Structural transformations of the nanoconfined water at high pressures: a potential mechanism of trigger effects in the subduction zones

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Water is one of the most common compounds in the Earth crust. In subduction zones, water captured in nanoscale pores of hydrophilic oceanic minerals can be carried to the depths of the upper mantle and the transition zone. In the nano-confined state, water exhibits properties that differ from the water in the free bulk state, especially under the extreme thermodynamic conditions of the subducted plate. The structure and properties of the nanopore walls at the molecular level are significant factors that determine the structure and properties of nanoconfined water, including its phase transformations with increasing lithostatic pressure. Phase transformations of the water, which are accompanied by a stepwise, abrupt changes in its mechanical properties, and hence the properties of the entire water-saturated mineral, can be a potential mechanism of trigger effects in subduction zones.

In the present study, the molecular level structure and phase transformations of nanoconfined water within model minerals with hydrophilic and hydrophobic surface are investigated in the pressure range up to 10 GPa. Using the molecular dynamics simulations, it was shown that the mineral surface polarity significantly affects the physical properties of nanoconfined water in the pressure range considered. In particular, the water confined in a hydrophilic nanopore, a phase transition from a liquid phase to a HCP crystal was observed at pressure 3.0 GPa, and HCP to FCC transformation at 6.7 GPa. At the same time, water in the artificial hydrophobic mineral with similar atomic structure but significantly reduced partial charges on mineral atoms behaves radically different: water doesn't form HCP lattice and transforms directly from the liquid phase to the FCC phase at 3.0 GPa. We show that the phase transformations of water in the nanopores of minerals are accompanied by a stepwise reversible increase in the compressibility of water up to 1-1.5 orders of magnitude. Such strong transient variations in the compressibility of water can cause significant variations in the effective stiffness of watered rock and can trigger a dynamic rupture and accompanying seismic effects.

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