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Twinning elements of 2-nd order derived from crystal lattice parameters in central-symmetrical ferroelastics

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The algorithm for determination of possible second order twinning laws–mirror planes and twofold axes is presented. The method is applicable for center-symmetrical ferroelastics and/or twins with non-zero obliquity. The proposed algorithm allows to determine twinning elements using only known crystal lattice parameters without additional analysis of correlation of para- and ferroelastic phase point groups or using other theoretical methods of twin structure forecast.

Представлен алгоритм определения возможных законов двойникования плоскостей зеркального отражения и осей 2-го порядка. Данный метод может быть применен к центросимметричным сегнетоэластикам и/или двойникам с ненулевым отклонением. Предложенный алгоритм позволяет найти элементы двойникования, используя только известные параметры кристаллической решетки без дополнительного анализа соотношения точечных групп пара- и сегнетоэластичных фаз или других теоретических методов определения параметров двойниковой структуры.

Physical and chemical properties of crystalline materials are directly related to their global crystal structure as well as to their microstructure. Specific features of some crystalline materials causes the subdivision thereof into ferroelastic, ferroelectric domains known as twins and hence, a further type of real structure appears referred to as domain structure. The domains are crystalline areas consisting of the same material joined together by certain symmetry element, which does not belong to the space group symmetry of a single domain of the sample. The different domains are equivalent in energy. The ferroelastic structure inherent in domains complicates essentially the crystal structure investigation and the determination of their physical and chemical properties, especially the anisotropies. The behavior of domains may strongly influence the material properties, for example, the configuration of the magnetic domain structure in solid solutions of rare earth manganites [1]. The interaction of defects in oxide sublattice with domain boundaries determines a series of physical properties in materials with perovskite-like structure, which have found numerous technical applications in last years. Among those, there is a large group of compounds having unique dielectric, ferroelectric properties [2–5], as well as ionic [6, 7] and high-temperature conductivity [8].

Twinning has long been considered to be one of the most serious potential hindrances to structure determination. The twinning can significantly complicate the structure solution/refinement process. Numerous definitions, approaches and computer programs specifically intended for the data processing and real structure determination of twinned crystals were developed [9–11]. These methods can be helpful only when a crystallographer has correctly identified the twinning laws.

An informative and often used investigation method of domain structure is electron microscopy, which supplies high resolution on submicron as well as submillimeter scale [12–15]. Furthermore, possibility of parallel use of selective electron diffraction in different areas of sample makes it possible to find orientation of the selected zones. At the same time, for interpretation of obtained images, a complicated simulation is necessary [16] when different symmetry models of connection (twinning elements) between investigated orientation states should be postulated. This, in part, demands complicated and time-consuming analysis of possible configurations of ferroelastic domain structure using theoretical group analysis [17], method of spontaneous strain tensors (Sapriel's method) [18] or theory of mechanical twinning [19, 20]. Neglecting of these theoretical methods often results in incorrect interpretation.

The purpose of this work is to provide the fundamental concepts and algorithm for determination of possible second order twinning laws — mirror planes and twofold axes. The method presented is applicable for center-symmetrical ferroelastics and/or so-called twins with non-zero obliquity.

Fundamental concepts. Domains can originate in three different ways: 1) when the nuclei are collided during crystal growth and a new domain is added to the face of an already existing domain, but has an orientation different from the first domain; 2) when a pre-existent crystal undergoes a polymorphic transformation due to a temperature change; 3) can be induced by some applied external (mechanical, electrical) fields.

In literature [21], there are several definitions of twinning, which depend on delimitation conception. One of the oldest classifications is the "crystallographic-mineralogical", which was summarized in [22]. Based upon their diffraction patterns, twinned crystals may be grouped into four general categories: merohedral, reticular merohedral, pseudo-merohedral and reticular pseudo-merohedral. A coarser classification was introduced in [23], where zero-obliquity twins (Twin Lattice Symmetry: TLS) and non-zero obliquity twins (Twin Lattice Quasi Symmetry: TLQS) are distinguished. This classification puts more emphasis on the role of a specific parameter, the twin obliquity w, which is responsible for the splitting of the reflections in the diffraction pattern of a twinned sample. A more detailed description of the "crystallographic-mineralogical" classification is presented, for example, at [21, 24].

