

Raman study of FeSiO₃ polymorphs across phase transitions

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Synthetic orthorhombic (opx, SG Pbc_a) and low-pressure monoclinic (LP-P21/c) FeSiO₃ pyroxenes were employed to perform Raman scattering measurement up to ~ 20 GPa. These two polymorphs are known of going through the displacive phase transitions at high pressure; from LP-P21/c to C2/c [1] and from Pbc_a to HP-P21/c [2,3]. Upon compression, when the LP-P21/c phase transformed to C2/c, the characteristic change in the doublet presented between 600 and 700 cm⁻¹ in P21/c phase merging to a single peak in C2/c phase was observed [4]. In addition to the Raman patterns showed dramatically changed between the frequency range of 100 to 500 cm⁻¹. Moreover, a Raman mode softening behaviour was observed at ~148cm⁻¹ when the pressure reached ~13 GPa. As for opx phase, the pattern remained similar feature till ~7 GPa. Above 7 GPa the major changes were observed below 200 cm⁻¹ and the peak at 1066 cm⁻¹. A peak splitting at the position near 680~700 cm⁻¹ was observed. The change should be related to the transition from Pbc_a to HP-P21/c, revealed by previous study [5]. The transition of Pbc_a to HP-P21/c also induced a velocity softening behaviour onset of phase transition at pressure of 7 GPa [6].

[1] Angel et al. (1992) *Nature* **358**, 322-324. [2]Zhang et a. (2012) *Am. Miner.* **97**, 1070-1074. [3]Dera et al. (2013) *Phys. Earth Planet.Inter.*, **221**,12-51. [4] Ross & Reynard (1999) *Eur. J. Mineral*, **11**, 585-589. [5] Zhang et al.(2013) *Am. Miner.* **98**, 986-992.[6] Kung & Li (2014) *J. Phy. Chem. C*, **118**, 12410-12419.