International Tables for Crystallography (2006). Vol. B, Section 4.6.2.3, pp. 489–490.

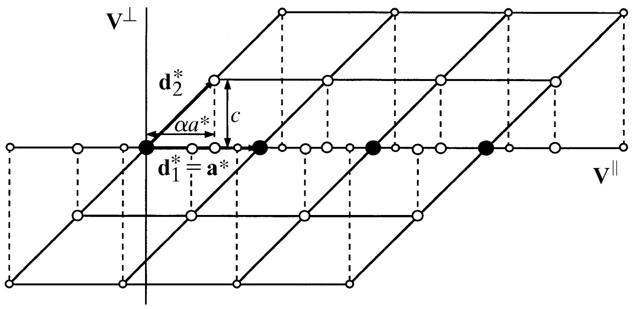

Fig. 4.6.2.3. Schematic representation of the 2D reciprocal-space embedding of the 1D sinusoidally modulated structure depicted in Figs. 4.6.2.1 and 4.6.2.2. Main reflections are marked by filled circles and satellite reflections by open circles. The sizes of the circles are roughly related to the reflection intensities. The actual 1D diffraction pattern of the 1D MS results from a projection of the 2D reciprocal space onto the parallel space. The correspondence between 2D reciprocal-lattice positions and their projected images is indicated by dashed lines.

shearing the 2D lattice Σ with a shear matrix S_m:

$$\mathbf{d}'_i = \sum_{j=1}^{2} S_{mij}\mathbf{d}_j, \text{ with } S_m = \begin{pmatrix} 1 & -x \\ 0 & 1 \end{pmatrix}_D \text{ and } x = \alpha' - \alpha,$$

$$\mathbf{d}'_1 = \mathbf{d}_1 - x\mathbf{d}_2 = \begin{pmatrix} a \\ -\alpha \end{pmatrix}_V - (\alpha' - \alpha)\begin{pmatrix} 0 \\ 1 \end{pmatrix}_V = \begin{pmatrix} a \\ -\alpha' \end{pmatrix}_V,$$

$$\mathbf{d}'_2 = \mathbf{d}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_V.$$

The subscript D (V) following the shear matrix indicates that it is acting on the D (V) basis. The shear matrix does not change the distances between the atoms in the basic structure. In reciprocal space, using the inverted and transposed shear matrix, one obtains

$$\mathbf{d}_i^{*\prime} = \sum_{j=1}^{2} (S_m^{-1})_{ij}^T \mathbf{d}_j^*, \text{ with } (S_m^{-1})^T = \begin{pmatrix} 1 & 0 \\ x & 1 \end{pmatrix}_D \text{ and } x = \alpha' - \alpha,$$

$$\mathbf{d}_1^{*\prime} = \mathbf{d}_1^* = \begin{pmatrix} a^* \\ 0 \end{pmatrix}_V,$$

$$\mathbf{d}_2^{*\prime} = x\mathbf{d}_1^* + \mathbf{d}_2^* = (\alpha' - \alpha)\begin{pmatrix} a^* \\ 0 \end{pmatrix}_V + \begin{pmatrix} \alpha a^* \\ 1 \end{pmatrix}_V = \begin{pmatrix} \alpha' a^* \\ 1 \end{pmatrix}_V.$$

4.6.2.3. *1D composite structures*

In the simplest case, a *composite structure* (CS) consists of two intergrown periodic structures with mutually incommensurate lattices. Owing to mutual interactions, each subsystem may be modulated with the period of the other. Consequently, CSs can be considered as coherent intergrowths of two or more incommensurately modulated substructures. The substructures have at least the origin of their reciprocal lattices in common. However, in all known cases, at least one common reciprocal-lattice plane exists. This means that at least one particular projection of the composite structure exhibits full lattice periodicity.