Another ("physical") definition of domains is based on phenomenological concept of transformation twins. In 1969, K.Aizu [25] has introduced a special definition "ferroics" into solid state physics. According to his definition, ferroics are a class of crystalline solids in which two or more orientation states (domains) can appear in the absence of external magnetic, electric or mechanical fields and switch from one to another under magnetic (ferromagnetics), electric (ferroelectrics) fields and mechanical stress (ferroelastics) or their combination. For characterization of ferroics, Aizu introduced also the concept of "species", which includes two point groups. The first is a certain nonferroic point group G, which was referred to as the "prototype". The second is a point group F of ferroic phase being considered, which can be considered as a slight modification of the "prototype" phase. The symmetry of ferromagnetic domains is characterized by specific magnetic groups, which are combination (integration) of space groups with specific magnetic symmetry element — time-inversion, and it will be not further considered in this work.

It was shown [17] that the comparison of point groups (the symmetry elements thereof) of the G prototype phase and F ferroic one allows to determine the number of possible domains (domain states), symmetry elements, which connect these states, and the orientation of some (not all) possible domain walls. If F is the point group of the D_1 orientation state and g_j is the operation transforming from the D_1 state to the D_j state (including D_1), then the set of all operations connecting D_1 and D_j is $g_i \cdot F$. This means that each state D_j has its corresponding left coset H_i of the subgroup F in which G can be expressed [17]:

$$G = H_1 + H_2 + \dots + H_q, \qquad (1)$$

where $H_i = g_i \cdot F$ and $i = 1 \dots q$. Here, the number q of possible orientation states in the ferroic phase is equal to the order of the G point group in the prototype phase divided by the order of the F subgroup in the ferroic phase: $q = n_G/n_F$.

Strain-free domain walls can exist between two orientation states only when corresponding "connection" elements $g_j \in H_i$

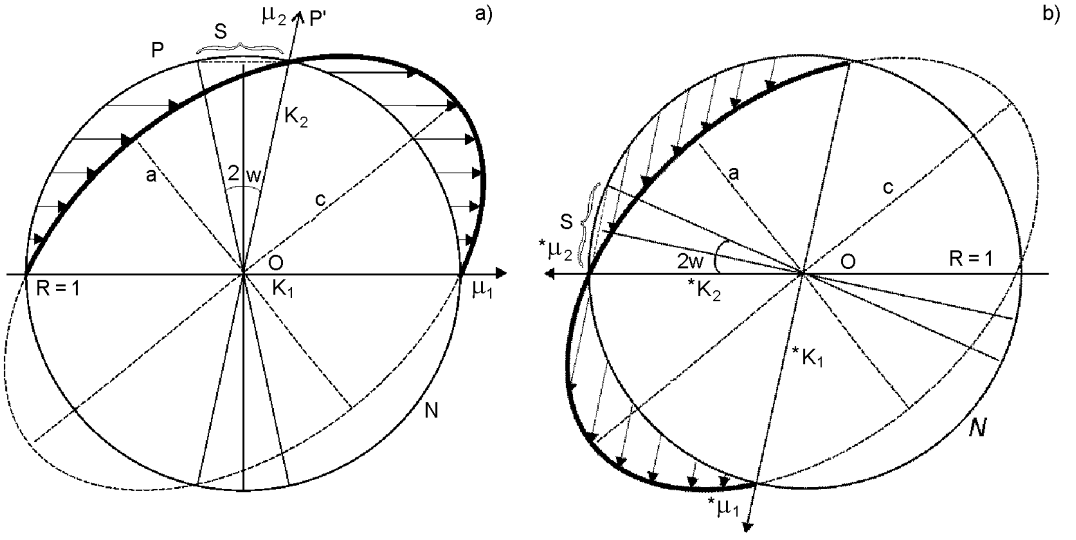

Fig. 1. Conjugated systems of twinning and twinning elements: K_1 is the composition plane; μ_1, the shear direction; K_2, the second circular cross-section; μ_2, the axis of the principal zone; N, the displacement plane (the plane of the Figure); s, the displacement value.

