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# Toward a coherent model for the melting behavior of the deep Earth's mantle

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## 41 1. ABSTRACT

42 Knowledge of melting properties is critical to predict the nature and the fate of melts produced  
43 in the deep mantle. Early in the Earth's history, melting properties controlled the magma ocean  
44 crystallization, which potentially induced chemical segregation in distinct reservoirs. Today, partial  
45 melting most probably occurs in the lowermost mantle as well as at mid upper-mantle depths, which  
46 control important aspects of mantle dynamics, including some types of volcanism. Unfortunately,  
47 despite major experimental and theoretical efforts, major controversies remain about several aspects  
48 of mantle melting. For example, the liquidus of the mantle was reported (for peridotitic or chondritic-  
49 type composition) with a temperature difference of  $\sim 1000$  K at high mantle depths. Also, the Fe  
50 partitioning coefficient ( $D_{\text{Fe}}^{\text{Bg/melt}}$ ) between bridgmanite (Bg, the major lower mantle mineral) and a  
51 melt was reported between  $\sim 0.1$  and  $\sim 0.5$ , for a mantle depth of  $\sim 2000$  km. Until now, these  
52 uncertainties had prevented the construction of a coherent picture of the melting behavior of the deep  
53 mantle.

54 In this article, we perform a critical review of previous works and develop a coherent, semi-  
55 quantitative, model. We first address the melting curve of Bg with the help of original experimental  
56 measurements, which yields a constraint on the volume change upon melting ( $\Delta V_m$ ). Secondly, we  
57 apply a basic thermodynamical approach to discuss the melting behavior of mineralogical  
58 assemblages made of fractions of Bg,  $\text{CaSiO}_3$ -perovskite and  $(\text{Mg,Fe})\text{O}$ -ferropericlasite. Our analysis  
59 yields quantitative constraints on the  $\text{SiO}_2$ -content in the pseudo-eutectic melt and the degree of  
60 partial melting ( $F$ ) as a function of pressure, temperature and mantle composition; For examples, we  
61 find that  $F$  could be more than 40% at the solidus temperature, except if the presence of volatile  
62 elements induces incipient melting. We then discuss the melt buoyancy in a partial molten lower  
63 mantle as a function of pressure,  $F$  and  $D_{\text{Fe}}^{\text{Bg/melt}}$ . In the lower mantle, density inversions (i.e. sinking  
64 melts) appear to be restricted to low  $F$  values and highest mantle pressures.

65 The coherent melting model has direct geophysical implications: (i) In the early Earth, the magma  
66 ocean crystallization could not occur for a core temperature higher than  $\sim 5400$  K at the core-mantle  
67 boundary (CMB). This temperature corresponds to the melting of pure Bg at 135 GPa. For a mantle  
68 composition more realistic than pure Bg, the right CMB temperature for magma ocean crystallization  
69 could have been as low as  $\sim 4400$  K. (ii) There are converging arguments for the formation of a  
70 relatively homogeneous mantle after magma ocean crystallization. In particular, we predict the bulk  
71 crystallization of a relatively large mantle fraction, when the temperature becomes lower than the  
72 pseudo-eutectic temperature. Some chemical segregation could still be possible as a result of some  
73 Bg segregation in the lowermost mantle during the first stage of the magma ocean crystallization, and  
74 due to a much later descent of very low  $F$ , Fe-enriched, melts toward the CMB. (iii) The descent of  
75 such melts could still take place today. Their formation should be related to incipient mantle  
76 melting due to the presence of volatile elements. Even though, these melts can only be denser than  
77 the mantle (at high mantle depths) if the controversial value of  $D_{\text{Fe}}^{\text{Bg/melt}}$  is indeed as low as suggested  
78 by some experimental studies. This type of melts could contribute to produce ultra-low seismic  
79 velocity anomalies in the lowermost mantle.

