High-pressure behavior of kyanite: Compressibility and structural deformations

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ABSTRACT

The lattice parameters of kyanite were measured at various pressures up to about 60 kbar by single-crystal X-ray diffraction in a diamond anvil cell. Unit-cell dimensions decreased linearly with an almost uniform rate:

\[ \beta_a = 2.00(8) \times 10^{-4}, \beta_b = 1.90(4) \times 10^{-4}, \beta_c = 2.00(4) \times 10^{-4} \text{ kbar}^{-1}. \]

The principal compressibility coefficients were \( \beta_a = 2.23 \times 10^{-4}, \beta_b = 2.04 \times 10^{-4}, \beta_c = 1.65 \times 10^{-4} \text{ kbar}^{-1} \), with \( \beta_c \) forming an angle of 35° with the c axis. \( K_0 \), calculated by fitting pressure-volume data to a third-order Birch-Murnaghan equation of state, was 1560(100) kbar, with \( K' = 5.6(5.5) \); when \( K' \) was set at 4, \( K_0 \) became 1600(30) kbar.

Structural refinements were carried out on data collected at 0.001 kbar with the crystal in air and at 0.1, 25.4, 37, and 47 kbar with the crystal in the diamond anvil cell. Whereas the Si tetrahedra and Al4 octahedron were incompressible in this \( P \)-range, the polyhedral bulk modulus for Al1 and Al2 was 1280(150) kbar and 2380(200) kbar for Al3. These octahedra became more regular with increasing pressure.

The almost isotropic compression pattern was due to the many shared edges between the polyhedra, uniformly distributed in the cell. The evolution of Al-Al separation showed that the largest reduction regarded the Al2-Al3 and Al2-Al4 distances, whereas the average Al1-Al2 distance was almost unchanged, resulting from linkage with Si tetrahedra having rigid edges. The result was that the largest reduction did not occur along the c axis but along the Al4-Al1–Al2-Al3 directions.

The geometrical structural invariance, expressed by the \( \beta_c/\alpha_c \) ratio and obtained from the average compressibility and average thermal expansion of the cell volume (Winter and Ghose 1979), was 23 °C/kbar. The following equation of state, which applies in crustal \( P-T \) conditions, may be defined as: \( V/V_0 = 1 + 3.00(7) \times 10^{-3} T - 5.8(1) \times 10^{-5} P \), where \( T \) is in °C and \( P \) in kbar.

The present volume-pressure data support multi-anvil experiments by Schmidt et al. (1997) defining the \( P-T \) conditions necessary for decomposition of kyanite into stishovite + corundum.

INTRODUCTION

Kyanite, andalusite, and sillimanite, the three polymorphs of Al2SiO5, are extensively used to characterize metamorphic rocks. Although the petrologic literature contains numerous attempts at localizing the exact position of the triple point in the \( T-P \) stability diagram of andalusite-sillimanite-kyanite, small changes in thermodynamic properties greatly influence the position of Al2SiO5 phase transitions, and the precise stability fields of the three polymorphs are still uncertain.

Kyanite is the high-pressure polymorph of Al2SiO5. In nature, kyanite is a common accessory mineral in eclogite-facies rocks in both metabasaltic and metasedimentary bulk compositions. When such crustal rock types are subducted, kyanite is involved in several breakdown reactions that increase its abundance at pressures higher than 20 kbar. These reactions involve paragonite (Chatterjee 1972), zoisite and lawsonite (Poli and Schmidt 1995), pumpellyite (Schreyer 1988) in mafic rocks, and chloritoid and staurolite in metagreywackes or metapelites (Schreyer 1988).

Neither kyanite nor corundum is reported from typical mantle compositions, i.e., lherzolites or harzburgites. As long as its structure remains stable (to ca. 200 kbar), garnet is capable of hosting the alumina present in an average upper mantle. However, when the subducted slab is disrupted at or below the transition zone, accretion of fertilized peridotite is expected (Ringwood 1991), and Al-phases other than garnet probably play a major role in mantle evolution. Furthermore, in experiments in a laser-heated diamond-anvil cell, Ahmed-Zaid and Madon (1991) identified a new high-pressure form of Al2SiO5. This phase, with a structure similar to that of V2O5, was proposed as...