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A first-principles calculation of the elastic and vibrational anomalies of lizardite under pressure

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ABSTRACT

Lizardite, being one of three serpentine minerals is of considerable interest in connection with understanding the geological processes occurring at subduction zones where serpentinized ocean floor is recycled into the Earth's mantle. The crystal structure, elasticity, and vibrational properties of lizardite under pressure were determined using first-principles techniques. Above 10 GPa, a stable and a metastable structures were obtained. The hydrogen bond geometry of the stable structure indicates the disappearance of hydrogen bonds above 10 GPa, whereas the metastable structure does not show any noticeable change of the hydrogen bond strength throughout the pressure range up to 20 GPa. At 10 GPa, a very sudden softening of the elastic constants was observed for the stable structure, which is associated with a slight change in the compressibility of the *c* axis. This elastic softening causes a sudden reduction in the seismic velocities v_P and v_ϕ by about 16 and 24%, respectively. These velocities then steeply increase with further compression. Shear velocity v_S, on the other hand, gradually decreases with pressure and then abruptly increases about 14% at 10 GPa. The calculated OH stretching frequencies also increase suddenly at ~10 GPa. Previous Raman measurement reported that the highest OH stretching frequencies also increase steeply above 6 GPa. Therefore, there is a possibility that this elastic anomaly can be observed experimentally at about 6 GPa.

Keywords: Lizardite, first principles, elasticity, vibration, high pressure