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Pressure-induced phase transitions in coesite

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ABSTRACT

High-pressure behavior of coesite was studied on single crystals using diamond-anvil cells with neon as the pressure-transmitting medium by means of in situ Raman spectroscopy up to pressures of ~51 GPa. The experimental observations were complemented with theoretical computations of the Raman spectra under similar pressure conditions. We find that coesite undergoes two phase transitions and does not become amorphous at least up to ~51 GPa. The first phase transition (coesite I to coesite II) is reversible and occurs around 23 GPa. The second transition (coesite II to coesite III) at about 35 GPa is also reversible but involves a large hysteresis. Samples recovered from the highest pressure achieved, ~51 GPa, show Raman spectra of the initial coesite. The ab initio calculations gave insight into the initiation mechanism of the first phase transition, implying, from the analysis of unstable phonon modes, that it is probably a displacive phase transition due to shearing of the four-membered rings of SiO_4 tetrahedra upon compression. The transition to the lowest-symmetry phase, coesite III, is possibly a first-order phase transition that leads to a very distinct structure. None of the metastable high-pressure phases of coesite has been previously studied and it was widely accepted that coesite undergoes pressure-induced amorphization at significantly lower pressures (30 GPa). The study of the high-pressure behavior of coesite is important to better constrain the metastable phase diagram of silica. Further crystallographic investigations are necessary for characterizing the structures of these metastable coesite forms. Crystalline or amorphous metastable phases derived from coesite under high-pressure conditions are of particular interest because they can be used as potential tracers of peak transient pressures (stress) reached in processes such as impacts or faulting.

Keywords: Silica, coesite, high-pressure polymorph, metastable, diamond-anvil cell, high-pressure Raman spectra