

Elastic properties of orthoenstatite and its high-pressure phase and implications for the origin of low V_p/V_s zones and the X discontinuity

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The composition of the Earth's interior is critical in understanding the origin and evolution of the Earth and its geodynamics. Orthopyroxene (opx) is an important component for the upper mantle both in the pyrolite model and in the piclogite model. Opx will transform to the high-pressure phase (HPCEN). The transformation has been related to the X discontinuity. Furthermore, much evidence suggests the local enrichment of opx in the upper mantle. Therefore, the elastic properties are fundamental for an understanding of chemical compositions and dynamics of the upper mantle.

We obtained the elastic properties of orthoenstatite (MgSiO_3), Mg end-member orthopyroxene with space group Pbc_a, and its high-pressure phase (HPCEN) up to 20 GPa and 2000 K using first principle calculations with local density approximation (LDA). The calculated results¹ are in good agreement with previously available experimental measurements and theoretical results. Both the bulk and shear modulus of orthoenstatite show noticeable nonlinear pressure dependence, and the softening of shear wave velocities is prominent at high pressure. Meanwhile, orthoenstatite exhibits a negative temperature derivate of V_p/V_s ratios. This is different from other upper mantle minerals such as olivine, ringwoodite and garnet, whose V_p/V_s increases with increasing temperature. Compared to other major minerals in the upper mantle, orthoenstatite shows the lowest compressional velocities, shear velocities, and V_p/V_s (<1.7) ratio up to a depth of ~ 200 km. Recently, many seismic studies have observed unusual low V_p/V_s (below 1.72) zones in the subduction mantle wedge, and orthopyroxene has been proposed to be a possible interpretation of this unusual observation. However, this explanation is still under debate because no experimental or calculated elastic data at the conditions of the upper mantle are so far available. Our calculations show that V_s and the V_p/V_s ratio of orthoenstatite under mantle wedge conditions (2-3 GPa and 1073-1723 K) are consistent with the unusual seismic observations of V_p/V_s in a subduction mantle wedge. Therefore, the enrichment of orthopyroxene may potentially account for the observed low V_p/V_s in the mantle wedge¹. The phase transformation from orthoenstatite to HPCEN caused an increase in V_p ~3.5% and in V_s ~5%. Thus the transformation cannot result in an X discontinuity for a normal pyrolytic mantle composition. But in the area where opx is significantly enriched, the possibility that the X discontinuity resulted from the transformation cannot be ruled out.

References

¹Qian et al., 2018. Elasticity of Orthoenstatite at High Pressure and Temperature: Implications for the Origin of Low V_p/V_s Zones in the Mantle Wedge. *Geophysical Research Letters* 45, 665-673.