Fig. 3.4.4.5. Transmission electron microscopy (TEM) image of the incommensurate triangular ($3-q$ modulated) phase of quartz. The black and white triangles correspond to domains with domain states $\mathbf{S}_1$ and $\mathbf{S}_2$, and the transition regions between black and white areas to domain walls (discommensurations). For a domain wall of a certain orientation there are no reversed domain walls with the same orientation but reversed order of black and white; the walls are, therefore, non-reversible. Domain walls in regions with regular triangular structures are related by 120 and 240° rotations about the z direction and carry parallel spontaneous polarizations (see text). Triangular structures in two regions (blocks) with different orientations of the triangles are related *e.g.* by 2_x and carry, therefore, antiparallel spontaneous polarizations and behave macroscopically as two ferroelectric domains with antiparallel spontaneous polarization. Courtesy of E. Snoeck, CEMES, Toulouse and P. Saint-Grégoire, Université de Toulon.

ture in which these six symmetry-related wall orientations still prevail (Van Landuyt *et al.*, 1985).

3.4.4.5. *Ferroelastic domain twins and walls. Ferroelastic twin laws*

As explained in Section 3.4.3.6, from a domain pair $(\mathbf{S}_1, \mathbf{S}_j)$ of ferroelastic single-domain states with two perpendicular equally deformed planes p and p' one can form four different ferroelastic twins (see Fig. 3.4.3.8). Two mutually reversed twins $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ and $(\mathbf{S}_j|\mathbf{n}|\mathbf{S}_1)$ have the same twin symmetry $\mathsf{T}_{1j}(p)$ and the same symmetry $\overline{\mathsf{J}}_{1j}(p)$ of the twin pair $(\mathbf{S}_1, \mathbf{S}_j|\mathbf{n}|\mathbf{S}_j, \mathbf{S}_1)$. The *ferroelastic twin laws* can be expressed by the layer group $\overline{\mathsf{J}}_{1j}(p)$ or, in a less complete way (without specification of reversibility), by the twin symmetry $\mathsf{T}_{1j}(p)$. The same holds for two mutually reversed twins $(\mathbf{S}_1|\mathbf{n}'|\mathbf{S}_j)$ and $(\mathbf{S}_j|\mathbf{n}'|\mathbf{S}_1)$ with a twin plane p' perpendicular to p.

Table 3.4.4.6 summarizes possible symmetries T_{1j} of ferroelastic domain twins and corresponding ferroelastic twin laws $\overline{\mathsf{J}}_{1j}$. Letters V and W signify strain-dependent and strain-independent (with a fixed orientation) domain walls, respectively. The classification of domain walls and twins is defined in Table 3.4.4.3. The last column contains twinning groups $K_{1j}(F_1)$ of ordered domain pairs $(\mathbf{S}_1, \mathbf{S}_j)$ from which these twins can be formed. The symbol of K_{1j} is followed by a symbol of the group F_1 given in square brackets. The twinning group $K_{1j}(F_1)$ specifies, up to two cases, a class of equivalent domain pairs [orbit $G(\mathbf{S}_1, \mathbf{S}_j)$] (see Section 3.4.3.4). More details on particular cases (orientation of domain walls, disorientation angle, twin axis) can be found in synoptic Table 3.4.3.6. From this table follow two general conclusions:

(1) All layer groups describing the symmetry of compatible ferroelastic domain walls are polar groups, therefore *all compatible ferroelastic domain walls in dielectric crystals can be spontaneously polarized*. The direction of the spontaneous polarization is parallel to the intersection of the wall plane p and the plane of shear (*i.e.* a plane perpendicular to the axis of the ferroelastic domain pair, see Fig. 3.4.3.5*b* and Section 3.4.3.6.2).

(2) *Domain twin* $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_j)$ *formed in the parent clamping approximation from a single-domain pair* $(\mathbf{S}_1, \mathbf{S}_j)$ *and the relaxed domain twin* $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_j^-)$ *with disoriented domain states have the same symmetry groups* T_{1j} and $\overline{\mathsf{J}}_{1j}$.

