Physics and chemistry of $CaIrO_3$-type postperovskite phase

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It was widely believed that some 75 vol.% of the Earth's lower mantle is made of Fe- and Al-bearing $MgSiO_3$ perovskite. Recently, we showed that at pressures and temperatures of the D'' layer $MgSiO_3$ transforms from perovskite into a $CaIrO_3$–structured phase (space group *Cmcm*) [1]. Its physical and chemical properties can explain many puzzling properties of the D'' layer. The phase change from the Mg-perovskite to $CaIrO_3$–type bearing assemblage in a pyrolitic mantle composition was observed at 2700 km depth and 2600 K. The phase boundary in the natural mantle composition was determined to be P (GPa) = 124 + 0.008 x (T (K) – 2500) [2]. Accoriding to the high-pressure experiments, the adiabatic temperature gradient in the lower mantle is estimated to be 0.31 K/km. This value is in good agreement with those estimated by theoritical approachs in previous studies. The compressibility of $CaIrO_3$–type $MgSiO_3$ was also measured. Pressure-volume data could be fitted to the Birch-Murnaghan equation of state with K_0 = 236 GPa, when K_0' was set to 4 [3]. The partition coefficients and the effect of some elements on the phase equilibrium between the orthorhombic $MgSiO_3$ perovskite and $CaIrO_3$-type $MgSiO_3$ were estimated from *ab initio* calculations [2]. Most elements, such as Al, Be, Ca, Sr, Ba, Ni, are much more soluble in the perovskite phase. In conrast, Fe is more souble in the $CaIrO_3$–type phase. We also estimated the electrical conductivity at the base of the lower mantle. Surprisingly, we find that the high electrical conductivity layer could exsit at the CMB [4]. After the formation of the Earth, the D" layer could not exist, because the mantle temperature was too high to stabilize the $CaIrO_3$–type phase. As the mantle temperature decreased in the Earth's histry, the D" layer appearred gradually. Our experimental and theoretical results indicate that the D" layer consists of a $CaIrO_3$-type bearing assemblage which is likely to have significant effect on the chemical and thermal evolution of the Earth's mantle.

References

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