

High-pressure single-crystal structural analysis of AlSiO₃OH phase egg

**KIRSTEN SCHULZE^{1,*}, MARTHA G. PAMATO², ALEXANDER KURNOSOV¹, TIZIANA BOFFA BALLARAN¹,
KONSTANTIN GLAZYRIN³, ANNA PAKHOMOVA³, AND HAUKE MARQUARDT^{1,4}**

¹Bayerisches Geoinstitut, University Bayreuth, 95440 Bayreuth, Germany

²Department of Earth Sciences, University College London, WC1E 6BT London, U.K.

³FS-PE, Deutsches Elektronen Synchrotron, Hamburg 22607, Germany

⁴Department of Earth Sciences, University of Oxford, OX1 3AN Oxford, U.K.

ABSTRACT

We present the first equation of state and structure refinements at high pressure of single-crystal phase egg, AlSiO₃OH. Phase egg is a member of the Al₂O₃-SiO₂-H₂O system, which contains phases that may be stable along a typical mantle geotherm (Fukuyama et al. 2017) and are good candidates for water transport into Earth's deep mantle. Single-crystal synchrotron X-ray diffraction was performed up to 23 GPa. We observe the **b** axis to be the most compressible direction and the β angle to decrease up to 16 GPa and then to remain constant at a value of $\sim 97.8^\circ$ up to the maximum experimental pressure reached. Structure refinements performed at low pressures reveal a distorted octahedron around the silicon atom due to one of the six Si-O bond lengths being significantly larger than the other five. The length of this specific Si-O4 bond rapidly decreases with increasing pressure leading to a more regular octahedron at pressures above 16 GPa. We identified the shortening of the Si-O4 bond and the contraction of the vacant space between octahedral units where the hydrogen atoms are assumed to lie as the major components of the compression mechanism of AlSiO₃OH phase egg.

Keywords: Phase egg, single-crystal, X-ray diffraction, compressibility, structure refinement