Preliminary data on the real perovksite (CaTiO3) phase diagram

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Abstract

The high-pressure *Pbnm*-perovskite structure of MgSiO3 is the most abundant mineral in the Earth's mantle. At pressure exceeding 120 GPa at high-temperature, a post-perovskite transition to a *Cmcm*-CaIrO3-structure of MgSiO3 has been shown by several authors. The same transition has been described in numerous other perovskite-structured compounds but a significant diversity of phases and transition paths have been reported in literature. Even iron and aluminium bearing MgSiO3 perovskites do not have a simple transition from *Pbnm*-perovskite to *Cmcm*-CaIrO3 showing intermediate phases often yet poorly understood.

In order to get a better insight on the different possible transition regimes in the complex silicate perovskite system, we have investigated the transformations at high pressure and high temperature of the actual perovskite mineral, CaTiO3. Moreover, as this compound already crystallizes in a *Pbnm*-perovskite structure at 1 bar and 300 K, it might present post post perovskite transitions at lower pressures than in MgSiO3. We have thus carried out *in-situ* X-ray diffraction experiments at the ID27 beamline of the european synchrotron radiation facility using laser-heated diamond-anvil cells.

We have first obtained a 300 K equation of state up to 110 GPa in Neon pressure transmitting medium. The results are in good agreement with previous literature data up to 55 GPa (Guennou et al., 2010 *Physical Review B 82 (13), pp.134101*) but we observed a change in compression regime at 60 GPa. Below 60 GPa, upon laser heating, CaTiO3 transforms

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to the *Pm-3m*- cubic perovskite with a positive slope in pressure-temperature coordinates. If however the pressure exceeds 60 GPa, a new phase appears which is not *Cmcm*-CaIrO3- but instead polytypes of *Pbnm*-perovskite and *Cmcm*-CaIrO3 structures which have already been reported in literature in the silicate perovskite system (*Tschauner et al., 2008, Amer. Mineral. (93) 533-539*). Then, at higher pressure, laser-heating experiments have been carried out up to 160 GPa, revealing a new structure which has not been identified yet. Implications of these results for the evolution of perovskite structure in terrestrial planets will be discussed with special emphasis on transition widths and slopes.