares the diffraction patterns for the two Spectre tile-vertex representations with the reciprocal-space origin at the centres. Superficially, the pattern from the tile vertices [Fig. 2(a)] resembles a periodic array of diffused concentric rings, each with an intense sharp spot in the middle. About the origin, the pattern superficially appears to have a point symmetry of $12m$, inconsistent with 2-periodicity. Closer inspection reveals that the repeating features are not identical, and the symmetry reduces to point group 6 about the origin, with no periodicity or mirror lines.

The pattern for the tile centroids [Fig. 2(b)] shows a different intensity distribution. Again, upon closer examination, the full pattern reduces to point symmetry 6 about the

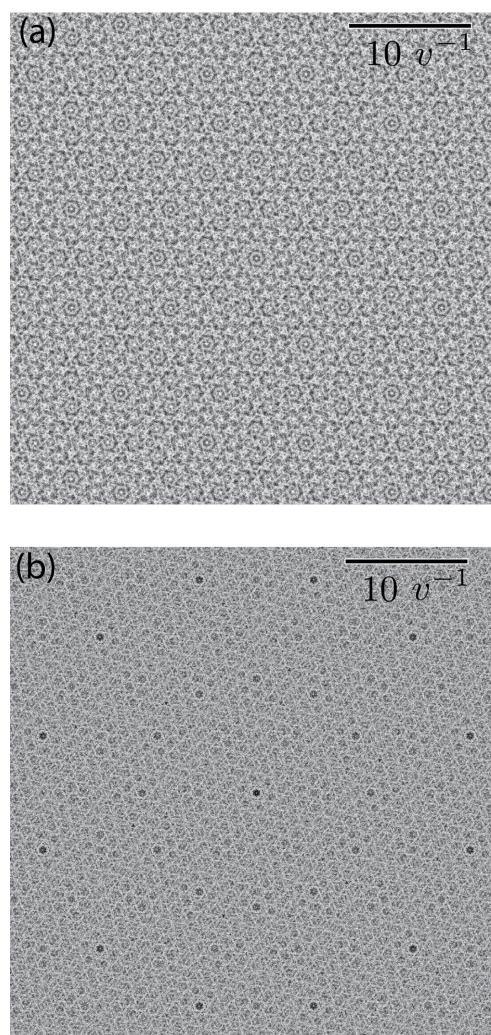


Figure 2

(a) The diffraction pattern (as log intensity) from a circular region of the Spectre tiling, radius $6000v$, with 20 698 280 point-scatterer tile vertices. (b) The diffraction pattern from the areal centroids. Both patterns have sixfold point symmetry about the origin (at the pattern centres), with no mirror symmetry, and are chiral. The recurring features are at different reciprocal locations between the two patterns, consistent with the aperiodic tiling structure. Unlike the Hat monotile, the diffracted intensity of the Spectre monotile is aperiodic.

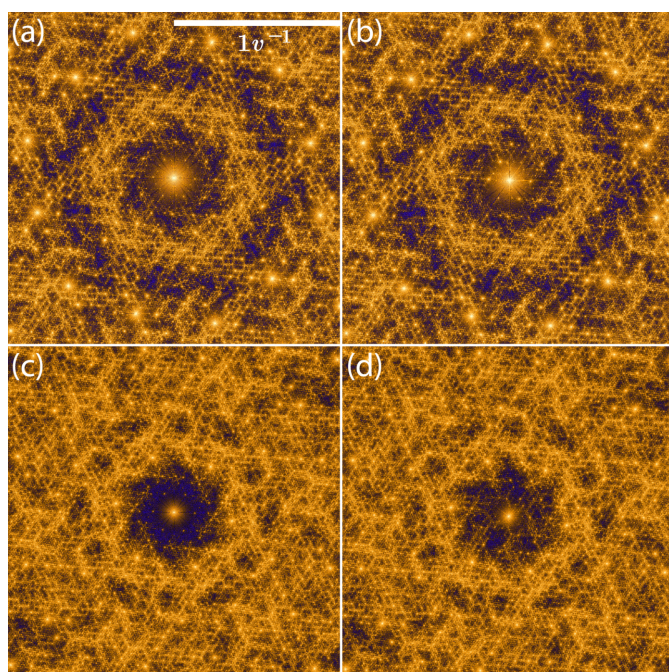


Figure 3

Comparison of similar motifs appearing in the diffraction of the Spectre tiling. The logarithm of intensity is displayed using the ICA colour lookup table in the program *ImageJ*: yellow is high log intensity, dark blue is low log intensity. The top row is the diffraction from tile vertices, the bottom row from tile areal centroids. (a) The region around the origin, $(0, 0) v^{-1}$ for tile vertices. (b) The region centred near $(10.97, 10.97) v^{-1}$ for tile vertices. (c) The region around the origin, $(0, 0) v^{-1}$ for tile areal centroids. (d) The region centred near $(12.69, 12.67) v^{-1}$ for tile areal centroids. Despite many similarities, the ‘repeating’ motifs are subtly different in each case. The sixfold chiral symmetry of the patterns about the origin is clear in (a) and (c) but is absent in (b) and (d).