## 80 **2. INTRODUCTION**

### 81 **2.1. MELTING IN THE EARLY EARTH'S MANTLE**

82 Within the first 100 million years of the Earth's history, the giant Moon forming impact (MFI)  
83 melted the Earth almost entirely (Nakajima and Stevenson, 2015). The release of energy induced by  
84 the gravitational segregation of the impactor's core could have potentially heated the Earth's core by  
85 3500–4000 degrees above the temperature reached prior to the giant impact (Herzberg et al., 2010;  
86 Nakajima and Stevenson, 2015; Rubie et al., 2015). It could have led to a core-mantle boundary  
87 (CMB) temperature of the order of 6000 K (Davies et al., 2015; Labrosse, 2015; Nakagawa and  
88 Tackley, 2010), well above the mantle solidus of ~4150 K (Andrault et al., 2011; Fiquet et al., 2010).  
89 Therefore, the MFI could have caused intensive melting of the mantle at all depths. However,  
90 geochemical evidences point out to large scale isotopic heterogeneities that seem to have survived  
91 the episode of MFI. For example, the excess in  $^{182}\text{W}$  (produced by the decay of  $^{182}\text{Hf}$ ) measured in  
92 2.7 Ga-old komatiites requires a large-scale magmatic differentiation during the first 30 Ma of the  
93 Solar system's history (Touboul et al., 2012). The difference in Xenon isotopic composition between  
94 MORBs and the Icelandic plume (Mukhopadhyay, 2012), also indicates two sources with distinct  
95 isotopic composition. Finally, geodynamical arguments suggest the presence of an unmixed and  
96 primordial material in the deep mantle (Davaille, 1999; Kellogg et al., 1999). Therefore, it is unlikely  
97 that primordial mantle temperatures exceeded the liquidus throughout the mantle.

98 A low viscosity of the magma-ocean is expected to induce vigorous and turbulent convective  
99 flow, favoring a homogeneous mixing. In the meantime, heat flux at the magma ocean surface could  
100 have been as high as  $\sim 10^6 \text{ W/m}^2$ , which suggests a very fast crystallization, within  $\sim 10^3$  years after  
101 the MFI (Solomatov, 2007). Longer time scales for cooling are also possible, due to the possible  
102 formation of an opaque atmosphere at the Earth's surface preventing heat loss, or other geodynamical  
103 complications, such as physical or chemical mantle layering, etc. (Lebrun et al., 2013; Sleep et al.,  
104 2014). On the other hand, petrological analyses of Archean and Proterozoic basalts preserved on the  
105 Earth's surface show primary magma compositions compatible with mantle potential temperatures  
106 ( $T_p$ ) of only 200–300 degrees higher than today (Herzberg et al., 2010). A similar temperature change  
107 is reported between Archean tonalite-trondhjemite-granodiorite associations of 4.0 to 2.5 Ga old  
108 (Martin and Moyen, 2002). Such a modest difference of mantle temperature compared to the present  
109 situation suggests a relatively rapid mantle cooling just after the MFI.

110 Finally, it has been suggested that a basal magma ocean (BMO) could have lasted in the  
111 lowermost mantle for very long times, billions of years, in correlation with an outer-core temperature  
112 significantly higher than the mantle solidus (e.g. (Labrosse, 2015)). This issue remains largely  
113 debated, however, because geodynamical models do not explain what could prevent such a hot core  
114 from rapid cooling (Monteux et al., 2016; Nakagawa and Tackley, 2010)).

### 115 **2.2. EVIDENCES FOR MANTLE MELTING TODAY**

116 In the upper mantle, seismic and magneto-telluric profiles present prominent anomalies, in  
117 particular at depths between 80 and 200 km (e.g. (Romanowicz, 1995)). Low velocity anomalies have  
118 also been reported atop the 410-km mantle discontinuity (Song et al., 2004; Tauzin et al., 2010). Low  
119 degree partial melting has often been advocated to explain these anomalies (Revenaugh and Sipkin,  
120 1994), as thermochemical effects alone cannot explain the magnitude of the geophysical anomalies.  
121 The possible mechanisms for mantle melting, however, are many. As for the temperature profile,  
122 anchor points of the geotherm are provided by phase transformations in major mantle minerals,

123 typically olivine, the constituent responsible for the seismic discontinuities between 410 and 660 km  
124 depths. It yields a potential temperature ( $T_p$ ) of  $\sim 1600$  K, which corresponds to the extrapolation to  
125 the Earth's surface of the adiabatic temperature profile passing through these anchor points (Katsura  
126 et al., 2010). Such a mantle geotherm plots at significantly lower temperatures compared to the  
127 melting curve of the peridotitic mantle determined experimentally (Litasov and Ohtani, 2002; Zhang  
128 and Herzberg, 1994). Noticeable exceptions exist, for example at mantle ridges, where the adiabatic  
129 decompression of the mantle leads to melting in the asthenosphere. On the other hand, in order to  
130 invoke melting at higher depths one has to invoke either higher temperatures (such as for OIB,  
131 Oceanic Island Basalts), or volatiles that depress the solidus (e.g. (Hirschmann et al., 1999)).

