Bridgmanite to post-perovskite partitioning of Fe-Al-components

C.E. MOHN[1], R.G. TRØNNES[1,2]

[1]Centre for Earth Evolution and Dynamics, Univ. Oslo
[2]Natural History Museum, Univ. Oslo

Multi-configurational Monte Carlo methods with density functional theory was used to investigate the phase relations of coexisting bridgmanite (bm) and post-perovskite (ppv) in the systems $MgSiO_3$-$FeSiO_3$ (MS-FS), $MgSiO_3$-$FeAlO_3$ (MS-FA) and $MgSiO_3$-Al_2O_3 (MS-AA). The pressure of the bm-ppv transition in pure MS at 3000 K is 127.4 GPa and the Clapeyron slope is 9.7 MPa/K. The FS and FA components partition into ppv, but the MS-FA phase loop in pressure-composition space is narrow and flat compared to the MS-FS loop. The stability limits of single-phase bm at 3000 K are about 120 and 116 GPa for 10 and 20 mol% FS, and about 122.5 and 121.3 GPa for 10 and 20 mol% FA, respectively. Coexisting bm-ppv pairs have 20 and 34 mol% FS and 20 and 24 mol% FA in the two systems.

In the MS-AA system bm and ppv coexist with $MgAl_2O_4$ (Ca-ferrite structure) + SiO_2 above 70 GPa [e.g. 1]. Although the solubility of AA in bm increases considerably in the 27-45 GPa range [2], it seems to drop below 10 mol% in the 70-130 GPa range. Although AA partitions into bm, the bm-ppv phase loop is narrow and flat.

The slow crystallisation of a thermally insulated basal magma ocean (BMO) was probably accompanied by supply of silica from the core and transfer of Fe-oxides to the core [3]. The stagnant E'-layer of the outermost core might provide a trace of the core-BMO exhange [4]. The exchange would maintain high Si/Mg and Mg/Fe ratios in the shrinking BMO, suppress ferropericlase crystallisation, extend the crystallisation of $MgSiO_3$-dominated bm and enrich the BMO in alumina. The low AA solubility in bm might favour late-stage bm cumulates with a high FA/FS ratio from the most Fe-enriched BMO, possibly resulting in basal LLSVP-layers (large low S-wave velocity provinces) with about 16 mol% FA+FS [3]. A recent study [5] concludes that ppv might be stable up to 300 km above the core-mantle boundary, even in the LLSVPs. Therefore, the large positive dp/dT slope of the bm-ppv transition and an estimated temperature excess of 750 K in the LLSVPs relative to the ambient D"-zone require LLSVP-material with high FS content and FS/FA ratio. Ppv-bearing basaltic material, possibly above base cumulates with FA-dominated bm might satisfy this requirement [3].

[1] Stixrude & Lithgow-Bertelloni (2011) *GJI* **44**, 8303. [2] Liu et al. (2017) *JGR* **122**, 7775. [3] Trønnes et al. (2019) *Tectonophys*.10.021. [4] Brodholt & Badro (2017) *GRL* **44**, 8303. [5] Koelemeijer et al. (2018) *EPSL* **494**, 226.

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