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On the Orientation of the Thermal and Compositional Strain Ellipsoids in Feldspars

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Abstract

A program has been written for the rigorous calculation of strain ellipsoids in triclinic crystals using lattice parameters for two homogeneous states of the crystal. The orientations and magnitudes of the thermal and compositional strain ellipsoids in feldspars have been calculated as examples. Because of the low precision and lack of multiple measurements for the thermal strain, curves were fitted to the cell parameters by hand. The results obtained are interesting and indicate the need for multiple precise measurements to obtain higher precision.

The thermal expansion behavior of the plagioclases is markedly anisotropic, clearly triclinic, and very similar for all compositions with the exceptions of anorthite below 400°C ($P \rightarrow I$ inversion) and high albite above 950°C (triclinic-monoclinic transformation). The directions of the principal axes are determined by variations in the cell angles as well as the cell edges, and the principal axes lie far from the directions of the unit cell axes. One of the coefficients α_3 is always negative. The values for the principal expansion coefficients are $9 < \alpha_1 < 45$, $0 < \alpha_2 < 15$, and $-24 < \alpha_3 < 0 \times 10^{-6}$ deg^{-1}, the coefficients decreasing in the series albite-anorthite. The thermal expansion ellipsoid of the potassium feldspars is nearly uniaxial and highly prolate, α_1 lying near [301].

The compositional strain ellipsoids in the series $NaAlSi_3O_8$–$KAlSi_3O_8$ have been calculated and for the end members are initially similar in orientation to their thermal strain ellipsoids, with intermediate positions for the intermediate compositions.

Introduction

If the lattice parameters are known for two homogeneous states of a crystal, it is possible to determine the strain on passing from one to the other and to calculate a strain ellipsoid. This strain may be caused by a change of temperature, composition, hydrostatic pressure, *etc*, so that one obtains a thermal, compositional, or compressional strain ellipsoid. The theory and method of calculation for thermal strain is developed in the next section. However, the program can be used for any type of strain.

Theory and Method of Calculation

The Thermal Expansion Tensor

Thermal expansion is a strain and this physical phenomenon is represented by a second rank tensor, D. The vector $\mathbf{v}_0$ is transformed into a vector $\mathbf{v}$ by the relation $\mathbf{v} = D\mathbf{v}_0$, $\mathbf{v}$ and $\mathbf{v}_0$ not generally being parallel. The coefficients α_{ij} of the thermal expansion tensor depend on the temperature. They can be defined at a temperature T, if the deformation of the crystal produced by a variation of temperature ΔT about T is known. As with all second-rank tensors, a representative quadric (which can be an ellipsoid or a hyperboloid, in general) corresponds to the thermal expansion tensor. The equation of this quadric referred to its principal axes is:

$$\alpha_1 \Delta T x_1^2 + \alpha_2 \Delta T x_2^2 + \alpha_3 \Delta T x_3^2 = 1$$

where α_1, α_2, and α_3 are the principal thermal expansion coefficients.

The Thermal Expansion Ellipsoid

The macroscopic aspects of thermal expansion are described by means of the thermal expansion ellipsoid. If at a temperature T, one were to cut a sphere of unit radius out of a crystal, this sphere would change in general into an ellipsoid at a temperature $T + \Delta T$. Any radius vector of the sphere would change in length to $1 + \alpha\Delta T$ where α is the thermal expansion coefficient in that direction. The coefficient α depends on the nature of the crystal and on the temperature and pressure and may be positive or negative. Three principal coefficients α_1, α_2, and α_3 correspond to the three axes x_1, x_2, and x_3 of the ellipsoid. By convention $\alpha_1 > \alpha_2 > \alpha_3$. The equation of the ellipsoid is:

$$(1 + \alpha_1 \Delta T)x_1^2 + (1 + \alpha_2 \Delta T)x_2^2 + (1 + \alpha_3 \Delta T)x_3^2 = 1$$

The isobaric volume expansion coefficient α_p is given by

$$\alpha_p = \alpha_1 + \alpha_2 + \alpha_3$$

The representative quadric of the thermal expansion tensor and the thermal expansion ellipsoid are two different surfaces with the same principal axial directions, the semi-axes being $\alpha_1 \Delta T$, $\alpha_2 \Delta T$, and $\alpha_3 \Delta T$ and $(1 + \alpha_1 \Delta T)$, $(1 + \alpha_2 \Delta T)$, and $(1 + \alpha_3 \Delta T)$, respectively.

