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Rotation of Domain States in Ferroelastic Domain Structures

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Abstract

This work deals with misfit angles, which are observable in ferroelastic phase transitions. In the literature the misfit angles were calculated for six different ferroelastic phase transitions, where there is only one possible misfit angle. In this work the method for obtaining all misfit angles (for the cases where there is more than one possible) is introduced. Also the expressions for all possible misfit angles for each ferroelastic species are given.

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1. Introduction

In a ferroelastic structure, several ferroelastic *domain states* can be formed [1]. These states have the same crystal structure and differ only in the orientation with respect to the coordinate system of the paraelastic phase. Since all domain states are energetically equivalent, they can coexist in the same crystal. The ferroelastic domains and domain walls can be well observed in a polarized-light microscope [2]. When only a single domain is formed in the ferroelastic structure, its single domain state has a prominent crystallographic orientation, and is referred to as the *ideal domain state*. In a multi-domain structure the orientations of the domain states differ from the orientations of the corresponding ideal domain states.

The domain walls between two ferroelastic domains that satisfy the conditions of the strain compatibility are then referred to as *permissible domain walls*. These domain walls must contain all directions for which the change in length of any infinitesimal vector of the prototype, due to spontaneous strain, is equal in the two adjacent domains [1]. If the existence of a permissible domain wall between two domains is possible, then there are always two planes in which the permissible domain walls can be formed. Furthermore, these two planes are always perpendicular to each other [1]. If the permissible domain walls cannot exist, then the two domain states will join only when external stress is applied. The boundaries between the two domain states are then not well-defined planes, often irregular, curved or diffuse, with internal stresses and dislocations. In this work we will consider only the cases when a permissible domain wall can be formed.

To form a domain wall between two ferroelastic domains a certain rotation of the corresponding ideal domain states of the adjacent domains is necessary [3, 4]. The aim of this work is to calculate all possible angles, the so-called *misfit angles*, at which the ideal domain states could be rotated in order to form the permissible domain wall. The magnitude of these angles depends on the spontaneous strain and on the relation between the two domain states. In Ref. [4] the angles have been calculated for six different phase transitions. In this work, these calculations are performed for all possible ferroelastic phase transitions.

2. Spontaneous strain tensor

The spontaneous strain tensor is defined in such a way that the volume of the prototype does not change after the spontaneous strain, although in reality the volume changes due to thermal expansion. The spontaneous strain tensor accounts only for the change in the crystal structure. This condition is expressed in the following formula [5]:

$$\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = 0, \tag{1}$$

where ε_{ii} are the main diagonal components of the spontaneous strain tensor.

As is shown in Ref. [6] the form of the spontaneous strain tensor depends only on the groups of symmetry P of the prototypic phase and E of the ferroelastic phase, respectively. Then we define the F-operations as the operations that are in P but not in E. The F-operations represent the symmetries that were lost in the phase transition. Any domain state of the ferroelastic structure has all the symmetries of the group of symmetry E. The F-operations transform one domain state into the other domain states. Tables for the forms of spontaneous strain tensors for all domain states for each ferroelastic phase transition can be found in Ref. [7].

Generally, there is more than one operation that transforms one certain domain state S^1 into another domain state S^2 (the quantities for different domain states are denoted by superscripts behind the symbols of the quantities). If one of the F-operations is a mirror plane or a twofold axis, then this plane, or the plane perpendicular to the twofold axis is going to be the W permissible domain wall, because it satisfies all the conditions. The W' wall is going to be perpendicular to the W wall. The exact orientation of the W' wall depends on the exact values of the components of the spontaneous strain tensor [1].

