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 is dissolved into (Mg,Fe)SiO_3 in the Earth's lower mantle. Existence of aluminum in $MgSiO_3$ is thought to change the volumes, elasticities and stability relations of perovskite and post perovskite. Previously we reported the phase relations and physical properties of pure $MgSiO_3$ and Al_2O_3 at high P, T conditions by means of first principles techniques. The theoretically determined post perovskite transition pressures of end-member $MgSiO_3$ and Al_2O_3 are relatively similar ($MgSiO_3$:˜100 GPa, Al_2O_3:˜110 GPa). However, the phase diagram of Al-bearing $MgSiO_3$ reported both experimentally and theoretically shows that Al drastically increases the post perovskite transition pressures [+5 GPa by 3.125 mol% Al_2O_3 (Akber-Knutson et al.2005, Zhang and Oganov 2006), +15 GPa by 25mol% Al_2O_3 (Tateno et al. 2005)] with significant co-existence regions. This suggests non-monotonical effect of Al on the post perovskite stability. Here we investigate systematically the effect of Al on $MgSiO_3$ at the wide range of Al concentration and the high P, T conditions by first principles calculation.

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