of the direct and reciprocal $(3+d)$ lattices (Janner & Janssen, 1980*b*)

$$\Sigma^*: \begin{cases} \mathbf{a}_i^* & = (\mathbf{a}_i^*, \mathbf{0}) & i = 1, \ldots, 3 \\ \mathbf{a}_{3+j}^* & = (\mathbf{a}_{3+j}^*, \mathbf{e}_j^*) & j = 1, \ldots, d \end{cases}$$

$$\Sigma: \begin{cases} \mathbf{a}_i & = (\mathbf{a}_i, -\sum_{j=1}^{d} \sigma_{ji} \mathbf{e}_j) & i = 1, \ldots, 3 \\ \mathbf{a}_{3+j} & = (\mathbf{0}, \mathbf{e}_j) & j = 1, \ldots, d. \end{cases}$$

4.6.3.2.1. Indexing

The indexing of diffraction patterns of composite structures can be performed in the following way:

(1) find the minimum number of reciprocal lattices Λ_ν^* necessary to index the diffraction pattern;

(2) find a basis for M^*, the union of sublattices Λ_ν^*;

(3) find the appropriate superspace embedding.

The $(3+d)$ vectors $\mathbf{a}_i^*$ forming a basis for the 3D Fourier module $M^* = \{\sum_{i=1}^{3+d} h_i \mathbf{a}_i^*\}$ can be chosen such that $\mathbf{a}_1^*$, $\mathbf{a}_2^*$ and $\mathbf{a}_3^*$ are linearly independent. Then the remaining d vectors can be described as a linear combination of the first three, defining the $d \times 3$ matrix σ: $\mathbf{a}_{3+j}^* = \sum_{i=1}^{3+d} \sigma_{ji} \mathbf{a}_i^*$, $j = 1, \ldots, d$. This is formally equivalent to the reciprocal basis obtained for an IMS (see Section 4.6.3.1) and one can proceed in an analogous way to that for IMSs.

4.6.3.2.2. Diffraction symmetry

The symmetry of CSs can be described with basically the same formalism as used for IMSs. This is a consequence of the formally equivalent applicability of the higher-dimensional approach, in particular of the superspace-group theory developed for IMSs [see Janner & Janssen (1980*a*,*b*); van Smaalen (1991, 1992); Yamamoto (1992*a*)].

4.6.3.2.3. Structure factor

The structure factor $F(\mathbf{H})$ of a composite structure consists of the weighted contributions of the subsystem structure factors $F_\nu(\mathbf{H}_\nu)$:

$$F(\mathbf{H}) = \sum_\nu |J_\nu| F_\nu(\mathbf{H}_\nu);$$

$$F_\nu(\mathbf{H}) = \sum_{(R^\nu, \mathbf{t}^\nu)}^{\infty} \sum_{k=1}^{N'} \int_0^1 \mathrm{d}\bar{x}_{4,k}^\nu \ldots \int_0^1 \mathrm{d}\bar{x}_{3+d,k}^\nu f_k^\nu(\mathbf{H}^\parallel) p_k^\nu \times \exp\left(- \sum_{i,j=1}^{3+d} h_i^\nu [R^\nu B_{ijk}^\nu R^{\nu T}] h_j^\nu + 2\pi i \sum_{j=1}^{3+d} h_j^\nu R^\nu x_{jk}^\nu + h_j^\nu t_j^\nu \right),$$

with coefficients similar to those for IMSs.

The weights are the Jacobians of the transformations from $\mathbf{t}_\nu$ to $\mathbf{t}$, and $\mathbf{H}_\nu$ are the reflection indices with respect to the subsystem Fourier modules M_ν^* (van Smaalen, 1995, and references therein). The relative values of $|J_\nu|$, where $J_\nu = \det\left[(V_{d\nu} - \sigma_\nu \cdot Z_{d\nu})^{-1}\right]$, are related to the volume ratios of the contributing subsystems. The subsystem structure factors correspond to those for IMSs (see Section 4.6.3.1). Besides this formula, based on the publications of Yamamoto (1982) and van Smaalen (1995), different structure-factor equations have been discussed (Kato, 1990; Petricek, Maly, Coppens *et al.*, 1991).

4.6.3.3. Quasiperiodic structures (QSs)

4.6.3.3.1. 3D structures with 1D quasiperiodic order

Structures with quasiperiodic order in one dimension and lattice symmetry in the other two dimensions are the simplest representatives of quasicrystals. A few phases of this structure type have been identified experimentally (see Steurer, 1990). Since the Fibonacci chain represents the most important model of a 1D quasiperiodic structure, it will be used in this section to represent the quasiperiodic direction of 3D structures with 1D quasiperiodic order. As discussed in Section 4.6.2.4, 1D quasiperiodic structures are on the borderline between quasiperiodic and incommensurately modulated structures. They can be described using either of the two approaches. In the following, the quasiperiodic description will be preferred to take account of the scaling symmetry.