While calculating the misfit angle of the ideal domain states the spontaneous strain difference tensor δ_{ij} is introduced. It is defined as the difference of the spontaneous strain tensors of two different domain states

$$\delta = \varepsilon^1 - \varepsilon^2. \tag{2}$$

From (1) and (2) we can conclude that

$$\delta_{11} + \delta_{22} + \delta_{33} = 0. \tag{3}$$

The spontaneous strain tensor possesses the point inversion as a symmetry element and therefore the spontaneous strain tensors have the same form for all crystal classes belonging to the same Laue's group, since the classes differ only in the point inversion symmetry. From this one can conclude that it is not necessary to perform calculations for phase transitions between all possible crystal classes, but only for the 11 Laue's groups. Therefore, we need to perform calculations for only one of the crystal species corresponding to this phase transition and the result is valid for all other species that exhibit the same phase transition. For example, for the phase transition from Cubic 1 to Tetragonal 1 we have three possible ferroelastic species: $432F422, \bar{4}3mF\bar{4}2m, m3mF4/mmm$. If we take for example the species with the highest symmetry, which is the $m3mF4/mmm$ transition, the calculations would be the same for the other two species.

3. Calculation of the misfit angle

The misfit angle φ is the whole angle that the two domains have to rotate at in order to join in a permissible domain wall (see Fig. 1). Let $\Delta\varphi^1$, respectively $\Delta\varphi^2$ be the oriented angle (counterclockwise) at which the first domain state, respectively the second domain state rotates. The angle φ is then given as

$$\varphi = \Delta\varphi^2 - \Delta\varphi^1. \tag{4}$$

3.1. Geometrical approach

Let us show an example of calculating the misfit angle φ using geometrical methods. Let us consider the case of the species $4/mmmFmmm$.

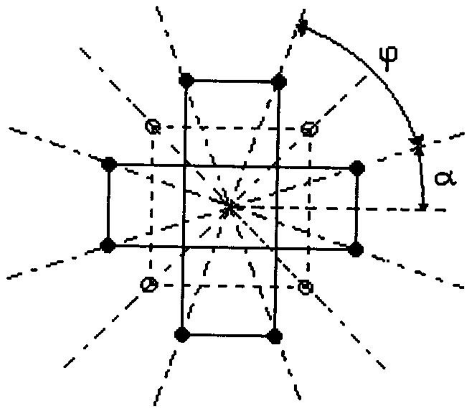

Fig. 1. The misfit angle in the case of $4/mmmFmmm$ (the magnitude of the strain is much smaller in reality).

In Ref. [7] we can find the form of the spontaneous strain tensor for the first domain state

$$\varepsilon^1 = \begin{pmatrix} -a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

In the prototypic structure, there is a fourfold axis of symmetry in the direction of the z axis. In the ferroelastic structure there is only a twofold axis of symmetry in the direction of the z axis. Therefore one of the F-operations is for example rotation about the z axis at the angle $90°$. Applying this operation on ε^1, we get the form of the spontaneous strain tensor for the second domain state

$$\varepsilon^2 = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The point with the coordinates in the prototypic structure $[x, y, z]$ is displaced to the point with the coordinates $[x', y', z']$ in the ferroelastic structure. These coordinates in both domain states can be expressed in terms of x, y, z and the spontaneous strain tensors

$$\text{DS1}: \qquad x' = x(1-a), \qquad y' = y(1+a), \qquad z' = z, \tag{5}$$

$$\text{DS2}: \qquad x' = x(1+a), \qquad y' = y(1-a), \qquad z' = z. \tag{6}$$

As we can see from this result, in the direction of the z axis there is no mechanical strain. Therefore we will limit our considerations to the plane $z = 0$. For our calculation it is best to consider a square lying in the plane that has its centre in the origin, and the sides parallel to the axes x, y, respectively. This square will be deformed into a rectangle. The whole situation is shown in Fig. 1. The centre of the square has coordinates [0,0,0] and the coordinates of the upper right vertex are [1,1,0]. From the calculations above we get the coordinates of the point in the first domain state $[1-a, 1+a, 0]$ and in the second domain state $[1+a, 1-a, 0]$. From the figure, it follows that

$$\varphi = 90° - 2\alpha. \tag{7}$$

From this equation we get

$$\tan(\varphi/2) = \tan(45° - \alpha) = \frac{1 - \tan\alpha}{1 + \tan\alpha} = a. \tag{8}$$

Since the value of a is very small in reality, we can use the approximation $\tan\ x \approx x$, therefore the result is

$$\varphi = 2a. \tag{9}$$

The geometrical approach can hardly be generalized and can lead to many difficulties, e.g. in the case of Cubic → Trigonal transition, when the trigonal axis is parallel to [111]. In fact the example shown above is probably the simplest case of a phase transition. Therefore we need to find a more general way of calculating the misfit angle. In the next section the algebraical approach is discussed in detail.

