

The structure of a strained intermediate microcline in cryptoperthitic association with twinned plagioclase

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Abstract

The crystal structure of a strained intermediate microcline ($a = 8.643$, $b = 12.929$, $c = 7.190\text{\AA}$; $\alpha = 90.1^\circ$, $\beta = 116.2^\circ$, $\gamma = 89.6^\circ$; $V = 720.6\text{\AA}^3$; $C\bar{1}$), intergrown as untwinned lamellae in a cryptoperthitic ternary feldspar of bulk composition $\text{Or}_{33}\text{Ab}_{58}\text{An}_8\text{Cn}_1$, has been refined to $R = 0.049$ using 893 reflections. The cryptoperthite is specimen K-235 from the Kûngnât syenites of SW Greenland. Unit-cell volume gives the best estimate of the composition of the microcline phase, $\text{Or}_{91}\text{Ab}_6\text{Cn}_3$, which constitutes ~ 36 percent of the bulk feldspar. The plagioclase composition, determined by mass balance, is approximately $\text{Ab}_{87}\text{An}_{13}$.

The plagioclase is twinned at a scale of 100–500Å on both albite- and pericline-twin laws, and special caution was required to exclude from the refinement diffracted peaks from the microcline lattice which overlapped with diffracted peaks from these four plagioclase lattices. In spite of the non-continuous, lamellar nature of the microcline phase in the cryptoperthite, the mosaic texture resulted in only $0.4^\circ 2\theta$ diffraction peak widths.

Due to its intergrowth with twinned plagioclase, the microcline is strained ($\Delta a = 0.30\text{\AA}$) in the manner described by Stewart and Wright (1974). This apparently does not prohibit the use of b - c and α^* - γ^* plots to estimate Al/Si distribution in the tetrahedral sites ($t_{10} \sim 0.51$, $t_{1m} \sim 0.35$, $t_{20} = t_{2m} \sim 0.07$ Al); mean T–O distances ($T_{10} = 1.671$, $T_{1m} = 1.651$, $T_{20} = 1.622$, $T_{2m} = 1.627\text{\AA}$) give similar values (0.47, 0.32, and 0.10 Al, respectively). Without a meaningful basis of comparison, the effects of strain on individual bond lengths and angles could not be evaluated quantitatively.

Introduction

In the past decade it has been shown that alkali feldspars, $(\text{K,Na})\text{AlSi}_3\text{O}_8$, can be characterized most satisfactorily by their lattice parameters. Wright and Stewart (1968) proposed a plot of the b and c cell edges (see Fig. 1) “because on such a graph points for samples of different composition but equivalent Al–Si order fall into more or less linear arrays regardless of the symmetry of the starting material” (Stewart, 1975). Samples of the same composition but different Al–Si order (e.g., the maximum microcline–high sanidine series) are arrayed on subparallel lines running between the limiting arrays for the completely ordered maximum microcline–low albite series and the disordered high sanidine–analbite (or high albite) series. Using data from crystal structure analyses, Stewart and Ribbe (1969) determined that relative position on the b - c plot very closely approximates the

total aluminum content of the T_1 tetrahedral sites, which are designated T_{10} and T_{1m} in triclinic alkali feldspars. Adopting the convention introduced by Kroll (1971), in which t_{10} represents the probability of finding aluminum in T_{10} , they contoured the b - c quadrilateral with lines of equal Al content in the T_1 sites: thus $t_{10} + t_{1m} = 1.00$ for the ordered series in which all the Al in the formula unit is concentrated in the T_{10} site and Si occupies the other three sites (i.e., $t_{10} = 1.00$; $t_{1m} = t_{20} = t_{2m} = 0.00$), and $t_{10} + t_{1m} = 0.50$ for the disordered series in which Al is randomly distributed over the four tetrahedral sites (i.e., $t_{10} = t_{1m} = t_{20} = t_{2m} = 0.25$).

Using data from homogeneous alkali feldspars, Stewart and Wright (1974) contoured the b - c plot for the a cell dimension, estimating a standard error for the contours of $\pm 0.02\text{\AA}$. They discussed in considerable detail a phenomenon which is especially common in cryptoperthitic intergrowths of two feldspar

phases, *viz.* "strained" feldspars, and they proposed an index of strain based on the difference between the observed a cell dimension and that estimated from the position of that specimen's b and c cell dimensions on the contoured b - c plot: $\Delta a = (a_{\text{obs}} - a_{\text{est}})$. They arbitrarily set $\Delta a > 0.05\text{Å}$ as the threshold for considering a feldspar to be strained.