The electron-density-distribution function $\rho(\mathbf{r})$ of a 1D quasiperiodically ordered 3D crystal can be represented by a 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 $\mathbf{H} = \sum_{i=1}^{3} h_i^\parallel \mathbf{a}_i^*$ with $h_1{}^\parallel \in \mathbb{R}$, $h_2{}^\parallel, h_3{}^\parallel \in \mathbb{Z}$ or with integer indexing $\mathbf{H} = \sum_{i=1}^{4} h_i \mathbf{a}_i^*$ with $h_i \in \mathbb{Z}$. The set of all vectors $\mathbf{H}$ forms a Fourier module $M^* = \{\mathbf{H}^\parallel = \sum_{i=1}^{4} h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ of rank 4 which can be decomposed into two rank 2 submodules $M^* = M_1^* \oplus M_2^*$. $M_1^* = \{h_1 \mathbf{a}_1^* + h_2 \mathbf{a}_2^*\}$ corresponds to a $\mathbb{Z}$ module of rank 2 in a 1D subspace, $M_2^* = \{h_3 \mathbf{a}_3^* + h_4 \mathbf{a}_4^*\}$ corresponds to a $\mathbb{Z}$ module of rank 2 in a 2D subspace. Consequently, the first submodule can be considered as a projection from a 2D reciprocal lattice, $M_1^* = \pi^\parallel(\Sigma^*)$, while the second submodule is of the form of a reciprocal lattice, $M_2^* = \Lambda^*$.

Hence, the reciprocal-basis vectors $\mathbf{a}_i^*$, $i = 1, \ldots, 4$, can be considered to be projections of reciprocal-basis vectors $\mathbf{d}_i^*$, $i = 1, \ldots, 4$, spanning a 4D reciprocal lattice, onto the physical space $\Sigma^* = \{\mathbf{H} = \sum_{i=1}^{4} h_i \mathbf{d}_i^* | h_i \in \mathbb{Z}\}$, with

$$\mathbf{d}_1^* = a_1^* \begin{pmatrix} 1 \\ -\tau \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{d}_2^* = a_1^* \begin{pmatrix} \tau \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{d}_3^* = a_3^* \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{d}_4^* = a_4^* \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

A direct lattice Σ with basis $\mathbf{d}_i$, $i = 1, \ldots, 4$ and $\mathbf{d}_i \cdot \mathbf{d}_j^* = \delta_{ij}$, can be constructed according to (compare Fig. 4.6.2.8) $\Sigma = \{\mathbf{r} = \sum_{i=1}^{4} m_i \mathbf{d}_i | m_i \in \mathbb{Z}\}$, with

$$\mathbf{d}_1 = \frac{1}{a_1^*(2+\tau)} \begin{pmatrix} 1 \\ -\tau \\ 0 \\ 0 \end{pmatrix}, \mathbf{d}_2 = \frac{1}{a_1^*(2+\tau)} \begin{pmatrix} \tau \\ 1 \\ 0 \\ 0 \end{pmatrix},$$

$$\mathbf{d}_3^* = \frac{1}{a_3^*} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{d}_4^* = \frac{1}{a_4^*} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Consequently, the structure in physical space $\mathbf{V}^\parallel$ is equivalent to a 3D section of the 4D hypercrystal.

4.6.3.3.1.1. Indexing

The reciprocal space of the Fibonacci chain is densely filled with Bragg reflections (Figs. 4.6.2.9 and 4.6.3.5). According to the nD embedding method, the shorter the parallel-space distance $\Delta\mathbf{H}^\parallel = \mathbf{H}_2^\parallel - \mathbf{H}_1^\parallel$ between two Bragg reflections, the larger the corresponding perpendicular-space distance $\Delta\mathbf{H}^\perp = \mathbf{H}_2^\perp - \mathbf{H}_1^\perp$ becomes. Since the structure factor $F(\mathbf{H})$ decreases rapidly as a

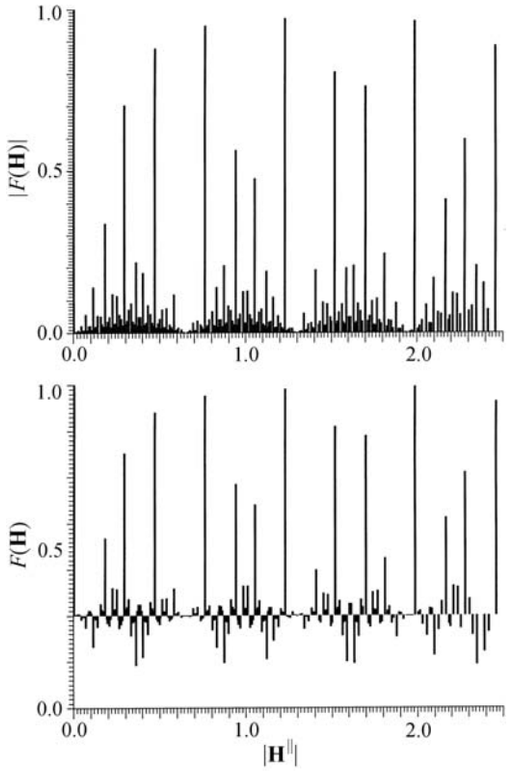

Fig. 4.6.3.5. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of a Fibonacci chain decorated with equal point atoms are shown as a function of the parallel-space component $|\mathbf{H}^{\parallel}|$ of the diffraction vector. The short distance in the Fibonacci chain is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