132       Temperatures in the lowermost mantle depart from the upper mantle geotherm as they are  
133 influenced by the heat flux coming from the core at the CMB. A large decrease ( $>10\%$ ) of shear wave  
134 velocities is reported in the D"-layer sitting just above the CMB. Even if alternative interpretations  
135 are possible, such as a solid-state origin (e.g. Fe-enriched (Mg,Fe)O (Wicks et al., 2010)), it strongly  
136 suggests occurrence of partial melting (e.g. (Herzberg et al., 2013; Rost et al., 2005)). Furthermore,  
137 the non-ubiquitous character of the seismic features in the D"-layer implies a CMB temperature lower  
138 than the mantle solidus. Otherwise, there would be a continuous melting line above the CMB. At the  
139 CMB pressure of 135 GPa, the solidus temperature of chondritic and peridotitic mantle was reported  
140 to be  $\sim 4150$  K (Andrault et al., 2011; Fiquet et al., 2010). There, where seismic anomalies appear,  
141 mantle partial melting could occur for different reasons: (i) presence of volatile elements, such as in  
142 the study of (Nomura et al., 2014) where their pyrolitic composition included  $\sim 400$  ppm  $H_2O$ , which  
143 lowered the solidus temperature to  $\sim 3570$  K. However, we note that a high water content is unlikely  
144 in the lower mantle, due to the limited capability of lower mantle minerals to store water below the  
145 660 km discontinuity (Bolfan-Casanova et al., 2003; Panero et al., 2015); (ii) the presence of an  
146 excess of silica has been invoked; Indeed, the solidus temperature at the CMB of a mid-ocean ridge  
147 basalt, was reported to be  $3800 (\pm 150)$  K, thus significantly lower than for the melting of the average  
148 mantle (Andrault et al., 2014). Presence of basalt in the lowermost mantle is supported by seismic  
149 tomography imaging deep descent of slabs toward the CMB (e.g. (van der Hilst and Karason, 1999));  
150 (iii) A very large amount of FeO could also lower the melting point of the mantle (Mao et al., 2005).  
151 Altogether, the non-ubiquitous seismic features in the D"-layer could very well be correlated to the  
152 presence of volatiles, basalt and/or high FeO concentration, together with a CMB temperature of  $4100$   
153 ( $\pm 200$ ) K (e.g. (Andrault et al., 2016)).

## 154 3. MELTING OF PURE BRIDGMANITE

### 155 3.1. IMPORTANT BRIDGMANITE PROPERTIES

156 MgO becomes extremely refractory with increasing pressure, with a melting point estimated at  
157 ~8000 K for a pressure of 135 GPa (Du and Lee, 2014). This contributes in making ferropericlase  
158 (Fp) the liquidus phase above 25 GPa, but only up to ~33 GPa, where Bg becomes the liquidus phase  
159 for mantle compositions (Ito et al., 2004). The melting curve of Bg dominates the topology of melting  
160 diagrams at high mantle depths. The role of Bg is further emphasized by a possible increase of Bg-  
161 content with increasing mantle depth, as the comparison between geophysical observations and  
162 experiments (e.g. (Murakami et al., 2012; Samuel et al., 2005)) suggest a mantle (Mg+Fe)/Si ratio  
163 closer to unity.

164 Mantle Bg can adopt chemical compositions ranging from (Mg,Fe)SiO<sub>3</sub>, produced after  
165 decomposition of olivine, to Al-bearing (Mg,Fe)SiO<sub>3</sub>, after the high pressure transformation of  
166 majoritic garnet below the 660 km discontinuity. A higher compositional variability could also come  
167 from the intrinsic high compliance of the Bg crystal structure, which composition can be decomposed  
168 in a number of (theoretical) end-members (MgSiO<sub>3</sub>, FeSiO<sub>3</sub>, FeAlO<sub>3</sub>, Al<sub>2</sub>O<sub>3</sub>, MgAlO<sub>2.5</sub>). It can adopt  
169 variable Mg/Si, Fe<sup>3+</sup>/ΣFe, Al/Fe ratios and Fe-content as a function of pressure, temperature, oxygen  
170 fugacity, and exchange with ferropericlase. (e.g. (Boujibar et al., 2016; Lauterbach et al., 2000)). The  
171 Bg crystal chemistry can thus vary with mantle depth (Andrault et al., 2007) and also laterally if the  
172 mantle presents significant heterogeneities. We also remind that the transition pressure from majoritic  
173 garnet to Bg increases significantly with the Al-content: compared to pure MgSiO<sub>3</sub>, an additional 3-  
174 4 GPa is required to produce Bg with ~10 wt% Al<sub>2</sub>O<sub>3</sub> (Akaogi and Ito, 1999; Irifune et al., 1996).

