Table 3.4.4.6. *Symmetry properties of ferroelastic domain twins and compatible domain walls*

T_{1j}	$\overline{\mathsf{J}}_{1j}$	Classification		$K_{1j}[F_1]$
1	$\underline{2}$	V	AR	$4^\star[2]$, $\bar{4}^\star[2]$, 6[2], $6/m[2]$
1	$\underline{2}$	V	AR	
1	$2^\star$	W	$AR^\star$	$2^\star[1]$, 422[2], $\bar{4}2m[m]$, 32[2], $\bar{3}m[m]$, 622[2], $\bar{6}m2[m]$, 432[222], $m\bar{3}m[mm2]$, $m\bar{3}m[2^\star_{xy}][mm2]$
$\underline{2}^\star$	$\underline{2}^\star$	V	SI	
1	$2^\star$	W	$AR^\star$	23[3], 432[4], 432[3], $m\bar{3}m[\bar{4}]$
$\underline{2}^\star$	$\underline{2}^\star$	W	SI	
1	$m^\star$	V	$AR^\star$	$m^\star[1]$, $4mm[m]$, $\bar{4}2m[2]$, $3m[m]$, $\bar{3}m[2]$, $6mm[m]$, $\bar{6}m2[2]$, $43m[mm2]$, $m\bar{3}m[222]$, $m\bar{3}m[m^\star_{xy}][m2m]$
$\underline{m}^\star$	$\underline{m}^\star$	W	SI	
1	$m^\star$	W	$AR^\star$	$m\bar{3}[3]$, $\bar{4}3m[\bar{4}]$, $\bar{4}3m[3]$, $m\bar{3}m[4]$
$\underline{m}^\star$	$\underline{m}^\star$	W	SI	
$\underline{2}^\star$	$2^\star\underline{2}^\star 2$	W	SR	$2^\star 2^\star 2[2]$, $4^\star 22^\star[222]$, $\bar{4}^\star 2^\star m[mm2]$, 622[222], $6/mmm[mm2]$, 432[422], 432[32], $m\bar{3}m[\bar{4}2m]$
$\underline{2}^\star$	$\underline{2}^\star 2^\star\underline{2}$	W	SR	
$\underline{2}^\star$	$\underline{2}^\star/m^\star$	V	SR	$2^\star/m^\star[\bar{1}]$, $4/mmm[2/m]$, $\bar{3}m[2/m]$, $6/mmm[2/m]$, $m\bar{3}m[mmm]$
$\underline{m}^\star$	$2^\star/\underline{m}^\star$	W	SR	
$\underline{2}^\star$	$\underline{2}^\star/m^\star$	W	SR	$m\bar{3}[\bar{3}]$, $m\bar{3}m[4/m]$, $m\bar{3}m[\bar{3}]$
$\underline{m}^\star$	$2^\star/\underline{m}^\star$	W	SR	
m	m	V	AI	$4/m[m]$, $\bar{6}[m]$, $6/m[m]$
m	m	V	AI	
m	$\underline{2}/m$	V	AR	$4^\star/m[2/m]$, $6/m[2/m]$
m	$\underline{2}/m$	V	AR	
$\underline{m}^\star$	$m^\star\underline{m}^\star 2$	W	SR	$m^\star m^\star 2[2]$, $4^\star mm^\star[mm2]$, $\bar{4}^\star 2m^\star[222]$, $6mm[mm2]$, $6/mmm[222]$, $43m[\bar{4}2m]$, $m\bar{3}m[422]$, $m\bar{3}m[32]$
$\underline{m}^\star$	$\underline{m}^\star m^\star 2$	W	SR	
m	$m^\star 2^\star m$	W	$AR^\star$	$m^\star 2^\star m[m]$, $4/mmm[2mm]$, $\bar{6}m2[m2m]$, $6/mmm[m2m]$, $\bar{4}3m[3m]$, $m\bar{3}m[4mm]$, $m\bar{3}m[\bar{4}2m]$, $m\bar{3}m[3m]$
$\underline{m}^\star\underline{2}^\star m$	$\underline{m}^\star\underline{2}^\star m$	W	SI	
$\underline{m}^\star\underline{2}^\star m$	$\underline{m}^\star m^\star m$	W	SR	$m^\star m^\star m[2/m]$, $4^\star/mmm^\star[mmm]$, $6/mmm[mmm]$, $m\bar{3}m[4/mmm]$, $m\bar{3}m[\bar{3}m]$
$2^\star\underline{m}^\star m$	$m^\star\underline{m}^\star m$	W	SR	

$$w = \sqrt{2\delta/\alpha(T_c - T)}. \quad (3.4.4.27)$$

This dependence, expressed in relative dimensionless variables ξ/w and η/η_0, is displayed in Fig. 3.4.4.6.