Determination of the Principal Expansion Coefficients and the Orientation of the Thermal Expansion Ellipsoid

The experimental data used came from X-ray diffraction diagrams at two different temperatures. The deformation of the crystal between T and $T + \Delta T$ can be calculated from the values of a, b, c, α, β, γ at these two temperatures. The coefficients α_{ij} of the thermal expansion tensor were calculated in the conventional right-handed coordinate system, where Oy_3 is parallel to c, Oy_2 parallel to b,* and Oy_1 perpendicular to b^* and c.

The coefficients α_{ij} were obtained by expressing the deformation of the crystal in the orthogonal system Oy_1, Oy_2, Oy_3, using the transformation matrix from the crystallographic system (a, b, c, α, β, γ) to the orthogonal system (Oy_1, Oy_2, Oy_3).

The coefficients α_{ij} obtained form a matrix, the eigenvectors of which are oriented parallel to the principal axes of the representative quadric. The direction cosines of the eigenvectors are the indices of the directions of the principal axes of the representative quadric and of the thermal expansion ellipsoid with respect to the orthogonal system Oy_1, Oy_2, Oy_3. By simple calculation, the polar angles ϕ and ρ of the stereographic projection and the crystallographic indices u, v, w of these directions are obtained. The lengths of the corresponding vectors (u**a** $+ v$**b** $+ w$**c**) at the temperatures T and $T + \Delta T$ are then calculated, from which are obtained the principal coefficients α_1, α_2, and α_3.

Program for the Calculations

The calculations, though not difficult, are extremely tedious, so that a program was written to carry them out. The input is the parameters a, b, c, α, β, γ at the two corresponding temperatures, the output is the directions of the principal axes of the thermal expansion ellipsoid in the orthogonal and crystallographic axial systems, as well as the thermal expansion coefficients. The program was written in Fortran IV with a memory less than 35 K; the listing and explanatory notice can be made available on request. Separate versions exist for triclinic or monoclinic crystals; the ellipsoid is fixed by symmetry in the other systems and the values of the principal coefficients are obtained directly.

As the only input is the two sets of parameters, the program can be used for any type of strain.

Input Data and Precision for the Feldspars

The program was applied to the feldspars as an example because sufficient data exist to calculate both thermal and compositional strain ellipsoids, though the precision of the high-temperature measurements is not high. In monoclinic feldspars one of the axes of the strain ellipsoid must coincide with the [010] direction at all temperatures, the other two lying in the (010) plane and having irrational indices. In triclinic feldspars there is no restriction on the orientation of the strain ellipsoid and its position may vary with temperature, pressure, and order.

The position of the thermal expansion ellipsoid in monoclinic adularia was calculated (Fizeau, 1868) up to 70°C, the major axis lying very near [301] and the other axes having negative coefficients. Beckenkamp (1881) indirectly calculated the position of the ellipsoid in triclinic anorthite from Vesuvius at three temperatures up to 200°C from measurements of interfacial angles and showed that its position changed as a function of temperature. Many measurements of variable quality exist for the thermal expansion of the feldspars, mostly by dilatometric methods in three nearly mutually perpendicular directions or in the three axial directions (see Saucier and Saplevitch, 1962, and Barth, 1969, for reviews). These measurements suffice, in general, to calculate roughly the volume expansion, but not the position and magnitude of the thermal expansion ellipsoid. Numerous X-ray determinations of the lattice parameters of triclinic feldspars up to 1000–1200°C are now available, from which the thermal expansion ellipsoid can be calculated.

The lattice parameters for a series of triclinic plagioclases up to 1000–1200°C are now available from X-ray powder diffraction: labradorite (Stewart *et al*, 1966), high and low albite (Stewart and von Limbach, 1967), ten natural and synthetic albites

(Grundy and Brown, 1969), and eight plagioclases (Grundy and Brown, 1974). No complete X-ray data exist for potassium feldspars or for alkali feldspars other than albite. The reciprocal lattice angles of microcline up to 1000°C are available, and they do not change at all within the error of measurement with the possible exception of γ^* (Grundy and Brown, 1967). However, results for the proportional axial expansions of adularia and microcline (Rosenholtz and Smith, 1941, 1942) are available.

This paper presents calculations of the orientations and magnitudes of the thermal expansion ellipsoid for eight plagioclases: anorthite from Monte Somma, F 109; bytownite from Crystal Bay, Minnesota, F 71; andesine from Valle Maggia, Switzerland, F 50; oligoclase from Mitchell County, F 36 (all from Grundy and Brown, 1973); and two low albites and two high albites (from Stewart and von Limbach, 1967, and Grundy and Brown, 1969). The four albites were chosen so that a comparison of precision could be obtained. In the case of the potassium feldspars, it was assumed that the cell angles do not change with temperature, and the results for the axial expansions for adularia and microcline (Rosenholtz and Smith 1941, 1942) were used in conjunction with the lattice parameters of high sanidine and maximum microcline (Orville, 1967). The results for the potassium feldspars at high temperature must be treated with caution, because of possible irreversible changes due to release of strain and to homogenization of perthitic albite during Rosenholtz and Smith's measurements (see, for example, Kôzu and Saiki, 1925).