### 175 3.2. PREVIOUS STUDIES OF BRIDGMANITE MELTING

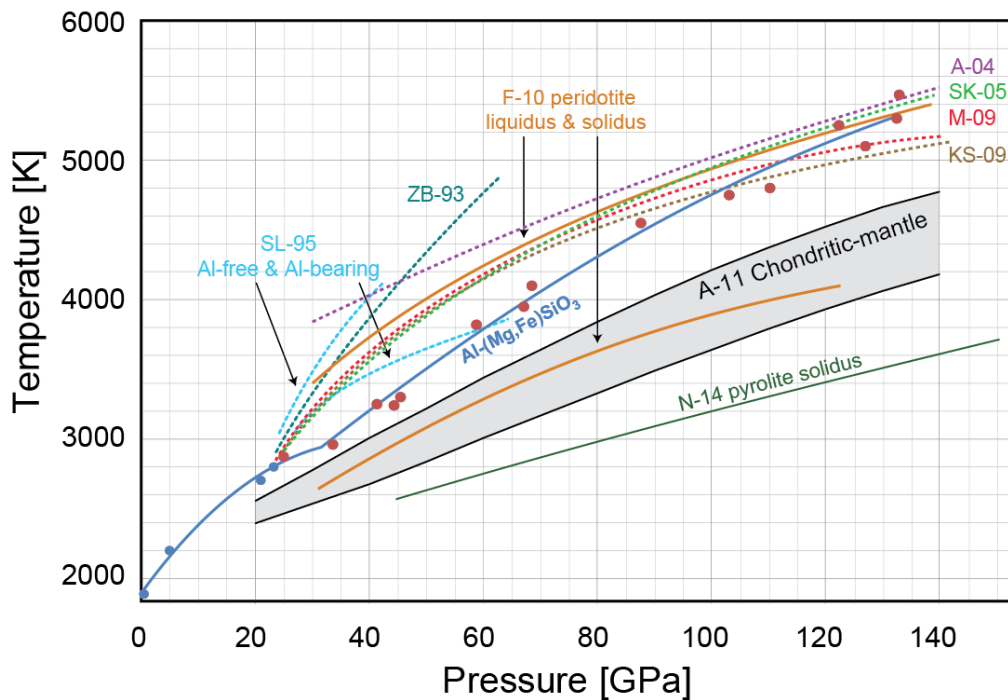
176 In early LH-DAC experiments, visual observations of the sample behavior were used as a major  
177 criterion to address the melting of Bg (Figure 1). Two studies performed on MgSiO<sub>3</sub> and (Mg,Fe)SiO<sub>3</sub>  
178 compositions agree for a steep melting curve above the transition zone pressure, at ~24 GPa (Shen  
179 and Lazor, 1995; Zerr and Boehler, 1993). On the other hand, comparison between the melting curves  
180 of MgSiO<sub>3</sub> and Mg<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub> evidences a significant melting temperature depletion, by ~300 K at 40  
181 GPa, due to the presence of Al (Shen and Lazor, 1995). Early works were limited to 60-70 GPa,  
182 compared to the 135 GPa prevailing at the CMB. Concerning melting of MgSiO<sub>3</sub> in the upper mantle,  
183 we note an important curvature of the melting line typical of the lower-density polymorphs (Katsura  
184 and Ito, 1990; Presnall and Gasparik, 1990). It can be related to a rapid decrease of the volume of  
185 melting ( $\Delta V_m$ ) with increasing pressure and, thus, a relatively high melt compressibility.

