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Phase stability, elastic behavior, and pressure-induced structural evolution of kalsilite: A ceramic material and high-*T*/high-*P* mineral

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Abstract

The phase stability, elastic behavior, and pressure-induced structural evolution of a natural metamorphic kalsilite (ideal formula $KAlSiO_4$) from Punalur (Kerala district in southern India), with $P31c$ symmetry and a K/Na molar ratio of ~350, has been investigated by in situ X-ray single-crystal diffraction up to ~7 GPa with a diamond-anvil cell under hydrostatic conditions. At high-pressure, a previously unreported iso-symmetric first-order phase transition occurs at ~3.5 GPa. The volume compression of the two phases is described by third-order Birch-Murnaghan equations-of-state: V_0 = 201.02(1) Å^3, K_{T0} = 59.7(5) GPa, K' = 3.5(3) for the low-*P* polymorph, and V_0 = 200.1(13) Å^3, K_{T0} = 44(8) GPa, K' = 6.4(20) for the high-*P* polymorph. The pressure-induced structural evolution in kalsilite up to 7 GPa appears to be completely reversible. The compression of both phases involves tetrahedral rotations around [0001], which close up the channels within the framework. In addition, compression of the low-pressure phase involves tilting of the tetrahedra. The major structural change at the phase transition is an increase in the tilting of the tetrahedra, but with a reversion of the tetrahedral rotations to the value found at ambient conditions. This behavior is in distinct contrast to that of nepheline, which has a tetrahedral framework of the same topology.

Keywords: Crystal structure, kalsilite, XRD data, single crystal, high pressure, compressibility, structural evolution, compressibility measurements