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# Equation of state and elasticity of the 3.65 Å phase: Implications for the X-discontinuity

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## Abstract

The 3.65 Å phase [$MgSi(OH)_6$] is likely to be formed by decomposition of the hydrous 10 Å phase [$Mg_3Si_4O_{10}(OH)_2 \cdot H_2O$] at pressures of 9–10 GPa. In this study, we use a combination of X-ray diffraction and *first-principles* simulations to constrain the equation of state and elasticity of the 3.65 Å phase. We find that the equation of state results for the 3.65 Å phase, from X-ray diffraction data are well represented by a third-order Birch-Murnaghan formulation, with $K_0$ = 83.0 (±1.0) GPa, $K_0'$ = 4.9 (±0.1), and $V_0$ = 194.52 (±0.02) Å$^3$. Based on the *first-principles* simulations, the full single-crystal elastic constant tensor with monoclinic symmetry shows significant anisotropy with the compressional $c_{11}$ = 156.2 GPa, $c_{22}$ = 169.4 GPa, $c_{33}$ = 189.3 GPa, the shear components $c_{44}$ = 55.9 GPa, $c_{55}$ = 58.5 GPa, $c_{66}$ = 74.8 GPa, and $c_{46}$ = 1.6 GPa; the off-diagonal components $c_{12}$ = 38.0 GPa, $c_{13}$ = 26.5 GPa, $c_{23}$ = 22.9 GPa, $c_{15}$ = 1.5 GPa, $c_{25}$ = 1.5 GPa, and $c_{35}$ = –1.9 GPa at zero pressure.

At depths corresponding to 270–330 km, the seismological X-discontinuity has been observed in certain regions. We find that the formation of 3.65 Å from layered hydrous magnesium silicates (LHMS) such as 10 Å angstrom phases occurs at around 9 GPa, i.e., coinciding with the seismic X-discontinuity. The LHMS phases have significant seismic anisotropy. Based on the full elastic constant tensor, although among the dense hydrous magnesium silicate (DHMS) phases, the 3.65 Å phase reveals considerably larger elastic anisotropy, it is significantly smaller than the LHMS phases. This change in seismic anisotropy in hydrous phases might be one of the plausible explanations for the seismic X-discontinuity.

**Keywords:** 3.65 Å phase, X-discontinuity, mantle hydration, elasticity, equation of state, high pressure