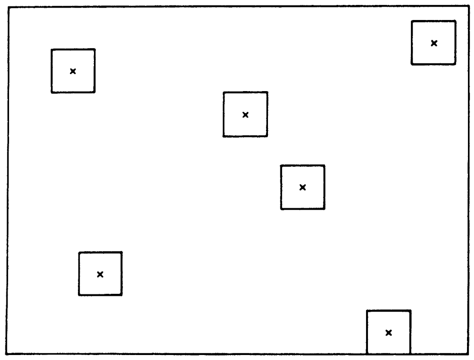

Fig. 4.2.3.1. Model of the two-dimensional distribution of point defects, causing changes in the surroundings.

$$d(\mathbf{r}) = \sum_{\mathbf{m}} \delta(\mathbf{r} - \mathbf{m}),$$

where **m** refers to the centres (crosses in Fig. 4.2.3.1) of the box functions. The problem is therefore defined by:

$$l(\mathbf{r}) * F_1(\mathbf{r}) + [l(\mathbf{r})b(\mathbf{r})] * [F_2(\mathbf{r}) - F_1(\mathbf{r})] * d(\mathbf{r}). \quad (4.2.3.20a)$$

The incorrect addition of $F_1(\mathbf{r})$ to the areas of clusters $F_2(\mathbf{r})$ is compensated by subtracting the same contribution from the second term in equation (4.2.3.20*a*). In order to determine the diffuse scattering the Fourier transformation of (4.2.3.20*a*) is performed:

$$L(\mathbf{H})F_1(\mathbf{H}) + [L(\mathbf{H}) * B(\mathbf{H})][F_2(\mathbf{H}) - F_1(\mathbf{H})]D(\mathbf{H}). \quad (4.2.3.20b)$$

The intensity is given by

$$|L(\mathbf{H})F_1(\mathbf{H}) + [L(\mathbf{H}) * B(\mathbf{H})][F_2(\mathbf{H}) - F_1(\mathbf{H})]D(\mathbf{H})|^2. \quad (4.2.3.20c)$$

Evaluation of equation (4.2.3.20*c*) yields three terms (c.c. means complex conjugate):

(i) $|L(\mathbf{H})F_1(\mathbf{H})|^2$

(ii) $\{[L(\mathbf{H})F_1(\mathbf{H})][L(\mathbf{H}) * B(\mathbf{H})] \times [F_2(\mathbf{H}) - F_1(\mathbf{H})]D(\mathbf{H}) + \text{c.c.}\}$

(iii) $|[L(\mathbf{H}) * B(\mathbf{H})][F_2(\mathbf{H}) - F_1(\mathbf{H})]D(\mathbf{H})|^2$.

The first two terms represent modulated lattices [multiplication of $L(\mathbf{H})$ by $F_1(\mathbf{H})$]. Consequently, they cannot contribute to diffuse scattering which is completely determined by the third term. Fourier transformation of this term gives [$l(\mathbf{r}) = l(-\mathbf{r})$; $b(\mathbf{r}) = b(-\mathbf{r})$; $\Delta F = F_2 - F_1$]:

$$\begin{aligned}&[l(\mathbf{r})b(\mathbf{r})] * \Delta F(\mathbf{r}) * d(\mathbf{r}) * [l(\mathbf{r})b(\mathbf{r})] * \Delta F^+(-\mathbf{r}) * d(-\mathbf{r})\\ &\quad = [l(\mathbf{r})b(\mathbf{r})] * [l(\mathbf{r})b(\mathbf{r})] * \Delta F(\mathbf{r}) * \Delta F^+(-\mathbf{r}) * d(\mathbf{r}) * d(-\mathbf{r})\\ &\quad = [l(\mathbf{r})t(\mathbf{r})] * \Delta F(\mathbf{r}) * \Delta F^+(-\mathbf{r}) * d(\mathbf{r}) * d(-\mathbf{r}). \quad (4.2.3.21a)\end{aligned}$$

According to equation (4.2.3.15) and its subsequent discussion the convolution of the two expressions in square brackets was replaced by $l(\mathbf{r})t(\mathbf{r})$, where $t(\mathbf{r})$ represents the 'pyramid' of *n*-fold height discussed above and *n* is the number of unit cells within $b(\mathbf{r})$. $d(\mathbf{r}) * d(-\mathbf{r})$ is the Patterson function of the distribution function $d(\mathbf{r})$. Its usefulness may be recognized by considering the two possible extreme solutions, namely the random and the strictly periodic distribution.

