International Tables for Crystallography (2013). Vol. D, Figure 3.4.3.6, p. 519.

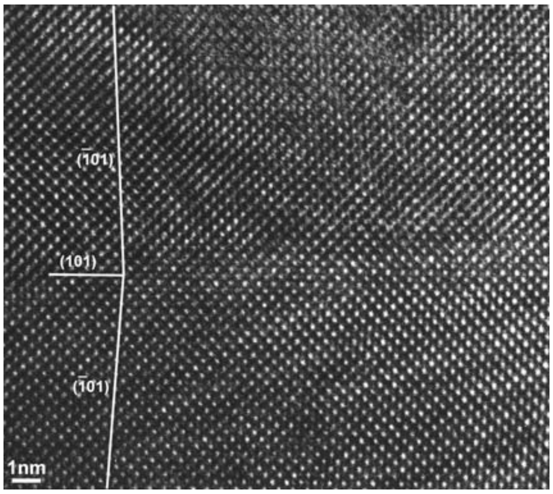

Fig. 3.4.3.6. High-resolution electron microscopy image of a ferroelastic twin in the orthorhombic phase of WO_3. Courtesy of H. Lemmens, EMAT, University of Antwerp.

angle between these planes equals 2ω, where ω is the shear angle (obliquity) of the ferroelastic twin.

Disorientations of domain states in a ferroelastic twin bring about a deviation of the optical indicatrix from a strictly perpendicular position. Owing to this effect, ferroelastic domains exhibit different colours in polarized light and can be easily visualized. This is illustrated for a domain structure of $YBa_2Cu_3O_{7-\delta}$ in Fig. 3.4.3.7. The symmetry descent $G = 4_z/m_zm_xm_{xy} \supset m_xm_ym_z = F_1 = F_2$ gives rise to two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$. The twinning group K_{12} of the non-trivial domain pair $(\mathbf{R}_1, \mathbf{R}_2)$ is

$$K_{12}[m_xm_ym_z] = J_{12}^{\star} = m_xm_ym_z \cup 4_z^{\star}\{2_xm_ym_z\} = 4_z^{\star}/m_zm_xm_{xy}^{\star}. \qquad (3.4.3.61)$$

The colour of a domain state observed in a polarized-light microscope depends on the orientation of the index ellipsoid (indicatrix) with respect to a fixed polarizer and analyser. This index ellipsoid transforms in the same way as the tensor of spontaneous strain, *i.e.* it has different orientations in ferroelastic domain states. Therefore, different ferroelastic domain states exhibit different colours: in Fig. 3.4.3.7, the blue and pink areas (with different orientations of the ellipse representing the spontaneous strain in the plane of of figure) correspond to two different ferroelastic domain states. A rotation of the crystal that does not change the orientation of ellipses (*e.g.* a 180° rotation about an axis parallel to the fourfold rotation axis) does not change the colours (ferroelastic domain states). If one neglects disorientations of ferroelastic domain states (see Section 3.4.3.6) – which are too small to be detected by polarized-light microscopy – then none of the operations of the group $F_1 = F_2 = m_xm_ym_z$ change the single-domain ferroelastic domain states $\mathbf{R}_1$, $\mathbf{R}_2$, hence there is no change in the colours of domain regions of the crystal. On the other hand, all operations with a star symbol (operations lost at the transition) exchange domain states $\mathbf{R}_1$ and $\mathbf{R}_2$, *i.e.* also exchange the two colours in the domain regions. The corresponding permutation is a transposition of two colours and this attribute is represented by a star attached to the symbol of the operation. This exchange of colours is nicely demonstrated in Fig. 3.4.3.7 where a $-90°$ rotation is accompanied by an exchange of the pink and blue colours in the domain regions (Schmid, 1991, 1993).

