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High-pressure deformation mechanism in scolecite: A combined computational-experimental study

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ABSTRACT

Pressure-induced structural modifications in scolecite were studied by means of in situ synchrotron X-ray powder diffraction and density functional computations. The experimental cell parameters were refined up to 8.5 GPa. Discontinuities in the slope of the unit-cell parameters vs. pressure dependence were observed; as a consequence, an increase in the slope of the linear pressure-volume dependence is observed at about 6 GPa, suggesting an enhanced compressibility at higher pressures. Weakening and broadening of the diffraction peaks reveals increasing structural disorder with pressure, preventing refinement of the lattice parameters above 8.5 GPa. Diffraction patterns collected during decompression show that the disorder is irreversible. Atomic coordinates within unit cells of different dimensions were determined by means of Car-Parrinello simulations. The discontinuous rise in compressibility at about 6 GPa is reproduced by the computation, allowing us to attribute it to re-organization of the hydrogen bonding network, with the formation of water dimers. Moreover we found that, with increasing pressure, the tetrahedral chains parallel to *c* rotate along their elongation axis and display an increasing twisting along a direction perpendicular to *c*. At the same time, we observed the compression of the channels. We discuss the modification of the Ca polyhedra under pressure, and the increase in coordination number (from 4 to 5) of one of the two Al atoms, resulting from the approach of a water molecule. We speculate that this last transformation triggers the irreversible disordering of the system.