accurately located at the reciprocal-lattice nodes. Diffuse diffraction phenomena are mostly neglected. This extrapolation to the existence of an ideal crystal is generally out of the question even if samples of very poor quality (high mosaicity, microdomain structure, defects, ...) are investigated.

The same practice is convenient for the determination of real aperiodic structures once the type of idealized aperiodic ordering is 'known'. Again, the global ordering principle is taken as a hard constraint. For instance, the question of whether a structure is commensurately or incommensurately modulated can only be answered within a given experimental resolution. Experimentally, the ratio of the wavelength of a modulation to the period of the underlying lattice can always be determined as a rational number only. Saying that a structure is incommensurately modulated, with the above ratio being an irrational number, simply means that the experimental results can be better understood, modelled and interpreted assuming an incommensurate modulation. For example, an incommensurate charge-density wave can be moved through an ideal crystal without changing the energy of the crystal. This is not so for a commensurate modulation. In some cases, the modulation period changes with temperature in discrete steps ('devil's staircase'), generating a series of commensurate superstructures ('lock-in structures'); in other cases, a continuous variation can be observed within the experimental resolution. The latter case will be described best by an incommensurately modulated structure.

However, if only the local structure of an aperiodic crystal is of interest, a structure analysis does not take much more experimental effort than for a regular crystal. In contrast, for the analysis of the global structure, *i.e.* the characterization of the type of its 'aperiodicity', diffraction experiments with the highest possible resolution are essential. Some problems connected with the structure analysis of aperiodic crystals are dealt with in Section 4.6.4.

To determine the long-range order – whether a real 'quasicrystal' is perfectly quasiperiodic, on average quasiperiodic, a crystalline approximant or a nanodomain structure – requires information from experiments that are sensitive to changes of the global structure. Hence, one needs diffraction experiments that allow the accurate determination of the spatial intensity distribution. Consequently, the limiting factors for such experiments are the maximum spatial and intensity resolution of the diffraction and detection equipment, as well as the size and quality of the sample. Nevertheless, the resolution available on state-of-the-art standard synchrotron-beamline equipment is sufficient to test whether the ordering of atoms in an aperiodic crystal reaches the same degree of perfection as found in high-quality silicon. Of course, the higher the sample quality the more necessary it is to account for dynamical diffraction effects such as reflection broadening and displacement. Otherwise, a misinterpretation may bias the global structure modelling.

The following sections present an aid to the characterization of aperiodic crystals based on information from diffraction experiments and give a survey of aperiodic crystals from the viewpoint of the experimentally accessible reciprocal space. Characteristic features of the diffraction patterns of the different types of aperiodic crystals are shown. A standard way of determining the metrics and finding the optimum nD embedding is described. Structure-factor formulae for general and special cases are given.

4.6.2. The n-dimensional description of aperiodic crystals

4.6.2.1. Basic concepts

An incommensurate modulation of a lattice-periodic structure destroys its translational symmetry in direct and reciprocal space. In the early seventies, a method was suggested by de Wolff (1974) for restoring the lost lattice symmetry by considering the diffraction pattern of an *incommensurately modulated structure* (IMS) as a projection of an nD reciprocal lattice upon the physical space. n, the dimension of the superspace, is always larger than or equal to d, the dimension of the physical space. This leads to a simple method for the description and characterization of IMSs as well as a variety of new possibilities in their structure analysis. The nD *embedding method* is well established today and can be applied to all aperiodic crystals with reciprocal-space structure equivalent to a $\mathbb{Z}$ module with finite rank n (Janssen, 1988). The dimension of the embedding space is determined by the rank of the $\mathbb{Z}$ module, *i.e.* by the number of reciprocal-basis vectors necessary to allow for indexing all Bragg reflections with integer numbers. The point symmetry of the 3D reciprocal space (Fourier spectrum) constrains the point symmetry of the nD reciprocal lattice and restricts the number of possible nD symmetry groups.

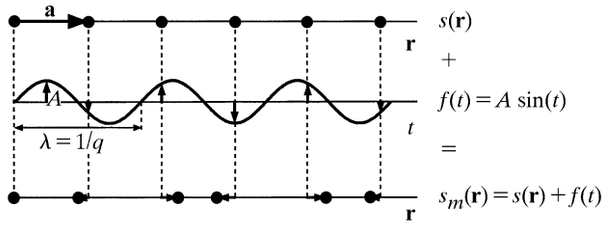

Fig. 4.6.2.1. The combination of a basic structure $s(\mathbf{r})$, with period a, and a sinusoidal modulation function $f(t)$, with amplitude A, period λ and $t = \mathbf{q} \cdot \mathbf{r}$, gives a modulated structure (MS) $s_m(\mathbf{r})$. The MS is aperiodic if a and λ are on incommensurate length scales. The filled circles represent atoms.

In the following sections, the nD descriptions of the four main classes of aperiodic crystals are demonstrated on simple 1D examples of incommensurately modulated phases, composite crystals, quasicrystals and structures with fractally shaped atomic surfaces. The main emphasis is placed on quasicrystals that show scaling symmetry, a new and unusual property in structural crystallography. A detailed discussion of the different types of 3D aperiodic crystals follows in Section 4.6.3.

4.6.2.2. 1D incommensurately modulated structures

A periodic deviation of atomic parameters from a reference structure (*basic structure*, BS) is called a *modulated structure* (MS). In the case of mutual incommensurability of the basic structure and the modulation period, the structure is called incommensurately modulated. Otherwise, it is called commensurately modulated. The modulated atomic parameters may be one or several of the following:

(a) coordinates,
(b) occupancy factors,
(c) thermal displacement parameters,
(d) orientation of the magnetic moment.

An incommensurately modulated structure can be described in a dual way by its *basic structure* $s(\mathbf{r})$ and a *modulation function* $f(t)$. This allows the structure-factor formula to be calculated and a full symmetry characterization employing representation theory to be performed (de Wolff, 1984). A more general method is the nD description: it relates the dD aperiodic incommensurately modulated structure to a periodic structure in nD space. This simplifies the symmetry analysis and structure-factor calculation, and allows more powerful structure-determination techniques.

The nD embedding method is demonstrated in the following 1D example of a displacively modulated structure. A basic structure $s(\mathbf{r}) = s(\mathbf{r} + n\mathbf{a})$, with period a and $n \in \mathbb{Z}$, is modulated by a function $f(t) = f(\mathbf{q} \cdot \mathbf{r}) = f(\alpha r) = f[\alpha r + (n a/\alpha)]$, with the satellite vector $\mathbf{q} = \alpha \mathbf{a}^*$, period $\lambda = 1/q = a/\alpha$, and α a rational or irrational number yielding a commensurately or incommensurately modulated structure $s_m(\mathbf{r})$ (Fig. 4.6.2.1).

If the 1D IMS and its 1D modulation function are properly combined in a 2D parameter space $\mathbf{V} = (\mathbf{V}^{\parallel}, \mathbf{V}^{\perp})$, a 2D lattice-

references