International Tables for Crystallography (2010). Vol. B, Section 4.6.2.5, pp. 597–598.

$$S_m = \frac{1}{2+\tau}\begin{pmatrix} \tau^2 + x\tau + 1 & -x \\ x\tau^2 & \tau^2 - x\tau + 1 \end{pmatrix}_D,$$

where $x = (n\tau - m)/(m\tau + n)$:

$$\mathbf{d}'_i = \sum_{j=1}^{2} S_{mij}\mathbf{d}_j;$$

$$\mathbf{d}'_1 = \frac{1}{2+\tau}\left[(\tau^2 + x\tau + 1)\mathbf{d}_1 - x\mathbf{d}_2\right]$$

$$= \frac{1}{(2+\tau)a^*}\begin{pmatrix} 1 \\ -\tau - x \end{pmatrix}_V$$

$$= \frac{1}{(2+\tau)a^*}\begin{pmatrix} 1 \\ -\dfrac{2n\tau + m\tau}{m\tau + n} \end{pmatrix}_V,$$

$$\mathbf{d}'_2 = \frac{1}{2+\tau}\left[x\tau^2\mathbf{d}_1 + (\tau^2 - x\tau + 1)\mathbf{d}_2\right]$$

$$= \frac{1}{(2+\tau)a^*}\begin{pmatrix} \tau \\ -x\tau + 1 \end{pmatrix}_V$$

$$= \frac{1}{(2+\tau)a^*}\begin{pmatrix} \tau \\ \dfrac{2m\tau - n\tau}{m\tau + n} \end{pmatrix}_V.$$

This shear matrix does not change the magnitudes of the intervals L and S. In reciprocal space the inverted and transposed shear matrix is applied on the reciprocal basis,

$$(S_m^{-1})^T = \frac{1}{2+\tau}\begin{pmatrix} \tau^2 - x\tau + 1 & -x\tau^2 \\ x & \tau^2 + x\tau + 1 \end{pmatrix}_D,$$

where $x = (n\tau - m)/(m\tau + n)$:

$$\mathbf{d}_i^{*\prime} = \sum_{j=1}^{2} (S_m^{-1})^T_{ij}\mathbf{d}_j^*;$$

$$\mathbf{d}_1^{*\prime} = \frac{1}{2+\tau}\left[(\tau^2 - x\tau + 1)\mathbf{d}_1^* - x\tau^2\mathbf{d}_2^*\right]$$

$$= a^*\begin{pmatrix} 1 - x\tau \\ -\tau \end{pmatrix}_V$$

$$= a^*\begin{pmatrix} \dfrac{2m\tau - n\tau}{m\tau + n} \\ -\tau \end{pmatrix}_V,$$

$$\mathbf{d}_2^{*\prime} = \frac{1}{2+\tau}\left[x\mathbf{d}_1^* + (\tau^2 + x\tau + 1)\mathbf{d}_2^*\right]$$

$$= a^*\begin{pmatrix} \tau + x \\ 1 \end{pmatrix}_V$$

$$= a^*\begin{pmatrix} \dfrac{2n\tau + m\tau}{m\tau + n} \\ 1 \end{pmatrix}_V.$$

The point $x_n(t)$ of the nth interval L or S of an infinite Fibonacci sequence is given by

$$x_n(t) = \{x_0 + n(3 - \tau) - (\tau - 1)[\mathrm{frac}(n\tau + t) - (1/2)]\}\mathrm{S},$$

where t is the phase of the modulation function $y(t) = (\tau - 1)[\mathrm{frac}(n\tau + t) - (1/2)]$ (Janssen, 1986). Thus, the Fibonacci sequence can also be dealt with as an incommensurately modulated structure. This is a consequence of the fact that for 1D structures only the crystallographic point symmetries 1 and $\bar{1}$ allow the existence of a periodic average structure.

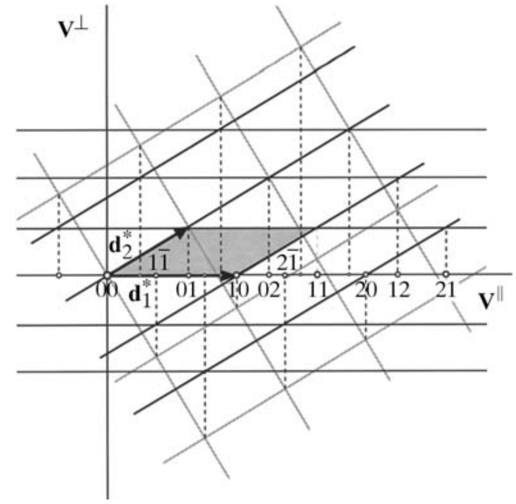

Fig. 4.6.2.10. Reciprocal space of the embedded Fibonacci chain as a modulated structure. Several main and satellite reflections are indexed. The square reciprocal lattice of the quasicrystal description illustrated in Fig. 4.6.2.9 is indicated by grey lines. The reflections located on $\mathbf{V}^\parallel$ can be considered to be projected either from the 2D square lattice of the embedding as for a QS or from the 2D oblique lattice of the embedding as for an IMS.

