

Strain in triclinic alkali feldspars: a crystal structure study

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Abstract

The crystal structure of a homogeneous unstrained intermediate microcline has been refined to $R = 0.043$ using 2183 reflections ($I > 2\sigma$) collected with an automated single-crystal X-ray diffractometer. Its composition ($\text{Or}_{89}\text{Ab}_{11}\text{Cn}_1$) and structural state ($t_1o = 0.54$, $t_1m = 0.32$, $t_2o = t_2m = 0.07$) are similar to those of the strained intermediate microcline (coherently exsolved from a cryptoperthitic ternary feldspar) for which the refined structure was reported by Ribbe (1979). A comparison of the two structures has led to a preliminary assessment of the crystallographic effects of strain in terms of bond lengths and bond angles, including a crystallographic explanation of strained lattice parameters.

Relative to corresponding sites in the strained feldspar, $\langle T_1O-O \rangle$ is larger in the unstrained feldspar by 0.010\AA , whereas the T_1m and T_2O sites are the same size, and $\langle T_2m-O \rangle$ in the unstrained feldspar is slightly smaller. As pointed out by many previous workers, coherent exsolution of the strained feldspar parallel to $(\bar{6}01)$ requires compression of b and c in the K-rich phase, with a concomitant expansion of a predicted by elasticity theory. Our results support these predictions. The strained a cell dimension is longer by 0.019\AA due to an extension of the double crankshaft chain by rotation of tetrahedra about c^* and lengthening of the $O_{Cm}-O_{Bm}$ and $O_{Bm}-O_{Cm}$ tetrahedral edges. These tetrahedral rotations about c^* and accompanying tilts about a result in the shortening of the b cell edge in the strained feldspar by 0.046\AA . The c cell edge of the strained feldspar is shorter by 0.015\AA due principally to the smaller size of the T_2O site.

With the exception of compression along c , previous predictions that feldspars respond to stress by tilting of tetrahedra rather than by alteration of $\langle T-O \rangle$ distances, and that the potassium site is a "soft" site, are confirmed. Envisioning tetrahedral tilts in terms of changes in $T-O-T$ angles does not lead to an accurate perception of the geometrical changes that accompany coherent strain.

Introduction

Over the past two decades, strained feldspars have been the subject of a number of studies aimed at elucidating the causes and the crystallographic effects of strain. Smith (1961) and Wright and Stewart (1968) recognized the existence of "anomalous" feldspars with a cell dimensions and (201) spacings inordinately large with respect to b and c , and explained the anomalous character as strain arising from the coherent or semicoherent intergrowth of potassic and sodic phases. In using Δa as a measure of strain, Stewart and Wright (1974) proposed that a feldspar for which Δa (observed a minus a predicted from their $b-c$ plot) exceeded 0.05\AA be considered strained. Robin (1974), Tullis (1975), Tullis and Yund (1979), and Yund and Tullis (1983) have considered coherency strain within the framework of elasticity the-

ory in order, among other things, to correct for strain in the unit cell parameters of coherently exsolved monoclinic feldspars. Ribbe (1979) refined the crystal structure of a strained intermediate microcline coherently and cryptoperthitically intergrown with a twinned albitic phase, but because there was no refinement of an unstrained feldspar of similar composition and structural state, he was unable to ascertain the crystallographic effects of strain in terms of individual bond lengths and bond angles.

In examining powder diffraction data for a suite of alkali feldspars collected from the Little Cottonwood Stock near Salt Lake City, Utah, we recognized that these minerals were of nearly the same composition and structural state as Ribbe's strained specimen. Strains ranged from $\Delta a = 0.01\text{\AA}$ to $\Delta a = 0.15\text{\AA}$, whereas Δa for Ribbe's feldspar was 0.30\AA . This suggested the possibility of determining the crystallographic effects of strain by comparing Ribbe's data with the refined structure of one of these feldspars.

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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4	0	0	118	126	8	4	4	26	26	-5	9	0	67	-66	4	14	0	29	-29
6	0	0	79	82	10	4	0	20	-19	-3	9	0	30	29	6	14	0	12	-13
8	0	0	4	-2	-11	5	0	16	16	-1	9	0	55	-55	8	14	0	6	-5
10	0	0	41	41	-9	5	0	22	22	1	9	0	46	-45	-7	15	0	9	11
-9	1	0	25	-26	-7	5	0	13	13	3	9	0	25	24	-3	15	0	9	9
-7	1	0	60	63	-5	5	0	55	50	5	9	0	67	-66	-1	15	0	6	-6
-5	1	0	18	-17	-3	5	0	10	10	7	9	0	25	25	1	15	0	6	1
-3	1	0	58	62	-1	5	0	5	-2	9	9	0	36	-36	3	15	0	7	6
-1	1	0	14	17	3	5	0	55	52	-8	10	0	7	6	5	15	0	4	-1
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-4	2	0	38	-41	0	6	0	169	162	-9	11	0	20	21	-1	17	0	3	-6
-2	2	0	148	-147	2	6	0	42	42	-7	11	0	53	53	1	17	0	33	34
0	2	0	21	-28	4	6	0	56	56	-5	11	0	7	5	3	17	0	18	-18
2	2	0	153	-147	6	6	0	38	39	-3	11	0	9	7	5	17	0	6	-4
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8	2	0	14	-14	-9	7	0	24	25	5	11	0	20	20	4	18	0	37	-39
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-9	3	0	21	-22	-5	7	0	19	18	9	11	0	18	17	-1	19	0	18	-22
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3	3	0	27	18	9	7	0	34	34	8	12	0	20	20	0	18	0	12	-11
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7	3	0	42	-44	-8	8	0	40	-40	-5	13	0	4	3	-5	17	0	2	5
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11	3	0	15	-14	-4	8	0	29	-30	-1	13	0	11	-12	-1	17	0	10	-10
-8	4	0	24	-25	-2	8	0	173	-166	1	13	0	11	-11	1	17	0	8	9
-6	4	0	37	-40	0	8	0	70	68	3	13	0	24	-25	3	17	0	3	-8
-4	4	0	21	-23	2	8	0	175	-170	7	13	0	28	-27	5	17	0	17	0
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4	4	0	19	-21	10	8	0	10	11	-2	14	0	30	-29	0	16	0	8	-7
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

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2-10	1	1	24	-33	-5	-5	1	4	1	7	-1	1	13	13	-4	4	1	74	73	8	8	1	32	31
4-10	1	1	6	5	-3	-5	1	54	-48	9	-1	1	2	-2	-2	4	1	123	-120	-7	9	1	10	-10
6-10	1	1	12	-12	-1	-5	1	71	64	-12	0	1	20	19	0	4	1	99	86	-5	9	1	5	-8
8-10	1	1	14	-13	-1	-5	1	54	-50	-10	0	1	22	21	2	4	1	88	-82	-3	9	1	3	-5
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-2	14	1	38	-39	-1	15	2	5	19	-7	-9	2	5	-2	7	-5	2	11	-12	-12	0	2	8	6
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-1	19	1	5	-3	4	12	2	18	18	7	-7	2	11	10	8	-2	2	30	31	-4	2	2	97	97
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

PAGE 4

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

PAGE 5

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

PAGE 6

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR VAF

PAGE 9

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR UAF

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H	K	L	FD	FC	H	K	L	FD	FC	H	K	L	FD	FC	H	K	L	FD	FC					
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