

An X-ray diffraction study of the pressure-induced hydration in cordierite at 4–5 GPa

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ABSTRACT

The elastic and structural behavior of natural cordierite compressed in aqueous medium up to 6 GPa was studied by means of in situ synchrotron powder diffraction with a diamond-anvil cell. In the range between 1–4 GPa the elastic behavior is regular and slightly anisotropic, with linear compressibilities $\beta_a:\beta_b:\beta_c = 4:4:5$, the most rigid **a-b** plane coinciding with the orientation of 6-membered rings. A distinct decrease of compressibility in the range of 4–5 GPa indicates a pressure-induced hydration (PIH), which is confirmed by the structure refinements. The addition of about 60% of the initial water content into the cordierite channels proceeds through positional disordering of the H₂O sites inside the channel cavity and a stepwise filling of the H₂O position inside the 6-membered rings, leading to the phase transition at about 4.7 GPa. The appearance of H₂O molecules inside 6-membered rings prevents their contraction and even causes their slight enlargement along the **a** direction, apparently related to the orientation of H-bonds. This results in an anisotropic deformation of the unit cell and an increase of the *a* parameter in the HP phase at 4.9 GPa, as well as a decrease of linear compressibility along **a** upon the further compression up to 6 GPa ($\beta_a:\beta_b:\beta_c = 5:9:10$).

Keywords: Cordierite, high pressure, compressibility, pressure-induced hydration, crystal structure