The embedding of the Fibonacci chain as an incommensurately modulated structure can be performed as follows:

(1) select a subset $\Lambda^* \subset M^*$ of strong reflections for main reflections $\mathbf{H} = h\mathbf{a}^*, h \in \mathbb{Z}$;

(2) define a satellite vector $\mathbf{q} = \alpha\mathbf{a}^*$ pointing from each main reflection to the next satellite reflection.

One possible way of indexing based on the same $\mathbf{a}^*$ as defined above is illustrated in Fig. 4.6.2.10. The scattering vector is given by $\mathbf{H}^\parallel = h(\tau + 1)\mathbf{a}^* + mq$, where $\mathbf{q} = \tau\mathbf{a}^*$, or, in the 2D representation, $\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^*$, where

$$\mathbf{d}_1^* = a^*\begin{pmatrix} 1 + \tau \\ 0 \end{pmatrix}_V$$

and

$$\mathbf{d}_2^* = a^*\begin{pmatrix} \tau \\ 1 \end{pmatrix}_V,$$

with the direct basis

$$\mathbf{d}_1 = \frac{1}{a^*(1+\tau)}\begin{pmatrix} 1 \\ -\tau \end{pmatrix}_V, \quad \mathbf{d}_2 = \frac{1}{a^*}\begin{pmatrix} 0 \\ 1 \end{pmatrix}_V.$$

The modulation function is saw-tooth-like (Fig. 4.6.2.11).

4.6.2.5. 1D structures with fractal atomic surfaces

A 1D structure with a *fractal atomic surface* (Hausdorff dimension 0.9157...) can be derived from the Fibonacci sequence by squaring its substitution matrix S:

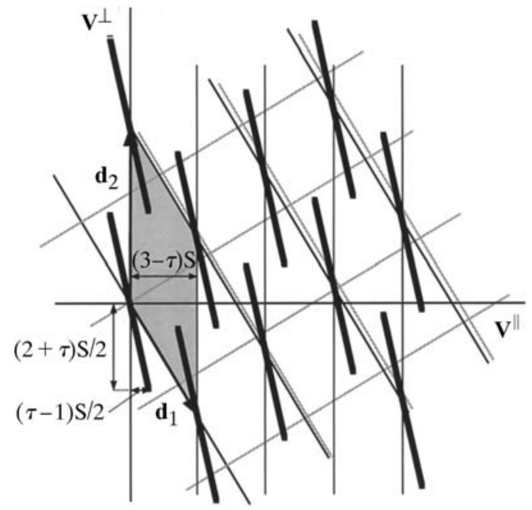

Fig. 4.6.2.11. 2D direct-space embedding of the Fibonacci chain as a modulated structure. The average period is $(3-\tau)$S. The square lattice in the quasicrystal description shown in Fig. 4.6.2.8 is indicated by grey lines. The rod-like atomic surfaces are now inclined relative to $\mathbf{V}^{\parallel}$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

$$\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix} = \begin{pmatrix} \mathrm{S}+\mathrm{L} \\ \mathrm{S}+2\mathrm{L} \end{pmatrix}$$
$$\text{with } S^2 = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix},$$

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

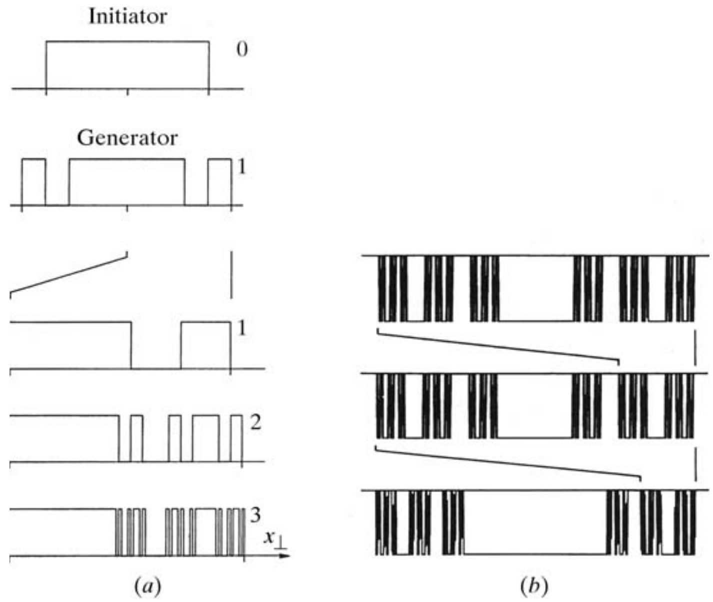

Fig. 4.6.2.12. (*a*) Three steps in the development of the fractal atomic surface of the squared Fibonacci sequence starting from an initiator and a generator. The action of the generator is to cut a piece from each side of the initiator and to add it where the initiator originally ended. This is repeated, 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).

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

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 (IMSs)

One-dimensionally modulated structures are the simplest representatives of IMSs. The vast majority of the one hundred or so IMSs known so far belong to this class (Cummins, 1990). However, there is also an increasing number of IMSs 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

references