American Mineralogist, Volume 98, pages 285–291, 2013

Pressure-induced structural transformations in the low-cristobalite form of $AlPO_4$

H.K. Poswal,[1,*] Nandini Garg,[1] Maddury Somayazulu,[2] and Surinder M. Sharma[1]

[1]High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India
[2]Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C. 20015, U.S.A.

Abstract

We have investigated the high-pressure behavior of low-cristobalite form of $AlPO_4$ (c-$AlPO_4$) using a combination of Raman scattering, synchrotron powder X-ray diffraction, and classical molecular dynamics simulations. Our experiments indicate that under non-hydrostatic conditions c-$AlPO_4$ initially transforms to a monoclinic phase, which then transforms to the *Cmcm* phase via an intermediate, disordered structure. In contrast, X-ray diffraction measurements made under hydrostatic conditions show that the ambient structure transforms directly to the *Cmcm* phase. Our classical molecular dynamics simulations, carried out under hydrostatic conditions, also show that c-$AlPO_4$ directly transforms to the *Cmcm* phase at ~13 GPa.

Keywords: Cristobalite, high pressure, Raman scattering, synchrotron X-ray diffraction, classical molecular dynamics, $AlPO_4$