The cell parameters are known only at 7 to 9 different temperatures from 25 to about 1000°C. The internal precision of one measurement at any one temperature is about 0.006–0.008 Å for the lengths and 0.05° for the angles (see original papers for individual precision). The differences in the parameters at two successive temperatures are of the order of, or less than the precision of, one measurement at one temperature. It is thus not reasonable to carry out the calculations using the raw data, and at the beginning we wondered if the calculations would be worth doing even after "smoothing" the data.

The data were "smoothed" in the following way: the parameters were plotted individually against temperature and smooth curves drawn by hand. It was assumed that no important structural changes occur during heating, except for high albite (specimen 307) and anorthite, so that the curves were drawn as simply as possible, avoiding inflection points. In most cases the curves were straight lines or gentle curves. Use of curve-fitting techniques was considered, but they are only justified if several sets of measurements exist for each temperature and if the form of the curve is known. It was decided that a better test of the uncertainties would be obtained from the coherence of the results themselves. Consequently, hand drawn curves were used, the values read from the curves every 25°C, and the calculations carried out for each sample at 30–35 mean temperatures for a fixed ΔT of 100°.

The uncertainty of the slope for a ΔT of say 100° depends on the precision of the parameters at T and $T + \Delta T$, but it is considerably reduced by drawing a curve which uses not only these two points but also others at temperatures outside the range. The analytic form for the parameter variation is unknown, but if it were a straight line from 25–1000°C, the uncertainty in the slope of the curve would be equal to twice $\delta p/975$, if δp is the error in the parameter. For a ΔT of 100°, the error in the slope would be the same, so that the error in the parameters read from the curves would be 1/5 of the original errors. Since the parameter variation with temperature is not linear in many cases, the uncertainty of the slope was considered to be twice as large, so that the uncertainty for a ΔT of 100° has been taken as 2/5 of the errors, *i.e.*, about 0.0025 Å for the lengths and 0.02° for the angles. The precision is obviously worse at the low and high temperature ends. This precision is not high but is sufficient to justify carrying out the calculations. In addition, the results of the calculations were plotted every 25° as a function of temperature and curves drawn neglecting the few aberrant points due to errors in the slopes. The errors in slopes are of course not cumulative.

An exact calculation of the precision in orientation and magnitude of the ellipsoid is difficult to obtain, since the smoothing procedure is complex. In the case of low albite, we compared our curve showing α_p as a function of temperature with the fitted curve of Stewart and von Limbach (1967, Fig. 5) for the same albite. The largest deviation between the two curves, 2.5×10^{-6} deg^{-1}, gives a measure of the uncertainty in the results. We tried to estimate the precision in the orientation and magnitude of the ellipsoid for this same low albite between 250 and 350°C by systematically varying all the parameters using all combinations with positive and negative values. The variations in the orientation of the axes of the ellipsoid and in the coefficients are α_1 : 18° and

1.0×10^{-6} deg^{-1}, α_2: 12° and 1.6×10^{-6} deg^{-1}, and α_3 : 11° and 2.1×10^{-6} deg^{-1} within the variation for α_v of 2.5×10^{-6} deg^{-1} determined above. The results in other cases would be different but would probably be within the limit of ±20° and $\pm 3 \times 10^{-6}$ deg^{-1} at the worst.

Results

The results obtained are presented chiefly as an example of the use of the program. However, even though the precision of the input data is low, the results show sufficient internal coherence to merit presentation (Table 1).

A measure of the coherence of the results is obtained by a comparison of two low albites and of two high albites (Figs. 2A, 2B) as calculated for totally different samples and by different investigators. Results for each pair are very similar in position and in trend. If the ellipsoid is nearly one of revolution (as is the case for microcline), the positions in the nearly circular section of the two minor axes are only roughly known, whereas their magnitude is well known.

The orientation of the thermal expansion ellipsoid is markedly triclinic and very similar in all plagioclases studied except for monalbite and anorthite at low temperature. At any given temperature, the variation in position of the axes for any one plagioclase is generally less than ±20° from the average position (and of the same order of magnitude) from that for all plagioclases at that temperature (Fig. 1).