function of $\mathbf{H}^{\perp}$ (Fig. 4.6.3.6), 'neighbouring' reflections of strong Bragg peaks are extremely weak and, consequently, the reciprocal space appears to be filled with *discrete* Bragg peaks even for low-resolution experiments.

This property allows an unambiguous identification of a correct set of reciprocal-basis vectors. However, infinitely many sets allowing a correct indexing of the diffraction pattern with integer indices exist. Nevertheless, an optimum basis (low indices are assigned to strong reflections) can be derived: the intensity distribution, not the metrics, characterizes the best choice of indexing. Once the minimum distance S in the structure is identified from chemical considerations, the reciprocal basis should be chosen as described in Section 4.6.2.4. It has to be kept in mind, however, that the identification of the metrics is not sufficient to distinguish in the 1D aperiodic case between an incommensurately modulated structure, a quasiperiodic structure or special kinds of structures with fractally shaped atomic surfaces.

A correct set of reciprocal-basis vectors can be identified in the following way:

(1) Find pairs of strong reflections whose physical-space diffraction vectors are related to each other by the factor τ.

(2) Index these reflections by assigning an appropriate value to a^*. This value should be derived from the shortest interatomic distance S expected in the structure.

(3) The reciprocal basis is correct if all observable Bragg reflections can be indexed with integer numbers.

4.6.3.3.1.2. Diffraction symmetry

The possible Laue symmetry group K^{3D} of the Fourier module $M^* = \{\mathbf{H}^{\parallel} = \sum_{i=1}^{4} h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ is any one of the direct product $K^{3D} = K^{2D} \otimes K^{1D} \otimes \bar{1}$. K^{2D} corresponds to one of the ten crystallographic 2D point groups, $K^{1D} = \{1\}$ in the general case of a quasiperiodic stacking of periodic layers. Consequently, the nine Laue groups $\bar{1}$, $2/m$, mmm, $4/m$, $4/mmm$, $\bar{3}$, $\bar{3}m$, $6/m$ and $6/mmm$ are possible. These are all 3D crystallographic Laue groups except for the two cubic ones.

The (unweighted) Fourier module shows only 2D lattice symmetry. In the third dimension, the submodule M_1^* remains invariant under the scaling symmetry operation $S^n M_1^* = \tau^n M_1^*$ with $n \in \mathbb{Z}$. The scaling symmetry operators S^n form an infinite group $s = \{\ldots, S^{-1}, S^0, S^1, \ldots\}$ of reciprocal-basis transformations S^n in superspace,

$$S^n = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_D^n, \quad S^{-1} = \begin{pmatrix} \bar{1} & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_D,$$

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

and act on the reciprocal basis $\mathbf{d}_i^*$ in superspace.

4.6.3.3.1.3. Structure factor

The structure factor of a periodic structure is defined as the Fourier transform of the density distribution $\rho(\mathbf{r})$ of its unit cell (UC):

$$F(\mathbf{H}) = \int_{\mathrm{UC}} \rho(\mathbf{r}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}) \, \mathrm{d}\mathbf{r}.$$

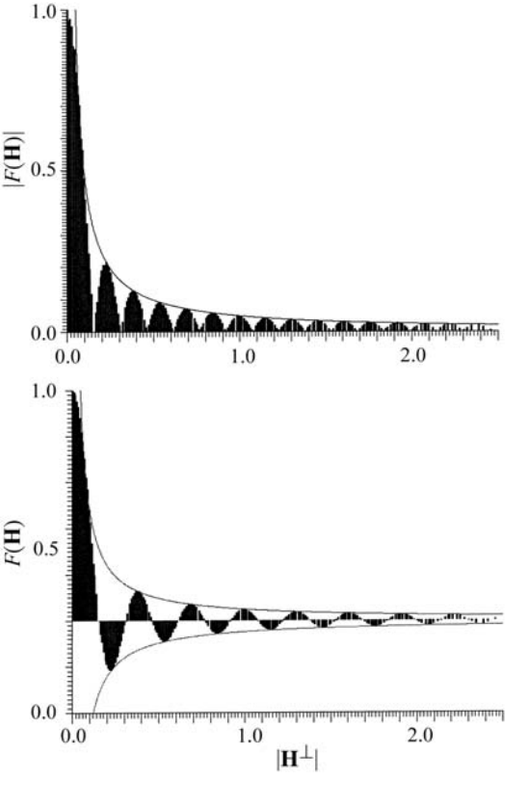

Fig. 4.6.3.6. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of a Fibonacci chain decorated with equal point atoms are shown as a function of the perpendicular-space component $|\mathbf{H}^{\perp}|$ of the diffraction vector. The short distance in the Fibonacci chain is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

