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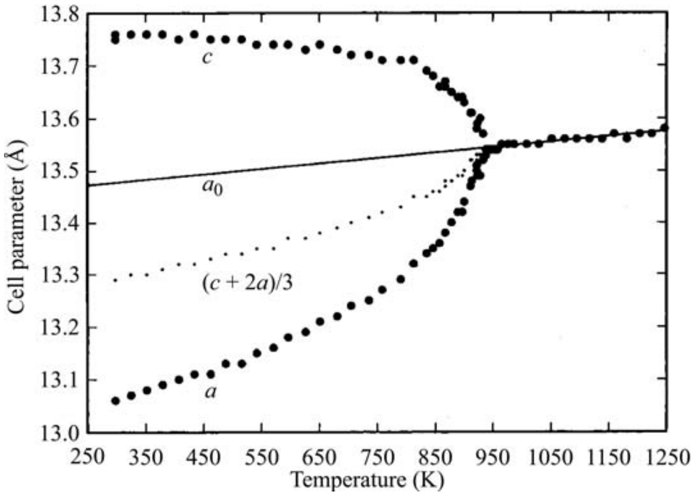

Fig. 3.4.3.4. Temperature dependence of lattice parameters in leucite. Courtesy of E. K. H Salje, University of Cambridge.

K_{1j} differs from the crystal family of the symmetry group F_1 of domain state $\mathbf{S}_1$,

$$\mathrm{Fam}K_{1j} \neq \mathrm{Fam}F_1. \qquad (3.4.3.43)$$

Before treating compatible domain walls and disorientations, we explain the basic concept of spontaneous strain.

3.4.3.6.1. *Spontaneous strain*

A *strain* describes a *change* of crystal shape (in a macroscopic description) or a change of the unit cell (in a microscopic description) under the influence of mechanical stress, temperature or electric field. If the relative changes are small, they can be described by a second-rank symmetric tensor $\mathbf{u}$ called the *Lagrangian strain*. The values of the strain components u_{ik}, $i, k = 1, 2, 3$ (or in matrix notation u_μ, $\mu = 1, \ldots, 6$) can be calculated from the 'undeformed' unit-cell parameters before deformation and 'deformed' unit-cell parameters after deformation (see Schlenker *et al.*, 1978; Salje, 1990; Carpenter *et al.*, 1998).

A *spontaneous strain* describes the change of an 'undeformed' unit cell of the high-symmetry phase into a 'deformed' unit cell of the low-symmetry phase. To exclude changes connected with thermal expansion, one demands that the parameters of the undeformed unit cell are those that the high-symmetry phase would have at the temperature at which parameters of the low-symmetry phase are measured. To determine these parameters directly is not possible, since the parameters of the high-symmetry phase can be measured only in the high-symmetry phase. One uses, therefore, different procedures in order to estimate values for the high-symmetry parameters under the external conditions to which the measured values of the low-symmetry phase refer (see *e.g.* Salje, 1990; Carpenter *et al.*, 1998). Three main strategies are illustrated using the example of leucite (see Fig. 3.4.3.4):

(i) The lattice parameters of the high-symmetry phase are extrapolated from values measured in the high-symmetry phase (a straight line a_0 in Fig. 3.4.3.4). This is a preferred approach.

(ii) For certain symmetry descents, it is possible to approximate the high-symmetry parameters in the low-symmetry phase by average values of the lattice parameters in the low-symmetry phase. Thus for example in cubic $\rightarrow$ tetragonal transitions one can take for the cubic lattice parameter $a_0 = (2a + c)/3$ (the dotted curve in Fig. 3.4.3.4), for cubic $\rightarrow$ orthorhombic transitions one may assume $a_0 = (abc)^{1/3}$, where a, b, c are the lattice parameters of the low-symmetry phase. Errors are introduced if there is a significant volume strain, as in leucite.

(iii) Thermal expansion is neglected and for the high-symmetry parameters in the low-symmetry phase one takes the lattice parameters measured in the high-symmetry phase as close as possible to the transition. This simplest method gives better results than average values in leucite, but in general may lead to significant errors.