With the exceptions of high albite and anorthite, the magnitudes of the three coefficients are also similar, with $\alpha_3 = -5 \pm 5 \times 10^{-6}$ deg^{-1}, $\alpha_2 = +8 \pm 6 \times 10^{-6}$ deg^{-1} in most cases, whereas α_1 diminishes from low albite ($+23 \pm 5 \times 10^{-6}$ deg^{-1}) to bytownite ($+11 \pm 3 \times 10^{-6}$ deg^{-1}). The values of the three coefficients are given for all feldspars in Table 1 at 300 and 600°C, where errors in smoothing the curves are smallest.

The orientations of the three axes of the thermal expansion ellipsoid for two high albites (Fig. 2A) overlap very closely. α_1 is oriented near [112] to [324], α_2 near $[\bar{4}11]$ to $[\bar{20}.1.1]$ and α_3 near $[1\bar{2}4]$. For specimen 307, as temperature is increased, the value of α_2 is almost unchanged (Fig. 4), whereas α_1 passes through a maximum and α_3 a minimum near 900°C. This temperature is 50°C below the transition temperature, since a range of 100°C was used for the calculations. No maximum is seen in α_v when the volume curve is smoothly extrapolated beyond 950°C.

TABLE 1. Magnitude and Orientation of the Coefficients of the Thermal Expansion Ellipsoid for Some Feldspars

Sample	An_{100}, F 109. Monte Somma, Italy		An_{76}, F 71. Crystal Bay, Minnesota		An_{36}, F 50. Valle Maggia, Switzerland		An_{22}, F 36. Mitchell Co., North Carolina		An_0, F 101. Amelia, Virginia	
Temp.	300°C	600°C	300°C	600°C	300°C	600°C	300°C	625°C	300°C	600°C
	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w
α_1	13 17 8 6	13 $\bar{30}$ $\bar{15}$ $\bar{8}$	9 29 14 15	11 8 3 3	19 19 9 18	19 8 6 19	17 28 13 30	22 29 13 30	20 17 6 16	25 17 5 14
α_2	2 $\bar{5}$ 3 6	2 $\bar{3}$ 2 6	0 $\bar{11}$ 3 4	6 $\bar{7}$ 5 5	6 $\bar{11}$ 4 9	13 $\bar{17}$ $\bar{3}$ 5	3 $\bar{17}$ 7 6	11 $\bar{14}$ 6 7	5 $\bar{11}$ 5 9	11 $\bar{9}$ 6 10
α_3	-2 14 $\bar{11}$ 10	-5 23 $\bar{15}$ 12	-4 4 $\bar{5}$ 4	-1 5 $\bar{8}$ 8	-5 8 $\bar{9}$ 17	-4 20 $\bar{17}$ 22	-5 1 $\bar{3}$ 7	-7 3 $\bar{7}$ 15	-1 6 $\bar{9}$ 16	-6 4 $\bar{8}$ 15
α_p	13	10	5	16	20	28	15	26	24	30