3.2. Algebraical approach

Let us consider the spontaneous strain tensor ε^1 for the first domain state and ε^2 for the second domain state. Now we will assume that there can exist a permissible domain wall between these two domain states. Let us consider an arbitrary vector $\boldsymbol{x}$ that lies in the domain wall. The elongation of this vector after the spontaneous strain in the individual domain states is (in Einstein's notation)

$$\text{DS1}: \qquad \Delta x^1 = \frac{\varepsilon^1_{ij} x_i x_j}{|\boldsymbol{x}|}, \tag{10}$$

$$\text{DS2}: \qquad \Delta x^2 = \frac{\varepsilon^2_{ij} x_i x_j}{|\boldsymbol{x}|}. \tag{11}$$

Since a permissible domain wall should be formed, it must hold

$$\Delta x^1 = \Delta x^2. \tag{12}$$

The equation of the permissible wall is then

$$(\varepsilon^1_{ij} - \varepsilon^2_{ij}) x_i x_j = 0 \tag{13}$$

and after substituting from (2) we get

$$\delta_{ij} x_i x_j = 0. \tag{14}$$

Equation (14) is the equation of the surface of a cone with the apex lying in the origin [1]. This solution, however, is not physically acceptable, because the domain wall must be independent of the choice of the origin. Therefore this solution must be rejected unless the cone surface degenerates into a plane. This condition is expressed as

$$\begin{vmatrix} \delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & \delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & \delta_{33} \end{vmatrix} = 0. \tag{15}$$

For very small deformations, which is our case, the misfit angle of the domain states is given as the eigenvalue of the spontaneous strain difference tensor.

The eigenvalues λ of the spontaneous strain difference tensor δ can be found as solutions of the secular equation

$$\lambda^3 - J_1 \lambda^2 + J_2 \lambda - J_3 = 0, \tag{16}$$

where $J_1 = \delta_{11} + \delta_{22} + \delta_{33}$, $J_2 = \begin{vmatrix} \delta_{11} & \delta_{12} \\ \delta_{21} & \delta_{22} \end{vmatrix} + \begin{vmatrix} \delta_{22} & \delta_{23} \\ \delta_{32} & \delta_{33} \end{vmatrix} + \begin{vmatrix} \delta_{11} & \delta_{13} \\ \delta_{31} & \delta_{33} \end{vmatrix}$, $J_3 = \begin{vmatrix} \delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & \delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & \delta_{33} \end{vmatrix}$. In our case, the equation will be simplified, since $J_1 = 0$ according to (3) and $J_3 = 0$ according to (15). Equation (16) then takes on the following form:

$$\lambda^3 + J_2 \lambda = 0. \tag{17}$$

Thus, the desired eigenvalues are

$$\lambda_1 = 0, \qquad \lambda_{2,3} = \pm\sqrt{-J_2}. \tag{18}$$

Therefore, the non-zero misfit angle is given as

$$\varphi = \pm\sqrt{-J_2}. \tag{19}$$

3.3. Calculating all possible angles for a phase transition

Using the above method, all possible misfit angles for all ferroelastic phase transitions were calculated. For each ferroelastic phase transition one must take all pairs of domain states. For each domain pair, it is necessary to calculate the spontaneous strain difference tensor, check if the determinant was zero, and if so, then calculate the misfit angle using the formula (19). In the list of results, all species belonging to the phase transition, the spontaneous strain for the first domain state and all possible misfit angles are listed for each phase transition.

