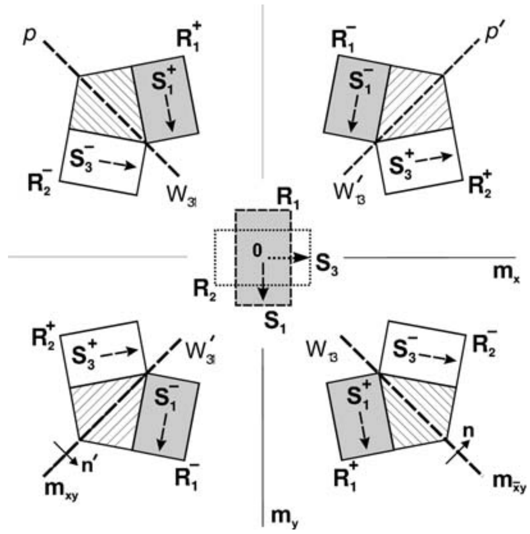

Fig. 3.4.3.8. Exploded view of four ferroelastic twins with disoriented ferroelastic domain states $\mathbf{R}_1^+$, $\mathbf{R}_2^-$ and $\mathbf{R}_1^-$, $\mathbf{R}_2^+$ formed from a single-domain pair $(\mathbf{S}_1, \mathbf{S}_2)$ (in the centre).

and positive sides of **n**, respectively, for which we have used letters Q_1 and Q_2, respectively. Then $(\mathbf{R}_1^+|$ and $|\mathbf{R}_2^-)$ represent domains $\mathbf{D}_1(\mathbf{R}_1^+, Q_1)$ and $\mathbf{D}_2(\mathbf{R}_2^-, Q_2)$, respectively. The symbol $(\mathbf{R}_1^+|\mathbf{R}_2^-)$ properly specifies a domain twin with a zero-thickness domain wall.

A domain wall can be considered as a domain twin with domain regions restricted to non-homogeneous parts near the plane p. For a domain wall in domain twin $(\mathbf{R}_1^+|\mathbf{R}_2^-)$ we shall use the symbol $[\mathbf{R}_1^+|\mathbf{R}_2^-]$, which expresses the fact that a domain wall of zero thickness needs the same specification as the domain twin.

If we exchange domain states in the twin $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$, we get a *reversed twin (wall)* with the symbol $(\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+)$. These two ferroelastic twins are depicted in the lower right and upper left parts of Fig. 3.4.3.8, where – for ferroelastic–non-ferroelectric twins – we neglect spontaneous polarization of ferroelastic domain states. The reversed twin $\mathbf{R}_2^-|\mathbf{n}'|\mathbf{R}_1^+$ has the opposite shear direction.

Twin and reversed twin can be, but may not be, crystallographically equivalent. Thus *e.g.* ferroelastic–non-ferroelectric twins $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$ and $(\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+)$ in Fig. 3.4.3.8 are equivalent, *e.g. via* 2_z, whereas ferroelastic–ferroelectric twins $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ and $(\mathbf{S}_3^-|\mathbf{n}|\mathbf{S}_1^+)$ are not equivalent, since there is no operation in the group K_{12} that would transform $(\mathbf{S}_1^+|\mathbf{n}|\mathbf{S}_3^-)$ into $(\mathbf{S}_3^-|\mathbf{n}|\mathbf{S}_1^+)$.

As we shall show in the next section, the symmetry group $\mathsf{T}_{12}(\mathbf{n})$ of a twin and the symmetry group $\mathsf{T}_{21}(\mathbf{n})$ of a reverse twin are equal,

$$\mathsf{T}_{12}(\mathbf{n}) = \mathsf{T}_{21}(\mathbf{n}). \qquad (3.4.3.66)$$

A sequence of repeating twins and reversed twins

$$\ldots \mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-|\mathbf{n}|\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^- \ldots \qquad (3.4.3.67)$$

forms a *lamellar ferroelastic domain structure* that is very common in ferroelastic phases (see *e.g.* Figs. 3.4.1.1 and 3.4.1.4).