Spontaneous strain has been examined in detail in many ferroic crystals by Carpenter *et al.* (1998).

Spontaneous strain can be divided into two parts: one that is different in all ferroelastic domain states and the other that is the same in all ferroelastic domain states. This division can be achieved by introducing a *modified strain tensor* (Aizu, 1970*b*), also called a *relative spontaneous strain* (Wadhawan, 2000):

$$\mathbf{u}^{(i)}_{(s)} = \mathbf{u}^{(i)} - \mathbf{u}^{(\mathrm{av})}_{(s)}, \qquad (3.4.3.44)$$

where $\mathbf{u}^{(i)}_{(s)}$ is the matrix of relative (modified) spontaneous strain in the ferroelastic domain state $\mathbf{R}_i$, $\mathbf{u}^{(i)}$ is the matrix of an 'absolute' spontaneous strain in the same ferroelastic domain state $\mathbf{R}_i$ and $\mathbf{u}^{(\mathrm{av})}_{(s)}$ is the matrix of an *average spontaneous strain* that is equal to the sum of the matrices of absolute spontaneous strains over all n_a ferroelastic domain states,

$$\mathbf{u}^{(\mathrm{av})} = \frac{1}{n_a}\sum_{j=1}^{n_a}\mathbf{u}^{(j)}. \qquad (3.4.3.45)$$

The relative spontaneous strain $\mathbf{b}^{(i)}_{(s)}$ is a *symmetry-breaking strain* that transforms according to a non-identity representation of the parent group G, whereas the average spontaneous strain is a *non-symmetry breaking strain* that transforms as the identity representation of G.

Example 3.4.3.6. We illustrate these concepts with the example of symmetry descent $4_z/m_zm_xm_{xy} \supset 2_xm_ym_z$ with two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ (see Fig. 3.4.2.2). The absolute spontaneous strain in the first ferroelastic domain state $\mathbf{R}_1$ is

$$\mathbf{u}^{(1)} = \begin{pmatrix} \frac{a-a_0}{a_0} & 0 & 0 \\ 0 & \frac{b-a_0}{a_0} & 0 \\ 0 & 0 & \frac{c-c_0}{c_0} \end{pmatrix} = \begin{pmatrix} u_{11} & 0 & 0 \\ 0 & u_{22} & 0 \\ 0 & 0 & u_{33} \end{pmatrix}, \qquad (3.4.3.46)$$

where a, b, c and a_0, b_0, c_0 are the lattice parameters of the orthorhombic and tetragonal phases, respectively.

The spontaneous strain $\mathbf{u}^{(2)}$ in domain state $\mathbf{R}_2$ is obtained by applying to $\mathbf{u}^{(1)}$ any switching operation that transforms $\mathbf{R}_1$ into $\mathbf{R}_2$ (see Table 3.4.2.1),

$$\mathbf{u}^{(2)} = \begin{pmatrix} u_{22} & 0 & 0 \\ 0 & u_{11} & 0 \\ 0 & 0 & u_{33} \end{pmatrix}. \qquad (3.4.3.47)$$

The average spontaneous strain is, according to equation (3.4.3.45),

$$\mathbf{u}^{(\mathrm{av})} = \tfrac{1}{2}\begin{pmatrix} u_{11}+u_{22} & 0 & 0 \\ 0 & u_{11}+u_{22} & 0 \\ 0 & 0 & u_{33}+u_{33} \end{pmatrix}. \qquad (3.4.3.48)$$

This deformation is invariant under any operation of G.