As an example, let us consider the phase transition Tetragonal 2 → Triclinic. The spontaneous strain tensors for the four possible domain states are as follows:

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \varepsilon^2 = \begin{pmatrix} a & -b & -d \\ -b & -a & c \\ -d & c & 0 \end{pmatrix},$$

$$\varepsilon^3 = \begin{pmatrix} -a & b & -c \\ b & a & -d \\ -c & -d & 0 \end{pmatrix}, \qquad \varepsilon^4 = \begin{pmatrix} a & -b & d \\ -b & -a & -c \\ d & -c & 0 \end{pmatrix}.$$

Now let us evaluate the spontaneous strain difference tensor for all possible pairs

$$\delta_{1,2} = \begin{pmatrix} -2a & 2b & c+d \\ 2b & 2a & d-c \\ c+d & d-c & 0 \end{pmatrix}, \qquad \delta_{1,3} = \begin{pmatrix} 0 & 0 & 2c \\ 0 & 0 & 2d \\ 2c & 2d & 0 \end{pmatrix},$$

$$\delta_{1,4} = \begin{pmatrix} -2a & 2b & c-d \\ 2b & 2a & c+d \\ c-d & c+d & 0 \end{pmatrix}, \qquad \delta_{2,3} = \begin{pmatrix} 2a & -2b & c-d \\ -2b & -2a & c+d \\ c-d & c+d & 0 \end{pmatrix},$$

$$\delta_{2,4} = \begin{pmatrix} 0 & 0 & -2d \\ 0 & 0 & 2c \\ -2d & 2c & 0 \end{pmatrix}, \qquad \delta_{3,4} = \begin{pmatrix} -2a & 2b & -c-d \\ 2b & 2a & c-d \\ -c-d & c-d & 0 \end{pmatrix}.$$

Only the cases of domain pairs S1, S3 and S2, S4 yield a zero determinant. For these pairs we get the same result and the only possible angle for this type of phase transition

$$\varphi = \pm 2\sqrt{c^2+d^2}.$$

4. List of results

Cubic 1 → Tetragonal 1
$432F422, \bar{4}3mF\bar{4}2m, m3mF4/mmm$
$x, y, z||$cubic axes; in S1, the tetragonal axis (ferr.)$||x$

$$\varepsilon^1 = \begin{pmatrix} -2b & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b \end{pmatrix}, \qquad \varphi = \pm 3|b|.$$

Cubic → Trigonal
$23F3, m3F\bar{3}, 432F32, \bar{4}3mF3m, m3mF\bar{3}m$
$x, y, z||$cubic axes; in S1, the trigonal axis (ferr.)$||[111]$

$$\varepsilon^1 = \begin{pmatrix} 0 & d & d \\ d & 0 & d \\ d & d & 0 \end{pmatrix}, \qquad \varphi = \pm 2\sqrt{2}|d|.$$

Cubic 1 → Orthorhombic (P)
$432F222, \bar{4}3mF222, m3mFmmm$
$x, y, z||$cubic axes

$$\varepsilon^1 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm|b-c|, \\ \varphi = \pm|a-c|, \\ \varphi = \pm|a-b|. \end{array}$$

Cubic 1 → Orthorhombic (S)
$432F222, \bar{4}3mF222, m3mFmmm$
$x, y, z||$cubic axes; in S1, the orthorhombic axis (ferr.)$||x$

$$\varepsilon^1 = \begin{pmatrix} -2b & 0 & 0 \\ 0 & b & d \\ 0 & d & b \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2|d|, \\ \varphi = \pm\sqrt{9b^2 + 2d^2}. \end{array}$$

Cubic 1 → Monoclinic (P)
$432F2(p), \bar{4}3mF2, m3mF2/m(p)$
$x, y, z||$cubic axes; in S1, 2 (ferr.)$||x$

$$\varepsilon^1 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & d \\ 0 & d & c \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2|d|, \\ \varphi = \pm|b-c|, \\ \varphi = \pm\sqrt{b^2 - 2bc + c^2 + 4d^2}, \\ \varphi = \pm\sqrt{a^2 - 2ab + b^2 + 2d^2}, \\ \varphi = \pm\sqrt{a^2 - 2ac + c^2 + 2d^2}. \end{array}$$