meet the condition of orientation state permutation. This means that if g_j applied to D_1 yields D_i, then the same operation g_j upon D_i should yield D_1, that indicates the equivalency of D_1 and D_j orientation states. Thus, the ambivalence condition [17] should be met to ensure that the condition of orientation states permutation is also fulfilled:

$$g_i^2 \in F. \qquad (2)$$

If the domains are connected with a mirror plane, this plane may be a composition plane W between corresponding domains. This is obvious from the fact that the repeated mirror reflection with respect to the same m plane results in the identical transformation E of an object in itself

$$m \times m = E. \qquad (3)$$

The 2nd order rotation also meets the ambivalence condition:

$$2 \times 2 = E. \qquad (4)$$

Hence, if there is a twofold axis among the elements connecting D_1 and D_i orientation states, the plane containing this axis may be a domain wall between these orientation states (S-wall). In contrast to W-walls, the orientation of this wall may have nonintegral Miller indices. In center-symmetrical ferroics, the left coset H_j can contain both the mirror plane and twofold axis which is perpendicular (in the prototype phase) to this plane:

$$\text{if } m \in H_j \text{ then } m \times C = 2 \text{ and } 2 \in H_j, \text{ because } C \in F, \qquad (5)$$

$$\text{if } 2 \in H_j \text{ then } 2 \times C = m \text{ and } m \in H_j, \text{ because } C \in F. \qquad (6)$$

It should be noted that center-symmetrical ferroics can be only ferroelastics. Ferroelastic domains can be switched from one domain state to another under mechanical stress of certain value and direction. The influence of a specifically oriented external mechanical stress can cause the shear of particular regions of the monodomain ferroelastic crystal and transform it into a bidomain sample. The relative position of two twin states can be formally described as a result of the uniform deformation through the simple shear, i.e., appearing of new ferroelastic (orientation) domain can be considered as the mechanical twinning. At the same time, twinning elements are point group symmetry elements lost at phase transition. Those are mirror planes and twofold axes of prototype phase. According to the "crystallographic-mineralogical" classification, the origination of such two domains is referred to as pseudo-merohedral twinning and characterized by a specific parameter, the *twin obliquity* ω [22].

The homogeneous strain is completely defined by an ellipsoid into which an imaginary sphere within the body is transformed (Fig. 1a). The K_1 twinning plane is a domain wall between a pair of orientation domains, with the first domain initially existing and the second one being formed through the twin shear from a certain region of the first domain. The second circular cross-section K_2 is a plane where all vectors do not change their lengths, however, being rotated at the $2w$ angle. The plane coincident with the Figure is called the displacement plane N. The trace of the intersection of the 2nd circular cross-section K_2 and the displacement plane N is denoted μ_2 and referred to as the principal zone axis [19, 20].

Fig. 1b shows that the same ellipsoid can be derived through the twin shear of cell sites at the same distance s in the direction μ_2. In this case, the composition (twinning) plane separating the distorted part (semi-ellipse) and non-distorted part of the crystal (semi-sphere) is the K_2 plane. In this new case, the second circular cross-section is K_1, and μ_1 is the axis of the principal zone. Hence, if there is a twin shear with elements K_1, K_2, μ_1 and μ_2 in the crystal, then another twin system with twin shear elements K_1^*, K_2^*, μ_1^* and μ_2^* may exist in the central-symmetric crystal:

$$K_1^* = K_2,\ K_2^* = K_1,\ \mu_1^* = \mu_2 \text{ and } \mu_2^* = \mu_1. \quad (7)$$

In the first case, the twin and the non-distorted part are separated by plane K_1, in the second case, by $K_1^* = K_2$. The plane K_1^* is almost perpendicular to plane K_1 for a small value s of the crystallographic shear. The twinning elements can be associated with planes and directions of the crystal cell taking into account the discrete atomic structure of the crystal. In the first case, if K_1 and μ_2 have integer Miller indices (HKL) and [UVW], then a new lattice formed by the twinning shear is connected with the non-displaced lattice by the mirror reflection relatively to plane K_1. In this case, the twin is called *reflection twin*. Then, according to (7), for another twin system, μ_1^* and K_2^* have integer Miller indices, and K_1^* and μ_2^* are irrational. In this case, the new lattice is connected with the lattice in the non-displaced region through the 180° rotation around $\mu_1^* = [UVW]$. This twin is called *rotation twin*, because twin states are connected by twofold axis. Such two twin systems are called corresponding twins with the same twin obliquity w for both reflection and rotation twins [19].