MacKenzie and Smith (1955) used an $\alpha^*-\gamma^*$ plot to describe the relative structural states of the triclinic alkali feldspars, and Stewart and Ribbe (1969) discovered that the $\alpha^*-\gamma^*$ quadrilateral could be contoured for the difference in Al content between the T_{10} and T_{1m} sites. Thus $t_{10} - t_{1m} = 1.00$ for the ordered maximum microcline-low albite series and 0.00 for the disordered high sanidine-high albite series. An alkali-exchange series with an invariant Al-Si distribution would extend parallel to these contours as Na/K is varied. In all monoclinic alkali feldspars t_{10} is equal to t_{1m} , thus $t_{10} - t_{1m} = 0.00$ and $\alpha^* = \gamma^* = 90^\circ$.

The a (or a^*) cell dimension is particularly sensitive to Na/K ratio and insensitive to Al-Si distribution among the four tetrahedral sites; consequently, it may be used to determine the composition of homogeneous alkali feldspars (Orville, 1967; Wright and Stewart, 1968). However, in individual phases of an exsolution intergrowth where structural coherency is in evidence, strain effects are manifested most strikingly by distortions of the a dimension, and values such as $\text{Ab}_{105}\text{Or}_{-5}$ or $\text{Ab}_{-10}\text{Or}_{110}$ may be predicted.

Smith (1961) suggested that the unit-cell volume should more reliably give the correct composition even in the presence of strain due to coherency. Thus Stewart and Wright (1974) recast an equation from Waldbaum and Thompson (1968) to be used in calculating orthoclase content from volume (V , in Å^3):

$$\text{Or}(\text{mol } \%) = \frac{0.2962 - \sqrt{0.953131 - 0.0013V}}{0.0018062}$$

However, the usefulness of this equation is limited by the fact that changes in Al-Si distribution affect b nearly twice as much as c (though in opposite directions), and therefore the "structural state" of the feldspar is not an entirely negligible consideration in the volume-composition relationship, especially for the low-high albite series.

With careful monitoring of diffraction data to exclude overlapping peaks, this study shows that it is possible to determine precisely the structure of one phase (intermediate microcline), intimately intergrown at the 100-500Å scale with another phase (plagioclase) which is twinned on two laws and has

four distinct orientations of its diffraction pattern. Having determined the crystal structure of this triclinic potassium feldspar with a strain index, $\Delta a = 0.30\text{Å}$, it is also possible to make preliminary assessments of the b - c and $\alpha^*-\gamma^*$ plots for determining Al-Si distributions in *strained* feldspars (see preliminary report by Ribbe and Gibbs, 1975).

The work of Keefer and Brown (1978) on a coherent intergrowth of monoclinic $\text{Or}_{65}\text{Ab}_{35}$ and pericline-twinned triclinic $\text{Or}_{22}\text{Ab}_{78}$ in a pegmatitic cryptoperthite (bulk composition $\text{Or}_{51}\text{Ab}_{48}\text{An}_1$) should be examined to obtain insight of a similar nature to the problems of such a study.

Experimental

The feldspar under consideration is from specimen K-235, a cryptoperthite from the eastern border group of the Kûngnât syenites, SW Greenland. Both MacKenzie and Smith (1962) and Stewart and Wright (1974) have studied this material. The former report (p. 85) an approximate bulk composition of $\text{Or}_{33}\text{Ab}_{58}\text{An}_8\text{Cn}_1$ and indicate from b -axis oscillation photographs that the potassium-rich phase is monoclinic and that the sodium-rich phase is albite- and pericline-twinned. The crystal used in this study differs in that the K-rich phase is triclinic (space group $C\bar{1}$) and the multiply-twinned plagioclase gives evidence of twin superlattices (scale 50-200Å), producing streaks through the X-ray reflections from the albite twin-related lattices. The textural features are illustrated (Fig. 1) in dark-field electron micrographs of grains of K-235 containing lamellae of monoclinic K-rich feldspars exsolved from the twinned plagioclase host.