Cubic 1 → Monoclinic (S)
$432F2(s), \bar{4}3mFm, m3mF2/m(s)$
$x, y, z||$cubic axes; in S1, the monoclinic axis$||[01\bar{1}]$

$$\varepsilon^1 = \begin{pmatrix} -2b & e & e \\ e & b & d \\ e & d & b \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{2}|e|, \\ \varphi = \pm 2\sqrt{d^2 + e^2}, \\ \varphi = \pm\sqrt{9b^2 + 2d^2 + 6e^2}, \\ \varphi = \pm\sqrt{9b^2 + 2d^2 + 4de + 2e^2}, \\ \varphi = \pm\sqrt{9b^2 + 2d^2 - 4de + 2e^2}. \end{array}$$

Cubic 1 → Triclinic
$432F1, \bar{4}3mF1, m3mF\bar{1}$
$x, y, z||$cubic axes

$$\varepsilon^1 = \begin{pmatrix} a & f & e \\ f & b & d \\ e & d & c \end{pmatrix}, \qquad \begin{array}{ll} \varphi = \pm 2\sqrt{e^2 + f^2}, & \varphi = \pm 2\sqrt{d^2 + f^2}, \\ \varphi = \pm 2\sqrt{d^2 + e^2}, & \varphi = \pm\sqrt{2}|e-f|, \\ \varphi = \pm\sqrt{2}|e+f|, & \varphi = \pm\sqrt{2}|d-e|, \\ \varphi = \pm\sqrt{2}|d+e|, & \varphi = \pm\sqrt{2}|d-f|, \\ \varphi = \pm\sqrt{2}|d+f|. & \end{array}$$

Cubic 2 → Orthorhombic
$23F222, m3Fmmm$
$x, y, z||$cubic axes

$$\varepsilon^1 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}, \text{ no permissible domain walls.}$$

Cubic 2 → Monoclinic
$23F2, m3F2/m$
$x, y, z||$cubic axes; in S1, 2 (ferr.)$||x$

$$\varepsilon^1 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & d \\ 0 & d & c \end{pmatrix}, \qquad \varphi = \pm 2|d|.$$

Cubic 2 → Triclinic
$23F1, m3F\bar{1}$
$x, y, z||$cubic axes

$$\varepsilon^1 = \begin{pmatrix} a & f & e \\ f & b & d \\ e & d & c \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{e^2 + f^2}, \\ \varphi = \pm 2\sqrt{d^2 + f^2}, \\ \varphi = \pm 2\sqrt{d^2 + e^2}. \end{array}$$

Hexagonal 1 → Orthorhombic
$622F22, 6mmFmm2, \bar{6}m2Fmm2, 6/mmmFmmm$
$z||6$ or $\bar{6}, x||2$ or $\perp m$; in S1, $x||$the orthorhombic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} -a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm\sqrt{3}|a|.$$

Hexagonal 1 → Monoclinic (P)
$622F2, 6mmF2, \bar{6}m2Fm, 6/mmmF2/m$
$z||6$ or $\bar{6}, x||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} -a & b & 0 \\ b & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2|b|, \\ \varphi = \pm\sqrt{3}\sqrt{a^2 + b^2}, \\ \varphi = \pm|\sqrt{3}a + b|, \\ \varphi = \pm\sqrt{3}\sqrt{a^2 + b^2}, \\ \varphi = \pm|\sqrt{3}a - b|. \end{array}$$

Hexagonal 1 → Monoclinic (S)
$622F2, 6mmF2, \bar{6}m2Fm, 6/mmmF2/m$
$z||6$ or $\bar{6}, y||2$ or $\perp m$; in S1, $y||$the monoclinic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} -a & 0 & c \\ 0 & a & 0 \\ c & 0 & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm\sqrt{3a^2 + c^2}, \\ \varphi = \pm\sqrt{3}\sqrt{a^2 + c^2}, \\ \varphi = \pm 2|c|, \\ \varphi = \pm\sqrt{3}\sqrt{a^2 + c^2}, \\ \varphi = \pm\sqrt{3a^2 + c^2}. \end{array}$$