If no fluctuations of domain sizes are admitted the minimum distance between two neighbouring domains is equal to the length of the domain in the corresponding direction. This means that the distribution function cannot be completely random. In one dimension the solution of a random distribution of particles of a given size on a finite length shows that the distribution functions exhibit periodicities depending on the average free volume of one particle (Zernike & Prins, 1927). Although the problem is more complicated in three dimensions, there should be no fundamental difference in the exact solutions.

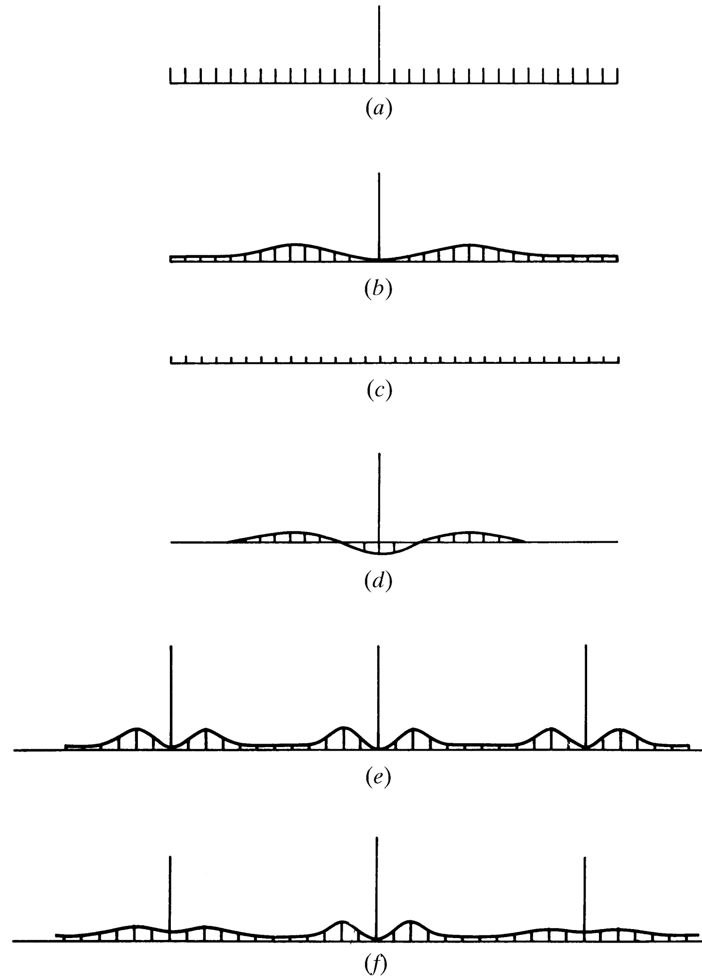

Fig. 4.2.3.2. One-dimensional Patterson functions of various point-defect distributions: (*a*) random distribution; (*b*) influence of finite volume of defects on the distribution function; (*c*), (*d*) decomposition of (*b*) into a periodic (*c*) and a convergent (*d*) part; (*e*) Fourier transform of (*c*) + (*d*); (*f*) changes of (*e*), if the centres of the defects show major deviations from the origins of the lattice.

On the other hand, it may be shown that the convolution of a pseudo-random distribution may be obtained if the average free volume is large. This is shown in Fig. 4.2.3.2(*a*) for the particular case of a cluster smaller than one unit cell. A strictly periodic distribution function (superstructure) may result, however, if the volume of the domain and the average free volume are equal. Obviously, the practical solution for the self-convolution of the distribution function (= Patterson function) lies somewhere in between, as shown in Fig. 4.2.3.2(*b*). If a harmonic periodicity damped by a Gaussian is assumed, this self-convolution of the distribution in real space may be considered to consist of two parts, as shown in Figs. 4.2.3.2(*c*), (*d*). Note that the two different solutions result in completely different diffraction patterns:

(i) The geometrically perfect lattice extends to distances which are large when compared with the correlation length of the distribution function. Then the Patterson function of the distribution function concentrates at the positions of the basic lattice, which is

references