This follows from simple reasoning: all twin symmetries T_{1j} in Table 3.4.4.6 have been derived in the parent clamping approximation and are expressed by the orthorhombic group $mm2$ or by some of its subgroups. As shown in Section 3.4.3.6.2, the maximal symmetry of a mechanically twinned crystal is also $mm2$. An additional simple shear accompanying the lifting of the parent clamping approximation cannot, therefore, decrease the symmetry $\mathsf{T}_{1j}(p)$ derived in the parent clamping approximation. In a similar way, one can prove the statement for the group $\overline{\mathsf{J}}_{1j}(p)$ of the twin pairs $(\mathbf{S}_1, \mathbf{S}_j|\mathbf{n}|\mathbf{S}_j, \mathbf{S}_1)$ and $(\mathbf{S}_1^+, \mathbf{S}_j^-|\mathbf{n}|\mathbf{S}_j^-, \mathbf{S}_1^+)$.

3.4.4.6. *Domain walls of finite thickness – continuous description*

A domain wall of zero thickness is a geometrical construct that enabled us to form a twin from a domain pair and to find a layer group that specifies the *maximal symmetry* of that twin. However, real domain walls have a finite, though small, thickness. Spatial changes of the structure within a wall may, or may not, lower the wall symmetry and can be conveniently described by a *phenomenological theory*.

We shall consider the simplest case of a one nonzero component η of the order parameter (see Section 3.1.2). Two nonzero equilibrium homogeneous values of $-\eta_0$ and $+\eta_0$ of this parameter correspond to two domain states $\mathbf{S}_1$ and $\mathbf{S}_2$. Spatial changes of the order parameter in a domain twin $(\mathbf{S}_1|\mathbf{n}|\mathbf{S}_2)$ with a zero-thickness domain wall are described by a step-like function $\eta(\xi) = -\eta_0$ for $\xi < 0$ and $\eta(\xi) = +\eta_0$ for $\xi > 0$, where ξ is the distance from the wall of zero thickness placed at $\xi = 0$.

A domain wall of finite thickness is described by a function $\eta(\xi)$ with limiting values $-\eta_0$ and η_0:

$$\lim_{\xi\to-\infty} \eta(\xi) = -\eta_0, \quad \lim_{\xi\to+\infty} \eta(\xi) = \eta_0. \qquad (3.4.4.23)$$

If the wall is symmetric, then the profile $\eta(\xi)$ in one half-space, say $\xi < 0$, determines the profile in the other half-space $\xi > 0$. For continuous $\eta(\xi)$ fulfilling conditions (3.4.4.23) this leads to the condition

$$\eta(\xi) = -\eta(-\xi), \qquad (3.4.4.24)$$

i.e. $\eta(\xi)$ must be an odd function. This requirement is fulfilled if there exists a non-trivial symmetry operation of a domain wall (twin): a side reversal ($\xi \to -\xi$) combined with an exchange of domain states [$\eta(\xi) \to -\eta(\xi)$] results in an identical wall profile.

A particular form of the wall profile $\eta(\xi)$ can be deduced from Landau theory. In the simplest case, the dependence $\eta(\xi)$ of the domain wall would minimize the free energy

$$\int_{-\infty}^{\infty} \left(\Phi_0 + \tfrac{1}{2}\alpha(T - T_c)\eta^2 + \tfrac{1}{4}\beta\eta^4 + \tfrac{1}{2}\delta\left(\tfrac{d^2\eta}{d\xi^2}\right)^2 \right) \mathrm{d}\xi, \qquad (3.4.4.25)$$

where α, β, δ are phenomenological coefficients and T and T_c are the temperature and the temperature of the phase transition, respectively. The first three terms correspond to the homogeneous part of the Landau free energy (see Section 3.2.1) and the last term expresses the energy of the spatially changing order parameter. This variational task with boundary conditions (3.4.4.23) has the following solution (see *e.g.* Salje, 1990, 2000*b*; Ishibashi, 1990; Strukov & Levanyuk, 1998)

$$\eta(\xi) = \eta_0 \tanh(\xi/w), \qquad (3.4.4.26)$$

where the value w specifies one half of the *effective thickness* $2w$ *of the domain wall* and is given by

references