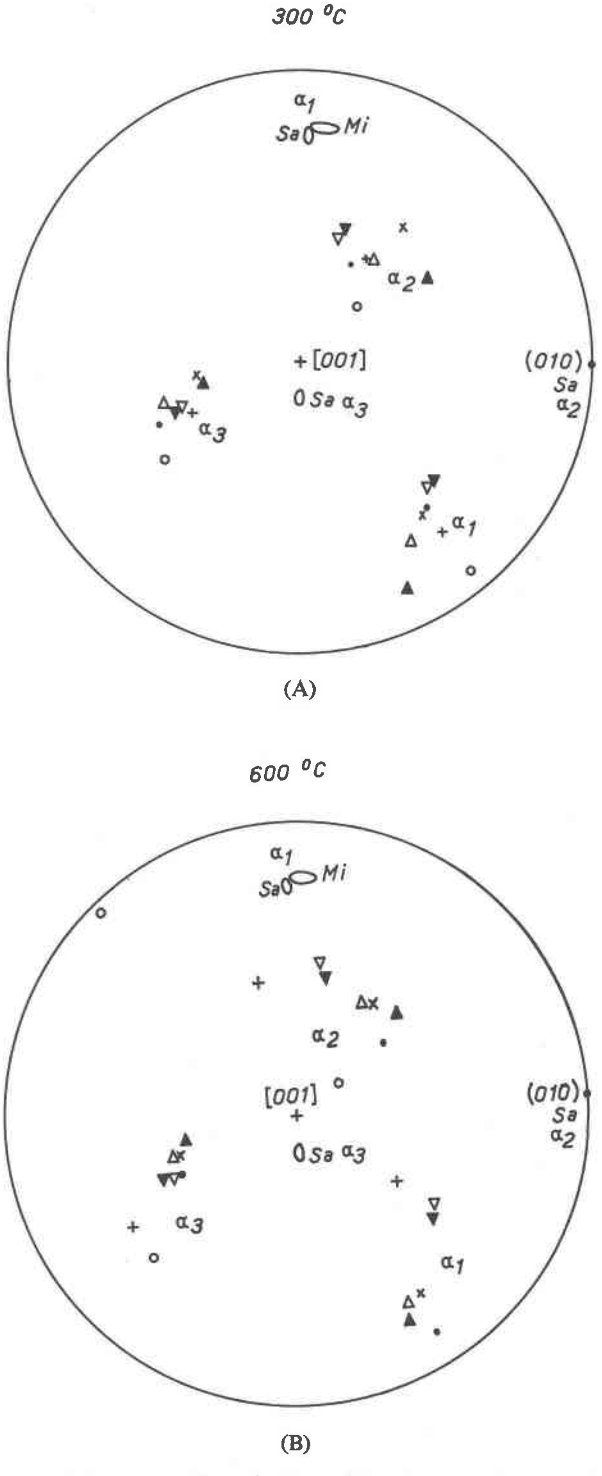
Sample	An_0, 1. Amelia, Virginia (Stewart and von Limbach)		An_0, 307. Synthetic 1000°C 2000 lbs/in^2, 66 h.		An_0, 2. Synthetic 925°C 3500 lbs/in^2, 3 h.		3. Microcline (see text)		4. Sanidine (see text)	
Temp.	300°C	600°C	300°C	600°C	300°C	600°C	300°C	600°C	300°C	600°C
	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w	mag. u v w
α_1	23 24 7 18	23 22 6 19	31 18 12 25	45 7 5 11	32 17 13 24	38 15 10 22	19 $\bar{11}$ 1 $\bar{3}$	20 $\bar{11}$ 1 $\bar{3}$	20 13 0 4	18 13 0 4
α_2	9 $\bar{16}$ 10 9	12 $\bar{11}$ 8 9	13 $\bar{19}$ 5 5	12 $\bar{19}$ 2 4	11 $\bar{17}$ 3 5	14 $\bar{18}$ 3 5	1 4 5 16	2 3 1 16	-1 0 1 0	1 0 1 0
α_3	-9 2 $\bar{5}$ 14	-3 2 $\bar{7}$ 14	-12 4 $\bar{7}$ 15	-24 6 $\bar{8}$ 17	-13 7 $\bar{8}$ 17	-20 6 $\bar{9}$ 16	-1 1 $\bar{6}$ 7	0 $\bar{1}$ $\bar{8}$ 2	-1 1 0 5	-1 1 0 5
α_p	23	32	32	33	30	32	19	22	18	18

The values for α_1, α_2, α_3, and α_v for the high albite of Stewart and von Limbach (1967) are identical to those of specimen 307 up to 600°C; beyond this temperature they show no maximum or minimum, as their sample, which was not fully disordered, did not become monoclinic (see Grundy and Brown, 1969; Kroll and Bambauer, 1971). The positions for α_1, α_2, and α_3 for monalbite (# 307) at 1000°C are also shown (Fig. 2A); the ellipsoid is nearly spherical compared to 900°C with $\alpha_1 \approx \alpha_2 \approx \alpha_3 \approx 8 \times 10^{-6}$ deg^{-1}. The great change in the coefficients below the triclinic/monoclinic symmetry transformation is due to the rapid variation in the angles α and γ. The change in the orientation of the ellipsoid at the symmetry change is discontinuous.

For two low albites (Fig. 2B), the variation in orientations of the three axes at a series of temperatures is greater than for the high albites. The values for the coefficients are given in Table 1. The orientations for bytownite F 71, for oligoclase F 36, and for andesine F 50 are similar.

Anorthite undergoes an apparent symmetry change from $P\bar{1}$ to $I\bar{1}$ at a temperature in the range 200–350°C (Brown, Hoffmann and Laves, 1963; Laves, Czank and Schulz, 1970). The orientations of the three axes are shown in Figure 2C. The major and minor axes, α_1 and α_3, change rapidly in position with temperature especially in the range 200–300°C. The low temperature positions for α_1 are close to those deduced by Beckenkamp (1881) from goniometric measurements, but the movement with temperature is different; the agreement is less good for α_2 and α_3. The changes in value of these coefficients with temperature (Fig. 5), show that α_1 and α_v have maximum values at 350–400°C, a value slightly above the probable temperature for the transition. The values of α_v suggest that the transition is of λ-type with "infinities" in the first order derivatives (Pippard, 1966). The volume versus temperature curve determined by Kôzu and Ueda (1933) is also in agreement with a λ-type transition. The cell volumes for anorthite from Vesuvius (Grundy and Brown, 1974; Czank and Schulz, 1971) are in agreement at room temperature and above 700°C. However, Czank and Schulz (1971) from single-crystal diffractometer measurements found a minimum in the volume near 200°C.