The domains formed through the twin shear from a certain region of the first domain D_1 in both cases (reflection and rotation twins) belong to the same state D_j, because they correspond to the same left coset H_j, which contains the mirror plane ($H_jK_jL_j$) as well as the twofold axis [$U_jV_jW_j$] (see eq.(5) and (6)).

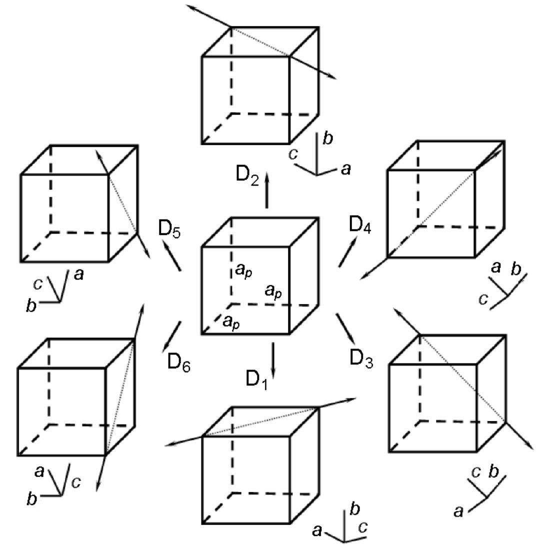

Fig. 2. The spatial orientation of domain (twinned) orientation states of a $La_{0.95}Sr_{0.05}Ga_{0.9}Mg_{0.1}O_{2.925}$ crystal in the orthorhombic phase and corresponding deformations of the perovskite cell.

The Miller indices for crystallographic planes of D_1 and D_j orientation states are connected by Mugge transformation [26]:

$$\begin{aligned} h_{ji} &= 2H_j(U_j \cdot h_{1i} + V_j \cdot k_{1i} + W_j \cdot l_{1i}) - \\ &\quad - h_{1i}(U_j \cdot H_j + V_j \cdot K_j + W_j \cdot L_j), \\ k_{ji} &= 2K_j(U_j \cdot h_{1i} + V_j \cdot k_{1i} + W_j \cdot l_{1i}) - \\ &\quad - k_{1i}(U_j \cdot H_j + V_j \cdot K_j + W_j \cdot L_j), \\ l_{ji} &= 2L_j(U_j \cdot h_{1i} + V_j \cdot k_{1i} + W_j \cdot l_{1i}) - \\ &\quad - l_{1i}(U_j \cdot H_j + V_j \cdot K_j + W_j \cdot L_j), \end{aligned} \quad (8)$$

where ($h_{1i}k_{1i}l_{1i}$) are Miller indices of the planes in orientation state D_1 and ($h_{ji}k_{ji}l_{ji}$), those in orientation state D_j, which appears after a shear. In the case when states D_1 and D_j are connected by mirror plane, ($H_jK_jL_j$) are the indices of composition plane K_1, [$U_jV_jW_j$] are indices of the axis of the principal zone μ_2. When the states are connected by twofold axis, ($H_jK_jL_j$) are indices of K_2^*, and [$U_jV_jW_j$] are indices of the shear direction μ_1^*.

Determination algorithm for the twinning elements. The proposed algorithm of twinning elements, determination is based on Aizus concept that considers the ferroelastic phase transition as a slight distortion of paraelastic (the prototype) unit cell with symmetry point group G. The resulting ferroelastic phase cell has point group F, which is subgroup of G. Furthermore, potential above-mentioned distortion can be realized in q ways, i.e., q different orientation states can appear within the ferroelastic phase, where $q = n_G/n_F$ [17]. The lattice sites (ions, atoms) which formed a crystallographic plane in paraelastic phase, in ferroelastic phase will also form a crystallographic plane with another space position depending on the mode of distortion, i.e. realized domain state. The planes in different states will be indexed differently, due to different orientations of the lattice basis. Nevertheless, in different states, the space disorientation of neogenic planes relatively to the positions of corresponding planes in paraelastic phase is very small due to minor displacements which is typical of ferroelastic phase transitions.

If we consider an arbitrary pair of crystallographic planes in paraelastic phase, then corresponding plane pairs can be found in all possible domain states of ferroelastic phase. Now, if we take into account that their space positions are close to those in paraelastic phase, then we can assert that the angles between above-mentioned pair of planes in all domain states of ferroelastic phase are close to that in paraelastic phase. As a rule, value of angle changes does not exceed few degrees for hard ferroelastics and is smaller than one degree for soft ones.

