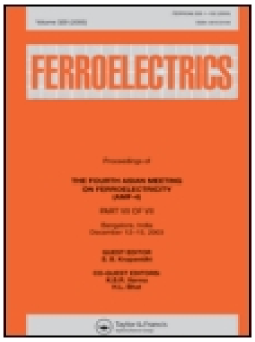

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EXAMINATION OF POINT GROUP SYMMETRIES OF NON-FERROELASTIC DOMAIN WALLS

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We recall how the symmetry properties of planar walls can be derived and how the orientational dependences of domain wall symmetry are related to simple crystal forms used in crystal morphology. We present a sample page of tables that contain symmetry properties of all crystallographically different non-ferroelastic domain walls in continuum description and on simple examples demonstrate how they can be used in discussing tensor properties of non-ferroelastic domain walls.

Key words: Non-ferroelastic domain structures, symmetry of domain walls, non-ferroelastic domain walls, tensor properties of domain walls, symmetry analysis of domain structures.

1. INTRODUCTION

Domain walls are thin, non-homogeneous transient regions connecting structures of two domains. Due to gradient effects domain walls can exhibit other physical properties than the bulks of adjacent domains. This has been demonstrated on the example of quartz where the existence of a spontaneous polarization of a wall joining two non-polar domains was first predicted theoretically[1] and later has been confirmed experimentally.[2]

Macroscopic physical properties of domain walls are described by material property tensors. The decisive components of these tensors can be deduced from the point group symmetry of the wall (described by a layer group) and the symmetry of the bulks of adjacent domains (expressed by an ordinary point group). Other layer groups describe local symmetries within the wall.

2. SYMMETRIES OF DOMAIN WALLS

A planar domain wall is an interface with orientation (hkl) between two domain states S_1 and S_2. We shall use for such a wall the symbol $(S_1(hkl)S_2)$ in which the domain state S_1 given first is on the inner side of the plane (hkl). The orientation can be also expressed by the outer normal $\mathbf{n}$ to the plane.

Derivation of the domain wall symmetry, described e.g. in Ref. 3-6, consists of the following steps:

(i) Find the symmetry group J_{12} of the unordered domain pair $\{S_1, S_2\}$. For non-ferroelastic domain pairs this group has the form[7]

$$J_{12} = F_1 + j_{12}^* F_1 \ , \tag{1}$$

where F_1 is the symmetry of S_1 and S_2, and j_{12}^* exchanges S_1 and S_2. Notice that S_1 and J_{12} specify the domain pair $\{S_1, S_2\}$ since $S_2 = j_{12}^* S_1$.

(ii) Determine the sectional layer group $\overline{J}_{12}$ of J_{12} along the plane (hkl) which has the form

$$\overline{J}_{12} = \widehat{F_1} + \underline{t}_{12}^* \widehat{F_1} + r_{1j}^* \widehat{F_1} + \underline{s}_{12} \widehat{F_1} \ , \tag{2}$$

where $\widehat{F_1}$ is the one-sided layer symmetry of the face (hkl) in F_1, $\underline{t}_{12}^*$ exchanges S_1 and S_2 and simultaneously transforms $\mathbf{n}$ into $-\mathbf{n}$, $\underline{s}_{12}$ reverses $\mathbf{n}$ into $-\mathbf{n}$, and r_{12}^* exchanges S_1 and S_2.

(iii) The symmetry group T_{12} of the wall $(S_1(hkl)S_2)$ consists of first two terms of Eq. (2),

$$T_{12} = \widehat{F_1} + \underline{t}_{12}^* \widehat{F_1} \ . \tag{3}$$

Walls with $T_{12} > \widehat{F_1}$ are called *symmetric walls* whereas for *asymmetric walls* $T_{12} = \widehat{F_1}$.

The last two cosets in Eq. (2) assemble operations that transform the wall $(S_1(hkl)S_2)$ into a *reversed wall* $(S_2(hkl)S_1)$ with opposite order of domain states adhering to the wall. Accordingly, one can distinguish *reversible walls* for which $\overline{J}_{12} > T_{12}$, and *irreversible walls* with $\overline{J}_{12} = T_{12}$.