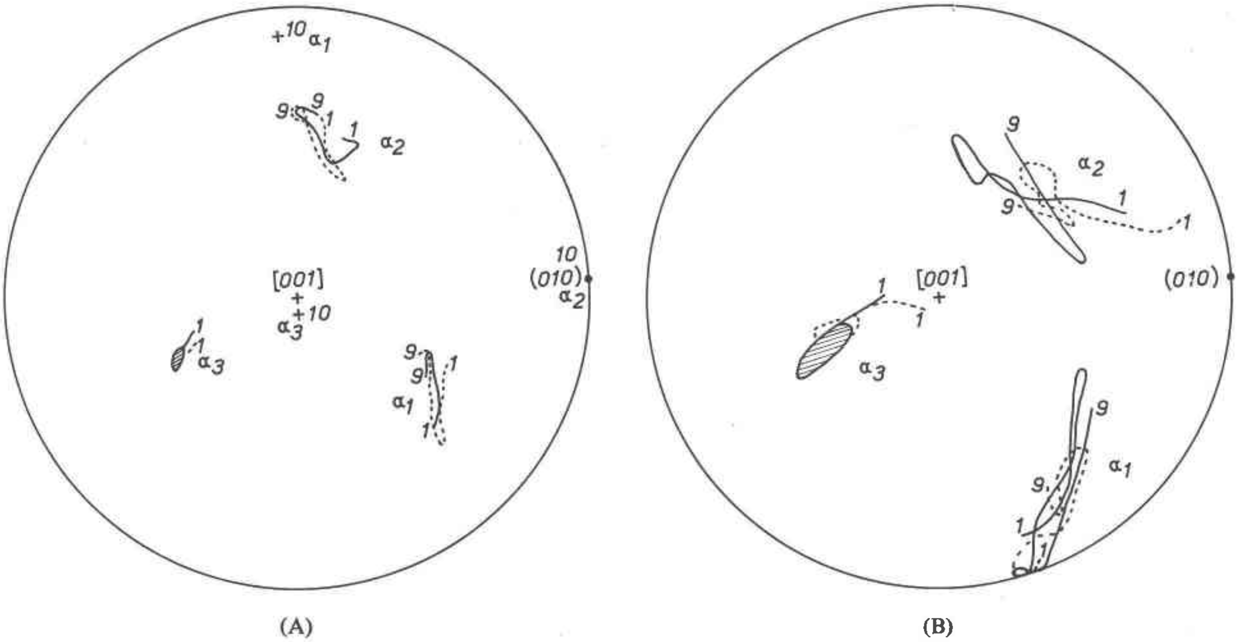
The thermal expansion of the potassium feldspars is extremely anisotropic and nearly uniaxial with $\alpha_2 \approx \alpha_3 \approx 0$ so that $\alpha_v \approx \alpha_1$ (Table 1). For sanidine the ellipsoid is nearly fixed in position and magnitude



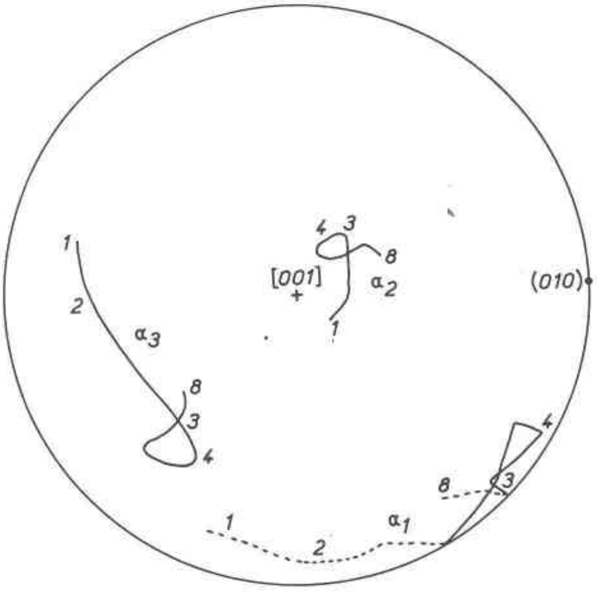
(A)

(B)

FIG. 1. Stereographic projections of the three axes (α_1, α_2, α_3) of the thermal expansion ellipsoid for the following plagioclases: An$_{100}$(symbol ○); An$_{78}$(●); An$_{36}$(+); An$_{22}$(×); low albite, An$_0$(△ and ▲); and high albite, An$_0$(▽ and ▼). The filled triangles represent albites from Stewart and von Limbach (1967). (A) For 300°C; (B) For 600°C.



