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The structure and elasticity of hydrogrossular under high pressure: Implications for the origin of the low-velocity zone in the mantle

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Abstract

Water is a critical component of the Earth and significantly affects key properties of the deep Earth. Hydrogrossular, a hydrous phase of garnet, is considered a potential water carrier in the mantle. This study employs first-principles methods to calculate the crystal structure and elastic properties of hydrogrossular garnets with different water contents at pressures up to 100 GPa. The results indicate that the density of hydrogrossular decreases linearly with increasing water content. The presence of water significantly reduces the elastic modulus and seismic velocity of hydrogrossular. The velocities of hydrogrossular phases with different water contents are lower than those of the Preliminary Reference Earth Model (PREM) at all depths in the mantle where low-velocity zones (LVZs) are present, suggesting that they may play a key role in the formation of LVZs in the mantle. Therefore, combining the newly proposed mantle uniform and the high content and low wave velocity of hydrogrossular, we propose that hydrogrossular might play a more important role in causing mantle LVZs than previously thought. The results provide new insight into the structure of the mantle.

Keywords: Elasticity, hydrogrossular, low-velocity zone in mantle, high pressure, first-principles simulation, Physics and Chemistry of Earth's Deep Mantle and Core