Similar considerations can be applied to the second equally deformed plane p' that is perpendicular to p. The two twins and corresponding compatible domain walls for the equally deformed plane p' have the symbols $(\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+)$ and $(\mathbf{R}_2^-|\mathbf{n}'|\mathbf{R}_1^+)$, and are also depicted in Fig. 3.4.3.8. The corresponding lamellar domain structure is

$$\ldots \mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+|\mathbf{n}'|\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+|\mathbf{n}'|\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+|\mathbf{n}'|\mathbf{R}_1^-|\mathbf{n}'|\mathbf{R}_2^+ \ldots . \qquad (3.4.3.68)$$

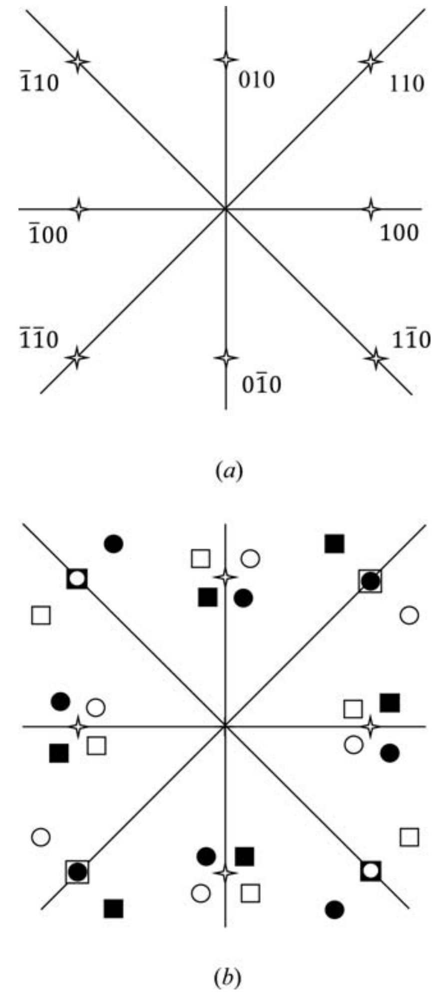

Fig. 3.4.3.9. Splitting of diffraction spots at a tetragonal-to-orthorhombic transition. (*a*) Fragment of the reciprocal lattice (stars) of the parent tetragonal phase. (*b*) Superposition of the reciprocal lattices of the four ferroelastic domains states in Fig. 3.4.3.8: $\mathbf{R}_1^+$ (reciprocal lattice black squares), $\mathbf{R}_1^-$ (reciprocal lattice black circles), $\mathbf{R}_2^+$ (reciprocal lattice white squares) and $\mathbf{R}_2^-$ (reciprocal lattice white circles).

Thus from one ferroelastic single-domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ depicted in the centre of Fig. 3.4.3.8 four different ferroelastic domain twins can be formed. It can be shown that these four twins have the same shear angle ω and the same amount of shear s. They differ only in the direction of the shear.

Four disoriented domain states $\mathbf{R}_1^-, \mathbf{R}_1^+$ and $\mathbf{R}_2^-, \mathbf{R}_2^+$ that appear in the four domain twins considered above are related by lost operations (*e.g.* diagonal, vertical and horizontal reflections), *i.e.* they are crystallographically equivalent. This result can readily be obtained if we consider the stabilizer of a disoriented domain state $\mathbf{R}_1^+$, which is $I_{4/mmm}(\mathbf{R}_1^+) = 2_z/m_z$. Then the number $n_a^{\rm dis}$ of disoriented ferroelastic domain states is given by

$$n_a^{\rm dis} = [G : I_g(\mathbf{R}_1^+)] = |4_z/m_z m_x m_{xy}| : |2_z/m_z| = 16 : 4 = 4. \qquad (3.4.3.69)$$

All these domain states appear in ferroelastic polydomain structures that contain coexisting lamellar structures (3.4.3.67) and (3.4.3.68).

Disoriented domain states in ferroelastic domain structures can be recognized by diffraction techniques (*e.g.* using an X-ray precession camera). The presence of these four disoriented domain states results in splitting of the diffraction spots of the high-symmetry tetragonal phase into four or two spots in the orthorhombic ferroelastic phase. This splitting is schematically depicted in Fig. 3.4.3.9. For more details see *e.g.* Shmyt'ko *et al.* (1987), Rosová *et al.* (1993), and Rosová (1999).