(A) (B)



(C)

FIG. 2. Stereographic projections showing positional changes of the axes of the thermal expansion ellipsoid between 100°C (point 1) and 900°C (point 9):

(A) For two high albites (the solid line represents sample 307, the dashed line represents the data for the high albite of Stewart and von Limbach). The plus signs represent sample 307 when monoclinic at 1000°C.

(B) For two low albites (the solid line represents sample F 101, the dashed line represents the low albite of Stewart and von Limbach).

(C) For anorthite from Monte Somma (dotted line corresponds to orientations with $\rho > 90°$).

over the whole temperature range with $\alpha_1 = 19 \pm 1 \times 10^{-6}$ deg^{-1} in a direction very near [301], $\alpha_2 = 0.5 \pm 0.5 \times 10^{-6}$ deg^{-1} near [105], and $\alpha_3 = -0.8 \pm 0.5 \times 10^{-6}$ deg^{-1} parallel to [010]. For microcline the major axis is also nearly fixed in position near $[\bar{1}\bar{1}.1.\bar{3}]$ with $\alpha_1 = 19 \pm 1 \times 10^{-6}$ deg^{-1} whereas α_2 and α_3 are nearly zero ($\pm 1 \times 10^{-6}$ deg^{-1}) and are spread out with temperature in a great circle with $[\bar{1}\bar{1}.1.\bar{3}]$ as pole, since very small relative changes in b and c have a large influence on the orientation of α_2 and α_3 (only α_1 shown on Fig. 1A, 1B).

The effect of an increase in temperature on the lattice parameters of albite and acid plagioclases resembles the effect of substitution of potassium at constant temperature (Grundy and Brown, 1969). The compositional strain ellipsoid for the substitution of K in low albite at room temperature (Fig. 3) was calculated from data from Orville (1967). Initially the orientation of the three compositional coefficients is very similar to the orientation of the thermal expansion coefficients in low and high albites. With increase in the Or content, the orientation approaches that of microcline, as might be expected. The values of α_1 and α_2 decrease and $\alpha_2 = \alpha_3 \to 0$ when the composition approaches that of microcline. The orientation of the ellipsoid in the high-albite/sanidine series (Orville, 1967) is also shown (Fig. 3), the coefficient α_1 passing through a maximum and that for α_3 through a minimum at the triclinic/monoclinic transformation for this series.

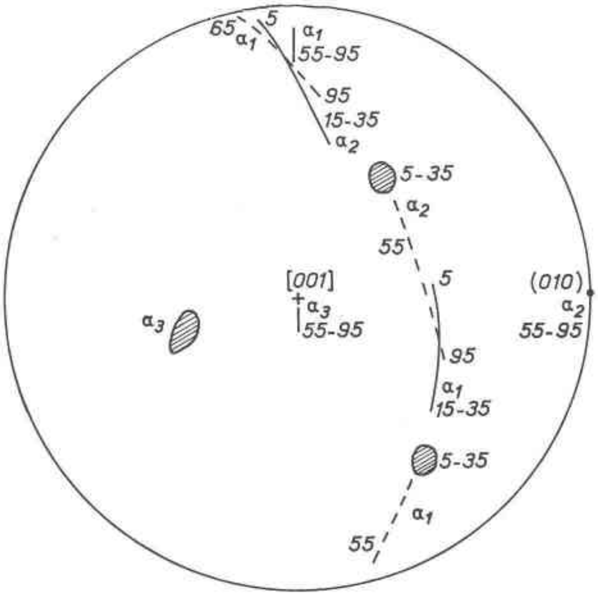


FIG 3. Stereographic projection of the three axes of the compositional strain ellipsoid. Dotted line for low albite to microcline; full line for high albite to sanidine. The composition is given in per cent Or for mean of 10% ranges. α_2 and α_1 are interchanged for the low series at Or_{95} and for the high series at Or_{15} and Or_{95}, the values being very nearly zero.

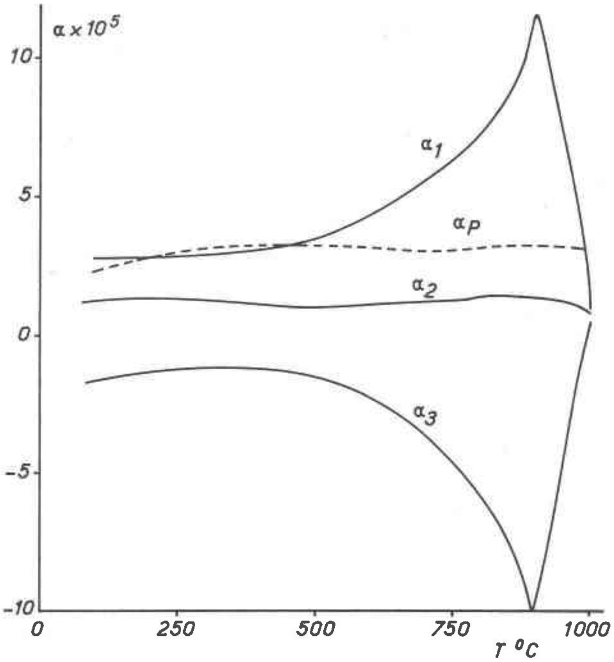


FIG 4. Thermal expansion coefficients for high albite, specimen 307. The great variation of α_1 and α_3 near 900°C corresponds to the symmetry transition.