The relative spontaneous strains in ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ are, according to equation (3.4.3.44),

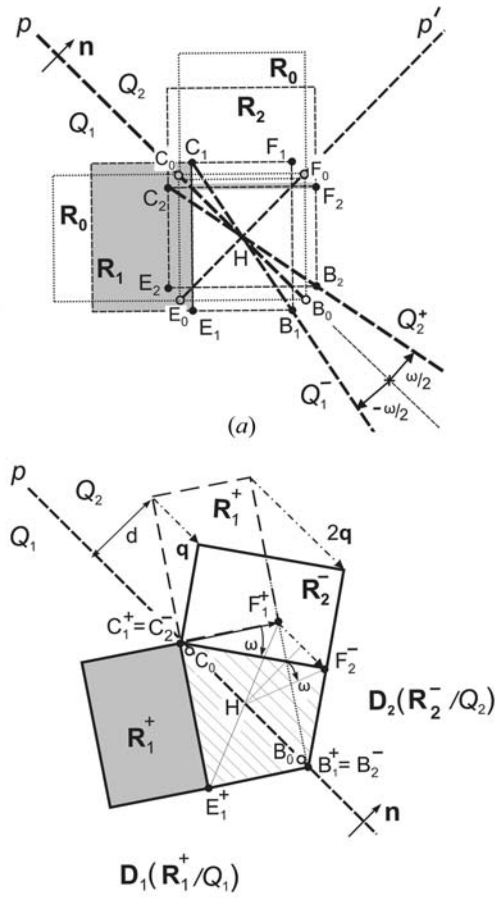

Fig. 3.4.3.5. Two ways of constructing a ferroelastic domain twin. (*a*) Formation of ferroelastic single-domain states $\mathbf{R}_1$, $\mathbf{R}_2$ from the parent phase state $\mathbf{R}_0$ and then rotating away these single-domain states through an angle $\pm\frac{1}{2}\omega$ about the domain-pair axis H so that disoriented ferroelastic domain states $\mathbf{R}_1^+$ and $\mathbf{R}_2^-$ meet along one of two perpendicular planes of equal deformation p or p'. (*b*) Formation of a ferroelastic twin from one ferroelastic domain state $\mathbf{R}_1^+$ by a simple shear deformation with a shear angle (obliquity) ω. For more details see the text.

$$\mathbf{u}_{(s)}^{(1)} = \mathbf{u}^{(1)} - \mathbf{u}^{(\mathrm{av})} = \begin{pmatrix} \frac{1}{2}(u_{11}-u_{22}) & 0 & 0 \\ 0 & -\frac{1}{2}(u_{11}-u_{22}) & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (3.4.3.49)$$

$$\mathbf{u}_{(s)}^{(2)} = \mathbf{u}^{(2)} - \mathbf{u}^{(\mathrm{av})} = \begin{pmatrix} -\frac{1}{2}(u_{11}-u_{22}) & 0 & 0 \\ 0 & \frac{1}{2}(u_{11}-u_{22}) & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (3.4.3.50)$$

Symmetry-breaking nonzero components of the relative spontaneous strain are identical, up to the factor $\frac{1}{2}$, with the secondary tensor parameters $\lambda_b^{(1)}$ and $\lambda_b^{(2)}$ of the transition $4_z/m_zm_xm_{xy} \supset 2_xm_ym_z$ with the stabilizer $I_{4_z/m_zm_xm_{xy}}(\mathbf{R}_1) = I_{4_z/m_zm_xm_{xy}}(\mathbf{R}_2) = m_xm_ym_z$. The non-symmetry-breaking component u_{33} does not appear in the relative spontaneous strain.

The form of relative spontaneous strains for all ferroelastic domain states of all full ferroelastic phases are listed in Aizu (1970*b*).

3.4.3.6.2. *Equally deformed planes of a ferroelastic domain pair*

We start with the example of a phase transition with the symmetry descent $G = 4_z/m_zm_xm_{xy} \supset 2_xm_ym_z$, which generates two ferroelastic single-domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ (see Fig. 3.4.2.2). An 'elementary cell' of the parent phase is represented in Fig. 3.4.3.5(*a*) by a square $B_0E_0C_0F_0$ and the corresponding domain state is denoted by $\mathbf{R}_0$.

In the ferroic phase, the square $B_0E_0C_0F_0$ can change either under spontaneous strain $\mathbf{u}^{(1)}$ into a spontaneously deformed rectangular cell $B_1E_1C_1F_1$ representing a domain state $\mathbf{R}_1$, or under a spontaneous strain $\mathbf{u}^{(2)}$ into rectangular $B_2E_2C_2F_2$ representing domain state $\mathbf{R}_2$. We shall use the letter $\mathbf{R}_0$ as a symbol of the parent phase and $\mathbf{R}_1$, $\mathbf{R}_2$ as symbols of two ferroelastic single-domain states.

