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In situ Raman spectroscopic investigation on the phase transition of grunerite at high pressures

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Abstract

Amphiboles are key rock-forming minerals and play a significant role in the subduction process. Grunerite $(Mg,Fe)_7Si_8O_{22}(OH)_2$, as an important ferromagnesian amphibole, is known to undergo a phase transition from monoclinic $C2/m$ to $P2_1/m$ structure at elevated pressures. This study investigates the phase transition of grunerite under high pressure using a diamond-anvil cell combined with in situ Raman spectroscopy, aiming to identify pressure-induced phase transitions and associated structural changes. We have identified mode splits of the OH stretching modes indicative of the $C2/m$ to $P2_1/m$ phase transition at ~1.46 GPa and observed another possible phase transition suggested by a discontinuity in the OH modes at ~17.81 GPa. The splitting of the OH stretching modes resulted from the distinct environments of two OH positions in the $P2_1/m$ structure, in comparison to the crystallographically identical OH positions in the $C2/m$ structure. We have also identified additional M-O modes in the lower-wavenumber spectrum range. The results provide new insights into the structural stability of grunerite under extreme geological conditions, contributing to a deeper understanding of metamorphic petrology and geodynamics.

Keywords: Grunerite, high pressure, Raman spectroscopy, OH stretching