Thermal expansion and high-temperature crystal chemistry of the Al₂SiO₆ polymorphs

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Seattle, Washington 98195

Abstract

The crystal structures of sillimanite and andalusite have been refined from intensity data collected at 25, 400, 600, 800, and 1000°C. R factors following refinement were 0.033±.002 and 0.029±.002 for the sillimanite and andalusite data sets respectively. For kyanite 2140, 1773, and 1741 reflections were measured at 25, 400, and 600°C, and the final R factors were 0.033, 0.031, and 0.036 respectively.

Unit-cell dimensions of all three polymorphs vary linearly with temperature. Although the unit-cell dimensions determined at room temperature agree within error limits with those of Skinner et al. (1961), significant deviations occur between the two data sets at elevated temperatures. All the Al octahedra exhibit considerable expansions with increasing temperature. In contrast, Al- or Si-tetrahedra in all three polymorphs remain relatively constant in size and shape as temperature is increased. Within the five-coordinated Al₆ polyhedron in andalusite the four short bonds remain relatively unchanged, whereas the longest bond, Al₆-O₅, expands considerably. The orientation of the long Al₆-O₅ bonds in sillimanite and andalusite, which are more expandable than the other octahedral Al-O bonds, determines the direction of maximum unit-cell expansion. The chains of fully stretched tetrahedra (and Al₄ trigonal bipyramids in andalusite) restrict expansion in the c axis direction for these two minerals. The greater number of shared octahedral edges in kyanite, as well as the lack of continuous tetrahedral chains, results in more evenly distributed coefficients of unit-cell expansion.

Polymorphic transitions involve major reconstructive transformations. In addition, the andalusite-sillimanite transition requires diffusive interchange of half the Si and Al₂ atoms. Consequently, although metastable coexistence of two or three polymorphs is commonly observed, coherent replacement textures are rare. The present volume-temperature data agree well with the experimentally-derived thermodynamic properties of the aluminum silicate minerals.

Introduction

Andalusite, kyanite, and sillimanite, the three Al₂SiO₆ polymorphs that commonly occur in metamorphosed pelitic sediments, have been the subject of a great deal of study in the fields of metamorphic and experimental petrology. Due to the small changes in thermodynamic properties associated with the polymorphic phase transitions, metastable coexistence of these phases is common, and the mode of occurrence and relative fields of stability of the polymorphs are not completely clear.

The crystal structures of sillimanite and andalusite were first determined by Taylor (1928, 1929), using estimated intensities from rotation photographs. The kyanite structure was deduced by inference from the staurolite structure by Naray-Szabo et al. (1929). From diffractometer-counter data, the structures of andalusite, sillimanite, and kyanite were refined by Burnham and Buerger (1961) and Burnham (1963a, b) respectively. Refinements of sillimanite and andalusite structures based on neutron diffraction data have been performed by Finger and Prince (1972). Thermal expansions of the three polymorphs were determined by Skinner et al. (1961), using the powder-diffraction technique with a heating stage.

We wish to relate the details of the crystal structures of the three polymorphs determined at elevated temperatures to the thermal expansion data, and thereby provide a basis for understanding the behav-
TABLE 5. Sillimanite, Andalusite, and Kyanite: Anisotropic thermal ellipsoids, axial lengths (Å) and isotropic equivalent temperature factors, $\Delta q^2$ (Å²) as a function of temperature.

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*Isotropic equivalent temperature factors, calculated from anisotropic temperature factors (Hamilton, 1959)
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The thermal expansion and the high temperature crystal chemistry of Al$_2$SiO$_5$ polymorphs

John X. Winter

and

Subrata Ghose

Department of Geological Sciences
University of Washington
Seattle, Washington 98195

Table A. Sillimanite, andalusite and kyanite: observed and calculated structure factors at various temperatures.
**TABLE 7. Continued**

<table>
<thead>
<tr>
<th></th>
<th>25°C</th>
<th>400°C</th>
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<td>$A_{12}-S_{11}$</td>
<td>125.49(9)</td>
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<td>$A_{22}-S_{11}$</td>
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"$A_{11}$ A-B" indicates the $O_{A1}-A_{11}-O_{B}$ angle etc.
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<th>Angle 2 (°)</th>
<th>Angle 3 (°)</th>
<th>Angle 4 (°)</th>
<th>Angle 5 (°)</th>
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**Note:** The above table represents a portion of the data from the document. The complete data includes various angles and their corresponding values, arranged in a tabular format. The table continues with similar entries, indicating a systematic approach to presenting the data.
<table>
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<th>θ (°)</th>
<th>3θ (°)</th>
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Ranges of (SIN[θ]/LAMBDA)**(1/2)

**[Table Continued]**

Results of Structure Factor Calculations

[Further details not legible]
calculated structure factors at various temperatures.

Table 4: Summary of structure and parameter observations and

Department of Geoscience

Substitute Chair

and

John A. Mercer

of the 0.5% position

The thermal expansion and the peak temperature crystal

diameter.
<table>
<thead>
<tr>
<th>Value</th>
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</table>

**Summary:**

- **Sample:** 990, 980, 970, 960, 950, 940, 930, 920, 910, 900
- **Preparation:** 99, 98, 97, 96, 95, 94, 93, 92, 91, 90

**Note:** The table above represents the results of a study on the preparation and weight of samples.
calculated structure factors at various temperatures.

Table 1: S111/121 and 121/111 structure and observed and

Department of Geological Sciences

Saratoga, Idaho

and

John R. Witter

of A12, A21, A121, and A211 polytypes

The thermal expansion and the high temperature crystal structure...
calculated structure factors at various temperatures.