The unmodulated (basic) 1D subsystems of a 1D incommensurate intergrowth structure can be related to each other in a 2D parameter space $\mathbf{V} = (\mathbf{V}^{\parallel}, \mathbf{V}^{\perp})$ (Fig. 4.6.2.4). The actual atoms result from the intersection of the physical space $\mathbf{V}^{\parallel}$ with the hypercrystal. The hyperatoms correspond to a convolution of the real atoms with infinite lines parallel to the basis vectors $\mathbf{d}_1$ and $\mathbf{d}_2$ of the 2D hyperlattice $\Sigma = \{\mathbf{r} = \sum_{i=1}^{2} n_i\mathbf{d}_i | n_i \in \mathbb{Z}\}$.

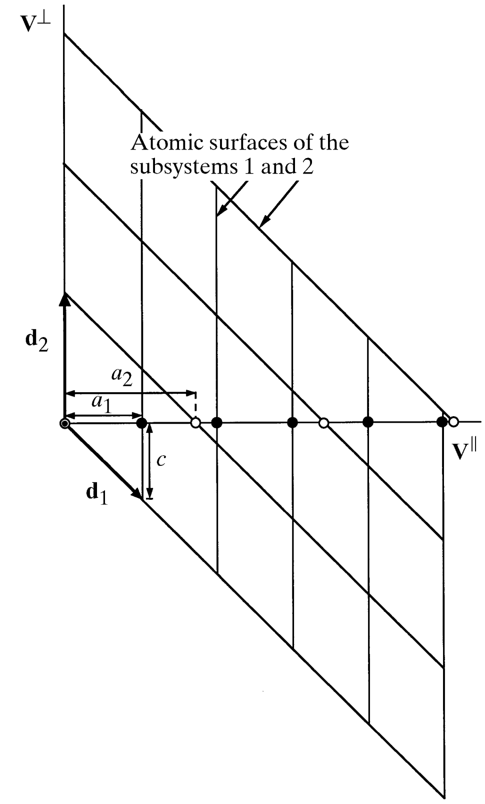

Fig. 4.6.2.4. 2D embedding of a 1D composite structure without mutual interaction of the subsystems. Filled and empty circles represent the atoms of the unmodulated substructures with periods a_1 and a_2, respectively. The atoms result from the parallel-space cut of the linear atomic surfaces parallel to $\mathbf{d}_1$ and $\mathbf{d}_2$.

An appropriate basis is given by

$$\mathbf{d}_1 = \begin{pmatrix} a_1 \\ -c \end{pmatrix}_V, \mathbf{d}_2 = \begin{pmatrix} 0 \\ c(a_2/a_1) \end{pmatrix}_V,$$

where a_1 and a_2 are the lattice parameters of the two substructures and c is an arbitrary constant. Taking into account the interactions between the subsystems, each one becomes modulated with the period of the other. Consequently, in the 2D description, the shape of the hyperatoms is determined by their modulation functions (Fig. 4.6.2.5).

A basis of the reciprocal lattice $\Sigma^* = \{\mathbf{H} = \sum_{i=1}^{2} h_i\mathbf{d}_i^* | h_i \in \mathbb{Z}\}$ can be obtained from the condition $\mathbf{d}_i \cdot \mathbf{d}_j^* = \delta_{ij}$:

$$\mathbf{d}_1^* = \begin{pmatrix} a_1^* \\ 0 \end{pmatrix}_V, \mathbf{d}_2^* = \begin{pmatrix} a_2^* \\ (a_2^*/ca_1^*) \end{pmatrix}_V.$$

The metric tensors for the reciprocal and the direct 2D lattices for $c = 1$ are

$$G^* = \begin{pmatrix} a_1^{*2} & a_1^* a_2^* \\ a_1^* a_2^* & (1 + a_1^{*2})(a_2^*/a_1^*)^2 \end{pmatrix} \text{ and } G = \begin{pmatrix} 1 + a_1^2 & -a_2/a_1 \\ -a_2/a_1 & (a_2/a_1)^2 \end{pmatrix}.$$

