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Anomalous elastic behavior of phase egg, $AlSiO_3(OH)$, at high pressures

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Abstract

Phase egg, [$AlSiO_3(OH)$], is an aluminosilicate hydrous mineral that is thermodynamically stable in lithological compositions represented by Al_2O_3-SiO_2-H_2O (ASH) ternary, i.e., a simplified ternary for the mineralogy of subducted sediments and continental crustal rocks. High-pressure and high-temperature experiments on lithological compositions resembling hydrated sedimentary layers in subducting slabs show that phase egg is stable up to pressures of 20–30 GPa, which translates to the transition zone to lower mantle depths. Thus, phase egg is a potential candidate for transporting water into the Earth's mantle transition zone. In this study, we use *first-principles* simulations based on density functional theory to explore the pressure dependence of crystal structure and how it influences energetics and elasticity. Our results indicate that phase egg exhibits anomalous behavior of the pressure dependence of the elasticity at mantle transition zone depths (~15 GPa). Such anomalous behavior in the elasticity is related to changes in the hydrogen bonding O-H···O configurations, which we delineate as a transition from a low-pressure to a high-pressure structure of phase egg. Full elastic constant tensors indicate that phase egg is very anisotropic resulting in a maximum anisotropy of compressional wave velocity, $Av_P \approx 30\%$ and of shear wave velocity, $Av_S \approx 17\%$ at zero pressures. Our results also indicate that the phase egg has one of the fastest bulk sound velocities (v_P and v_S) compared to other hydrous aluminous phases in the ASH ternary, which include topaz-OH, phase Pi, and δ-AlOOH. However, the bulk sound velocity of phase egg is slower than that of stishovite. At depths corresponding to the base of mantle transition zone, phase egg decomposes to a mixture of δ-AlOOH and stishovite. The changes in compressional Δv_P and shear Δv_S velocity associated with the decomposition is ~0.42% and –1.23%, respectively. Although phase egg may be limited to subducted sediments, it could hold several weight percentages of water along a normal mantle geotherm.

Keywords: Phase egg, equation of state, elasticity, anisotropy, symmetric hydrogen bonding, subduction zone