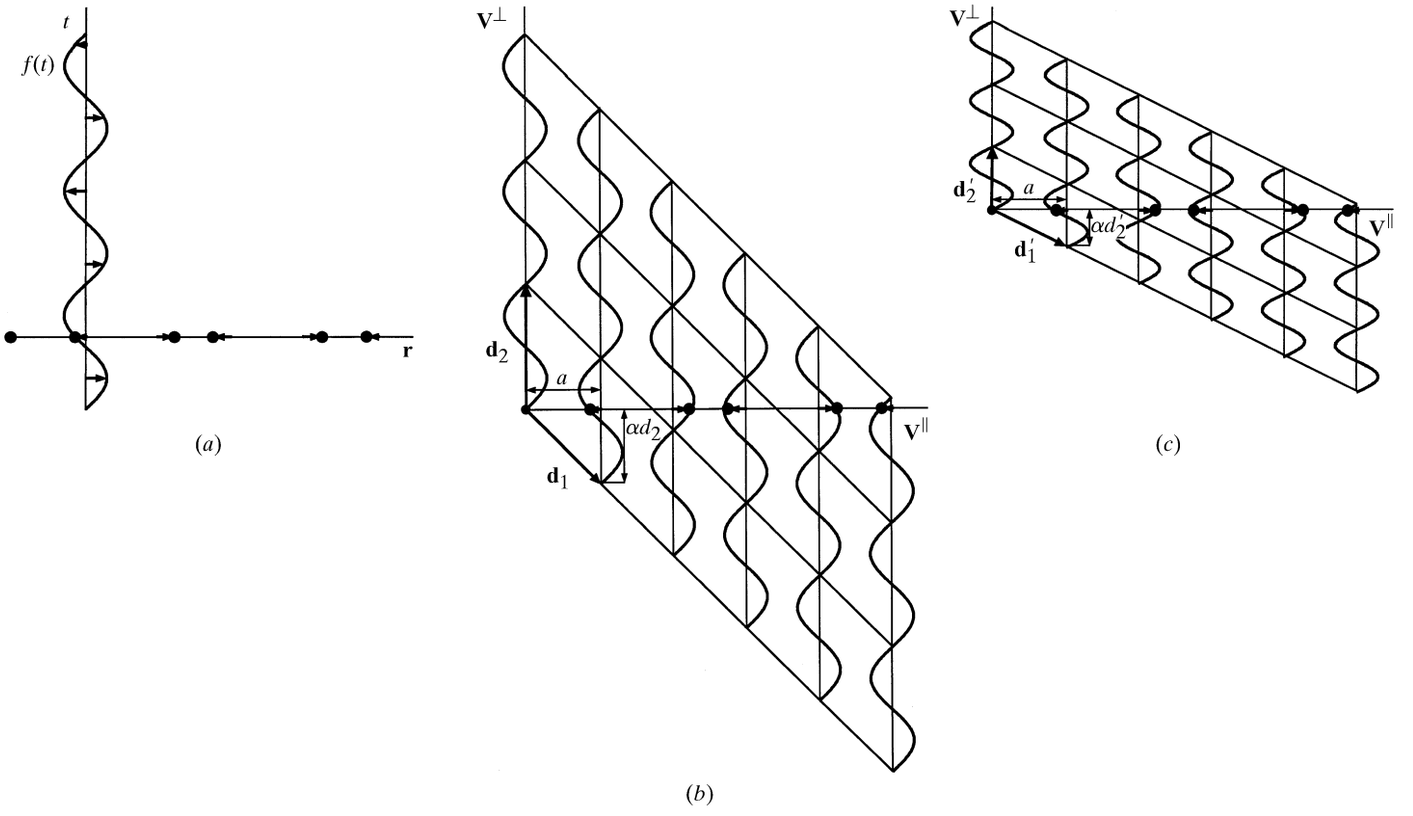

Fig. 4.6.2.2. 2D embedding of the sinusoidally modulated structure illustrated in Fig. 4.6.2.1. The correspondence between the actual displacement of an atom in the 1D structure and the modulation function defined in one additional dimension is illustrated in part (*a*). Adding to each atom its modulation function in this orthogonal dimension (perpendicular space $\mathbf{V}^{\perp}$) yields a periodic arrangement in 2D space $\mathbf{V}$, part (*b*). The MS results as a special section of the 2D periodic structure along the parallel space $\mathbf{V}^{\parallel}$. It is obvious from a comparison of (*b*) and (*c*) that the actual MS is independent of the perpendicular-space scale.

periodic structure results (Fig. 4.6.2.2). The actual atoms are generated by the intersection of the 1D physical (external, parallel) space $\mathbf{V}^{\parallel}$ with the continuous *hyperatoms*. The hyperatoms have the shape of the modulation function along the perpendicular (internal, complementary) space $\mathbf{V}^{\perp}$. They result from a convolution of the physical-space atoms with their modulation functions.