The same is valid in the case of the nD description of a quasiperiodic structure. The parallel- and perpendicular-space components are orthogonal to each other and can be separated. In the case of the 1D Fibonacci sequence, the Fourier transform of the parallel-space component of the electron-density distribution of a single atom gives the usual atomic scattering factor $f(\mathbf{H}^{\parallel})$. Parallel to $x^{\perp}$, $\rho(\mathbf{r})$ adopts values $\neq 0$ only within the interval $-(1+\tau)/[2a^*(2+\tau)] \leq x^{\perp} \leq (1+\tau)/[2a^*(2+\tau)]$ and one obtains

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})[a^*(2+\tau)]/(1+\tau) \times \int_{-(1+\tau)/[2a^*(2+\tau)]}^{+(1+\tau)/[2a^*(2+\tau)]} \exp(2\pi i \mathbf{H}^{\perp} \cdot x^{\perp})\, \mathrm{d}x^{\perp}.$$

The factor $[a^*(2+\tau)]/(1+\tau)$ results from the normalization of the structure factors to $F(\mathbf{0}) = f(0)$. With

$$\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^* + h_3\mathbf{d}_3^* + h_4\mathbf{d}_4^* = h_1a_1^*\begin{pmatrix}1\\-\tau\\0\\0\end{pmatrix} + h_2a_1^*\begin{pmatrix}\tau\\1\\0\\0\end{pmatrix} + h_3a_3^*\begin{pmatrix}0\\0\\1\\0\end{pmatrix} + h_4a_4^*\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

and $\mathbf{H}^{\perp} = a_1^*(-\tau h_1 + h_2)$ the integrand can be rewritten as

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})[a^*(2+\tau)]/(1+\tau) \times \int_{-(1+\tau)/[2a^*(2+\tau)]}^{+(1+\tau)/[2a^*(2+\tau)]} \exp[2\pi i(-\tau h_1 + h_2)x^{\perp}]\, \mathrm{d}x^{\perp},$$

yielding

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})(2+\tau)/[2\pi i(-\tau h_1 + h_2)(1+\tau)] \times \exp[2\pi i(-\tau h_1 + h_2)x^{\perp}]\Big|_{-(1+\tau)/[2a^*(2+\tau)]}^{+(1+\tau)/[2a^*(2+\tau)]}.$$

Using $\sin x = (\mathrm{e}^{ix} - \mathrm{e}^{-ix})/2i$ gives

$$F(\mathbf{H}) = f(\mathbf{H}^{\parallel})(2+\tau)/[\pi(-\tau h_1 + h_2)(1+\tau)] \times \sin[\pi(1+\tau)(-\tau h_1 + h_2)]/(2+\tau).$$

Thus, the structure factor has the form of the function $\sin(x)/x$ with x a perpendicular reciprocal-space coordinate. The upper and lower limiting curves of this function are given by the hyperbolae $\pm 1/x$ (Fig. 4.6.3.6). The continuous shape of $F(\mathbf{H})$ as a function of $\mathbf{H}^{\perp}$ allows the estimation of an overall temperature factor and atomic scattering factor for reflection-data normalization (compare Figs. 4.6.3.6 and 4.6.3.7).

In the case of a 3D crystal structure which is quasiperiodic in one direction, the structure factor can be written in the form

$$F(\mathbf{H}) = \sum_{k=1}^{n}\big[T_k(\mathbf{H})f_k(\mathbf{H}^{\parallel})g_k(\mathbf{H}^{\perp})\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_k)\big].$$

The sum runs over all n averaged hyperatoms in the 4D unit cell of the structure. The *geometric form factor* $g_k(\mathbf{H}^{\perp})$ corresponds to the Fourier transform of the kth atomic surface,