Let us consider as an example the ferroelastic transition $m3mFmmm$ ($q = 48/8 = 6$), which is typical of most perovskite-like ferroelastics, including, for example, rare earth gallates, aluminates, manganites, etc. The transformation can be considered as stretching of ideal perovskite cubic lattice along 6 different face diagonals of cube. Space orientations of these possible domain states in orthorhombic phase are shown in Fig. 2. In Fig. 3, two crystallographic planes $(100)_p$ and $(110)_p$ are marked in perovskite paraelastic lattice. At the phase transition to the D_1 state of ferroelastic phase, these planes become transformed into $(101)_o$ and $(100)_o$ planes, and in the case of D_2 state, into $(101)_o$ and $(001)_o$, respectively (Fig. 3). As is seen, the Miller indices of one plane $(100)_p$ are the same in both orientation states since that is just the plane being the boundary between the both states, while the second plane $(110)_p$ is transformed into crystallographic planes with different indices, $(100)_o$ or $(001)_o$ in setting of orthorhombic phase. For example, in LSGM05 crystal the angle between the marked planes forms $\alpha = 45°$ in paraelastic cubic phase, while it will be equal to $\alpha_1 = 44.798°$ in domain state D_1 and $\alpha_2 = 45.202°$ in D_2 state after phase transformation to orthorhombic structure. Hence, a difference between α_1 and α_2 is equal to 0.404° at room temperature.

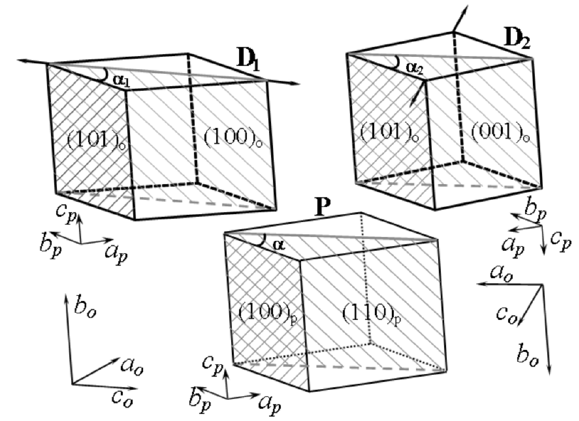

Fig. 3. Angle transformation between two crystallographic planes at ferroelastic phase transition. Two planes $(100)_p$ and $(110)_p$, marked in paraelastic cubic phase, are transformed into $(101)_o$ and $(100)_o$ of D_1 state and $(101)_o$ and $(001)_o$ of D_2 state in orthorhombic ferroelastic phase of LSGM crystal.

In the proposed algorithm, we use an indexing method of laue diffraction patterns, for example, see [27]. The indexing algorithm is based on determination of Cartesian coordinates for N spots in a Laue pattern (optimal value $N = 6$) and comparison of the angular distances separating the selected spots ($\alpha_1^{\mathrm{exp}}...\alpha_m^{\mathrm{exp}}$) calculated from the pattern with those calculated theoretically ($\alpha_1^{theor}...\alpha_m^{theor}$) starting from the known lattice parameters. For $N = 6$, $m = 15$ pairs of crystallographic planes are obtained. In the computer program, the process of spots indexing is realized by way of search of sets of angles ($\alpha_1^{theor}...\alpha_m^{theor}$), for which the angular distances α_i^{theor} fulfill next equation:

$$\alpha_i^{exp} - \varepsilon \le \alpha_i^{theor} \le \alpha_i^{exp} + \varepsilon, \tag{9}$$

where ε is a small fixed angle (tolerance). Parameter ε is preset by the user and does not exceed 1–3 degrees. As a result, a set of Miller indices for N crystallographic planes $(h_1k_1l_1)^{theor}$ ...$(h_Nk_Nl_N)^{theor}$ is determined.

The angles between these plane pairs are in the angle ranges meeting the condition (9). If the input value ε is relatively large, then more than one $(\alpha_1^{theor}...\alpha_m^{theor})$ set can be obtained, for which condition (9) is fulfilled.