origin with no mirror lines. Unusually for diffraction patterns, this pattern appears as a near-periodic array of dark dots within a grey background of diffused intensity. Importantly, the spacings between the near-periodic features of the two patterns are different. This is consistent with the absence of an underlying 2-periodic lattice associated with the Spectre tiling.

The diffracted wavefunction, $\psi(h, k)$, from large areas of the Spectre tiling, has threefold rotational symmetry (allowing for a linear phase gradient arising from the placement of the model origin). This reflects the presence of many local threefold structural centres in the tiling (see Fig. 1 for examples). The threefold-symmetric Fourier-transform wavefunction naturally has a centre of symmetry, with $\psi(-h, -k) = \exp(i\varphi)\psi^*(h, k)$, where φ is a phase related to the model’s origin of coordinates. Accordingly, the diffracted intensity inherits an additional twofold symmetry axis, $|\psi(-h, -k)|^2 = |\psi(h, k)|^2$, and exhibits an overall sixfold symmetry per Friedel’s law (Friedel, 1913).

Fig. 3 compares pairs of superficially repeating features of the patterns from the two structures. The logarithm of intensity is displayed using the ICA colour-lookup table in the program *ImageJ* (Schneider *et al.*, 2012). Fig. 3(a) shows the details about the origin of the tile-vertex pattern from a

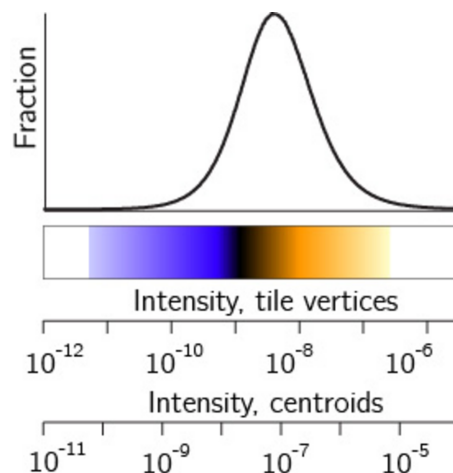


Figure 4

Top: the intensity-histogram shape for all four Spectre-tiling diffraction patterns in Fig. 3. Bottom: the intensity scales are set such that the bright peak at the origin of each pattern has unit intensity, 10^0 .

circular region of the Spectre tiling of radius $6000v$ containing 20 698 280 tile vertices. The point symmetry of 6 about the origin is evident, as is the absence of mirror lines. Fig. 3(b) shows a similar diffraction feature centred at reciprocal-lattice location $(10.97, 10.97) v^{-1}$. The two patterns are almost identical: the differences appear in the fine-scale details.

Similarly, the pair of patterns for the areal centroids from a region of radius $6000v$, containing 3 449 715 centroids [Figs.

