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Nonperiodic tessellation with eightfold rotational symmetry.

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Abstract

A tessellation with eightfold rotational symmetry was obtained by a self-similar subdivision of unit cells into rhombi and squares.

Early algebraic work to generate a two-dimensional quasi-lattice like the Penrose tessellation (Penrose, 1974) was carried out by de Bruijn (1981) and Mackay (1982). Since the discovery of a quasi-crystal of an Al-Mn alloy (Schechtman, Blech, Gratias & Cahn, 1984), several model structures of the quasi-lattice and its diffraction pattern have been studied by many authors (Hiraga, Hirabayashi, Inoue & Masumoto, 1985; Kimura, Hashimoto, Suzuki, Nagayama, Ino & Takeuchi, 1985; Levine & Steinhardt, 1984, *etc.*). There are two methods of obtaining a quasi-lattice; one is a projection of cubic cells in a higher-dimensional space to a lower one (Kramer & Neri, 1984; Duneau & Katz, 1985), and the other is a self-similar subdivision of unit cells constituting the tessellation (Mackay, 1982; Ogawa, 1985)

We obtained a tessellation with eightfold rotational symmetry by a self-similar subdividing operation of two kinds of cells, a rhombus and a square. Each unit cell is derived by dividing a regular octagon, which is uniquely divided into 16 rhombi and eight squares with eightfold symmetry at the center. In this subdividing operation the rhombus is divided into four squares and six rhombi, and the square into six squares and eight rhombi respectively (Fig. 1). The first-generation pattern of the square has a rhombic assembly with eightfold symmetry in its center and that of the acute rhombus includes a regular sub-octagon which consists of two squares and four rhombi, as shown by the shaded area of Fig. 1, having mirror symmetry. Therefore eight different tessellations could be derived using the two kinds of subdivided unit cells obtained by rotating the sub-octagon about the center. The tessellation after n self-similar subdividing operations is called the nth-generation pattern.

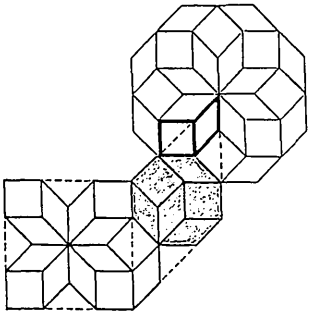

Fig. 1. First-generation pattern derived from division of a regular octagon.

The ratio of the number of squares to rhombi for the nth generation with n tending to infinity is obtained by solving a recurrence formula. Let S_n be the number of squares and R_n be the number of rhombi in the nth generation. Then the recurrence formula written in matrix form is

$$\mathbf{X}_n = A\mathbf{X}_{n-1} = A^n\mathbf{X}_0. \tag{1}$$

Here $\mathbf{X}_n$ is a column vector given by

$$\mathbf{X}_n = \begin{bmatrix} S_n \\ R_n \end{bmatrix} \tag{2}$$

with $S_0 = 1$ and $R_0 = 1$, and A is a matrix

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \tag{3}$$

with $a_{11} = 6$, $a_{12} = 8$, $a_{21} = 4$, $a_{22} = 6$. After a simple calculation we obtain A^n:

$$A^n = \begin{bmatrix} \frac{1}{2}\{(6+4\sqrt{2})^n + (6-4\sqrt{2})^n\} & \frac{\sqrt{2}}{2}\{(6+4\sqrt{2})^n - (6-4\sqrt{2})^n\} \\ \frac{\sqrt{2}}{4}\{(6+4\sqrt{2})^n - (6-4\sqrt{2})^n\} & \frac{1}{2}\{(6+4\sqrt{2})^n + (6-4\sqrt{2})^n\} \end{bmatrix}. \tag{4}$$

The ratios of the number of nth-generation squares to rhombi are s_n in a square, r_n in a rhombus, and t_n in a pattern of both added together, where

$$s_n = a_{11}^{(n)}/a_{12}^{(n)}, \qquad r_n = a_{21}^{(n)}/a_{22}^{(n)},$$
$$t_n = (a_{11}^{(n)} + a_{21}^{(n)})/(a_{12}^{(n)} + a_{22}^{(n)}). \tag{5}$$

