Multimegabar phase relations of major Earth and planetary materials

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Recent improvements in detection methods have allowed for the discovery of terrestrial exoplanets with 1–10 times Earth's mass, so-called 'super-Earths'. However, their interior is currently highly unclear, because understanding of the ultrahigh-pressure phase relations of major Earth and planetary materials is still quite limited. Those should be clarified before developing models of the internal structures of such objects. In this study, we tried to establish the ultrahigh-pressure and temperature phase relations of some silicates by means of *ab initio* techniques.

It has been known that silica (SiO_2) shows a sequential phase evolution from quartz, coesite, stishovite, $CaCl_2$, α-PbO_2 and pyrite (modified fluorite) with elevating pressure. However, further denser phases are still underdetermined, although studies on some low-pressure analogs have suggested an orthorhombic cotunnite phase as the final high-pressure phase. After examining several dense structure types with AX_2 compound, we successfully discovered a new phase transformation of pyrite type SiO_2 at multi-megabar condition to an unexpected hexagonal structure, which possesses high and relatively regular nine-fold coordinated Si. Similar phase transitions were also predicted in other dioxide compounds, and we finally succeeded in identifying one of them experimentally.

Then, we investigated high-pressure stabilities of some important silicate compounds ($MgSiO_3$ and $CaSiO_3$) and elucidated that the new phase change in silica could initiate breakdown of these silicates to oxide mixtures in the conditions relevant to the mantle of super-Earths and the core of giant planets. Thsy would lead to various complexities in their internal structures. Our calculations show that relatively large density jump is expected associated with the breakdown of $MgSiO_3$ post-perovskite, while the breakdown of $CaSiO_3$ yields an metallic oxide phase. Based on the results, we try to make a standard internal structure model of terrestrial exoplanets.

Research supported by JSPS Grant-in-Aid for Scientific Research Grants 20001005 and 21740379 and the Ehime Univ G-COE program 'Deep Earth Mineralogy'.

Subduction cycling of C-O-H volatiles from sediment melting

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Sediment subduction is a key mechanism of crustal recycling and mantle-exosphere exchange of C-O-H fluids. Thus high pressure melting systematics of C-O-H bearing pelite is important. While experimental data on the melting relations of alumina-rich pelites became recently available to 23.5 GPa [1, 2], those of alumina-poor pelites are limited to 3 GPa [3, 4]. To completely understand the deep cycling of water and carbon dioxide via sediment subduction, we performed new melting experiments on a silica and alumina-poor, water-undersaturated and carbonate-saturated pelite up to 7 GPa.

Piston cylinder and multi-anvil experiments are performed at 3-7 GPa and 800-1150 °C using a model pelite composition containing 1 wt.% H_2O and 5 wt.% CO_2 in Au capsules. We bracketed the solidus temperatures, at 800-850 °C at 3 GPa, at 900-1000 °C at 5 GPa, and <1100 °C at 7 GPa. Cpx, garnet, and coesite are present in all the experiments, and subsolidus phases also include rutile, phengite, and calcite$_{ss}$ at 3 GPa and 800 °C and joined by kyanite at 5 GPa and 900 °C. The near-solidus melts at 3 GPa, 850 °C are hydrous rhyolite, whereas those at 5 GPa, 1000 °C and 7 GPa, 1100 °C are K-rich carbonatitic. At 5 GPa and 1100 °C, both silicate and carbonatite melts were present. The phengite-out boundary is located between 850 and 900 °C at 3 GPa and 1000 and 1100 °C at 5 GPa, and phengite was not present at 7 GPa and 1100 °C. The solidus constrained in our study is 50-100 °C lower than the previous experiments on pelitic compositions [1, 2].

Comparison of our melting boundaries with thermal models of slab surface temperatures suggests that water-undersaturated, carbonated pelite solidus is located near the *P-T* trajectories of warm subduction zones. Hence subducting pelite in cold to intermediate subducting zones likely survives melting-induced devolatilization up to ~200 km. Hot subduction, on the other hand, may lead to supply of K-rich carbonatitic melt flux to deep sub-arc mantle wedge.

[1] Thomsen & Schmidt (2008) *EPSL* **267**, 17–31. [2] Grassi & Schmidt (2011) *J. Petrol.* **52**, 765–789. [3] Tsuno & Dasgupta (2011) *Contrib. Mineral. Petrol.* **161**, 743–763. [4] Tsuno & Dasgupta (submitted) *EPSL*.