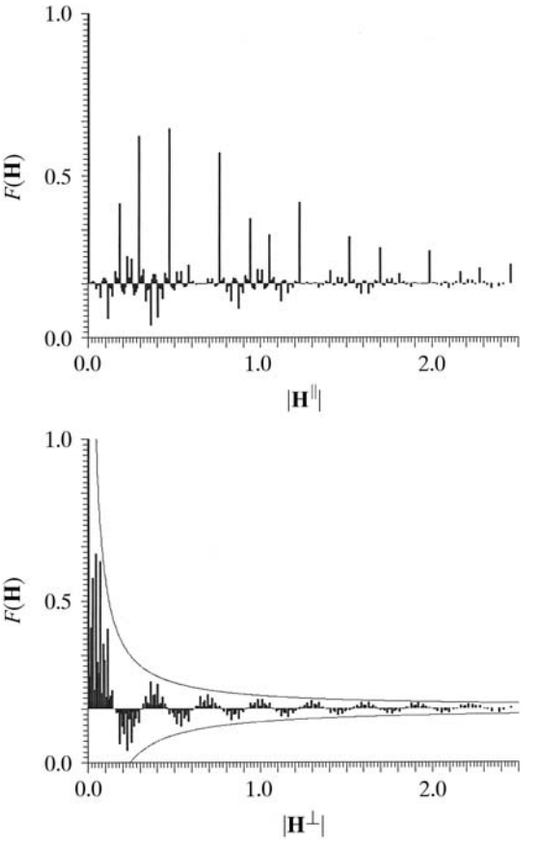

Fig. 4.6.3.7. The structure factors $F(\mathbf{H})$ of the Fibonacci chain decorated with aluminium atoms (U_{overall} = 0.005 Å^2) as a function of the parallel (above) and the perpendicular (below) component of the diffraction vector. The short distance is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

$$g_k(\mathbf{H}^{\perp}) = (1/A_{\mathrm{UC}}^{\perp})\int_{A_k}\exp(2\pi i\mathbf{H}^{\perp}\cdot\mathbf{r}^{\perp})\ \mathrm{d}\mathbf{r}^{\perp},$$

normalized to $A_{\mathrm{UC}}^{\perp}$, the area of the 2D unit cell projected upon $\mathbf{V}^{\perp}$, and A_k, the area of the kth atomic surface.

The atomic temperature factor $T_k(\mathbf{H})$ can also have perpendicular-space components. Assuming only harmonic (static or dynamic) displacements in parallel and perpendicular space one obtains, in analogy to the usual expression (Willis & Pryor, 1975),

$$T_k(\mathbf{H}) = T_k(\mathbf{H}^{\parallel}, \mathbf{H}^{\perp}) = \exp(-2\pi^2\mathbf{H}^{\parallel T}\langle\mathbf{u}_i^{\parallel}\mathbf{u}_j^{\parallel T}\rangle\mathbf{H}^{\parallel})\exp(-2\pi^2\mathbf{H}^{\perp T}\langle\mathbf{u}_i^{\perp}\mathbf{u}_j^{\perp T}\rangle\mathbf{H}^{\perp}),$$

with

$$\langle\mathbf{u}_i^{\parallel}\mathbf{u}_j^{\parallel T}\rangle = \begin{pmatrix}\langle\mathbf{u}_1^{\parallel 2}\rangle & \langle\mathbf{u}_1^{\parallel}\cdot\mathbf{u}_2^{\parallel T}\rangle & \langle\mathbf{u}_1^{\parallel}\cdot\mathbf{u}_3^{\parallel T}\rangle\\ \langle\mathbf{u}_2^{\parallel}\cdot\mathbf{u}_1^{\parallel T}\rangle & \langle\mathbf{u}_2^{\parallel 2}\rangle & \langle\mathbf{u}_2^{\parallel}\cdot\mathbf{u}_3^{\parallel T}\rangle\\ \langle\mathbf{u}_3^{\parallel}\cdot\mathbf{u}_1^{\parallel T}\rangle & \langle\mathbf{u}_3^{\parallel}\cdot\mathbf{u}_2^{\parallel T}\rangle & \langle\mathbf{u}_3^{\parallel 2}\rangle\end{pmatrix}$$

and $\langle\mathbf{u}_i^{\perp}\mathbf{u}_j^{\perp T}\rangle = \langle\mathbf{u}_4^{\perp}\rangle$.

The elements of the type $\langle\mathbf{u}_i\cdot\mathbf{u}_j^T\rangle$ represent the average values of the atomic displacements along the ith axis times the displacement along the jth axis on the V basis.

4.6.3.3.1.4. Intensity statistics

In the following, only the properties of the quasiperiodic component of the 3D structure, namely the Fourier module M_1^*,