There is an alternative method for determining left cosets of the sectional layer group $\overline{J}_{12}$ based on the analysis of simple forms associated with symmetry groups F_1 and J_{12} .

By application of all the symmetry operations of a group F_1 on assigned plane $\rho(hkl)$ we get a set of symmetrically equivalent planes $\{\rho\}_{F_1}$. These planes restrict in space a convex polyhedron (open or closed) which is called *simple form* $sf(F_1)_\rho$.

The symmetry group of $J_{12} = F_1 + j_{12}^* F_1$ can be treated as a dichromatic (e.g. black and white) group. Then the simple form associated with group J_{12} can be decomposed into the simple form associated with F_1 (white faces) and geometrically egual polyhedron associated with the left coset $j_{12}^* F_1$ (grey faces), see Fig. 1.

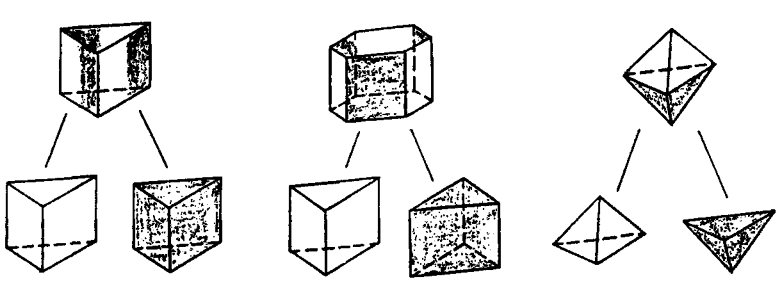


Figure 1: Decomposition of $sf(J_{12})_\rho$ into $sf(F_1)_\rho$ and $sf(j_{12}^* F_1)_\rho$.

If a plane of sectional layer group $\overline{J}_{12}$ is parallel to one face of the simple form associated with J_{12}, using colour and geometrical symmetry of the corresponding isohedron we can determine which left coset of $\overline{J}_{12}$ is (non)empty, see Table 1.

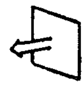
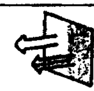
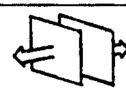
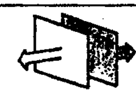
left coset	corresponding faces	
$\widehat{F}_1$	single, one-colour face	 or 
$\underline{r}^*_{12}\widehat{F}_1$	single, two-colour face	
$\underline{s}_{12}\widehat{F}_1$	two parallel faces having the same colour	 or 
$\underline{t}^*_{12}\widehat{F}_1$	two parallel faces with different colours	

Table 1: Left cosets of $\overline{J}_{12}$ and corresponding types of faces. Arrow-heads represent outer normals.

3. SYSTEMATIC EXAMINATION OF LAYER SYMMETRIES FOR ALL NON-EQUIVALENT NON-FERROELASTIC WALLS

All non-ferroelastic domain pairs and their symmetries J_{12} are listed in Ref. 7. For each domain pair the crystallographically different wall orientations can be deduced from simple crystal forms that are given in Ref. 8. For all different cases we have determined the sectional layer group $\overline{J}_{12}$ and its decomposition (2) which contains all essential information on wall symmetry. In Table 2 we summarize number of walls according to their classification symmetric-asymmetric and reversible-irreversible.

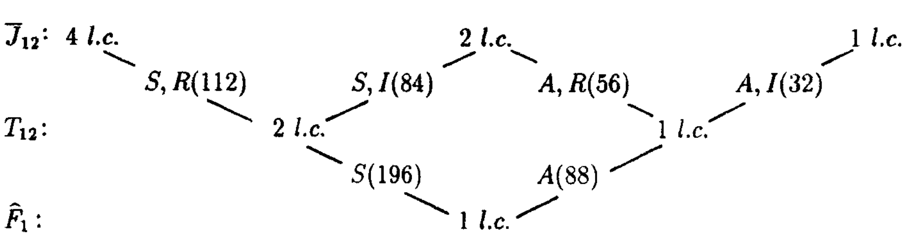


Table 2: Number of left cosets (l.c.) and corresponding types of domain walls.
R = reversible I = irreversible S = symmetrical A = asymmetrical
(n) = number of non-equivalent walls of the given type

Explicit results of the systematic analysis are available in form of tables which will be published elsewhere. In Table 3 we give as an illustration a shortened presentation for several domain pairs which describe the situation in TGS ($J_{12} = 2/m^*$), quartz ($J_{12} = 6^*22^*$) and a simple example of a ferroelectric domain wall discussed below ($J_{12} = mm^*m$).

