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Raman scattering and Cr^{3+} luminescence study on the structural behavior of δ-AlOOH at high pressures

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Abstract

δ-AlOOH is regarded as a potential water carrier that is stable in the Earth's lower mantle down to the core-mantle boundary along the cold slab geotherm; thus, knowledge of its structural evolution under high pressure is very important for understanding water transport in the Earth's interior. In this work, we conducted Raman scattering and luminescence spectroscopic experiments on δ-AlOOH at pressures up to 34.6 and 22.1 GPa, respectively. From the collected Raman spectra, significant changes in the pressure dependence of the frequencies of Raman-active modes were observed at ~8 GPa, with several modes displaying softening behavior. In particular, the soft A_1 mode, which corresponds to a lattice vibration of the AlO_6 octahedron correlated to OH stretching vibrations, decreases rapidly with increasing pressure and shows a trend of approaching 0 cm^{-1} at ~9 GPa according to a quadratic polynomial extrapolation. These results provide clear Raman-scattering spectroscopic evidence for the $P2_1nm$-to-$Pnnm$ structural transition. Similarly, the phase transition was also observed in the luminescence spectra of Cr^{3+} in both powder and single-crystal δ-AlOOH samples, characterized by abrupt changes in the pressure dependences of the wavelength of the R-lines and sidebands across the $P2_1nm$-to-$Pnnm$ transition. The continuous decrease in R_2-R_1 splitting with pressure indicated that the distortion of the AlO_6 octahedron was suppressed under compression. No abnormal features were clearly observed in our Raman or luminescence spectra at ~18 GPa, where the ordered symmetrization or fully centered state with hydrogen located at the midpoint of the hydrogen bond was observed by a previous neutron diffraction study. However, some subtle changes in Raman and luminescence spectra indicated that the ordered symmetrization state might form at around 16 GPa.

Keywords: δ-AlOOH, phase transition, Raman spectra, luminescence, high pressure