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Incorporation of Mg in phase Egg, $AlSiO_3OH$: Toward a new polymorph of phase H, $MgSiH_2O_4$, a carrier of water in the deep mantle

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Abstract

The crystal structure and chemical composition of a crystal of Mg-bearing phase Egg with a general formula $M^{3+}_{1-x}M^{2+}_{x}SiO_4H_{1+x}$ (M^{3+} = Al, Cr; M^{2+} = Mg, Fe), where $x = 0.35$, produced by subsolidus reaction at 24 GPa and 1400 °C of components of subducted oceanic slabs (peridotite, basalt, and sediment), was analyzed by electron microprobe and single-crystal X-ray diffraction. Neglecting the enlarged unit cell and the consequent expansion of the coordination polyhedra (as expected for Mg substitution for Al), the compound was found to be topologically identical to phase Egg, $AlSiO_3OH$, space group $P2_1/n$, with lattice parameters $a = 7.2681(8)$, $b = 4.3723(5)$, $c = 7.1229(7)$ Å, $\beta = 99.123(8)°$, $V = 223.49(4)$ Å^3, and $Z = 4$. Bond-valence considerations lead to hypothesize the presence of hydroxyl groups only, thereby excluding the presence of the molecular water that would be present in the hypothetical end-member $MgSiO_3 \cdot H_2O$. We thus demonstrate that phase Egg, considered as one of the main players in the water cycle of the mantle, can incorporate large amounts of Mg in its structure and that there exists a solid solution with a new hypothetical $MgSiH_2O_4$ end-member, according to the substitution $Al^{3+} \leftrightarrow Mg^{2+} + H^+$. The new hypothetical $MgSiH_2O_4$ end-member would be a polymorph of phase H, a leading candidate for delivering significant water into the deepest part of the lower mantle.

Keywords: phase Egg, phase H, hydrous dense magnesium silicate, sample synthesis, electron microprobe analysis, X-ray diffraction, crystal structure