

Elasticity and phase transformation at high pressure in coesite from experiments and first-principles calculations

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ABSTRACT

The crystal structure and equation of state of coesite (space group $C2/c$) and its high-pressure polymorph coesite-II (space group $P2_1/n$) under pressure have been studied using X-ray powder diffraction in a diamond-anvil cell (DAC) up to 31 GPa at room-temperature and first-principles calculations at 0 K up to 45 GPa. New diffraction peaks appear above 20 GPa, indicating the formation of coesite-II structure. The calculated enthalpies provide theoretical support for the pressure-induced phase transformation from coesite to coesite-II at ~ 21.4 GPa. Compared with coesite, the coesite-II structure is characterized by a “doubled” b -axis and the breakdown of the linear Si1-O1-Si1 angle in coesite into two distinct angles—one is $\sim 176^\circ$, close to linear, whereas the other decreases by 22 to 158° . Coesite is very anisotropic with the a -axis the shortest and twice more compressible than the b - and c -axis. By comparison, coesite-II is not so anisotropic with similar compressibilities in its a -, b -, and c -axis. As analyzed by a third-order Eulerian finite strain equation of state, the bulk modulus of coesite at 21.4 GPa is 182.3 GPa, and that of coesite-II is 140.8 GPa, indicating that coesite-II is much more compressible than coesite. The existence of coesite-II in the coldest subduction zone will change the elasticity and anisotropic properties of the subducting materials dramatically.

Keywords: Coesite, phase transition, diamond-anvil cell, first-principles calculation