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SiO2の新しい高密度相の発見とスーパー地球の内部構造

A New Dense Phase of Silica Initiating Silicates Breakdown in Super-Earths

土屋 卓久[1*], 土屋 旬[1]

Taku Tsuchiya[1*], Jun Tsuhciya[1]

[1]愛媛大学

[1]Ehime University

It has been known that silica (SiO_2) shows a sequential phase evolution from quartz, coesite, stishovite, $CaCl_2$, a-$PbO_2$and pyrite (modified fluorite) with elevating pressure (e.g., Teter et al., 1998; Tsuchiya et al., 2004a). However, further denser phases are still underdetermined, although studies on some low-pressure analogs such as TiO_2(Dubrovinskaia et al., 2001) and MgF_2(Haines et al., 2001) have suggested the cotunnite phase as the final high-pressure phase. In order to elucidate the post-pyrite phase of silica, we performed structure search based on the ab initio computation method (Tsuchiya et al., 2004b). After examining several dense structure types with AX_2compound, we successfully discovered a new phase transformation of pyrite type SiO_2at multi-megabar condition to an unexpected hexagonal phase, which possesses quite high nine-fold coordinated Si and eclipses the cotunnite stability field in the entire pressure range up to 2000 GPa. We subsequently investigated high-pressure stabilities of some important silicate compounds ($MgSiO_3$and $CaSiO_3$) and found that the new phase change in silica could initiate breakdown of these silicates to oxide mixtures at the pressures relevant to the interior of super-Earths and exoplanets. High-P,T phase boundaries, density and elasticity changes associated with the new phase transitions, which are the most fundamental information to understand the structure and dynamics of giant planets, will be presented in detail.

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