Perovskite and post perovskite phase relation in the $MgSiO_3$-Al_2O_3 system

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It has been believed that a few mol% Al_2O_3 would dissolve into (Mg,Fe)SiO_3 in the Earth's lower mantle. Existence of aluminum in $MgSiO_3$ is thought to change the volumes, elasticity and stability relations of perovskite (Pv) and post perovskite (pPV). The phase diagram of Al-bearing $MgSiO_3$ reported both experimentally and theoretically shows that Al drastically increases the pPV transition pressures with significant Pv+pPV co-existence regions. The large two phase loops are however irreconcilable to the transition seismically detectable as the D" discontinuity. Here we investigated finite temperature high-pressure phase equilibria in the $MgSiO_3$-Al_2O_3 system based on the density functional first principles method with multiple configuration sampling of solid solution structures. Through the calculations, interesting structural relationship between Pv and Rh_2O_3(II) was also discovered.

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