

4. DIFFUSE SCATTERING AND RELATED TOPICS

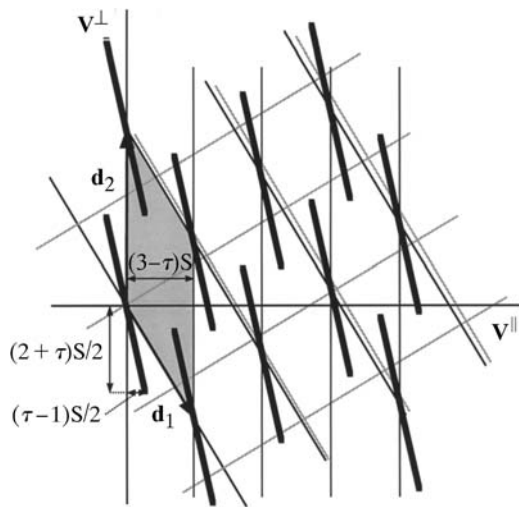


Fig. 4.6.2.11. 2D direct-space embedding of the Fibonacci chain as a modulated structure. The average period is $(3 - \tau)S$. The square lattice in the quasicrystal description shown in Fig. 4.6.2.8 is indicated by grey lines. The rod-like atomic surfaces are now inclined relative to V^{\parallel} and arranged so as to give a saw-tooth modulation wave.

$$\begin{pmatrix} S \\ L \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} S \\ L \end{pmatrix} = \begin{pmatrix} S + L \\ S + 2L \end{pmatrix}$$

with $S^2 = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$,

corresponding to the substitution rule $S \rightarrow SL, L \rightarrow LLS$ as well as two other non-equivalent ones (see Janssen, 1995). The eigenvalues λ_i are obtained by calculating

$$\det |S - \lambda I| = 0.$$

The evaluation of the determinant gives the characteristic polynomial

$$\lambda^2 - 3\lambda + 1 = 0,$$

with the solutions $\lambda_{1,2} = [3 \pm (5)^{1/2}]/2$, with $\lambda_1 = \tau^2$ and $\lambda_2 = 1/\tau^2 = 2 - \tau$, and the same eigenvectors

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ \tau \end{pmatrix}, \quad \mathbf{w}_2 = \begin{pmatrix} 1 \\ -1/\tau \end{pmatrix}$$

as for the Fibonacci sequence. Rewriting the eigenvalue equation gives

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ \tau \end{pmatrix} = \begin{pmatrix} \tau + 1 \\ 2\tau + 1 \end{pmatrix} = \begin{pmatrix} \tau^2 \\ \tau^3 \end{pmatrix} = \tau^2 \begin{pmatrix} 1 \\ \tau \end{pmatrix}.$$

Identifying the eigenvector

$$\begin{pmatrix} 1 \\ \tau \end{pmatrix}$$

with

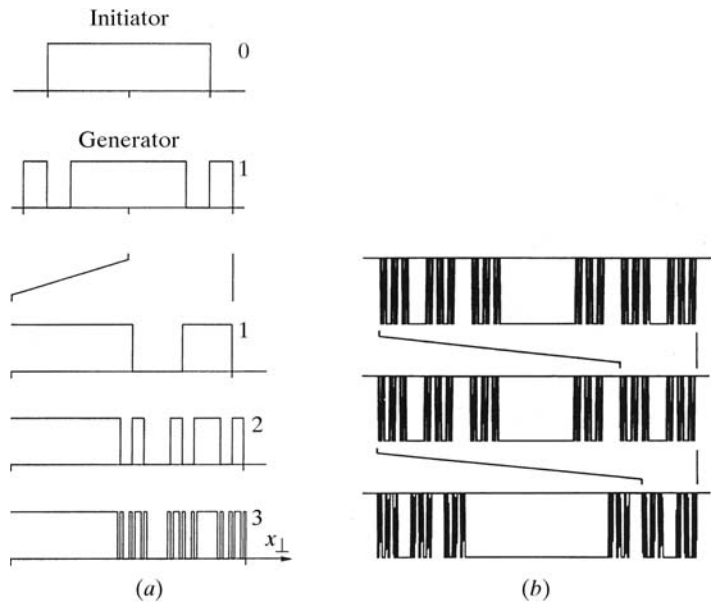


Fig. 4.6.2.12. (a) Three steps in the development of the fractal atomic surface of the squared Fibonacci sequence starting from an initiator and a generator. The action of the generator is to cut a piece from each side of the initiator and to add it where the initiator originally ended. This is repeated, cutting thinner and thinner pieces each time from the generated structures. (b) Magnification sequence of the fractal atomic surface illustrating its self-similarity. Each successive figure represents a magnification of a selected portion of the previous figure (from Zobetz, 1993).

$$\begin{pmatrix} S \\ L \end{pmatrix}$$

shows that the infinite 1D sequence $s(\mathbf{r})$ multiplied by powers of its eigenvalue τ^2 (scaling operation) remains invariant (each new lattice point coincides with one of the original lattice):

$$s(\tau^2 \mathbf{r}) = s(\mathbf{r}).$$

The fractal sequence can be described on the same reciprocal and direct bases as the Fibonacci sequence. The only difference in the 2D direct-space description is the fractal character of the perpendicular-space component of the hyperatoms (Fig. 4.6.2.12) (see Zobetz, 1993).

4.6.3. Reciprocal-space images

4.6.3.1. Incommensurately modulated structures (IMs)

One-dimensionally modulated structures are the simplest representatives of IMs. The vast majority of the one hundred or so IMs known so far belong to this class (Cummins, 1990). However, there is also an increasing number of IMs with 2D or 3D modulation. The dimension d of the modulation is defined by the number of rationally independent modulation wavevectors (satellite vectors) \mathbf{q}_i (Fig. 4.6.3.1). The electron-density function of a dD modulated 3D crystal can be represented by the Fourier series

$$\rho(\mathbf{r}) = (1/V) \sum_{\mathbf{H}} F(\mathbf{H}) \exp(-2\pi i \mathbf{H} \cdot \mathbf{r}).$$

The Fourier coefficients (*structure factors*) $F(\mathbf{H})$ differ from zero only for reciprocal-space vectors $\mathbf{H} = \sum_{i=1}^3 h_i \mathbf{a}_i^* + \sum_{j=1}^d m_j \mathbf{q}_j = \sum_{i=1}^{3+d} h_i \mathbf{a}_i^*$ with $h_i, m_j \in \mathbb{Z}$. The d satellite vectors are given by $\mathbf{q}_j = \mathbf{a}_{3+j}^* = \sum_{i=1}^3 \alpha_{ij} \mathbf{a}_i^*$, with α_{ij} a $3 \times d$ matrix σ . In the case of an