In the proposed algorithm, we have modified abovementioned method for Laue pattern indexing. The user inputs Miller indices for N arbitrary crystallographic planes $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$ and then the program calculates m angular distances $(\alpha_1^{ref}...\alpha_m^{ref})$ between all pairs of planes using known lattice parameters. The calculated set of angular distances $(\alpha_1^{ref}...\alpha_m^{ref})$ is accepted as $(\alpha_1^{exp}...\alpha_m^{exp})$ and then the standard process of indexing is continued. For example, if we input N planes $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$, including planes $(101)_o$ and $(100)_o$ (we conditionally accept state D_1 as the reference domain state $D_1 = D_{ref}$), then in the set of calculated angles $(\alpha_1^{ref}...\alpha_m^{ref})$ we obtain $\alpha_k^{ref} = 44.798°$. At the end of indexing procedure, the same set $(h_1k_1l_1)^{ref}$ ... $(h_Nk_Nl_N)^{ref}$ with planes $(101)_o$ and $(100)_o$ will be obtained. Besides, since a tolerance ε was input, for example, $\varepsilon = 0.5°$, then one more set $(h_1k_1l_1)^{ref2}$ ...$(h_Nk_Nl_N)^{ref2}$ including planes $(101)_o$ and $(001)_o$ will be obtained. That is, apart from the set $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$ input by the user, that corresponds to state D_1, we obtain second set of planes (second solution), which corresponds to state D_2.

In this example, the angle between the planes is 45° in paraelastic cubic phase. But, if we input some planes $(h_1k_1l_1)^{ref}$ ... $(h_Nk_Nl_N)^{ref}$, for which the angles are smaller than 45°, then the differences between angles for planes of different ferroelastic domain states are also less than the difference $\alpha_1 - \alpha_2 = 0.404°$. In essence, for an LSGM crystal, 6 solutions were already obtained at tolerance $\varepsilon = 0.2°$ and conformable selection of input set $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$. These 6 different sets of plane indices correspond to 6 different states of ferroelastic orthorhombic phase in LSGM crystal (Fig. 2).

Due to small spontaneous deformation of paraelastic lattice, which is typical for ferroelastics, we obtain q sets of plane indices $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$, $(h_1k_1l_1)^{ref2}$ ...$(h_Nk_Nl_N)^{ref2}$ $(h_1k_1l_1)^{refq}$ ...$(h_Nk_Nl_N)^{refq}$ when performing the proposed "indexing" procedure. These q solutions correspond to q possible domain states in ferroelastic phase. It is significant that planes $(h_jk_jl_j)^{ref}$, $(h_jk_jl_j)^{ref2}$ ...$(h_jk_jl_j)^{refn}$ are created from the same plane of paraelastic phase $(h_jk_jl_j)^{proto}$, where $j = 1...N$, and mutually connected by equation of Mugge (8).

The obtained sets $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$, $(h_1k_1l_1)^{ref2}$ ...$(h_Nk_Nl_N)^{ref2}$ $(h_1k_1l_1)^{refn}$ ...$(h_Nk_Nl_N)^{refn}$, are further used to determine the 2nd order symmetry elements of, i.e., indices of mirror planes $(H_jK_jL_j)$ and twofold axes $[U_jV_jW_j]$ from equations of Mugge (8) for all possible domain pairs, for example, D_1 and D_j, where $j = 1...q$. Because at the end of proposed "indexing" we obtain N planes for every solution, we can write N Mugge equations (8), which connect mutually the plane indices of j-th solution $(h_1k_1l_1)^{refj}$ ...$(h_Nk_Nl_N)^{refj}$ with indices of the first (reference) one $(h_1k_1l_1)^{ref}$ ...$(h_Nk_Nl_N)^{ref}$. For N planes, we can build $3 \times N$ linear equations with only six unknown indices H_j, K_j, L_j and U_j, V_j, W_j. The unknown indices are inscribed in the equations in the form of 9 corresponding products H_jU_j, H_jV_j, H_jW_j, K_jU_j, K_jV_j, K_jW_j, L_jU_j, L_jV_j and L_jW_j. In order to get a linear equation system, we propose to create an equation system from 9 equations using indices of only three planes from N obtained ones:

