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LETTER

Partition of Al between Phase D and Phase H at high pressure: Results from a simultaneous structure refinement of the two phases coexisting in a unique grain

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ABSTRACT

The crystal structure of the two dense hydrous magnesium silicates Phase D, $MgSi_2H_2O_6$, and Phase H, $MgSiH_2O_4$, synthesized at 45 GPa and 1000 °C and coexisting in the same micrometer-sized grain, was investigated by single-crystal X-ray diffraction to study the preferential partition of Al between the two structures. In agreement with the literature, Phase D was found to be trigonal, space group $P\overline{3}1m$, with lattice parameters a = 4.752(2), c = 4.314(2) Å, V = 84.37(6) Å^3 (R_1 = 0.020), and Phase H was found to be orthorhombic, space group *Pnnm*, with lattice parameters a = 4.730(2), b = 4.324(2), c = 2.843(2) Å, V = 58.15(5) Å^3 (R_1 = 0.024). The estimated proportion (vol%) of the two phases from the refinement is $27(2)_{PhD} - 73_{PhH}$. The analysis of the geometric details of the two structures shows that Phase D hosts almost all the Al available, whereas Phase H is nearly identical to pure $MgSiH_2O_4$. Overexposed electron-microprobe X-ray maps of the same grain used for the X-ray diffraction study together with WDS spots on the two phases confirmed the structural results. Thus, our results suggest that when Phase D and Phase H coexist, Al is strongly partitioned into Phase D at the expense of coexisting Phase H. At pressure above ~50 GPa, where Phase D is no longer stable, Phase H is able to incorporate the high aluminum contents present in hydrous peridotitic compositions in the deep lower mantle and be stabilized at the expense of Phase D and magnesium silicate perovskite.

Keywords: Phase D, Phase H, aluminum, dense hydrous magnesium silicates, lower mantle, crystal structure, synthesis