Stewart and Wright (1974, p. 365) report the presence of two potassium feldspars in their powdered sample of K-235. A few diffraction peaks attributable to triclinic K-feldspar were observed in the powder pattern from which the lattice parameters of only the dominant monoclinic K-rich phase (space group $C2/m$) and the triclinic plagioclase could be refined. The crystal chosen for structure refinement contains the untwinned triclinic K-feldspar in addition to the twinned albite. The lattice parameters of the triclinic phase, determined by least-squares refinement using 26 carefully centered reflections on a Picker FACS-1 four-circle diffractometer, are listed in Table 1, together with those reported by Stewart and Wright (1974) for the monoclinic K-feldspar and the triclinic plagioclase.

Intensities from the untwinned intermediate microcline phase of a cryptoperthitic crystal ($\sim 0.15 \times 0.15$

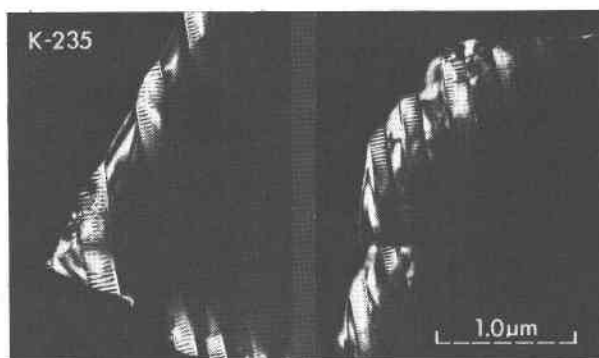


Fig. 1. Dark-field transmission electron micrographs of the K-235 cryptoperthite showing lamellae of twinned plagioclase (bright) intergrown with triclinic potassium feldspar (dark, out of contrast).

$\times 0.22$ mm) were collected using Nb-filtered Mo radiation ($\lambda = 0.71069\text{\AA}$) on an automated Picker four-circle diffractometer. Each reflection ($2\theta \leq 50^\circ$) was monitored on a strip chart during the $\theta - 2\theta$ scan so that at least the obviously overlapping peaks (204 of them) from the twinned plagioclase phase could be eliminated from the least-squares refinement. Note that although this so-called "single crystal" of microcline is made up of ~ 100 distinct lamellae (see Fig. 1), the mosaic texture of the collection of these lamellae resulted in only 0.4° broadening of the diffraction peaks. The data were corrected for Lorentz and polarization effects but not for absorption ($\mu = 14.6 \text{ cm}^{-1}$). In addition another 107 peaks, most suffering from diffraction amplification due to undetected peak overlap, were removed from the data set at successive stages in the refinement on the basis of values of $(F_{\text{obs}} - F_{\text{calc}})/\sigma_{\text{obs}}$ in excess of 5.0. In the final full-matrix least-squares refinement 893 reflections with values $F_{\text{obs}} > 1\sigma_{\text{obs}}$ were used, and the anisotropic model (118 parameters) gave an unweighted R factor of 0.049.

Atomic coordinates and anisotropic temperature factors and their isotropic equivalents (along with the thermal ellipsoid data for the potassium atom) are listed in Table 2, and interatomic distances and inter-bond angles in Table 3. Table 4 contains observed and calculated structure factors¹.

Discussion of results

Composition of individual phases

The bulk composition of the K-235 specimen is $\text{Or}_{33}\text{Ab}_{58}\text{An}_8\text{Cn}_1$ (MacKenzie and Smith, 1962). Because all the barium represented by the one mole percent celsian (Cn) component may be assumed to be in the potassium-rich phase [as expected from the studies of Corlett and Ribbe (1967)], it seems reasonable to assume that eight- or nine-coordinated Ba^{2+} (radius $\sim 1.4\text{\AA}$) has the same relative effect on lattice parameters as K^{1+} (radius $\sim 1.5\text{\AA}$) and that any estimates of composition based on a^* or volume will give (Or + Cn) content, rather than just Or content. From the cell volumes listed in Table 1, $(\text{Or} + \text{Cn})_{64}\text{Ab}_8$ is predicted for the composition of the triclinic microcline and $(\text{Or} + \text{Cn})_{87}\text{Ab}_{13}$ for the monoclinic K-feldspar (Stewart and Wright, 1974, p. 365). The predicted composition of the plagioclase is Or_{-10} , but given the "problem" with Stewart and Wright's lattice parameters for this phase (pointed out in the footnote to Table 1) and the fact that it contains substantial anorthite (An), attempts to estimate the composition of the plagioclase by methods other than mass balance must be disregarded.