F_1	J_{1j}	(hkl)	$\hat{F}_1$	$\underline{s}_{1j}$	r^*_{1j}	$\underline{t}^*_{1j}$	T_{1j}	$\bar{J}_{1j}$
2	$2/m^*$	(001)	2_z			$\underline{\bar{1}}^*$	$2_z/\underline{m}^*_z$	$2_z/\underline{m}^*_z$
		$(hk0)$	1	$\underline{2}_z$	m^*_z	$\underline{\bar{1}}^*$	$\underline{\bar{1}}^*$	$\underline{2}_z/m^*_z$
		(hkl)	1			$\underline{\bar{1}}^*$	$\underline{\bar{1}}^*$	$\underline{\bar{1}}^*$
$m2m$	mm^*m	(010)	$m_x2_ym_z$			$\underline{\bar{1}}^*$	$\underline{2}^*_x/m_x2_y/\underline{m}^*_y\underline{2}^*_z/m_z$	$\underline{2}^*_x/m_x2_y/\underline{m}^*_y\underline{2}^*_z/m_z$
		(100)	m_z	$\underline{2}_y$	2^*_x	$\underline{\bar{1}}^*$	$\underline{2}^*_z/m_z$	$2^*_x/\underline{m}_x\underline{2}_y/m^*_y\underline{2}^*_z/m_z$
		(001)	m_x	$\underline{2}_y$	2^*_z	$\underline{\bar{1}}^*$	$\underline{2}^*_x/m_x$	$\underline{2}^*_x/m_x\underline{2}_y/m^*_y2^*_z/\underline{m}_z$
		$(k0h)$	1	$\underline{2}_y$	m^*_y	$\underline{\bar{1}}^*$	$\underline{\bar{1}}^*$	$\underline{2}_y/m^*_y$
		$(0lh)$	m_x			$\underline{\bar{1}}^*$	$\underline{2}^*_x/m_x$	$\underline{2}^*_y/m_y$
		$(kl0)$	m_z			$\underline{\bar{1}}^*$	$\underline{2}^*_z/m_z$	$\underline{2}^*_x/m_x$
		(hkl)	1			$\underline{\bar{1}}^*$	$\underline{\bar{1}}^*$	$\underline{\bar{1}}^*$
32	6^*22^*	(0001)	3_z	$\underline{2}_{10}$	2^*_z	$\underline{2}^*_{12}$	$3_z1\underline{2}^*_{12}$	$6^*_z\underline{2}_{10}\underline{2}^*_{12}$
		$(2\bar{1}\bar{1}0)$	2_{10}			$\underline{2}^*_z$	$2_{10}\underline{2}^*_{12}\underline{2}^*_z$	$2_{10}\underline{2}^*_{12}\underline{2}^*_z$
		$(01\bar{1}0)$	1	$\underline{2}_{10}$	2^*_{12}	$\underline{2}^*_z$	$\underline{2}^*_z$	$\underline{2}_{10}2^*_{12}\underline{2}^*_z$
		$(2h\bar{h}\bar{h}l)$	1			$\underline{2}^*_{12}$	$\underline{2}^*_{12}$	$\underline{2}^*_{12}$
		$(0h\bar{h}l)$	1	$\underline{2}_{10}$			1	$\underline{2}_{10}$
		$(hki0)$	1			$\underline{2}^*_z$	$\underline{2}^*_z$	$\underline{2}^*_z$
		$(hkil)$	1				1	1

Table 3: Sample page of tables of symmetry properties of non-ferroelastic domain walls.

