

## 4. DIFFUSE SCATTERING AND RELATED TOPICS

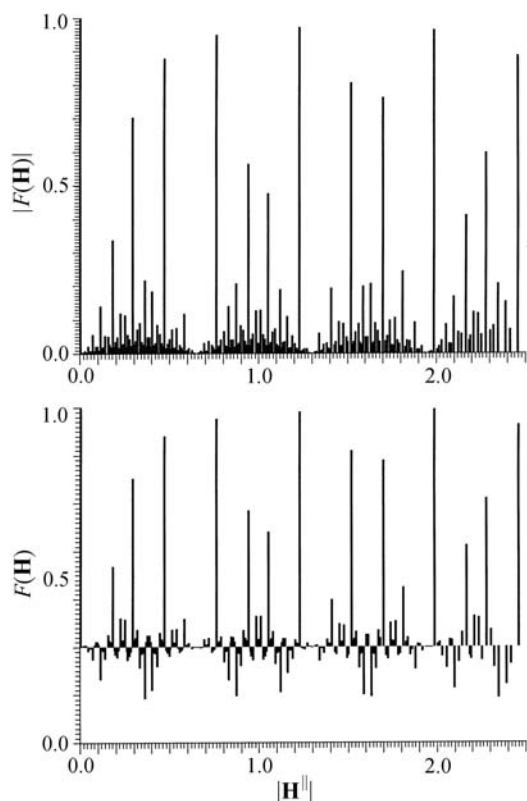


Fig. 4.6.3.5. The structure factors  $F(\mathbf{H})$  (below) and their magnitudes  $|F(\mathbf{H})|$  (above) of a Fibonacci chain decorated with equal point atoms are shown as a function of the parallel-space component  $|\mathbf{H}^{\parallel}|$  of the diffraction vector. The short distance in the Fibonacci chain is  $S = 2.5 \text{ \AA}$ , all structure factors within  $0 \leq |\mathbf{H}| \leq 2.5 \text{ \AA}^{-1}$  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  $\tau$ .
- (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  $K^{3D} = K^{2D} \otimes K^{1D} \otimes 1$ .  $K^{2D}$  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  $s = \{\dots, S^{-1}, S^0, S^1, \dots\}$  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):

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

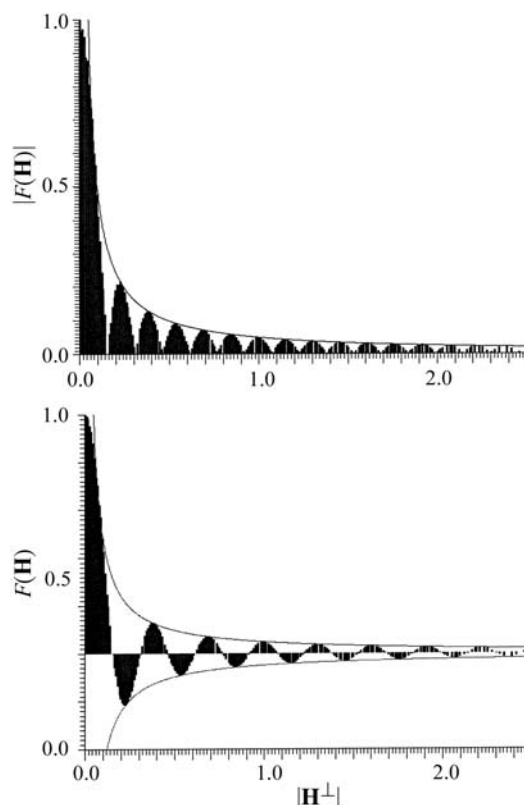


Fig. 4.6.3.6. The structure factors  $F(\mathbf{H})$  (below) and their magnitudes  $|F(\mathbf{H})|$  (above) of a Fibonacci chain decorated with equal point atoms are shown as a function of the perpendicular-space component  $|\mathbf{H}^{\perp}|$  of the diffraction vector. The short distance in the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