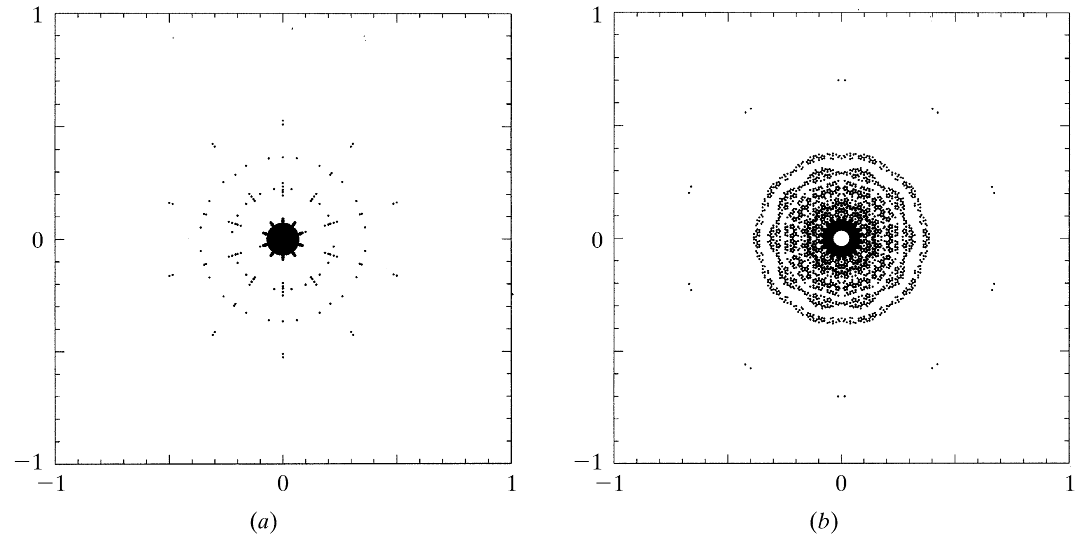

Fig. 4.6.3.37. Perpendicular-space distribution of (*a*) positive and (*b*) negative structure factors of the 3D Penrose tiling of the 6D *P* lattice type decorated with point atoms (edge lengths of the Penrose unit rhombohedra $a_r = 5.0$ Å). The magnitudes of the structure factors are indicated by the diameters of the filled circles. All reflections are shown within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \leq h_i \leq 6, i = 1, \ldots, 6$.

4.6.4. Experimental aspects of the reciprocal-space analysis of aperiodic crystals

4.6.4.1. *Data-collection strategies*

Theoretically, aperiodic crystals show an infinite number of reflections within a given diffraction angle, contrary to periodic crystals. The number of reflections to be included in a structure analysis of a *periodic* crystal may be very high (one million for virus crystals, for instance) but there is no ambiguity in the selection of reflections to be collected: all Bragg reflections within a limiting sphere in reciprocal space, usually given by $0 \leq \sin\theta/\lambda \leq 0.7$ Å^{-1}, are used. All reflections, observed and unobserved, are included to fit a reliable structure model.

However, for *aperiodic* crystals it is not possible to collect the infinite number of dense Bragg reflections within $0 \leq \sin\theta/\lambda \leq 0.7$ Å^{-1}. The number of observable reflections within this limiting sphere depends only on the spatial and intensity resolution.

What happens if not all reflections are included in a structure analysis? How important is the contribution of reflections with large perpendicular-space components of the diffraction vector which are weak but densely distributed? These problems are illustrated using the example of the Fibonacci sequence. An infinite model structure consisting of Al atoms with isotropic thermal parameter $B = 1$ Å^2, and distances S = 2.5 Å and L = τ S, was used for the calculations (Table 4.6.4.1).

It turns out that 92.6% of the total diffracted intensity of 161 322 reflections is included in the 44 strongest reflections and 99.2% in the strongest 425 reflections. It is remarkable, however, that in all the experimental data for icosahedral and decagonal quasicrystals collected so far, rarely more than 20 to 50 reflections along reciprocal-lattice lines corresponding to net planes with Fibonacci-

Table 4.6.4.1. *Intensity statistics of the Fibonacci chain for a total of 161 322 reflections with* $-1000 \leq h_i \leq 1000$ *and* $0 \leq \sin\theta/\lambda \leq 2$ Å^{-1}

In the upper line, the number of reflections in the respective interval is given; in the lower line the partial sums $\sum I(\mathbf{H})$ of the intensities $I(\mathbf{H})$ are given as a percentage of the total diffracted intensity. The $F(00)$ reflection is not included in the sums.

	$F(\mathbf{H})/F(\mathbf{H})_{\max} \geq 0.1$	$0.1 > F(\mathbf{H})/F(\mathbf{H})_{\max} \geq 0.01$	$0.01 > F(\mathbf{H})/F(\mathbf{H})_{\max} \geq 0.001$	$F(\mathbf{H})/F(\mathbf{H})_{\max} < 0.001$
$0 \leq \sin\theta/\lambda \leq 0.2$ Å^{-1}	17	148	1505	14 511
$\sum I(\mathbf{H})$	52.53%	2.56%	0.27%	0.03%
$0.2 \leq \sin\theta/\lambda \leq 0.4$ Å^{-1}	11	107	1066	14 998
$\sum I(\mathbf{H})$	27.03%	2.03%	0.19%	0.02%
$0.4 \leq \sin\theta/\lambda \leq 0.6$ Å^{-1}	9	64	654	15 456
$\sum I(\mathbf{H})$	9.84%	0.96%	0.12%	0.01%
$0.6 \leq \sin\theta/\lambda \leq 0.8$ Å^{-1}	6	27	326	15 823
$\sum I(\mathbf{H})$	2.94%	0.34%	0.07%	0.01%
$0.8 \leq \sin\theta/\lambda \leq 2$ Å^{-1}	1	35	338	96 720
$\sum I(\mathbf{H})$	0.23%	0.79%	0.06%	0.01%
Total sum	44	381	3389	157 508
	92.57%	6.67%	0.70%	0.06%

references