1.4. Thermal expansion

By H. Küppers

1.4.1. Definition, symmetry and representation surfaces

If the temperature T of a solid is raised by an amount ΔT, a deformation takes place that is described by the strain tensor u_{ij}:

$$u_{ij} = \alpha_{ij}\Delta T. \qquad (1.4.1.1)$$

The quantities α_{ij} are the coefficients of thermal expansion. They have dimensions of T^{-1} and are usually given in units of 10^{-6} K^{-1}. Since u_{ij} is a symmetrical polar tensor of second rank and T is a scalar, α_{ij} is a symmetrical polar tensor of second rank ($\alpha_{ij} = \alpha_{ji}$). According to the properties of the strain tensor u_{ij} (*cf.* Section 1.3.1.3.2), the 'volume thermal expansion', β, is given by the (invariant) trace of the 'linear' coefficients α_{ij}.

$$\beta = \frac{1}{V}\frac{\Delta V}{\Delta T} = \alpha_{11} + \alpha_{22} + \alpha_{33} = \text{trace } (\alpha_{ij}). \qquad (1.4.1.2)$$

The magnitudes of thermal expansion in different directions, α'_{11}, can be visualized in the following ways:

(1) The representation quadric (*cf.* Section 1.1.3.5.2)

$$\alpha_{ij}x_ix_j = C \qquad (1.4.1.3)$$

can be transformed to principal axes X_1, X_2 and X_3 with principal values α_1, α_2 and α_3:

$$\alpha_1X_1^2 + \alpha_2X_2^2 + \alpha_3X_3^2 = C.$$

The length of any radius vector leading to the surface of the quadric ($C = 1$) represents the reciprocal of the square root of thermal expansion along that direction, $\alpha'_{11} = a_{1i}a_{1j}\alpha_{ij}$ (a_{kl} are the direction cosines of the particular direction).

If all α_i are positive, the quadric ($C = +1$) is represented by an ellipsoid, whose semiaxes have lengths $1/\sqrt{\alpha_i}$. In this case, the square of the reciprocal length of radius vector $\mathbf{r}$, r^{-2}, represents the amount of positive expansion in the particular direction, *i.e.* a *dilation* with increasing temperature. If all α_i are negative, C is set to -1. Then, the quadric is again an ellipsoid, and r^{-2} represents a negative expansion, *i.e.* a *contraction* with increasing temperature.

If the α_i have different signs, the quadric is a hyperboloid. The asymptotic cone represents directions along which no thermal expansion occurs ($\alpha'_{11} = 0$).

If one of the α_i is negative, let us first choose $C = +1$. Then, the hyperboloid has one (belt-like) sheet (*cf.* Fig. 1.3.1.3) and the squares of reciprocal lengths of radius vectors leading to points on this sheet represent positive expansions (dilatations) along the particular directions. Along directions where the hyperboloid has no real values, negative expansions occur. To visualize these, C is set to -1. The resulting hyperboloid has two (cap-like) sheets (*cf.* Fig. 1.3.1.3) and r^{-2} represents the amount of contraction along the particular direction.

If two of the α_i are negative, the situation is complementary to the previous case.

(2) A crystal sample having spherical shape (radius = 1 at temperature T) will change shape, after a temperature increase ΔT, to an ellipsoid with principal axes $(1 + \alpha_1\Delta T)$, $(1 + \alpha_2\Delta T)$ and $(1 + \alpha_3\Delta T)$. This 'strain ellipsoid' is represented by the formula

$$\frac{X_1^2}{(1+\alpha_1\Delta T)^2} + \frac{X_2^2}{(1+\alpha_2\Delta T)^2} + \frac{X_3^2}{(1+\alpha_3\Delta T)^2} = 1.$$

Whereas the strain quadric (1.4.1.3) may be a real or imaginary ellipsoid or a hyperboloid, the strain ellipsoid is always a real ellipsoid.

(3) The magnitude of thermal expansion in a certain direction (the longitudinal effect), α'_{11}, if plotted as radius vector, yields an oval:

$$(\alpha_1X_1^2 + \alpha_2X_2^2 + \alpha_3X_3^2)^2 = (X_1^2 + X_2^2 + X_3^2)^3.$$

If spherical coordinates (φ, ϑ) are used to specify the direction, the length of $\mathbf{r}$ is

$$|\mathbf{r}| = \alpha'_{11} = (\alpha_1\cos^2\varphi + \alpha_2\sin^2\varphi)\sin^2\vartheta + \alpha_3\cos^2\vartheta. \qquad (1.4.1.4)$$

Sections through this representation surface are called polar diagrams.

The three possible graphical representations are shown in Fig. 1.4.1.1.

The maximum number of independent components of the tensor α_{ij} is six (in the triclinic system). With increasing symmetry, this number decreases as described in Chapter 1.1. Accordingly, the directions and lengths of the principal axes of the representation surfaces are restricted as described in Chapter 1.3 (*e.g.* in hexagonal, trigonal and tetragonal crystals, the representation surfaces are rotational sheets and the rotation axis is parallel to the n-fold axis). The essential results of these symmetry considerations, as deduced in Chapter 1.1 and relevant for thermal expansion, are compiled in Table 1.4.1.1.

The coefficients of thermal expansion depend on temperature. Therefore, the directions of the principal axes of the quadrics in triclinic and monoclinic crystals change with temperature (except the principal axis parallel to the twofold axis in monoclinic crystals).

The thermal expansion of a polycrystalline material can be approximately calculated if the α_{ij} tensor of the single crystal is known. Assuming that the grains are small and of comparable size, and that the orientations of the crystallites are randomly distributed, the following average of α'_{11} [(1.4.1.4)] can be calculated:

$$\bar{\alpha} = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \alpha'_{11}\sin\vartheta\,\mathrm{d}\vartheta\,\mathrm{d}\varphi = \tfrac{1}{3}(\alpha_1 + \alpha_2 + \alpha_3).$$

If the polycrystal consists of different phases, a similar procedure can be performed if the contribution of each phase is considered with an appropriate weight.

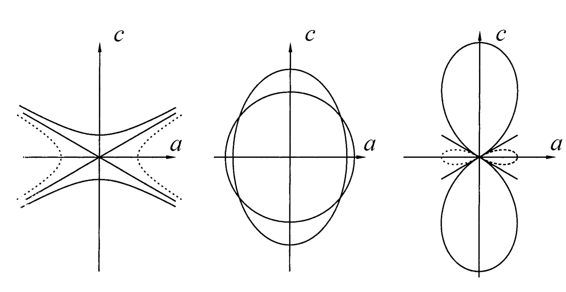

Fig. 1.4.1.1. Sections (*ac* plane) of representation surfaces for a trigonal (or tetragonal or hexagonal) crystal with $\alpha_{11} = \alpha_{22} = -1$ and $\alpha_{33} = +3 \times 10^{-5}$ K^{-1} (similar to calcite). (*a*) Quadric, (*b*) strain ellipsoid (greatly exaggerated), (*c*) polar diagram. The *c* axis is the axis of revolution. Sectors with negative expansions are dashed.

  references