If one substitutes the relevant matrix elements of (4) into (5), and lets n approach infinity, then the ratios s_n, r_n and t_n converge to $\sqrt{2}/2$. This irrational number proves that the

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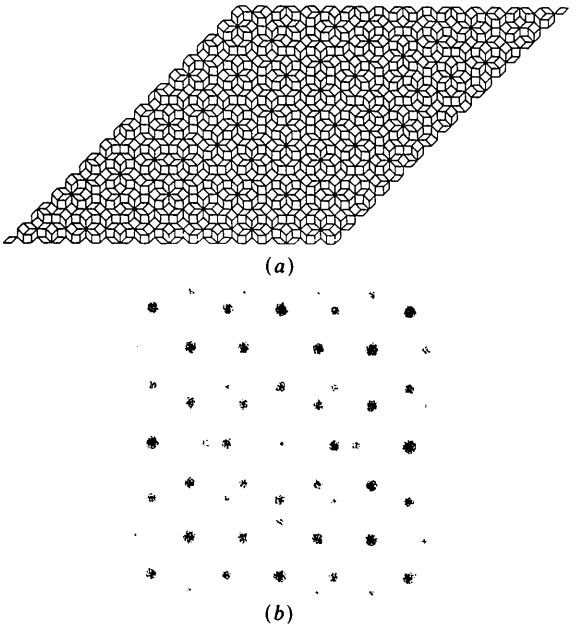

(*a*)

(*b*)

Fig. 2. (*a*) Octagonal tessellation in rhombic cell. (*b*) Diffraction pattern of lattice points about the center of Fig. 2(*a*).

octagonal tessellation pattern is non-periodic, as in the case of pentagonal tessellation (Mackay, 1981). The ratio of similarity from *n*th to $(n+1)$th generation for this tessellation is $1/(2+\sqrt{2})$.

As far as we know the eightfold symmetry diffraction pattern of a non-periodic structure has not yet been reported. The diffraction pattern (Fig. 2*b*) of the tessellation shown in Fig. 2(*a*) was calculated by a FFT algorithm assuming that point-like atoms of 1423 are located at lattice points about the center of the rhombic cell. All the coordinates of lattice points in the *n*th-generation pattern can be computed from those of the zeroth-generation pattern by applying the self-similar subdividing operation recursively.

In Fig. 2(*b*) we can also see sharp Bragg-like peaks with eightfold symmetry as expected, which might prove that the tessellation is a two-dimensional quasi-lattice.

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A reciprocal-space method for calculating a molecular envelope using the algorithm of B. C. Wang.

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Abstract

A method is described to determine the molecular envelope from an isomorphous replacement phased electron density map using the reciprocal-space equivalent of B. C. Wang's algorithm [Wang (1985). In *Methods in Enzymology*, Vol. 115: *Diffraction Methods for Biological Macromolecules*, edited by H. Wyckoff, C. H. W. Hirs & S. N. Timasheff. New York: Academic Press.]. In the case of chloramphenicol acetyl transferase the computation time was reduced from 35 h (using the real-space algorithm) to 40 min.

A suite of programs designed to improve the quality of protein electron density maps has recently been developed and distributed by B. C. Wang and colleagues (Wang, 1985). The basis of their method is to use the electron density map to determine a molecular envelope and then to set the electron density in the solvent region to a constant value (solvent flattening) and apply a positivity constraint to the electron density in the protein region. The modified electron density map is Fourier transformed, and the resulting phases combined with the original single isomorphous replacement (or multiple isomorphous replacement) phase information. The combined phases are then used to calculate a new electron density map, and the whole procedure is repeated iteratively until there is no further improvement in the quality of the electron density.

The solvent flattening part of this procedure has been used successfully in the structure determination of human alpha-1 proteinase inhibitor (Loebermann, Tokuoka, Deisenhofer & Huber, 1984), the photosynthetic reaction centre (Deisenhofer, Epp, Miki, Huber & Michel, 1984) and a light-harvesting biliprotein (Schirmer, Bode, Huber, Sidler & Zuber, 1985), all at 3 Å resolution, and similar results have been obtained by Wang and colleagues in the structure determination of cytochrome c5 at 2·5 Å resolution (Carter, Melis, O'Donnell, Burgess, Furey, Wang & Stout, 1985) as well as a number of structures at lower

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