It can be shown (Shuvalov *et al.*, 1985; Dudnik & Shuvalov, 1989) that for small spontaneous strains the amount of shear s and the angle ω can be calculated from the second invariant Λ_2 of the differential tensor Δu_{ik}:

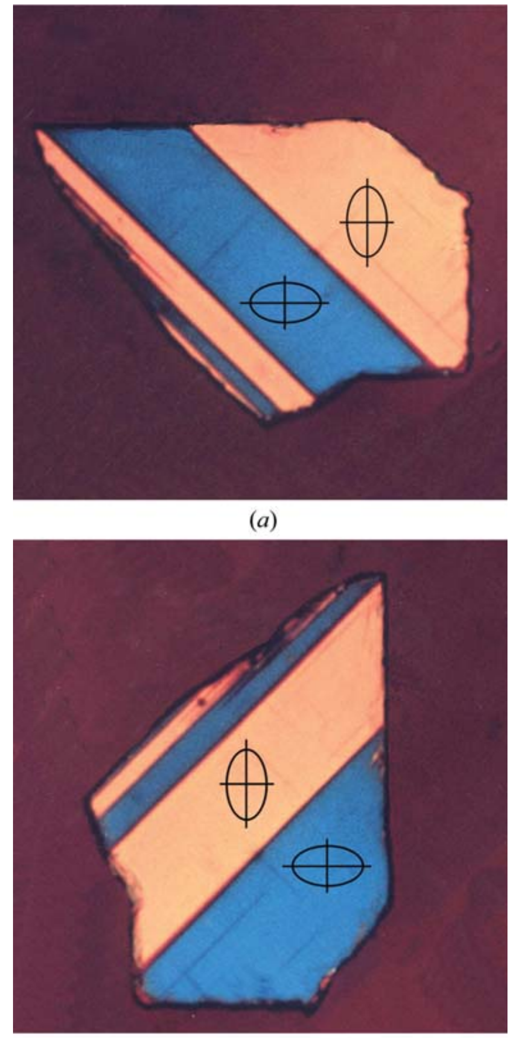

Fig. 3.4.3.7. Ferroelastic twins in a very thin $YBa_2Cu_3O_{7-\delta}$ crystal observed in a polarized-light microscope. Courtesy of H. Schmid, Université de Geneve.

$$s = 2\sqrt{-\Lambda_2}, \qquad (3.4.3.62)$$

$$\omega = \sqrt{-\Lambda_2}, \qquad (3.4.3.63)$$

where

$$\Lambda_2 = \begin{vmatrix} \Delta u_{11} & \Delta u_{12} \\ \Delta u_{21} & \Delta u_{22} \end{vmatrix} + \begin{vmatrix} \Delta u_{22} & \Delta u_{23} \\ \Delta u_{32} & \Delta u_{33} \end{vmatrix} + \begin{vmatrix} \Delta u_{11} & \Delta u_{13} \\ \Delta u_{31} & \Delta u_{33} \end{vmatrix}. \qquad (3.4.3.64)$$

In our example, where there are only two nonzero components of the differential spontaneous strain tensor [see equation (3.4.3.58)], the second invariant $\Lambda_2 = -(\Delta u_{11}\Delta u_{22}) = -(u_{22} - u_{11})^2$ and the angle ω is

$$\omega = \pm|u_{22} - u_{11}|. \qquad (3.4.3.65)$$

In this case, the angle ω can also be expressed as $\omega = \pi/2 - 2\arctan a/b$, where a and b are lattice parameters of the orthorhombic phase (Schmid *et al.*, 1988).

The shear angle ω ranges in ferroelastic crystals from minutes to degrees (see *e.g.* Schmid *et al.*, 1988; Dudnik & Shuvalov, 1989).

Each equally deformed plane gives rise to two compatible domain walls of the same orientation but with opposite sequence of domain states on each side of the plane. We shall use for a *simple domain twin* with a planar wall a symbol $(\mathbf{R}_1^+|\mathbf{n}|\mathbf{R}_2^-)$ in which $\mathbf{n}$ denotes the normal to the wall. The bra–ket symbol (| and |) represents the half-space domain regions on the negative

references