The composition of the microcline phase is (Or +

¹ To obtain a copy of Table 4, order Document AM-79-091 from the Mineralogical Society of America Business Office, 1909 K St., N.W., Washington, D.C. 20006. Please remit \$1.00 in advance for a copy of the microfiche.

Table 1. Lattice parameters for the three phases found in specimen K-235. Standard errors (1σ) are given in parentheses and refer to the last decimal place

Phase, space group	a	b	c	α	β	γ	α^*	γ^*	v
Triclinic K-feldspar, $C\bar{1}$	8.643(3) \AA	12.929(4) \AA	7.190(3) \AA	90.13(3) $^\circ$	116.24(3) $^\circ$	89.60(3) $^\circ$	90.05 $^\circ$	90.38 $^\circ$	720.6 \AA^3
**Monoclinic K-feldspar, $C2/m$	8.624(4)	12.918(4)	7.187(2)	90.00	116.23(4)	90.00	90.00	90.00	718.2
**Triclinic plagioclase, $C\bar{1}$	8.126(6)	12.782(7)	7.155(11)	94.24(13)	117.45(12)	87.82(10)	86.35	90.26	657.9

** Based on powder diffraction data reported by Stewart and Wright (1974) in which a few triclinic K-phase lines were observed. The plagioclase parameters were obtained from a 13-peak refinement (Stewart, personal comm.); b is anomalously large (by $\sim 1^\circ$ compared to "normal" Na-feldspars), and the volume smaller than "normal" feldspars by an amount ($\sim 5 \text{ \AA}^3$) corresponding almost exactly to the 1° difference in b .

Table 2. Fractional atomic coordinates, isotropic equivalent temperature factors (B , Å^2), and anisotropic temperature factors (β_{ij} , $\times 10^4$)

Atom	x	y	z	B	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K	0.2867(2)*	0.9985(1)	0.1406(3)	2.3	70(3)*	38(1)	155(5)	3(1)	39(3)	2(2)
T ₁ O	0.0095(2)	0.1844(1)	0.2225(3)	0.9	51(3)	9(1)	64(4)	2(1)	31(3)	2(1)
T ₁ m	0.0091(2)	0.8168(1)	0.2249(3)	0.9	52(3)	7(1)	63(4)	6(1)	29(3)	5(2)
T ₂ O	0.7105(2)	0.1184(1)	0.3413(3)	1.0	54(3)	5(1)	76(4)	1(1)	28(3)	6(2)
T ₂ m	0.7095(2)	0.8826(1)	0.3433(3)	1.1	54(3)	7(1)	87(4)	1(1)	28(3)	1(2)
O _A 1	0.0005(6)	0.1440(4)	0.9977(7)	2.1	111(9)	18(3)	159(13)	0(4)	66(9)	6(5)
O _A 2	0.6382(6)	0.0011(4)	0.2809(7)	2.0	92(9)	18(3)	119(12)	4(4)	18(8)	9(4)
O _B 0	0.8251(7)	0.1472(4)	0.2228(7)	2.4	103(10)	38(3)	159(14)	-11(5)	78(10)	6(5)
O _B m	0.8278(7)	0.8534(4)	0.2274(8)	2.5	108(10)	43(4)	140(13)	2(5)	68(9)	-0(5)
O _C 0	0.0367(6)	0.3116(4)	0.2580(7)	2.0	80(9)	21(3)	150(12)	-3(4)	46(9)	-9(5)
O _C m	0.0378(6)	0.6903(3)	0.2602(7)	1.8	78(8)	14(3)	141(12)	4(4)	39(8)	9(5)
O _D 0	0.1815(6)	0.1240(3)	0.4075(7)	1.9	109(9)	12(3)	126(12)	1(4)	40(9)	6(4)
O _D m	0.1790(6)	0.8749(3)	0.4085(7)	2.0	96(9)	16(3)	135(13)	2(4)	38(9)	0(5)

r.m.s. components of thermal displacement along principal axes (r) and thermal ellipsoid orientation for K

r	r.m.s. displacement	Angle ($^\circ$) with respect to		
		a	b	c
1	0.145(3)*	26(3)	98(4)	92(3)
2	0.179(3)	98(7)	172(5)	88(15)
3	0.187(3)	114(4)	88(15)	3(12)

* *e.s.d.*'s, given in parentheses, refer to the last decimal place.

