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# Seismic signature of the upper continental crust: Implications from the thermoelastic properties of liebermannite and K-hollandite II

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## Abstract

Thermoelastic properties of upper continental crust or terrigenous sediments (similar composition to the upper continental crust) are the basis for identifying them and investigating their fate in the Earth's mantle. Potassium feldspar, one of the most abundant minerals in the upper continental crust, transforms to liebermannite under high-pressure conditions, which subsequently transitions to its high-pressure phase, K-hollandite II. However, the thermoelastic properties of liebermannite and K-hollandite II remain unknown. This study employs first-principles calculations to determine their equations of state and elastic properties under high temperatures and pressures. Elastic moduli of both liebermannite and K-hollandite II exhibit strong nonlinear pressure and temperature dependencies. Liebermannite experiences shear instability and unusually large $V_S$ anisotropy (~200%) before its transition to K-hollandite II. The shear instability shifts to higher pressures at higher temperatures with a slope of ~3.8 MPa/K and generates a ~50% $V_S$ jump from liebermannite to K-hollandite II. We find that the upper continental crust exhibits higher velocities than the surrounding mantle to ~550 km, which explains the high-velocity anomalies observed under continent-continent collision zones. At the top of the lower mantle, the softening of liebermannite's shear modulus turns the upper continental crust into a low-velocity body with potential seismic anisotropy, and the liebermannite to K-hollandite II phase transition leads to a large velocity contrast, causing the upper continental crust to appear again as high-velocity anomalies. Therefore, the presence of upper continental crust could be a reasonable explanation for strong anisotropy around low-velocity scatterers at the top of the lower mantle. At depths greater than ~800 km, both oceanic and upper continental crust have higher velocities than the surrounding mantle, but because their velocities are similar, distinguishing them is challenging.

**Keywords:** Elasticity, first-principles calculations, liebermannite, K-hollandite II, continental crust