

Silica phase transitions: implications for deep mantle dynamics and silica crystallisation in the proto-core

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Supplementary material: Crystal structures of β -stishovite, seifertite and pyrite-structured silica. The common structural units are SiO_6 -octahedra, which are variably linked and oriented. The crystallographic axes are uniformly color-coded: a, red; b, green; c, blue.

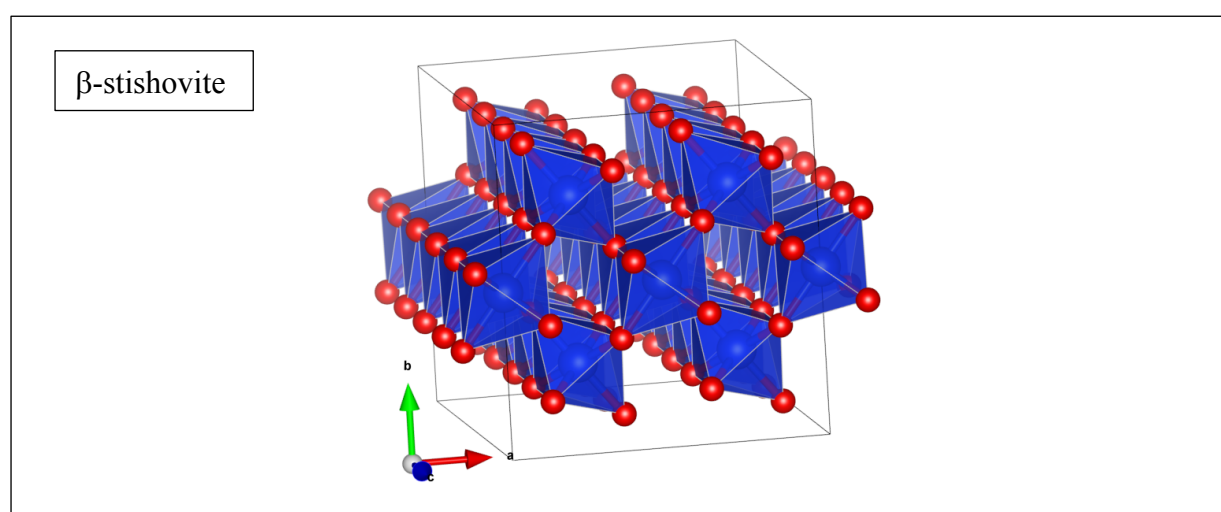


Fig. S1: Edge-sharing SiO_6 -octahedra along the c-axis form ac-layers normal to the b-axis. Two alternating ac-layers, made of oppositely tilted SiO_6 -octahedra, are connected by corner-sharing octahedra.

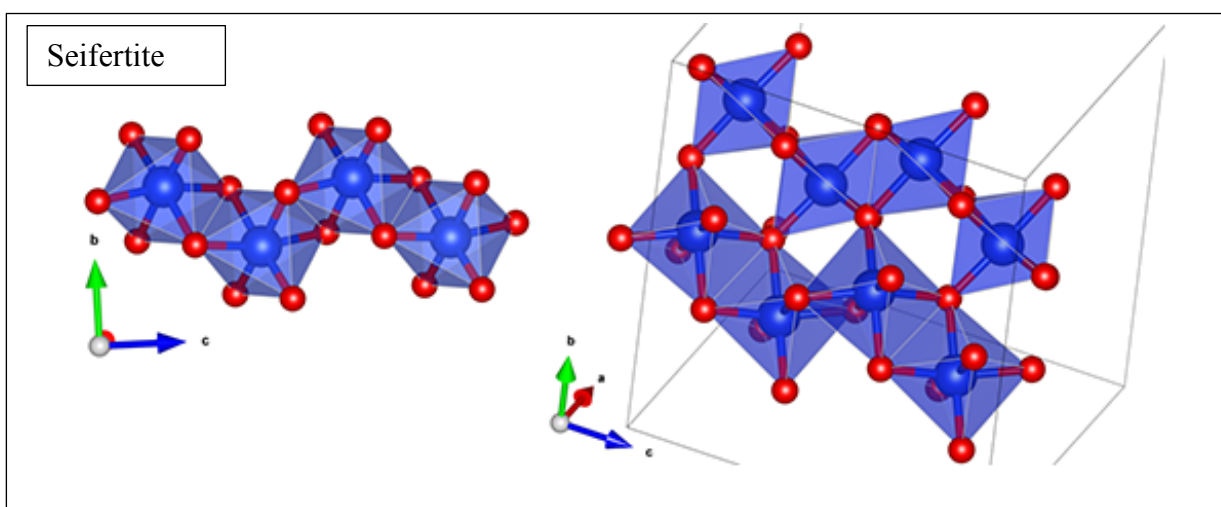


Fig. S2: Edge-sharing SiO_6 -octahedra form octahedral layers parallel to the bc-plane. Each of the edge-sharing octahedra along the c-axis is rotated relative to its neighbors, forming a zig-zag pattern. The bc-layers are connected to each other along the a-axis by corner-linked octahedra.

Pyrite-structured silica

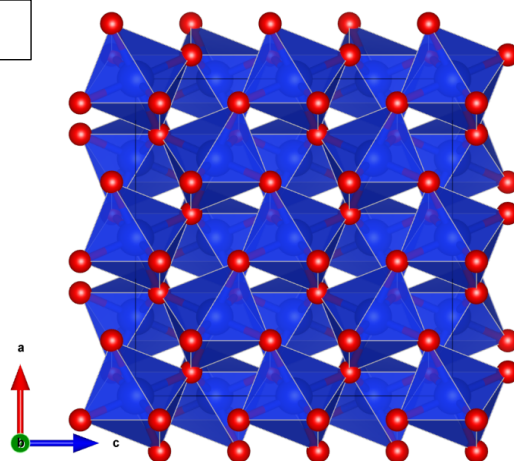


Fig. S3: All of the SiO_6 -octahedra are corner-linked in the pyrite-type silica phase. Each corner of the SiO_6 -octahedra are connected to another two octahedra. This close-packing may be the reason for higher entropy reflected by phonon-DOS.