Discussion

The calculation of the thermal expansion ellipsoid is rigorous, the uncertainties in the result being due solely to the uncertainties in the parameters. If the lattice parameters were known more precisely with multiple measurements at many temperatures, curve fitting techniques would be justified and the orientation of the thermal expansion ellipsoid would be known with high precision.

The program was written to obtain information which is not immediately obvious in the case of a triclinic crystal, because of the important role of variations in the cell angles. The calculations seem justified by the reasonable coherence of the data, namely, the close similarity of the results for two different low and high albites and for the plagioclases in general.

One surprising result is that one at least of the principal axes of the thermal expansion ellipsoid is always negative at all temperatures for all triclinic feldspars (with a few trivial exceptions). This is understandable *a posteriori*: because of the large proportional reduction in the cell angle, α, one of the diagonals in the $b - c$ plane diminishes with increasing temperature. Secondly, the thermal expansion behavior of the plagioclases is distinctly not pseudo-monoclinic, except for monalbite. For all feldspars, the relative movements with temperature for α_1 and α_2 are much greater than for α_3, which is nearly fixed

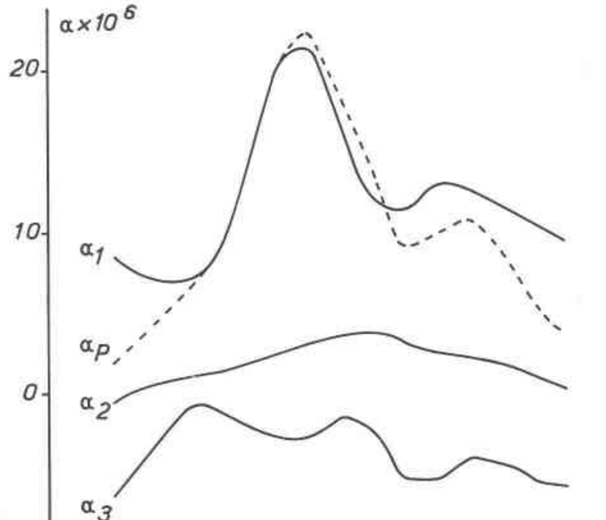


FIG. 5. Thermal expansion coefficients for anorthite, F 109. The α_p variation suggests a λ-type transition. The variation in α_3 is near the limit of error.

in position, except for anorthite. Thirdly, the orientation of the ellipsoid is broadly the same in all plagioclases (except for monalbite and anorthite at low temperature) and distinctly different from that in potassium feldspars.

The thermal expansion coefficient for the volume, α_v, decreases in the series high-albite–low-albite, albite-potassium feldspar, and albite-anorthite. The structure of albite is more fully collapsed at room temperature than that of potassium feldspar, so should have a larger value for the coefficient α_v (Taylor, 1972). For the same reason glasses have a smaller value for α_v than the more fully collapsed crystals of the same composition (for measurements on glasses, see Arndt and Häberle, 1973). The value of α_v decreases with increase in anorthite content for plagioclase crystals or glasses of the same composition, probably because the (Al, Si)-O framework is more rigid in the presence of divalent Ca than monovalent Na. This is true because Ca-O bonds are somewhat stronger than Na-O bonds as evidenced by shorter bond lengths and smaller temperature factors for Ca in anorthite than for Na in albite.

Note Added in Proof

The manuscript for this article was submitted in August, 1972. Since this date, articles have appeared by Y. Ohashi and C. W. Burnham (1973), *Am. Mineral.*, **58,** 843–849; and Y. Ohashi and L. W. Finger (1973), *Carnegie Inst. Wash. Year Book,* **72,** 569–573. Ohashi and Finger calculated the positions of the strain ellipsoids for compositional strain (data from Orville, 1967), for thermal strain (Stewart and von Limbach, 1967) and for order/disorder strain. Their results for the first two strains are essentially similar to ours; any differences must come from our use of smoothing techniques, whereas they used the raw data. Their calculated standard errors are in some cases quite large.

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