

High pressure polymorphism of Al+H-bearing SiO₂: ab initio investigation

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Stishovite has been reported to be a possible carrier and reservoir of water in the deep mantle, when Si⁴⁺ is substituted by Al³⁺ and H⁺ (Pawly et al. 1993). This Al+H bearing SiO₂ system can be considered as the solid solution between SiO₂ and AlOOH end-members. The rutile type SiO₂ (stishovite) has known to transform into the CaCl₂ type at about 50 GPa, then the CaCl₂ phase into alpha-PbO₂ at about 100 GPa and further into the pyrite phase above 200 GPa (e.g., Tsuchiya et al., 2004; Kuwayama et al., 2005). In the case of AlOOH, the diaspore transforms into delta-AlOOH which has the CaCl₂ type AlO₆ framework with hydrogen atoms in its interstitial spaces above about 18 GPa. We have recently found a new phase transition at about 170 GPa from delta-AlOOH to the pyrite type structure. In this AlOOH case, alpha-PbO₂ type structure is found not stabilized, being different from SiO₂. Therefore, we can expect that effects of Al+H on the high pressure polymorphism of SiO₂ as follows: 1) decrease the transition pressure from rutile to CaCl₂ type structure, 2) lower the transition pressure from alpha-PbO₂ to pyrite type structure, and 3) narrow the stability of alpha-PbO₂. In order to verify this anticipation, we determine the stable Al+H defect structures in SiO₂ polymorphs and estimate the high-pressure polymorphic relation of Al+H bearing SiO₂.

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