$$\begin{vmatrix} h_{j1} \\ k_{j1} \\ l_{j1} \\ h_{j2} \\ k_{j2} \\ l_{j2} \\ h_{j3} \\ k_{j3} \\ l_{j3} \end{vmatrix} = \begin{vmatrix} h_{11} & 2k_{11} & 2l_{11} & 0 & -h_{11} & 0 & 0 & 0 & -h_{11} \\ -k_{11} & 0 & 0 & 2h_{11} & k_{11} & 2l_{11} & 0 & 0 & -k_{11} \\ -l_{11} & 0 & 0 & 0 & -l_{11} & 0 & 2h_{11} & 2k_{11} & l_{11} \\ h_{12} & 2k_{12} & 2l_{12} & 0 & -h_{12} & 0 & 0 & 0 & -h_{12} \\ -k_{12} & 0 & 0 & 2h_{12} & k_{12} & 2l_{12} & 0 & 0 & -k_{12} \\ -l_{12} & 0 & 0 & 0 & -l_{12} & 0 & 2h_{12} & 2k_{12} & l_{12} \\ h_{13} & 2k_{13} & 2l_{13} & 0 & -h_{13} & 0 & 0 & 0 & -h_{13} \\ -k_{13} & 0 & 0 & 2h_{13} & k_{13} & 2l_{13} & 0 & 0 & -k_{13} \\ -l_{13} & 0 & 0 & 0 & -l_{13} & 0 & 2h_{13} & 2k_{13} & l_{13} \end{vmatrix} \times \begin{vmatrix} H_jU_j \\ H_jV_j \\ H_jW_j \\ K_jU_j \\ K_jV_j \\ K_jW_j \\ L_jU_j \\ K_jV_j \\ L_jW_j \end{vmatrix}, \quad \mathbf{(10)}$$

where h_{11}, k_{11}, l_{11}, h_{12}, $k_{12\mathrm{d}}$, l_{12}, h_{13}, k_{13}, l_{13} and h_{j1}, k_{j1}, l_{j1d}, h_{j2}, k_{j2}, l_{j2}, h_{j3}, k_{j3}, l_{j3} are Miller indices of first three planes in the first (reference) and j-th solutions. The selected three planes should not belong to the same crystallographic zone, because in this case, indices of selected planes h_{11}, k_{11}, l_{11}, h_{12}, k_{12}, l_{12}, h_{13}, k_{13}, l_{13} and respectively h_{j1}, k_{j1}, l_{j1}, h_{j2}, k_{j2}, l_{j2}, h_{j3}, k_{j3}, l_{j3} are linearly independent and the determinant is not equal zero. For determination of such system, the known Kramer approach can be used.

The above-mentioned equation system can be formed for an arbitrary pair of solutions obtained after the "indexing" procedure. But, it is not needed to find twinning elements for all possible pairs of states, i.e. solutions. It is enough to determine the twinning elements between the reference D_1

and other domain states D_j, i. e., state pairs D_1-D_2, ... D_1-D_q, since for other pairs, the same twinning elements will be obtained. This follows from principle of domain state equivalence, because any arbitrary domain from q possible orientation states of ferroelastic phase can be selected as a reference domain.

If we use a large tolerance value ε, then among all the solutions, those with crystallographic planes that are close to "reference" planes and are not connected by equation of Mugge (8) may appear. This situation may arise in case of "hard" ferroelastics when a large value of tolerance ε is needed to be input. To sort out these solutions, we should take into account that indices H_j, K_j, L_j and U_j, V_j, W_j must be integers according to theory of mechanical twinning [19, 20, 26]. For "non-twin" solutions, we obtain rational indices H_j, K_j, L_j and U_j, V_j, W_j.

To conclude, the proposed algorithm allows to determine twinning elements in central-symmetrical ferroelastics using only known lattice parameters without additional analysis of correlation of para- and ferroelastic point groups or using other theoretical methods of twin structure forecast, for example, Sapriel method, etc. [17, 18].

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Визначення елементів двійникування 2-го порядку у центросиметричних сегнетоеластиках за параметрами кристалічної гратки

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Метою роботи є представлення алгоритму визначення можливих законів двійникування — площин дзеркального відображення та осей 2-го порядку. Даний метод може бути застосований до центросиметричних сегнетоеластиків та/або двійникування з ненульовим відхиленням. Запропонований алгоритм дозволяє знайти елементи двійникування, використовуючи тільки відомі параметри кристалічної гратки без додаткового аналізу співвідношень точкових груп пара- та сегнетоеластичних фаз чи інших теоретичних методів передбачення параметрів двійникової структури.