

TWO NEW POLYMORPHS IN THE POOL OF (Li,Sc)-PYROXENE STRUCTURES

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Pyroxenes are among the most abundant minerals in the upper mantle. Knowledge of their high-pressure behavior is of particular interest, since phase transitions of pyroxenes are discussed as being responsible for discontinuities in seismic wave propagation (e.g. WOODLAND, 1998). As the compression behavior of pyroxenes does not follow the bulk modulus – unit cell volume relationship for isostructural compounds proposed by ANDERSON & ANDERSON (1970) for isostructural compounds, but strongly depends on chemical compositions (e.g. ENDE et al., 2020), systematic studies seem inevitable to predict their high-pressure behavior. Germanate-analogue phases have already been in the focus early, as the larger Ge atoms were supposed to provide easier access to equivalent high-pressure phases.

In this context in-situ compression studies were conducted on synthetic crystals of α -LiScGe₂O₆ (LSG) orthopyroxenes using Raman spectroscopy as well as single-crystal X-ray diffraction. The purpose of this study is to understand the stability criteria from a structural perspective, any polymorphism, and the mechanisms of the underlying transitions in non-ambient pressure conditions.

In compression studies below 10 GPa on LSG crystals an orthopyroxene- (OEn-*Pbca*) to post-orthopyroxene (pOEn-*P2₁/c*) transition has been discovered and found to be the second example of this type of transformation (ENDE et al., 2020). However, by a further increase in pressure for the α -phase two more phase transitions were observed between 9.9 and 10.4 GPa as well as around 14 GPa. The first transition was an expected transition from a monoclinic low-clinoenstatite (LCEn-*P2₁/c*) to a monoclinic high-pressure clinoenstatite (HP-CEn-*C2/c*) not known for LSG before. Nevertheless, the second transition, visible with Raman spectroscopy and single crystal X-ray diffraction, follows the first transition with only ~ 4 GPa pressure increase and therewith considerably lower pressure as expected. While a structure determination of the first modification was successful using in-situ diffraction data the structure of the second new phase could not be determined reliably even after a quenching from high-P conditions. However, a twinned and still monoclinic new high-pressure clinoenstatite unit cell was found most probably preserving the *C2/c* space group.

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