

Transformation pathways of single-crystal coesite on compression and decompression

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As one of the most abundant natural compounds, polymorphs of SiO₂ and their phase transitions have been of great interest. Here, we discover new transformation pathways of single-crystal coesite on compression and decompression at room temperature, by means of single-crystal X-ray diffraction and Raman experiments. The transition from coesite to metastable phases is observed at pressures 22~38 GPa. Pressure-induced amorphization occurs above 38 GPa and persists up to 50 GPa. The behaviors of coesite on compression are consistent with previous power XRD and Raman results (Hemley 1987; Hemley et al., 1988), but different from discovery from Hu et al. (2015). Hu et al. reported a new phase transition of coesite to post-stishovite (*P2/c*) above 32 GPa with coexisted metastable phases at 26-40 GPa by single-crystal XRD and theoretical calculations. In addition, the pressure-induced amorphization is unquenchable and the decompressed phase at ambient conditions is coesite. While, Hemley et al. (1987 and 1988) found that the amorphous SiO₂ at high pressure is quenchable. The new transformation pathways of single-crystal coesite in this work provide new insights into the high-pressure behavior of SiO₂.

Reference

- Hemley, R., 1987. Pressure Dependence of Raman Spectra of SiO₂ Polymorphs: α -Quartz, Coesite, and Stishovite. *High-Pressure Research in Mineral Physics: a Volume in Honor of Syun-iti Akimoto*, 347-359.
- Hemley, R., Jephcoat, A., Mao, H.K., Ming, L., Manghnani, M., 1988. Pressure-induced amorphization of crystalline silica. *Nature* 334, 52-54.
- Hu, Q., Shu, J.-F., Cadien, A., Meng, Y., Yang, W., Sheng, H., Mao, H.-K., 2015. Polymorphic phase transition mechanism of compressed coesite. *Nat. Commun.* 6.