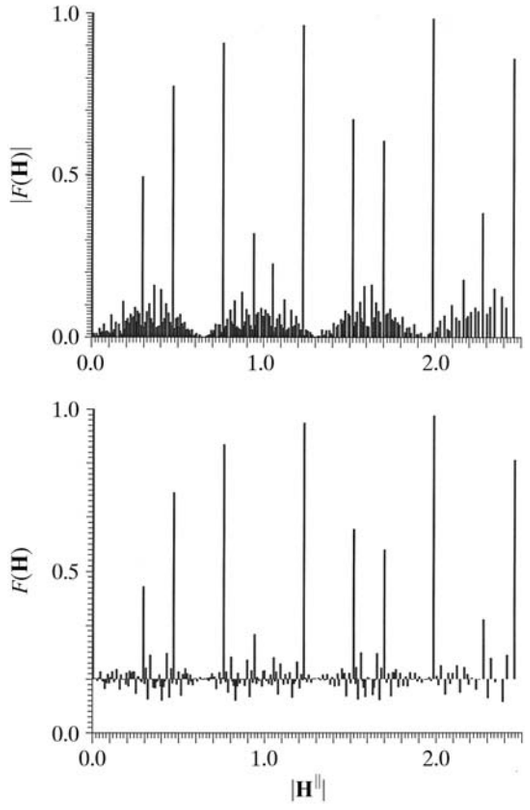

Fig. 4.6.3.8. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of the squared Fibonacci chain decorated with equal point atoms are shown as a function of the parallel-space component $|\mathbf{H}^{\parallel}|$ of the diffraction vector. The short distance is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

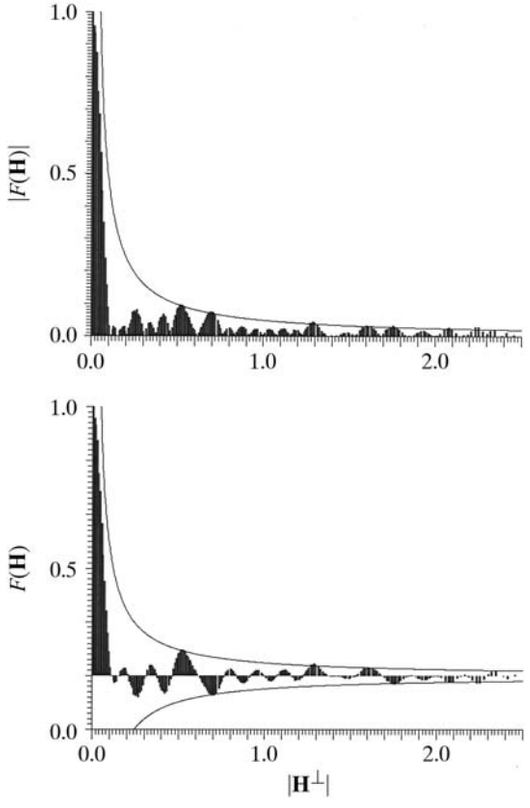

Fig. 4.6.3.9. The structure factors $F(\mathbf{H})$ (below) and their magnitudes $|F(\mathbf{H})|$ (above) of the squared Fibonacci chain decorated with equal point atoms are shown as a function of the perpendicular-space component $|\mathbf{H}^{\perp}|$ of the diffraction vector. The short distance is S = 2.5 Å, all structure factors within $0 \leq |\mathbf{H}| \leq 2.5$ Å^{-1} have been calculated and normalized to $F(00) = 1$.

are discussed. The intensities $I(\mathbf{H})$ of the Fibonacci chain decorated with point atoms are only a function of the perpendicular-space component of the diffraction vector. $|F(\mathbf{H})|$ and $F(\mathbf{H})$ are illustrated in Figs. 4.6.3.5 and 4.6.3.6 as a function of $\mathbf{H}^{\parallel}$ and of $\mathbf{H}^{\perp}$. The distribution of $|F(\mathbf{H})|$ as a function of their frequencies clearly resembles a centric distribution, as can be expected from the centrosymmetric 2D subunit cell. The shape of the distribution function depends on the radius $H_{\max}$ of the limiting sphere in reciprocal space. The number of weak reflections increases with the square of $H_{\max}$, that of strong reflections only linearly (strong reflections always have small $\mathbf{H}^{\perp}$ components).

The weighted reciprocal space of the Fibonacci sequence contains an infinite number of Bragg reflections within a limited region of the physical space. Contrary to the diffraction pattern of a periodic structure consisting of point atoms on the lattice nodes, the Bragg reflections show intensities depending on the perpendicular-space components of their diffraction vectors.

The reciprocal space of a sequence generated from hyperatoms with fractally shaped atomic surfaces (squared Fibonacci sequence) is very similar to that of the Fibonacci sequence (Figs. 4.6.3.8 and 4.6.3.9). However, there are significantly more weak reflections in the diffraction pattern of the 'fractal' sequence, caused by the geometric form factor.

4.6.3.3.1.5. Relationships between structure factors at symmetry-related points of the Fourier image

The two possible point-symmetry groups in the 1D quasiperiodic case, $K^{1D} = 1$ and $K^{1D} = \bar{1}$, relate the structure factors to

$$1: \qquad F(\mathbf{H}) = -F(\bar{\mathbf{H}}),$$
$$\bar{1}: \qquad F(\mathbf{H}) = F(\bar{\mathbf{H}}).$$

A 3D structure with 1D quasiperiodicity results from the stacking of atomic layers with distances following a quasiperiodic sequence. The point groups K^{3D} describing the symmetry of such structures result from the direct product $K^{3D} = K^{2D} \otimes K^{1D}$. K^{2D} corresponds to one of the ten crystallographic 2D point groups, K^{1D} can be $\{1\}$ or $\{1, m\}$. Consequently, 18 3D point groups are possible.