A basis $\mathbf{d}_1, \mathbf{d}_2$ (D basis) of the 2D hyperlattice $\Sigma = \{\mathbf{r} = \sum_{i=1}^{2} n_i \mathbf{d}_i | n_i \in \mathbb{Z}\}$ is given by

$$\mathbf{d}_1 = \begin{pmatrix} a \\ -\alpha/c \end{pmatrix}_V, \mathbf{d}_2 = \begin{pmatrix} 0 \\ 1/c \end{pmatrix}_V,$$

where a is the translation period of the BS and c is an arbitrary constant. The components of the basis vectors are given on a 2D orthogonal coordinate system (V basis). The components of the basis vector $\mathbf{d}_1$ are simply the parallel-space period a of the BS and α times the perpendicular-space component of the basis vector $\mathbf{d}_2$. The vector $\mathbf{d}_2$ is always parallel to the perpendicular space and its length is one period of the modulation function in arbitrary units (this is expressed by the arbitrary factor $1/c$). An atom at position $\mathbf{r}$ of the BS is displaced by an amount given by the modulation function $f(t)$, with $f(t) = f(\mathbf{q} \cdot \mathbf{r})$. Hence, the perpendicular-space variable t has to adopt the value $\mathbf{q} \cdot \mathbf{r} = \alpha \mathbf{a}^* \cdot r\mathbf{a} = \alpha r$ for the physical-space variable $\mathbf{r}$. This can be achieved by assigning the slope α to the basis vector $\mathbf{d}_1$. The choice of the parameter c has no influence on the actual MS, *i.e.* the way in which the 2D structure is cut by the parallel space (Fig. 4.6.2.2*c*).

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

$$\mathbf{d}_1^* = \begin{pmatrix} a^* \\ 0 \end{pmatrix}_V, \mathbf{d}_2^* = \begin{pmatrix} \alpha a^* \\ c \end{pmatrix}_V,$$

with $a^* = 1/a$. The metric tensors for the reciprocal and direct 2D lattices for $c = 1$ are

$$G^* = \begin{pmatrix} a^{*2} & \alpha a^{*2} \\ \alpha a^{*2} & 1 + \alpha^2 a^{*2} \end{pmatrix} \quad \text{and} \quad G = \begin{pmatrix} a^2 + \alpha^2 & -\alpha \\ -\alpha & 1 \end{pmatrix}.$$

The choice of an arbitrary number for c has no influence on the metrics of the physical-space components of the IMS in direct or reciprocal space.

The Fourier transform of the *hypercrystal* depicted in Fig. 4.6.2.2 gives the weighted reciprocal lattice shown in Fig. 4.6.2.3. The 1D diffraction pattern $M^* = \{\mathbf{H}^{\parallel} = \sum_{i=1}^{2} h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ in physical space is obtained by a projection of the weighted 2D reciprocal lattice Σ^* along $\mathbf{V}^{\perp}$ as the Fourier transform of a section in direct space corresponds to a projection in reciprocal space and *vice versa*:

$$M^* = \{\mathbf{H}^{\parallel}\} \xleftarrow{\text{projection } \pi^{\parallel} \text{ onto } \mathbf{V}^{\parallel}} \Sigma^* = \{\mathbf{H} = (\mathbf{H}^{\parallel}, \mathbf{H}^{\perp})\}.$$

Reciprocal-lattice points lying in physical space are referred to as *main reflections*, all others as *satellite reflections*. All Bragg reflections can be indexed with integer numbers h_1, h_2 in the 2D description $\mathbf{H} = h_1 \mathbf{d}_1^* + h_2 \mathbf{d}_2^*$. In the physical-space description, the diffraction vector can be written as $\mathbf{H}^{\parallel} = h\mathbf{a}^* + m\mathbf{q} = \mathbf{a}^*(h_1 + \alpha h_2)$, with $\mathbf{q} = \alpha \mathbf{a}^*$ for the satellite vector and $m \in \mathbb{Z}$ the order of the satellite reflection. For a detailed discussion of the