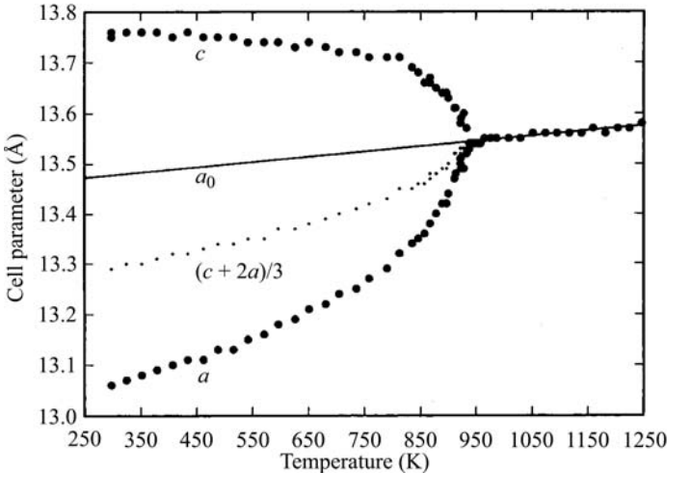

Fig. 3.4.3.4. Temperature dependence of lattice parameters in leucite. Courtesy of E. K. H Salje, University of Cambridge.

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

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

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 **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):

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

where $\mathbf{u}_{(s)}^{(i)}$ 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 $\mathbf{u}_{(s)}^{(\text{av})}$ 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,

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

The relative spontaneous strain $\mathbf{b}_{(s)}^{(i)}$ 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 $4_z/m_z m_x m_{xy} \supset 2_x m_y m_z$ 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),

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

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),