the intensities of satellites. Since this position determines the origin of the unit cells in the sublattice, we have to choose this origin for the calculation of $F(\mathbf{H})$ and $\Delta F(\mathbf{H})$. This involves phase factors which are meaningless for integral values of $\mathbf{H}$, (i) if the average $\langle F(\mathbf{H})\rangle$ refers to different structures with arbitrary origin, or (ii), which is important for practical cases, where no change occurs in the origin of related structures for neighbouring domains which are bound to an origin by general convention (*e.g.* a centre of symmetry). This statement is no longer true for non-integral values of $\mathbf{H}$ which are needed for the calculation of intensities of satellites. The intensities of satellites become different for different positions of the interface, even in the absence of a relative displacement between neighbouring domains with respect to an origin by convention. This statement may be extended to non-periodic distribution functions. Consequently, one may conclude that the study of diffuse scattering yields information on the interfacial scattering. For slightly different structures at the interface two cases are important:

(i) the two structures are related by symmetry (*e.g.* by a twin law); and

(ii) the difference between the two structures cannot be described by a symmetry operation.

In structures based on the same sublattice, the first case seems to be more important, because two different structures with the same sublattice are improbable. In the first case there is an identical sublattice if the symmetry operation in question does not influence the plane of intergrowth, *e.g.* a mirror plane should coincide with the plane of intergrowth. Since we have two inequivalent mirror planes in any sublattice, there are two such planes. It is assumed that no more than one unit cell of both domains at the interface has a slightly different structure without any change of geometry of the unit cell, and the number of unit cells is equal because of the equivalence of both domain structures (twins). Fig. 4.2.3.4(*a*) shows a picture of this model; Figs. 4.2.3.4(*b*), (*c*) explain that this structure may be described by two contributions:

(i) The first term is already given by equation (4.2.3.23) for $N_1 = N_2$, consequently odd orders of satellites only are observed.

(ii) The second term may be described by a superlattice containing $2N_1$ cells with an alternating arrangement of interfaces, correlated by the relevant plane of symmetry.

In real space the second term may be constructed by convolution of the one-dimensional superlattice with two difference structures displaced by $\mp N_1/2$ units of the sublattice; its Fourier transformation yields

$$L_s(\mathbf{H})\{\Delta F_i(\mathbf{H})\exp\{2\pi i N_1 H/2\} + \Delta F_i'(\mathbf{H})\exp\{-2\pi i N_1 H/2\}\}, \qquad (4.2.3.24)$$

where $\Delta F_i, \Delta F_i'$ correspond to the Fourier transforms of the contributions shown in Fig. 4.2.3.4(*c*). Since $H = \nu/N_1$ there are alternating contributions to the νth satellite, which may be calculated more accurately by taking into account the symmetry operations. The important difference between equations (4.2.3.23) and (4.2.3.24) is the missing decrease in intensity with increasing order of satellites. Consequently one may conclude that the interface contributes to low- and high-order satellites as well, but its influence prevails for high-order satellites. Similar considerations may be made for two- and three-dimensional distributions of domains. A great variety of extinction rules may be found depending on the type of order approximated by the distribution under investigation.

(5) *Two kinds of lamellar domains with variable size distribution*

Obviously the preceding discussion of the diffuse scattering from domains is restricted to more or less small fluctuations of domain sizes. This is specifically valid if the most probable domain size

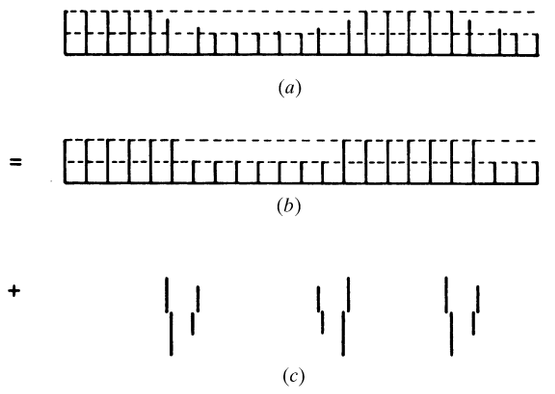

Fig. 4.2.3.4. Influence of distortions at the boundary of domains, and separation into two parts; for discussion see text.