Let us now choose in the parent phase a vector $\overrightarrow{HB_0}$. This vector changes into $\overrightarrow{HB_1}$ in ferroelastic domain state $\mathbf{R}_1$ and into $\overrightarrow{HB_2}$ in ferroelastic domain state $\mathbf{R}_1$. We see that the resulting vectors $\overrightarrow{HB_1}$ and $\overrightarrow{HB_2}$ have different direction but equal length: $|\overrightarrow{HB_1}| = |\overrightarrow{HB_2}|$. This consideration holds for any vector in the plane p, which can therefore be called an *equally deformed plane* (EDP). One can find that the perpendicular plane p' is also an equally deformed plane, but there is no other plane with this property.

The intersection of the two perpendicular equally deformed planes p and p' is a line called an *axis of the ferroelastic domain pair* ($\mathbf{R}_1$, $\mathbf{R}_2$) (in Fig. 3.4.3.5 it is a line at H perpendicular to the paper). This axis is the only line in which any vector chosen in the parent phase exhibits equal deformation and has its direction unchanged in both single-domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ of a ferroelastic domain pair.

This consideration can be expressed analytically as follows (Fousek & Janovec, 1969; Sapriel, 1975). We choose in the parent phase a plane p and a unit vector $\mathbf{v}(x_1, x_2, x_3)$ in this plane. The changes of lengths of this vector in the two ferroelastic domain states $\mathbf{R}_1$ and $\mathbf{R}_2$ are $u_{ik}^{(1)}x_ix_k$ and $u_{ik}^{(2)}x_ix_k$, respectively, where $u_{ik}^{(1)}$ and $u_{ik}^{(2)}$ are spontaneous strains in $\mathbf{R}_1$ and $\mathbf{R}_2$, respectively (see *e.g.* Nye, 1985). (We are using the Einstein summation convention: when a letter suffix occurs twice in the same term, summation with respect to that suffix is to be understood.) If these changes are equal, *i.e.* if

$$u_{ik}^{(1)}x_ix_k = u_{ik}^{(2)}x_ix_k, \quad (3.4.3.51)$$

for any vector $\mathbf{v}(x_1, x_2, x_3)$ in the plane p, then this plane will be an equally deformed plane. If we introduce a *differential spontaneous strain*

$$\Delta u_{ik} \equiv u_{ik}^{(2)} - u_{ik}^{(1)}, \quad i, k = 1, 2, 3, \quad (3.4.3.52)$$

the condition (3.4.3.51) can be rewritten as

$$\Delta u_{ik}x_ix_j = 0. \quad (3.4.3.53)$$

This equation describes a cone with the apex at the origin. The cone degenerates into two planes if the determinant of the differential spontaneous strain tensor equals zero,

$$\det\Delta u_{ik} = 0. \quad (3.4.3.54)$$

If this condition is satisfied, two solutions of (3.4.3.53) exist:

$$Ax_1 + Bx_2 + Cx_3 = 0, \quad A'x_1 + B'x_2 + C'x_3 = 0. \quad (3.4.3.55)$$

These are equations of two planes p and p' passing through the origin. Their normal vectors are $\mathbf{n} = [ABC]$ and $\mathbf{n}' = [A'B'C']$. It can be shown that from the equation

$$\Delta u_{11} + \Delta u_{22} + \Delta u_{33} = 0, \quad (3.4.3.56)$$

which holds for the trace of the matrix $\det\Delta u_{ik}$, it follows that these two planes are perpendicular:

$$AA' + BB' + CC' = 0. \quad (3.4.3.57)$$

The intersection of these equally deformed planes (3.4.3.53) is the *axis* $\mathbf{h}$ *of the ferroelastic domain pair* ($\mathbf{R}_1$, $\mathbf{R}_2$).