Alkali Feldspar Unit-Cell Parameters at Liquid Nitrogen Temperatures: Low Temperature Limits of the Displacive Transformation

TIMOTHY L. GROVE, AND ROBERT M. HAZEN

Department of Geological Sciences, Harvard University, Hoffinan Laboratory, Cambridge, Massachusetts 02138

Abstract

Unit-cell parameters of analbite, low albite, high sanidine, maximum microcline, and adularia have been determined at room and liquid nitrogen temperatures. In all feldspars b and π are unchanged in this temperature interval, while a undergoes significant contraction. Interaxial angles show little change in low albite, maximum microcline, and high sanidine, though analbite displays a significant increase in α and γ (and thus an increase in obliquity) with decreasing temperature. An increase in γ of adularia from 90.00° to 90.07° may indicate a low-temperature displacive transformation from a monoclinic to a triclinic phase.

Introduction

The distribution of aluminum and silicon among the tetrahedrally coordinated equipoints in the alkali feldspar structure and the size of the alkali cations that occupy the interstices of the Al-Si-O framework help determine the symmetry of the feldspar structure (see, e.g., Smith, 1970). The topologic symmetry of the alkali feldspar structure is C2/m. However, distortions of the tetrahedral framework and/or differences in the distribution of aluminum and silicon amongst the tetrahedral sites may reduce the symmetry to triclinic, as is the case for microcline and analbite.

High-temperature X-ray crystallographic studies of alkali feldspars show that continuous changes occur as a function of increasing temperature. The high-temperature X-ray powder diffraction experiments of Grundy and Brown (1969) and Stewart and von Limbach (1967) determined the magnitude of these modifications in low albite to analbite. High temperature single crystal data on microcline to 1200°C have been presented by Grundy and Brown (1967). Continuous modifications of the feldspar structure as a function of temperature may lead to changes in symmetry. Upon heating, analbite approaches monoclinic symmetry continuously, and at 980°C a displacive transformation takes place from C1 to C2/m (Grundy and Brown, 1967). Other similar displacive transformations have been found in feldspars that have an Al-Si distribution consistent with monoclinic symmetry (Kroll and Bambauer, 1971; Grove and Ito, 1973; Nager, Bambauer, and Hoffmann, 1970).

The purpose of this low temperature study was to determine the magnitudes of continuous changes in cell dimensions of alkali feldspars having different structural states. Two monoclinic alkali feldspars were observed to see if a displacive transformation could be induced at low temperatures. Three triclinic alkali feldspars were studied at low temperature to determine the lower attainable limits of the continuous changes in lattice geometry.

Experimental

Specimens of five alkali feldspars—analbite, low albite, high sanidine, maximum microcline, and adularia—were generously provided by Dr. Guy Hovis (Hovis, 1974; Thompson, Waldbaum, and Hovis, 1974). From each of these samples an untwined, equi-dimensional single crystal approximately 200 μm in diameter was selected. Optical examination showed all five crystals to be clear, colorless, and unaltered, while X-ray photographs revealed each feldspar to have sharp and unsplit diffraction maxima. A list of specimens' localities, compositions, and structural states is given in Table 1.

Each feldspar crystal was mounted and centered on our four-circle, computer-controlled Picker diffractometer. The orientations of twelve strong reflections with 2θ greater than 35° (MoKα radiation), representing all octants of reciprocal space,
were measured at both positive and negative 2θ. Room temperature (23°C) unit-cell parameters were refined from this orientation data using the Picker least-squares orientation program (Busing and Levy, 1967). In all cases these cell parameters agreed within experimental error with values determined from powder diffraction data (Hovis, 1974; Thompson et al., 1974; Orville, 1967; Hovis, unpublished data).

(Liquid nitrogen temperature (77K) was achieved and maintained using a Cryo-Tip refrigerator system manufactured by Air Products and Chemicals, Inc. The crystal is mounted on a copper pin and is surrounded by a thin-walled beryllium vacuum shroud. The copper pin maintains contact with a small chamber of liquid nitrogen, which refrigerates the pin and crystal by conduction. The crystal temperature was monitored continuously using a copper-constantan thermocouple positioned beneath the specimen in the refrigeration pin, and was found to vary no more than 2°C from the minimum of -198°C. The feldspar crystals were first allowed to equilibrate for two hours at liquid nitrogen temperature. Experimental procedures for determining unit-cell parameters at low temperature were identical to those used at room temperature. After twelve diffraction maxima were measured, the initial two reflections were remeasured to confirm that the feldspar crystals had not altered in orientation. In all cases the initial and final orientations agreed within 0.02°.