does not differ markedly from the average size. The condition is violated in the case of order–disorder phenomena. It may happen that the smallest ordered area is the most probable one, although the average is considerably larger. This may be shown for a lamellar structure of two types of layers correlated by a (conditional) pair probability $p_{\mu\mu'}(\mathbf{1})$. As shown below, a pair at distance $\mathbf{m}$ occurs with the probability $p_\mu p_{\mu\mu'}(\mathbf{m})$ which may be derived from the pair-probability of nearest neighbours $p_\mu p_{\mu\mu'}(\mathbf{1})$. (In fact only one component of vector $\mathbf{m}$ is relevant in this context.) The problem will be restricted to two kinds of layers $(\mu, \mu' = 1, 2)$. Furthermore, it will be symmetric in the sense that the pair probabilities obey the following rules

$$p_{11}(\mathbf{m}) = p_{22}(\mathbf{m}), \quad p_{12}(\mathbf{m}) = p_{21}(\mathbf{m}). \qquad (4.2.3.25)$$

It may be derived from equation (4.2.3.25) that the *a priori* probabilities p_μ of a single layer are $\frac{1}{2}$ and

$$p_{11}(\mathbf{0}) = p_{22}(\mathbf{0}) = 1, \quad p_{12}(\mathbf{0}) = p_{21}(\mathbf{0}) = 0.$$

With these definitions and the general relation

$$p_{11}(\mathbf{m}) + p_{12}(\mathbf{m}) = p_{22}(\mathbf{m}) + p_{21}(\mathbf{m}) = 1$$

the *a priori* probability of a domain containing m layers of type 1 may be calculated with the aid of $p_{11}(\mathbf{1})$ $[0 \le p_{11}(\mathbf{1}) \le 1]$:

$$p_\mu = \tfrac{1}{2} p_{11}(\mathbf{1})^{m-1}[1 - p_{11}(\mathbf{1})]. \qquad (4.2.3.26)$$

Hence the most probable size of domains is a single layer because a similar relation holds for layers of type 2. Since the average thickness of domains is strongly dependent on $p_{11}(\mathbf{1})$ [infinite for $p_{11}(\mathbf{1}) = 1$, and one layer for $p_{11}(\mathbf{1}) = 0$] it may become very large in the latter case. Consequently there are extremely large fluctuations if $p_{11}(\mathbf{1})$ is small, but different from zero.

It may be concluded from equation (4.2.3.26) that the function $p_{11}(\mathbf{m})$ decreases monotonically with increasing $\mathbf{m}$, approaching $\frac{1}{2}$ with $\mathbf{m} \to \infty$. Apparently this cannot be true for a finite crystal if $p_{11}(\mathbf{m})$ is unity (structure of two types of domains) or zero (superstructure of alternating layers). In either case the crystal should consist of a single domain of type 1 or 2, or one of the possible superstructures 1212 . . ., 2121 . . ., respectively. Hence one has to differentiate between long-range order, where two equivalent solutions have to be considered, and short-range order, where $p_{11}(\mathbf{m})$ approaches the *a priori* probability $\frac{1}{2}$ for large m. This behaviour of $p_{11}(\mathbf{m})$ and $p_{12}(\mathbf{m})$, which may also be expressed by equivalent correlation functions, is shown in Figs. 4.2.3.5(*a*) (short-range order) and 4.2.3.5(*b*) (long-range order). $p_{11}(\mathbf{m})$ approaches $\frac{1}{2} + s$ for large m with $s = 0$ in the case of short-range order, while $p_{12}(\mathbf{m})$ becomes $\frac{1}{2} - s$. Obviously a strict correlation between $p_{11}(\mathbf{1})$ and s exists which has to be calculated. For a qualitative

references