Since 1D quasiperiodic sequences can be described generically as incommensurately modulated structures, their possible point and space groups are equivalent to a subset of the (3 + 1)D superspace groups for IMSs with satellite vectors of the type (00γ), *i.e.* $\mathbf{q} = \gamma\mathbf{c}^*$, for the quasiperiodic direction [001] (Janssen *et al.*, 2004).

From the scaling properties of the Fibonacci sequence, some relationships between structure factors can be derived. Scaling the physical-space structure by a factor τ^n, $n \in \mathbb{Z}$, corresponds to a scaling of the perpendicular space by the inverse factor $(-\tau)^{-n}$. For the scaling of the corresponding reciprocal subspaces, the inverse factors compared to the direct spaces have to be applied.

The set of vectors $\mathbf{r}$, defining the vertices of a Fibonacci sequence $s(\mathbf{r})$, multiplied by a factor τ coincides with a subset of the vectors defining the vertices of the original sequence (Fig. 4.6.3.10). The residual vertices correspond to a particular decoration of the scaled sequence, *i.e.* the sequence $\tau^2 s(\mathbf{r})$. The Fourier transform of the sequence $s(\mathbf{r})$ then can be written as the sum of the Fourier transforms of the sequences $\tau s(\mathbf{r})$ and $\tau^2 s(\mathbf{r})$;

$$\sum_k \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_k) = \sum_k \exp(2\pi i \mathbf{H} \tau \mathbf{r}_k) + \sum_k \exp[2\pi i \mathbf{H}(\tau^2 \mathbf{r}_k + \tau)].$$

In terms of structure factors, this can be reformulated as

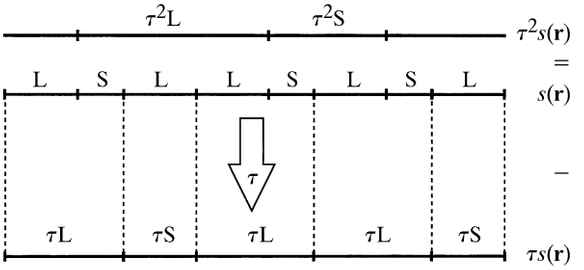

Fig. 4.6.3.10. Part ... LSLLSLSL ... of a Fibonacci sequence $s(\mathbf{r})$ before and after scaling by the factor τ. L is mapped onto τL, S onto τS = L. The vertices of the new sequence are a subset of those of the original sequence (the correspondence is indicated by dashed lines). The residual vertices $\tau^2 s(\mathbf{r})$, which give when decorating $\tau s(\mathbf{r})$ the Fibonacci sequence $s(\mathbf{r})$, form a Fibonacci sequence scaled by a factor τ^2.

$$F(\mathbf{H}) = F(\tau\mathbf{H}) + \exp(2\pi i\tau\mathbf{H})F(\tau^2\mathbf{H}).$$

Hence, phases of structure factors that are related by scaling symmetry can be determined from each other.

Further scaling relationships in reciprocal space exist: scaling a diffraction vector

$$\mathbf{H} = h_1\mathbf{d}_1^* + h_2\mathbf{d}_2^* = h_1 a^* \begin{pmatrix} 1 \\ -\tau \end{pmatrix}_V + h_2 a^* \begin{pmatrix} \tau \\ 1 \end{pmatrix}_V$$

with the matrix

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

$$\begin{aligned} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}_D &= \begin{pmatrix} F_n & F_{n+1} \\ F_{n+1} & F_{n+2} \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}_D \\ &= \begin{pmatrix} F_n h_1 + F_{n+1} h_2 \\ F_{n+1} h_1 + F_{n+2} h_2 \end{pmatrix}_D, \end{aligned}$$

increases the magnitudes of structure factors assigned to this particular diffraction vector $\mathbf{H}$,

$$\left|F(S^n\mathbf{H})\right| > \left|F(S^{n-1}\mathbf{H})\right| > \ldots > \left|F(S\mathbf{H})\right| > \left|F(\mathbf{H})\right|.$$