$\text{Cn}_{94}\text{Ab}_6$ and the Or/Cn ratio given in the bulk analysis is 33/1. Thus its appropriate formula is $\text{Or}_{91}\text{Cn}_3\text{Ab}_6$. If the assumptions are made that no K remains in solid solution in the plagioclase and that no Ca is in the alkali feldspar, then by simple mass balance calculations the plagioclase phase has a composition

$$\text{Or}_{33}\text{Cn}_1\text{Ab}_{58}\text{An}_8 - 0.36(\text{Or}_{91}\text{Cn}_3\text{Ab}_6) \\ = \text{Ab}_{56}\text{An}_8/0.64 = \text{Ab}_{87}\text{An}_{13}$$

If the plagioclase contains as much as 3 mole percent Or, then the calculation is

$$\text{Or}_{33}\text{Cn}_1\text{Ab}_{58}\text{An}_8 - 0.34(\text{Or}_{91}\text{Cn}_3\text{Ab}_6) \\ = \text{Or}_2\text{Ab}_{56}\text{An}_8/0.66 = \text{Or}_3\text{Ab}_{85}\text{An}_{12}$$

In either case the microcline constitutes ~35 percent of the bulk and the plagioclase ~65 percent.

In conjunction with their study of the structures of intergrown sanidine ($\text{Or}_{86}\text{Ab}_{86}$) and high albite ($\text{Or}_{22}\text{Ab}_{78}$), Keefer and Brown (1978) have discussed at length the problems that yet remain in accurately determining the compositions of strained feldspars in cryptoperthitic association. Even the models of Robin (1974) and Tullis (1975), designed for use with intergrowths of two untwinned monoclinic phases in

the system Ab-Or, have limitations imposed by a lack of understanding of the elastic properties of feldspars at the high temperatures where spinodal decomposition or nucleation begins. Fortunately, in the case of the K-235 cryptoperthite, not much is lost by an incorrect estimation of the composition of the microcline phase: whether it has 6 or 16 mole percent albite does not particularly affect the results discussed below². If the mean (K,Na,Ba)-O distance for the 9-coordinated large cation polyhedron is any measure of the size of the average cation occupying it, it is reassuring to observe that the value of 2.974Å for K-235 microcline is actually larger than those in other K-rich feldspars, whose values range between 2.956 and 2.971Å (as opposed to 2.80Å for a comparable 9-coordinated Na-O polyhedron in high albite).

The structure of the microcline phase

Tables 1-4 contain data for our discussion of the structure of strained microcline from the K-235

² If the composition of the microcline were assumed to contain as much as 20 mole percent Ab, mass balance would require that it constitute 43 percent of the total bulk of the $\text{Or}_{33}\text{Ab}_{58}\text{An}_8\text{Cn}_1$ specimen, but the plagioclase composition would change only to $\text{Ab}_{86}\text{An}_{14}$.

Table 3. Interatomic distances (Å) and angles (°) for K-235 microcline (*e.s.d.*'s are 0.005Å on T-O and K-O distances, 0.007Å on O...O distances, and 0.3° on angles)