Hexagonal 1 → Triclinic
$622F1, 6mmF1, \bar{6}m2F1, 6/mmmF\bar{1}$
$z||6$ or $\bar{6}$, $x||2$ or $\perp m$; in S1, $x||$the hexagonal axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{b^2+c^2}, \\ \varphi = \pm 2\sqrt{b^2+d^2}, \\ \varphi = \pm 2\sqrt{c^2+d^2}, \\ \varphi = \pm\sqrt{3a^2+2\sqrt{3}ab+b^2+3c^2+2\sqrt{3}cd+d^2}, \\ \varphi = \pm\sqrt{3a^2+2\sqrt{3}ab+b^2+c^2-2\sqrt{3}cd+3d^2}, \\ \varphi = \pm\sqrt{3a^2-2\sqrt{3}ab+b^2+3c^2-2\sqrt{3}cd+d^2}, \\ \varphi = \pm\sqrt{3a^2-2\sqrt{3}ab+b^2+c^2+2\sqrt{3}cd+3d^2}. \end{array}$$

Hexagonal 2 → Monoclinic
$6F2, \bar{6}Fm, 6/mF2/m$
$z||6$ or $\bar{6}$

$$\varepsilon^1 = \begin{pmatrix} -a & b & 0 \\ b & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm\sqrt{3(a^2+b^2)}.$$

Hexagonal 2 → Triclinic
$6F1, \bar{6}F1, 6/mF\bar{1}$
$z||6$ or $\bar{6}, x||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \varphi = \pm 2\sqrt{c^2+d^2}.$$

Tetragonal 1 → Orthorhombic (P)
$422F222, 4mmFmm2, \bar{4}2mF222, \bar{4}2mFmm2, 4/mmmFmmm$
$z||4$ or $\bar{4}, x||$the orthorhombic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} -a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm 2|a|.$$

Tetragonal 1 → Orthorhombic (S)
$422F222, 4mmFmm2, \bar{4}2mF222, \bar{4}2mFmm2, 4/mmmFmmm$
$z||4$ or $\bar{4}, x||2$ or $\perp m$; $x\langle 45^\circ\rangle$ the orthorhombic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} 0 & a & 0 \\ a & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm 2|a|.$$

Tetragonal 1 → Monoclinic (P)
$422F2, 4mmF2, \bar{4}2mF2, 4/mmm2/m$
$z||4$ or $\bar{4}, x||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} -a & b & 0 \\ b & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2|b|, \\ \varphi = \pm 2\sqrt{a^2+b^2}, \\ \varphi = \pm 2|a|. \end{array}$$

Tetragonal 1 → Monoclinic (S)
$422F2, 4mmF2, \bar{4}2mF2, 4/mmm2/m$
$z||4$ or $\bar{4}, y||2$ or $\perp m$; in S1, $y||$the monoclinic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} -a & 0 & b \\ 0 & a & 0 \\ b & 0 & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm\sqrt{2}\sqrt{2a^2 + b^2}, \\ \varphi = \pm 2|b|. \end{array}$$

Tetragonal 1 → Monoclinic (S)
$422F2, 4mmF2, \bar{4}2mF2, 4/mmm2/m$
$z||4$ or $\bar{4}, x||2$ or $\perp m$; $x\langle 45^\circ \rangle$ the monoclinic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} 0 & a & c \\ a & 0 & c \\ c & c & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{a^2 + c^2}, \\ \varphi = \pm 2\sqrt{2}|c|. \end{array}$$

Tetragonal 1 → Triclinic
$422F1, 4mmF1, \bar{4}2mF1, 4/mmmF\bar{1}$
$z||4$ or $\bar{4}, x||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{b^2 + c^2}, \\ \varphi = \pm 2\sqrt{b^2 + d^2}, \\ \varphi = \pm 2\sqrt{c^2 + d^2}, \\ \varphi = \pm\sqrt{2}\sqrt{2a^2 + c^2 - 2cd + d^2}, \\ \varphi = \pm\sqrt{2}\sqrt{2a^2 + c^2 + 2cd + d^2}. \end{array}$$