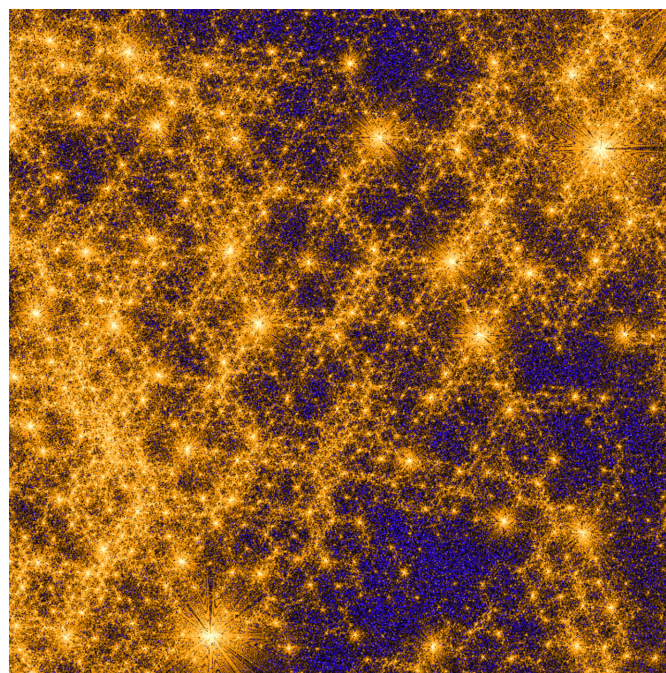


Figure 5

A close-up view of the log-intensity diffraction pattern from the tile vertices centred near reciprocal vector $(0.6, 0.0) v^{-1}$, to the right of the origin in Fig. 3(a). The reciprocal width of the square field of view is $0.189 v^{-1}$. The irregular hexagonal motif recurs at many length scales. The bright region on the left is part of the hexagonal band around the origin visible in Fig. 3(a). Yellow is high intensity, dark blue is low intensity.

3(c) and 3(d)], reveal similar subtle differences. The motif in Fig. 3(d) is centred at $(12.69, 12.67)v^{-1}$, a different location from the ‘repeated’ feature in the diffraction pattern from the tile vertices [Fig. 3(b)]. This is consistent with no 2-periodic lattice being associated with the Spectre tiling.

The log(intensity) histogram profile of the diffraction patterns from large numbers of vertices is approximately Gaussian for the vertices and centroids of the Spectre tiling (Fig. 4), as well as for the Hat tiling. The outlier intensities, far from the mean, do not fade away as quickly as a Gaussian. The ICA colour-lookup table used in Fig. 3 is also indicated. The log10 intensity scales given are calibrated such that the central peak at the origin in each set of patterns has unit intensity. This origin peak scales as N^2 , where N is the number of scatterers in the model.

As for the previously reported Hat tiling (Kaplan *et al.*, 2024), there is high-frequency detail, ‘diffused scattering’, in the diffraction patterns, which accounts for much of the histogram intensity spread, which is not visible at the printed resolution of Fig. 3. This detail sharpens up as the number of vertices in the model increases. We differentiate this from the term ‘diffuse scattering’, which is generally associated with defects in periodic systems or amorphous structures and does not sharpen as the model size increases. These aperiodic tilings, generated by simple rules, are perfectly ordered. Sharp diffraction speckles are expected at Fourier-space length scales proportional to the reciprocal of the model size.

Fig. 5 shows a zoomed-in region of the tile-vertices’ diffraction pattern centred at $(0.6, 0)v^{-1}$, close to the origin, spanning a reciprocal width of $0.189 v^{-1}$. 57 495 023 tile vertices in a disc of radius $10\,000v$ were used in the computation with a sampling of $5 \times 10^{-4} v^{-1}$ per pixel. Self-similar renderings of the hexagonal-ring motif appear at decreasing length scales, a characteristic feature of diffraction from aperiodic tilings (Senechal, 1995; Solomyak, 1997; Baake & Moody, 2000; O’Keeffe & Treacy, 2010; Baake & Grimm, 2013; Kellendonk *et al.*, 2015).

3. Conclusions

As reported earlier (Kaplan *et al.*, 2024), the Hat tiling aligns with a hexagonal lattice, so its diffraction pattern is periodic. Although closely related to the Hat tiling, the Spectre tiling does not align with any 2-periodic lattice, and we confirm that its diffraction pattern is strictly non-periodic despite a superficial appearance of periodicity. Like the Hat tiling, the Spectre tiling’s diffraction pattern contains self-similar

features at smaller length scales, which sharpen as the number of point scatterers increases.

Although the Hat and Spectre tilings are related, they are not combinatorially equivalent: there is no continuous bijection of the plane that transforms a tiling by Hats into a tiling by Spectres. A third 14-sided monotile shape, the ‘Turtle’, has been identified, which can also align aperiodically with the hexagonal 2-periodic **mta** tiling (Smith *et al.*, 2024b). Every tiling by Spectres can be continuously deformed into one by Hats distributed sparsely within Turtles or one by Turtles distributed sparsely within Hats.

Our computational methods use a ‘brute force’ summation of waves from large numbers of point scatterers into large reciprocal-space pixel arrays. Although effective and accurate, such methods are computationally laborious and inefficient for exploring large numbers of tile configurations. Diffraction from deformable, combinatorially equivalent families of monotiles could be explored more efficiently using recurrence relations for the diffraction amplitudes and phases, such as those developed by Socolar (2023). Parameterizing tile shapes should allow the evolution of the diffraction pattern in a region of reciprocal space to be followed efficiently as tiles are continuously deformed, possibly passing through 2-periodic resonances.

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