<u>T-O</u> distances		O-O distances		O-T-O angles
<u>T₁O tetrahedron</u>				
T ₁ O-O _A 1	1.667	O _A 1-O _B 0	2.662	105.9
-O _B 0	1.668	-O _C 0	2.788	113.6
-O _C 0	1.666	-O _D 0	2.668	105.6
-O _D 0	1.682	O _B 0-O _C 0	2.751	111.2
		-O _D 0	2.777	112.0
		O _C 0-O _D 0	2.717	108.5
Mean	1.671		2.727	109.5
<u>T₁m tetrahedron</u>				
T ₁ m-O _A 1	1.647	O _A 1-O _B m	2.635	106.5
-O _B m	1.642	-O _C m	2.759	113.3
-O _C m	1.655	-O _D m	2.644	106.1
-O _D m	1.661	O _B m-O _C m	2.714	110.8
		-O _D m	2.739	112.1
		O _C m-O _D m	2.683	108.0
Mean	1.651		2.695	109.5
<u>T₂O tetrahedron</u>				
T ₂ O-O _A 2	1.624	O _A 2-O _B 0	2.643	109.5
-O _B 0	1.612	-O _C m	2.569	104.4
-O _C m	1.627	-O _D m	2.635	108.4
-O _D m	1.624	O _B 0-O _C m	2.669	110.9
		-O _D m	2.683	112.0
		O _C m-O _D m	2.684	111.3
Mean	1.622		2.647	109.4
<u>T₂m tetrahedron</u>				
T ₂ m-O _A 2	1.639(5)	O _A 2-O _B m	2.646	108.5
-O _B m	1.622(5)	-O _C 0	2.592	104.9
-O _C 0	1.630(5)	-O _D 0	2.640	108.4
-O _D 0	1.616(5)	O _B m-O _C 0	2.680	111.0
		-O _D 0	2.677	111.5
		O _C 0-O _D 0	2.692	112.1
Mean	1.627		2.655	109.4
<u>K polyhedron</u>				
K-O _A 2	2.746(5)	T ₁ O-O _A 1-T ₁ m	144.8	
-O _A 1	2.900(5)	T ₂ O-O _A 2-T ₂ m	138.3	
-O _A 1	2.902(5)	T ₁ O-O _B 0-T ₂ O	151.7	
-O _D 0	2.942(5)	T ₁ m-O _B m-T ₂ m	153.0	
-O _D m	2.958(5)	T ₁ O-O _C 0-T ₂ m	131.6	
-O _B 0	3.014(5)	T ₁ m-O _C m-T ₂ O	131.7	
-O _B m	3.053(5)	T ₁ O-O _D 0-T ₂ m	141.1	
-O _C 0	3.089(5)	T ₁ m-O _D m-T ₂ O	141.8	
-O _C m	3.165(5)			
Mean	2.974 (CN=9)		141.8	

cryptoperthite. The first conclusion of interest is that the Al/Si distribution among the four non-equivalent tetrahedral sites apparently is as well estimated by the *b-c* and $\alpha^*-\gamma^*$ plots of Stewart and Ribbe (1969; revised by Stewart and Wright, 1974) as it is by the use of mean T-O bond lengths in a method suggested by Ribbe (1975). The calculations are detailed in Table 5. The mean bond lengths yield:

$$t_{1o} = 0.47; t_{1m} = 0.32; t_{2o} = t_{2m} = 0.10 \text{ Al}$$

The lattice parameters give the following average Al contents:

$$t_{1o} = 0.51; t_{1m} = 0.35; t_{2o} = t_{2m} = 0.07 \text{ Al}$$

These are well within the expected errors of estimate, given the assumptions and approximations involved in both methods. The literature discussing sources of errors in determining the Al/Si contents of tetrahedral sites stretches over a quarter of a century; ± 0.05 Al seems a reasonable estimate of errors by either method used here.

Perhaps it is less important to belabor the exact values of the probability of finding Al in each of the tetrahedral sites than to examine this intermediate microcline in context with the structures of other K-rich feldspars. This is most realistically done on a graph such as that in Figure 2, in which all the mean

Table 5. Estimates of Al/Si distribution in the microcline phase of the K-235 cryptoperthite

Using *b-c* and $\alpha^*-\gamma^*$ plots:

$$t_{1o} + t_{1m} = \Delta(bc) = \frac{c - 0.45132b - 1.22032}{1.6095 - 0.11252b} = 0.87$$

$$t_{1o} - t_{1m} = \Delta(\alpha^*\gamma^*) = \frac{\alpha^* - 1.99754\gamma^* + 89.77811}{0.24614\gamma^* - 26.8196} = 0.16$$

$$\text{Assume } t_{2o} = t_{2m} = 1/2(1 - t_{1o} - t_{1m})$$

$$t_{1o} = 0.51; t_{1m} = 0.35; t_{2o} = t_{2m} = 0.07$$

(Method of Stewart and Ribbe, 1969; equations from W.C. Luth)

Using mean T-O bond lengths:

$$\langle T_{1O-O} \rangle = 1.671 \text{ \AA} \quad \langle T_{1m-O} \rangle = 1.651 \text{ \AA}$$

$$\langle T_{2O-O} \rangle = 1.622 \text{ \AA} \quad \langle T_{2m-O} \rangle = 1.627 \text{ \AA}$$

$$t_{1o} - t_{1m} = (1.671 - 1.651)/0.130 = 0.15$$

$$t_{1o} - 1/2(t_{2o} + t_{2m}) = (1.671 - 1.624)/0.130 = 0.36$$

$$t_{1o} + t_{1m} + t_{2o} + t_{2m} = 1.00$$

$$t_{1o} = 0.47 \quad t_{1m} = 0.31 \quad t_{2o} = t_{2m} = 0.10$$

(Method of Ribbe, 1975, ch. 1, p. R-22)