The Fourier transforms of the hypercrystals depicted in Figs. 4.6.2.4 and 4.6.2.5 correspond to the weighted reciprocal lattices illustrated in Figs. 4.6.2.6 and 4.6.2.7. The 1D diffraction patterns $M^* = \{\mathbf{H}^{\parallel} = \sum_{i=1}^{2} h_i\mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ in physical space are obtained by a projection of the weighted 2D reciprocal lattices Σ^* upon $\mathbf{V}^{\parallel}$. All Bragg reflections can be indexed with integer numbers h_1, h_2 in both the 2D description $\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^*$ and in the 1D physical-space description with two parallel basis vectors $\mathbf{H}^{\parallel} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^*$.

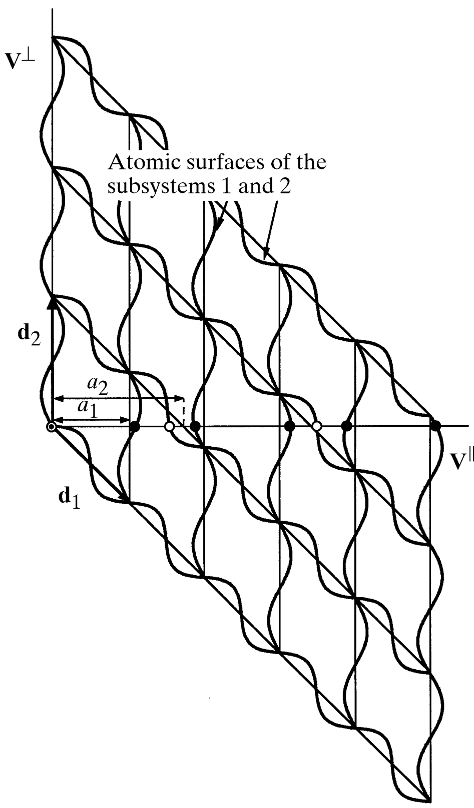

Fig. 4.6.2.5. 2D embedding of a 1D composite structure with mutual interaction of the subsystems causing modulations. Filled and empty circles represent the modulated substructures with periods a_1 and a_2 of the basic substructures, respectively. The atoms result from the parallel-space cut of the sinusoidal atomic surfaces running parallel to $\mathbf{d}_1$ and $\mathbf{d}_2$.

The reciprocal-lattice points $\mathbf{H} = h_1\mathbf{d}_1^*$ and $\mathbf{H} = h_2\mathbf{d}_2^*$, h_1, $h_2 \in \mathbb{Z}$, on the main axes $\mathbf{d}_1{}^*$ and $\mathbf{d}_2{}^*$ are the main reflections of the two substructures. All other reflections are referred to as satellite reflections. Their intensities differ from zero only in the case of modulated substructures. Each reflection of one subsystem coincides with exactly one reflection of the other subsystem.

4.6.2.4. *1D quasiperiodic structures*

The Fibonacci sequence, the best investigated example of a 1D quasiperiodic structure, can be obtained from the substitution rule σ: S $\rightarrow$ L, L $\rightarrow$ LS, replacing the letter S by L and the letter L by the word LS (see *e.g.* Luck *et al.*, 1993). Applying the substitution matrix

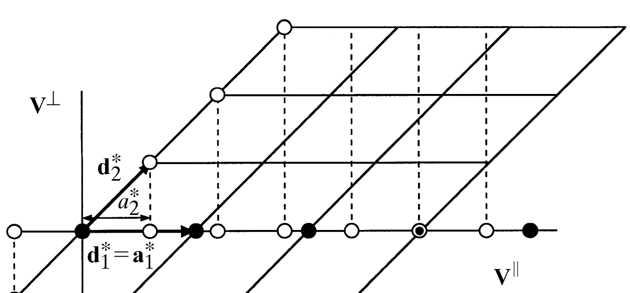

Fig. 4.6.2.6. Schematic representation of the reciprocal space of the embedded 1D composite structure depicted in Fig. 4.6.2.4. Filled and empty circles represent the reflections generated by the substructures with periods a_1 and a_2, respectively. The actual 1D diffraction pattern of the 1D CS results from a projection of the 2D reciprocal space onto the parallel space. The correspondence between 2D reciprocal-lattice positions and their projected images is indicated by dashed lines.