4. TENSOR PROPERTIES OF DOMAIN WALLS

The layer group T_{12} describes the *global symmetry* of the wall. Comparing T_{12} with the symmety F_1 of domain bulks one can infer in which tensor properties the domain wall differs from the adjacent domains. Thus from the Table 2 it follows e.g. for quartz with $J_{12} = G = 622$ and $F_1 = 32$ (non-polar domain states) that the walls $(S_1(hki0)S_2)$ have the symmetry $T_{12} = \underline{2}^*_z$ and can be, therefore, spontaneously polarized along z axis, up to a special orientation $(2\bar{1}\bar{1}0)$ in which the wall symmetry $T_{12} = 2_{10}\underline{2}^*_{12}\underline{2}^*_z$ precludes nonzero polarization. The walls with both these orientations are irreversible up to a special orientation $(01\bar{1}0)$ in which the wall is reversible. The fact that for irreversibe walls a wall $(S_1(hki0)S_2)$ and the reversed wall $(S_2(hki0)S_1)$ (which are not symmetrically equivalent) can have different energy is demonstrated on incommensurate structures of quartz[1,2] which consist of symmetrically equivalent domain walls only.

Local symmetries within the wall are determined by the following groups: The sectional layer group $\overline{J}_{12}$ expresses the symmetry of the central plane of a symmetrical wall, $\widehat{F}_1$ describes the symmetry of the off-center region and the group F_1 gives the symmetry of domain bulks S_1 and S_2. These symmetries provide constraints on possible changes of tensor properties within the wall. This is illustrated on a ferroelectric wall in Fig. 2. $F_1 = m2m$ allows for the spontaneous polarization $-P_{y0}$ and $+P_{y0}$ in S_1 and S_2, resp. The group $\overline{J}_{12} = \underline{m}_x m_y^* m_z$ requires zero polarization in the center of the wall. In off-center region $\widehat{F}_1 = m_z$ allows for gradient component $P_x \sim P_y(dP_y/dx)$. The wall is reversible.

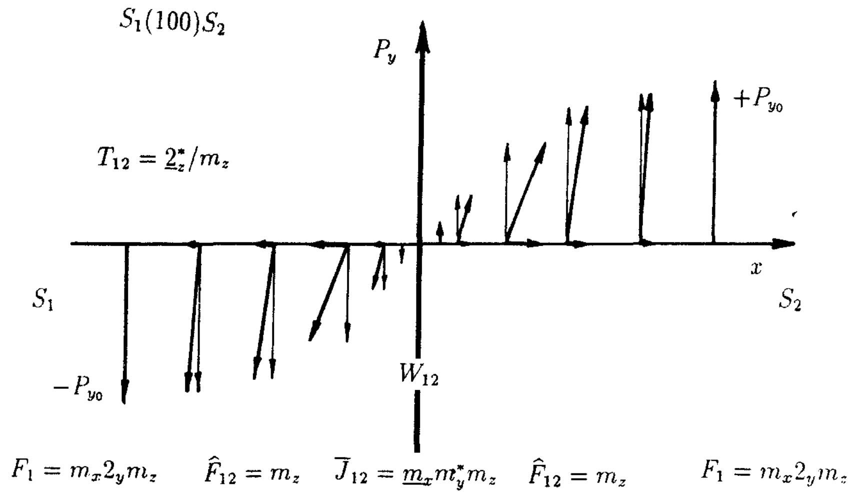


Figure 2: Example of polarization changes in a symmetric ferroelectric domain wall as they follow from local symmetries

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REFERENCES

1. M. B. Walker, R. J. Gooding, *Phys. Rev. B*, **32**, 7408 (1985).
2. E. Snoeck, P. Saint-Grégoire, V. Janovec, C. Roucau, *Ferroelectrics* **155**, 371 (1994).
3. V. Janovec, *Ferroelectrics*, **35**, 105 (1981).
4. Z. Zikmund, *Czech. J. Phys.*, B **34**, 932 (1984).
5. R. C. Pond and D. S. Vlachavas, *Proc.R. Soc. Lond.* A **386**, 95 (1983).
6. C. Kalonji, *J. de Physique*, C4, **46**, 249 (1985).
7. V. Janovec, L Richterová and D. B. Litvin, *Ferroelectrics*, **140**, 95 (1993).
8. *International Tables for Crystallography*, Ed. T. Hahn (Kluwer Academic Publishers, Dordrecht, 3rd Edition, 1992), Vol. A.