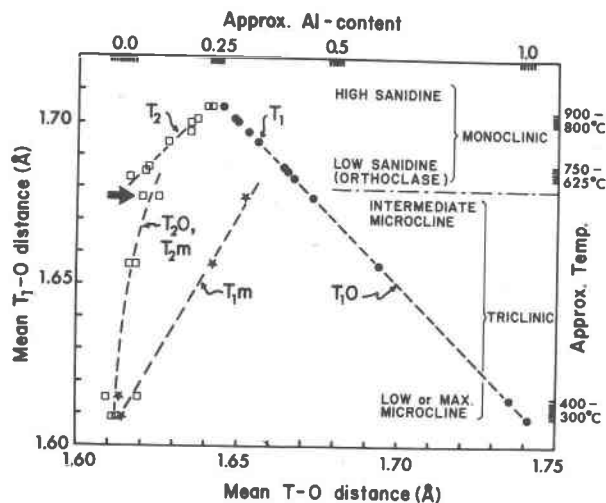


Fig. 2. A plot of the mean T -O distance as a function of the mean T_1 -O distance for the individual tetrahedra in potassium-rich feldspars as determined by crystal structure analyses. Approximate Al contents are indicated on the upper abscissa. Temperatures on the right-hand ordinate are from Stewart and Wright (1974), and their discussion of the significance of these values should be consulted. Data points for the K-235 intermediate microcline are on line with the arrow.

T -O distances are plotted as a function of the mean T_1 -O distance (T_1 O-O, in the case of triclinic feldspars). This avoids error-producing assumptions that might be involved in assigning Al occupancies to individual sites in the various structures. At the bottom of the figure are plotted data for the highly ordered maximum microclines, the lower one granitic in origin (Brown and Bailey, 1964), the higher authigenic (Finney and Bailey, 1964). Halfway up are the bond lengths for a slightly strained ($\Delta a = 0.07\text{\AA}$) microperthitic intermediate microcline (specimen U of Spencer, 1937; structure refined by Bailey, 1969). The K-235 microcline is the most nearly disordered of the four triclinic structures. Bond lengths for the T_1 and T_2 sites in even more highly disordered monoclinic K-feldspars are shown for a number of refinements reported in the literature.

The lines drawn on Figure 2 are not intended to represent a unique path of Al/Si segregation into non-equivalent T -sites as a function of temperature. Nor is it anywhere implied that there is such a path. Stewart and Wright (1974, p. 368ff.) have adequately discussed the thermal significance of Al/Si ordering, and their treatment of the ordering process in potassic feldspar in natural occurrences (p. 370ff.) has been supplemented by a summary of the structural aspects of ordering by Ribbe (1975, p. R22-28). Suffice it to say that the K-235 cryptoperthite has apparently

"equilibrated" at a temperature higher than Spencer's pegmatitic specimen U but not much different from certain of the microclines observed in a suite of rocks of K-feldspar + sillimanite grade from northwest Maine (Guidotti *et al.*, 1973; see discussion in Stewart and Wright, 1974, p. 371-373).

In seeking for some evidence of distortion in individual bond lengths or bond angles, the K-235 data were compared in detail with those of the unstrained maximum microclines and the slightly strained ($\Delta a = 0.07\text{\AA}$) intermediate microcline. Given that Al/Si distribution is different in each structure and that there are substantially larger T_2 -O bond length discrepancies in the two refinements of so-called "maximum" microcline than there are differences between similar bond lengths in Spencer U and K-235, it became evident that it would be impossible to assign the strain in K-235 to any particular bond length or bond angle distortions. Without a meaningful basis of comparison, this deduction will have to await structural studies of a comparably disordered, *unstrained* microcline.