**Results**

Unit-cell parameters and their estimated standard deviations for five alkali feldspars at 23°C and -198°C are presented in Table 1. In all cases b and β remain unchanged as temperature is lowered. The a dimension is significantly shortened at liquid nitrogen temperature in all the feldspars studied. An increase in obliquity is observed in analbite by a positive change in both a and γ. A similar change in the γ of adularia is observed and indicates a departure from monoclinic symmetry at low temperatures. Microcline, sanidine, and low albite show little change in interaxial angles during the 221°C temperature change, indicating that the room temperature structures probably represent frameworks with configurations near the lower limit of continuous change. Of the five feldspars studied, the interaxial angles of analbite show the greatest changes.

**Conclusions**

Our results are consistent with previous high temperature studies of alkali feldspars. With decreasing temperatures the triclinic minerals increase in obliquity, and cell parameters decrease. The rate of

---

**Table 1. Specimen Sources, Compositions, and Unit-Cell Parameters**

<table>
<thead>
<tr>
<th>Sample (Reference)</th>
<th>¯a/¯ab</th>
<th>T (°C)</th>
<th>a (Å)</th>
<th>b (Å)</th>
<th>c (Å)</th>
<th>α (°)</th>
<th>β (°)</th>
<th>γ (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adularia St. Gotthard, Switz. (Hovis, 1973; UNI-7007)</td>
<td>0.882</td>
<td>23</td>
<td>8.551(3)</td>
<td>22.971(4)</td>
<td>7.210(3)</td>
<td>90.00(3)</td>
<td>120.02(3)</td>
<td>90.00(2)</td>
</tr>
<tr>
<td>Maximum Microcline Hugo pegmatite, S.D. (Orville, 1967)</td>
<td>0.881</td>
<td>23</td>
<td>8.575(3)</td>
<td>22.952(4)</td>
<td>7.221(2)</td>
<td>90.64(3)</td>
<td>125.94(3)</td>
<td>87.75(2)</td>
</tr>
<tr>
<td>High Sanidine Lashier Cell, Germany Heated 560 hours @ 1050°C, 1 atm. (Hovis, 1973; UNI-7002)</td>
<td>0.847</td>
<td>23</td>
<td>8.545(2)</td>
<td>23.040(3)</td>
<td>7.173(2)</td>
<td>90.00(2)</td>
<td>120.00(2)</td>
<td>90.00(2)</td>
</tr>
<tr>
<td>Low Albite Amelsa Courthouse, Va. (Thompson et al., 1973)</td>
<td>0.016</td>
<td>23</td>
<td>8.132(2)</td>
<td>22.788(3)</td>
<td>7.160(2)</td>
<td>94.21(2)</td>
<td>116.58(2)</td>
<td>87.68(2)</td>
</tr>
<tr>
<td>Anorthite Heated Amelsa low albite 362 hours @ 1060°C, 1 atm. (Thompson et al., 1973)</td>
<td>0.016</td>
<td>23</td>
<td>8.163(2)</td>
<td>22.881(4)</td>
<td>7.112(3)</td>
<td>93.67(3)</td>
<td>116.49(3)</td>
<td>90.30(4)</td>
</tr>
</tbody>
</table>

* Parenthesized figures represent the estimated standard deviation (σ) in terms of least units cited for the value to the immediate left, thus 8.551(3) indicates an σ of 0.023.
contraction of cell edges and change of interaxial angles decreases at lower temperatures. Both the low temperature equilibrium forms of potassium and sodium feldspar undergo little change in interaxial angles over the temperature region from 23°C to -198°C, suggesting that the continuous changes which take place at elevated temperatures have nearly reached their lower limits at room temperature. In contrast, the high temperature polymorph of albite has not reached the lower bounds of its continuous change at room temperature, but increases significantly in obliquity at liquid nitrogen temperature. The experimentally determined change in γ found for the adularia is small but greater than one standard deviation and may indicate a low temperature displacive transformation from monoclinic to triclinic symmetry.

Acknowledgments

The authors gratefully acknowledge the contributions of Dr. Guy Hovis and Professor C. W. Burnham, who offered advice on experimental aspects of this study and carefully reviewed the manuscript. We also thank Professor James B. Thompson who first proposed this study. This research was supported by National Science Foundation Grant GA-12852 to Professor C. W. Burnham.

References


Manuscript received, March 25, 1974; accepted for publication, July 16, 1974.