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The influence of Al_2O_3 on the structural properties of $MgSiO_3$ akimotoite

Nicki C. Siersch[1,*,†], Giacomo Criniti[1,§], Alexander Kurnosov[1], Tiziana Boffa Ballaran[1], Zhaodong Liu[1,2,#], Takayuki Ishii[1,‡], Daniel J. Frost[1,‖], Tony Yu[3], and Yanbin Wang[3]

[1]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany
[2]State Key Laboratory of Superhard Materials, Jilin University, Changchun 13001, China
[3]Center for Advanced Radiation Sources, The University of Chicago, Chicago, Illinois 60637, U.S.A.

Abstract

Akimotoite, a $MgSiO_3$ polymorph present in the lower transition zone within ultramafic portions of subducting slabs and potentially also in the ambient mantle, will partition some amount of Al, raising the question of how this will affect its crystal structure and properties. In this study, a series of samples along the $MgSiO_3$-Al_2O_3 (akimotoite-corundum) solid solution have been investigated by means of single-crystal X-ray diffraction to examine their crystal chemistry. Results show a strong nonlinear behavior of the *a*- and *c*-axes as a function of Al content, which arises from fundamentally different accommodation mechanisms in the akimotoite and corundum structures. Furthermore, two Al_2O_3-bearing akimotoite samples were investigated at high pressure to determine the different compression mechanisms associated with Al substitution. Al_2O_3-bearing akimotoite becomes more compressible at least up to 20 mol% Al_2O_3, due likely to an increase in compressibility as the Al cation is incorporated into the SiO_6 octahedron. This observation is in strong contrast to the stiffer corundum end-member having a K_T = 250 GPa, which is larger than that of the akimotoite end-member [K_T = 205(1) GPa]. These findings have implications for mineral physics models of elastic properties, which have in the past assumed linear mixing behavior between the $MgSiO_3$ akimotoite and Al_2O_3 corundum end-members to calculate sound wave velocities for Al-bearing akimotoite at high pressure and temperature.

Keywords: Akimotoite, corundum, X-ray diffraction, high pressure, solid solution