The wall profile $\eta(\xi)$ expressed by solution (3.4.4.26) is an odd function of ξ,

$$\eta(-\xi) = \eta_0 \tanh(-\xi/w) = -\eta_0 \tanh(\xi/w) = -\eta(\xi), \quad (3.4.4.28)$$

and fulfils thus the condition (3.4.4.24) of a symmetric wall.

The wall thickness can be estimated from electron microscopy observations, or more precisely by a diffuse X-ray scattering technique (Locherer *et al.*, 1998). The effective thickness $2w$ [see equation (3.4.4.26)] in units of crystallographic repetition length A normal to the wall ranges from $2w/A = 2$ to $2w/A = 12$, *i.e.* $2w$ is about 10–100 nm (Salje, 2000*b*). The temperature dependence

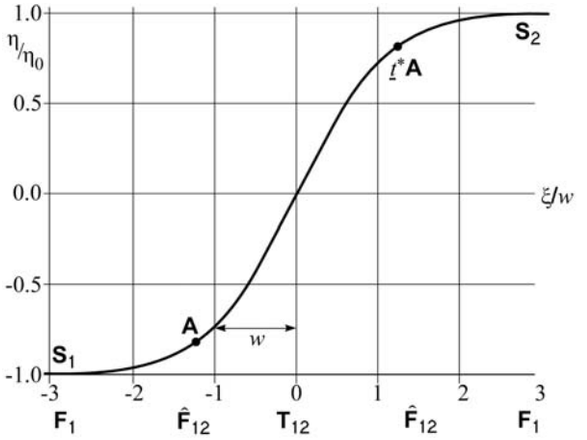

Fig. 3.4.4.6. Profile of the one-component order parameter $\eta(\xi)$ in a symmetric wall (S). The effective thickness of the wall is $2w$.

of the domain wall thickness expressed by equation (3.4.4.27) has been experimentally verified, *e.g.* on $LaAlO_3$ (Chrosch & Salje, 1999).

The energy σ of the domain wall per unit area equals the difference between the energy of the twin and the energy of the single-domain crystal. For a one nonzero component order parameter with the profile (3.4.4.26), the wall energy σ is given by (Strukov & Levanyuk, 1998)

$$\sigma = \int_{-\infty}^{\infty} \left[\Phi(\eta(\xi)) - \Phi(\eta_0)\right] \mathrm{d}\xi = \frac{2\sqrt{2\delta}}{3\beta}[\alpha(T_c - T)]^{3/2}, \quad (3.4.4.29)$$

where $2w$ is the effective thickness of the wall [see equation (3.4.4.27)] and the coefficients are defined in equation (3.4.4.25).

The order of magnitude of the wall energy σ of ferroelastic and non-ferroelastic domain walls is typically several millijoule per square metre (Salje, 2000*b*).

Example 3.4.4.3. In our example of a ferroelectric phase transition $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$, one can identify η with the P_1 component of spontaneous polarization and ξ with the axis y. One can verify in Fig. 3.4.4.6 that the symmetry $\mathsf{T}_{12}[010] = \underline{2}^\star_z/m_z$ of the twin $(\mathbf{S}_1[010]\mathbf{S}_2)$ with a zero-thickness domain wall is retained in the domain wall with symmetric profile (3.4.4.26): both non-trivial symmetry operations $\underline{2}^\star_z$ and $\underline{1}^\star$ transform the profile $\eta(y)$ into an identical function.

This example illustrates another feature of a symmetric wall: All non-trivial symmetry operations of the wall are located at the central plane $\xi = 0$ of the finite-thickness wall. The sectional group T_{12} of this plane thus expresses the *symmetry of the central layer* and also the *global symmetry* of a symmetric wall (twin). The *local symmetry* of the off-centre planes $\xi \neq 0$ is equal to the face group $\widehat{\mathsf{F}}_{12}$ of the the layer group T_{12} (in our example $\widehat{\mathsf{F}}_{12} = \{1, m_z\}$).