Summary

The refinement of the structure of a strained microcline in cryptoperthitic association with albite- and pericline-twinned plagioclase has not led to a detailed understanding of what bond lengths and/or bond angles account for the effects so clearly evidenced in the index of strain, $\Delta a = 0.30\text{\AA}$. However, the mean T -O bond lengths indicate that the Al/Si distribution in the non-equivalent tetrahedral sites may be reasonably well estimated using the b - c and $\alpha^*-\gamma^*$ plots of Stewart and Wright (1974), even though partially coherent microcline is highly distorted. Composition of the microcline is best estimated from its volume, using an equation from Waldbaum and Thompson (1968). Successful crystal-structure analysis of a composite crystal, interlaminated with another phase twinned on two laws (represented by four lattices in the diffraction pattern) should encourage further study of submicroscopic intergrowths and, in particular, coherent phases about which so little is known.

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References

- Bailey, S. W. (1969) Refinement of an intermediate microcline structure. *Am. Mineral.*, 54, 1540–1545.
- Brown, B. E. and S. W. Bailey (1964) The structure of maximum microcline. *Acta Crystallogr.*, 17, 1391–1400.
- Corlett, M. and P. H. Ribbe (1967) Electron probe microanalysis of minor elements in plagioclase feldspars. (Part III of laboratory investigations on plagioclases.) *Schweiz. Mineral. Petrogr. Mitt.*, 47, 317–332.
- Finney, J. J. and S. W. Bailey (1964) Crystal structure of an authigenic maximum microcline. *Z. Kristallogr.*, 119, 413–436.
- Guidotti, C. V., H. H. Herd and C. L. Tuttle (1973) Composition and structural state of K-feldspars from K-feldspar + sillimanite grade rocks in northwestern Maine. *Am. Mineral.*, 58, 705–716.
- Keefer, K. D. and G. E. Brown (1978) Crystal structures and compositions of sanidine and high albite in cryptoperthitic intergrowth. *Am. Mineral.*, 63, 1264–1273.
- Kroll, H. (1971) *Feldspäte im System $K[AlSi_3O_8]-Ca[Al_2Si_2O_8]$: Al, Si-Verteilung und Gitterparameter, Phasen-Transformationen und Chemismus*. Inaug-Diss. der Westfälischen Wilhelms-Universität, Münster.
- MacKenzie, W. S. and J. V. Smith (1955) The alkali feldspars: I. Orthoclase-micropertthites. *Am. Mineral.*, 40, 707–732.
- and ——— (1962) Single crystal X-ray studies of crypto- and micropertthites. *Norsk Geol. Tidsskr.*, 42/2, 72–103.
- Orville, P. M. (1967) Unit-cell parameters of the microcline-low albite and the sanidine-high albite solid solution series. *Am. Mineral.*, 52, 55–86.
- Ribbe, P. H. (Ed.) (1975) *Feldspar Mineralogy*. Mineralogical Society of America Short Course Notes, Vol. 2.
- and G. V. Gibbs (1975) The crystal structure of a strained intermediate microcline in cryptoperthitic association with low albite (abstr.). *Geol. Soc. Am. Abstracts with Programs*, 7, 1245.
- Robin, P.-Y. F. (1974) Stress and strain in cryptoperthite lamellae and the coherent solvus of alkali feldspars. *Am. Mineral.*, 59, 1299–1318.
- Smith, J. V. (1961) Explanation of strain and orientation effects in perthites. *Am. Mineral.*, 46, 1489–1493.
- Stewart, D. B. (1975) Lattice parameters, composition and Al/Si order in alkali feldspars. In P. H. Ribbe, Ed., *Feldspar Mineralogy*, Mineralogical Society of America Short Course Notes, Vol. 2, p. St-1–St-22.
- and P. H. Ribbe (1969) Structural explanation for variations in cell parameters of alkali feldspar with Al/Si ordering. *Am. J. Sci.*, 267-A, 444–462.
- and T. L. Wright (1974) Al/Si order and symmetry of natural alkali feldspars, and the relationship of strained cell parameters to bulk composition. *Bull. Soc. fr. Minéral. Cristallogr.*, 97, 356–377.
- Tullis, J. (1975) Elastic strain effects in coherent perthitic feldspars. *Contrib. Mineral. Petrol.*, 49, 83–91.
- Waldbaum, D. R. and J. B. Thompson, Jr. (1968) Mixing properties of sanidine crystalline solutions: II. Calculations based on volume data. *Am. Mineral.*, 53, 2000–2017.
- Wright, T. L. and D. B. Stewart (1968) X-ray and optical study of alkali feldspar: I. Determination of composition and structural state from refined unit-cell parameters and 2V. *Am. Mineral.*, 53, 38–87.

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