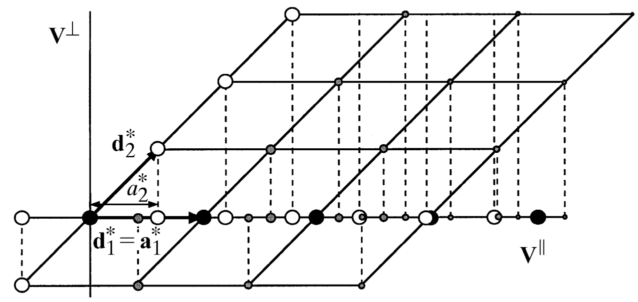

Fig. 4.6.2.7. Schematic representation of the reciprocal space of the embedded 1D composite structure depicted in Fig. 4.6.2.5. Filled and empty circles represent the main reflections of the two subsystems. The satellite reflections generated by the modulated substructures are shown as grey circles. The diameters of the circles are roughly proportional to the intensities of the reflections. The actual 1D diffraction pattern of the 1D CS results from a projection of the 2D reciprocal space onto the parallel space. The correspondence between 2D reciprocal-lattice positions and their projected images is indicated by dashed lines.

$$S = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$$

associated with σ, this rule can be written in the form

$$\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix} = \begin{pmatrix} \mathrm{L} \\ \mathrm{L}+\mathrm{S} \end{pmatrix}.$$

S gives the sum of letters, $\mathrm{L}+\mathrm{S} = \mathrm{S}+\mathrm{L}$, and not their order. Consequently, the same substitution matrix can also be applied, for instance, to the substitution σ': S $\rightarrow$ L, L $\rightarrow$ SL. The repeated action of S on the alphabet $A = \{\mathrm{S},\ \mathrm{L}\}$ yields the words $A_n = \sigma^n(\mathrm{S})$ and $B_n = \sigma^n(\mathrm{L}) = A_{n+1}$ as illustrated in Table 4.6.2.1. The frequencies of letters contained in the words A_n and B_n can be calculated by applying the nth power of the transposed substitution matrix on the unit vector. From

$$\begin{pmatrix} \nu_{n+1}^A \\ \nu_{n+1}^B \end{pmatrix} = S^T \begin{pmatrix} \nu_n^A \\ \nu_n^B \end{pmatrix}$$

it follows that

$$\begin{pmatrix} \nu_n^A \\ \nu_n^B \end{pmatrix} = (S^T)^n \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

In the case of the Fibonacci sequence, ν_n^B gives the total number of letters S and L, and ν_n^A the number of letters L.

An infinite Fibonacci sequence, *i.e.* a word B_n with $n \rightarrow \infty$, remains invariant under inflation (deflation). Inflation (deflation) means that the number of letters L, S increases (decreases) under the action of the (inverted) substitution matrix S. Inflation and deflation represent self-similarity (scaling) symmetry operations on the infinite Fibonacci sequence. A more detailed discussion of the scaling properties of the Fibonacci chain in direct and reciprocal space will be given later.

The Fibonacci numbers $F_n = F_{n-1} + F_{n-2}$ form a series with $\lim_{n\rightarrow\infty} (F_{n+1}/F_n) = \tau$ {the golden mean $\tau = [1 + (5)^{1/2}]/2 = 2\cos(\pi/5) = 1.618\ldots$}. The ratio of the frequencies of L and S in the Fibonacci sequence converges to τ if the sequence goes to infinity. The continued fraction expansion of the golden mean τ,