Tetragonal 2 → Monoclinic
$4F2, \bar{4}F2, 4/mF2/m$
$z||4$ or $\bar{4}$

$$\varepsilon^1 = \begin{pmatrix} -a & b & 0 \\ b & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm 2\sqrt{a^2 + b^2}.$$

Tetragonal 2 → Triclinic
$4F1, \bar{4}F1, 4/mF\bar{1}$
$z||4$ or $\bar{4}$

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \varphi = \pm 2\sqrt{c^2 + d^2}.$$

Trigonal 1 → Monoclinic
$32F2, 3mFm, \bar{3}mF2/m$
$z||3, y||2$ or $\perp m$; in S1, $y||$ the monoclinic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} -a & 0 & c \\ 0 & a & 0 \\ c & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm\sqrt{3(a^2 + c^2)}.$$

Tetragonal 1 → Monocpage Trigonal 1 → Triclinic
$32F1, 3mF1, \bar{3}mF\bar{1}$
$z||3, x||2$ or $x||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{b^2+c^2}, \\ \varphi = \pm\sqrt{3a^2 - 2\sqrt{3}ab + b^2 + (c+\sqrt{3}d)^2}, \\ \varphi = \pm\sqrt{3a^2 + 2\sqrt{3}ab + b^2 + (c-\sqrt{3}d)^2}. \end{array}$$

Trigonal 1 → Triclinic
$32F1, 3mF1, \bar{3}mF\bar{1}$
$z||3, y||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{b^2+d^2}, \\ \varphi = \pm\sqrt{3a^2 - 2\sqrt{3}ab + b^2 + 3c^2 - 2\sqrt{3}cd + d^2}, \\ \varphi = \pm\sqrt{3a^2 + 2\sqrt{3}ab + b^2 + 3c^2 + 2\sqrt{3}cd + d^2}. \end{array}$$

Trigonal 2 → Triclinic
$3F1, \bar{3}F\bar{1}$
$z||3$

$$\varepsilon^1 = \begin{pmatrix} -a & b & c \\ b & a & d \\ c & d & 0 \end{pmatrix}, \text{ no permissible domain walls.}$$

Orthorhombic → Monoclinic
$222F2, mm2F2, mm2Fm, mmmF2/m$
$x, y, z||$the orthorhombic axes; $y||$ the monoclinic axis (ferr.)

$$\varepsilon^1 = \begin{pmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 0 \end{pmatrix}, \qquad \varphi = \pm 2|b|.$$

Orthorhombic → Triclinic
$222F1, mm2F1, mmmF\bar{1}$
$x, y, z||$the orthorhombic axes

$$\varepsilon^1 = \begin{pmatrix} 0 & c & b \\ c & 0 & a \\ b & a & 0 \end{pmatrix}, \qquad \begin{array}{l} \varphi = \pm 2\sqrt{b^2+c^2}, \\ \varphi = \pm 2\sqrt{a^2+c^2}, \\ \varphi = \pm 2\sqrt{a^2+b^2}. \end{array}$$

Monoclinic → Triclinic
$2F1, mF1, 2/mF\bar{1}$
$y||2$ or $\perp m$

$$\varepsilon^1 = \begin{pmatrix} 0 & a & 0 \\ a & 0 & b \\ 0 & b & 0 \end{pmatrix}, \qquad \varphi = \pm 2\sqrt{a^2+b^2}.$$

5. Conclusion

The aim of this work was to calculate the misfit angles of domain states joining in a permissible planar domain wall, which satisfies all the conditions of mechanical compatibility. The explicit formulae, giving the result as a function of the spontaneous strain tensor for the first domain state, have been derived for all 30 possible types of ferroelastic phase transitions, in which the compatible domain wall can be formed. In the cases, where there are more than two possible ferroelastic domain states, all different pairs of domain states have been investigated. For six types of phase transitions the results correspond with the results obtained by Shuvalov et al. [4]. For the remaining 24, the explicit formulae for the misfit angles have not been published before.

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