This is due to the shrinking of the perpendicular-space component of the diffraction vector by powers of $(-\tau)^{-n}$ while expanding the parallel-space component by τ^n according to the eigenvalues τ and $-\tau^{-1}$ of S acting in the two eigenspaces $\mathbf{V}^{\parallel}$ and $\mathbf{V}^{\perp}$:

$$\begin{aligned} \pi^{\parallel}(S\mathbf{H}) &= (h_2 + \tau(h_1 + h_2))a^* = (\tau h_1 + h_2(\tau + 1))a^* \\ &= \tau(h_1 + \tau h_2)a^*, \\ \pi^{\perp}(S\mathbf{H}) &= (-\tau h_2 + h_1 + h_2)a^* = (h_1 - h_2(\tau - 1))a^* \\ &= -(1/\tau)(-\tau h_1 + h_2)a^*, \\ \left|F(\tau^n\mathbf{H}^{\parallel})\right| &> \left|F(\tau^{n-1}\mathbf{H}^{\parallel})\right| > \ldots > \left|F(\tau\mathbf{H}^{\parallel})\right| > \left|F(\mathbf{H}^{\parallel})\right|. \end{aligned}$$

Thus, for scaling n times we obtain

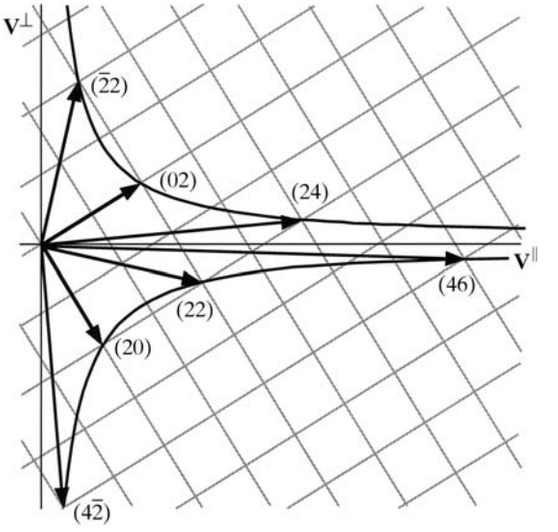

Fig. 4.6.3.11. Scaling operations of the Fibonacci sequence. The scaling operation S acts six times on the diffraction vector $\mathbf{H} = (4\bar{2})$ yielding the sequence $(4\bar{2}) \rightarrow (\bar{2}2) \rightarrow (20) \rightarrow (02) \rightarrow (22) \rightarrow (24) \rightarrow (46)$.

$$\begin{aligned} \pi^{\perp}(S^n\mathbf{H}) &= \left(-\tau\left(F_n h_1 + F_{n+1} h_2\right) + \left(F_{n+1} h_1 + F_{n+2} h_2\right)\right)a^* \\ &= \left(h_1\left(-\tau F_n + F_{n+1}\right) + h_2\left(-\tau F_{n+1} + F_{n+2}\right)\right)a^* \end{aligned}$$

with

$$\lim_{n\to\infty}\left(-\tau F_n + F_{n+1}\right) = 0 \text{ and } \lim_{n\to\infty}\left(-\tau F_{n+1} + F_{n+2}\right) = 0,$$

yielding eventually

$$\lim_{n\to\infty}\left(\pi^{\perp}(S^n\mathbf{H})\right) = 0 \text{ and } \lim_{n\to\infty}\left(F(S^n\mathbf{H})\right) = F(\mathbf{0}).$$

The scaling of the diffraction vectors $\mathbf{H}$ by S^n corresponds to a hyperbolic rotation (Janner, 1992) with angle $n\varphi$, where $\sinh\varphi = 1/2$ (Fig. 4.6.3.11):

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}^{2n} = \begin{pmatrix} \cosh 2n\varphi & \sinh 2n\varphi \\ \sinh 2n\varphi & \cosh 2n\varphi \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}^{2n+1} = \begin{pmatrix} \sinh[(2n+1)\varphi] & \cosh[(2n+1)\varphi] \\ \cosh[(2n+1)\varphi] & \sinh[(2n+1)\varphi] \end{pmatrix}.$$

4.6.3.3.2. Decagonal phases

A structure quasiperiodic in two dimensions, periodic in the third dimension and with decagonal diffraction symmetry is called a decagonal phase. Its holohedral Laue symmetry group is $K = 10/mmm$. All reciprocal-space vectors $\mathbf{H} \in M^*$ can be represented on a basis (V basis) $\mathbf{a}_i^* = a_i^*(\cos 2\pi i/5, \sin 2\pi i/5, 0)$, $i = 1, \ldots, 4$ and $\mathbf{a}_5^* = a_5^*(0, 0, 1)$ (Fig. 4.6.3.12) as $\mathbf{H} = \sum_{i=1}^{5} h_i\mathbf{a}_i^*$. The vector components refer to a Cartesian coordinate system in physical (parallel) space. Thus, from the number of independent reciprocal-basis vectors necessary to index the Bragg reflections with integer numbers, the dimension of the embedding space has to be at least five. This can also be shown in a different way (Hermann, 1949).

The set M^* of all vectors $\mathbf{H}$ remains invariant under the action of the symmetry operators of the point group $10/mmm$. The symmetry-adapted matrix representations for the point-group