186 Several theoretical works address the equation of state and the melting curve of Bg up to more  
187 than 135 GPa, using *ab initio* calculations (Figure 1). The MgSiO<sub>3</sub> end-member is generally studied,  
188 because such calculations encounter difficulties in addressing the role of transition elements and point  
189 defects (such as Al<sup>3+</sup>, Fe<sup>3+</sup>, etc.). In all calculations, the initial slope of the melting curve (above ~24  
190 GPa) is relatively steep. This points out to a relatively large volume of MgSiO<sub>3</sub>-Bg melting, which is  
191 dominated by the ~10% volume change at the transition from majoritic garnet to Bg at 660 km-depth  
192 (Yu et al., 2011). Based on the propagation of shock waves, MgSiO<sub>3</sub> melting was identified at 5000-  
193 5500 K for a pressure above 100 GPa (Akins et al., 2004; Mosenfelder et al., 2009). It was also  
194 suggested that the volume of Bg melting becomes very small at pressures typical of the lowermost  
195 mantle (Mosenfelder et al., 2009; Petitgirard et al., 2015).



196 **3.3. UPDATED MELTING CURVE OF BRIDGMANITE**

197 In this article, we report original measurements of the melting curve of a (Fe,Al)-bearing Bg  
 198 phase with  $\text{Fe}/(\text{Mg}+\text{Fe})=0.12$  and  $\text{Al}/\text{Fe}=0.9$ . We acknowledge that this composition corresponds to  
 199 relatively high Al and Fe contents compared to the expected composition for natural Bg. Experiments  
 200 were performed using LH-DAC coupled with *in situ* X-ray diffraction on the ID-27 beamline (ESRF,  
 201 France). All experimental methods are detailed in *Supplementary Materials*. At relatively low  
 202 pressures, the melting curve of this Bg appears significantly more flat than those reported for pure  
 203  $\text{MgSiO}_3$  (Figure 1). This observation tends to confirm a significant effect of Al on the melting slope,  
 204 as reported previously between Al-free and Al-bearing starting materials (Shen and Lazor, 1995). We  
 205 also find that the discontinuous increase of the melting curve slope, related to the majorite to Bg phase  
 206 transition, is not observed at  $\sim 24$  GPa, but instead at  $\sim 30$ - $35$  GPa for this (Fe,Al)-bearing composition.  
 207 This behavior can be logically related to extension to higher pressures of the garnet stability field in  
 208 the presence of Al, as described in previous works for Fe-free starting materials (Akaogi and Ito,  
 209 1999; Irifune et al., 1996). The relatively lower melting temperature of (Fe,Al)-bearing Bg in the 25-  
 210 35 GPa pressure range, compared to pure- $\text{MgSiO}_3$  and, most importantly, to other lower mantle  
 211 minerals such as MgO, explains why Bg is not the liquidus phase in this pressure range for typical  
 212 mantle compositions (Ito et al., 2004).



**Figure 1:** Melting curve of Bg inferred from different experimental and theoretical studies determined using LH-DAC for  $(\text{Mg}_{0.88}\text{Fe}_{0.12}\text{SiO}_3)$  (Zerr and Boehler, 1993),  $\text{MgSiO}_3$  and  $\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$  (Shen and Lazor, 1995), shock measurements for  $\text{MgSiO}_3$  (Akins et al., 2004; Mosenfelder et al., 2009) and *ab initio* calculations for  $\text{MgSiO}_3$  (e.g. (de Koker and Stixrude, 2009; Stixrude and Karki, 2005)). We also include experimental reports of solidus and liquidus of peridotite (Fiquet et al., 2010), chondritic-type mantle (Andrault et al., 2011) and pyrolite with  $\sim 400$  ppm  $\text{H}_2\text{O}$  (Nomura et al., 2014). Our new LH-DAC measurements performed from  $\sim 24$  to  $\sim 135$  GPa on a (Fe,Al)-rich Bg (red dots and blue guide for the eyes) plot in continuity with previous determinations of mantle melting performed at lower pressures using the large volume press (Blue dots, (Katsura and Ito, 1990; Presnall and Gasparik, 1990)).

214 At higher pressures, the slope of the (Fe,Al)-bearing Bg melting curve remains fairly constant up  
215 to the CMB pressure of 135 GPa, which contrasts with the flattening reported for MgSiO<sub>3</sub>. This makes  
216 the different available results to converge to a temperature of 5100-5500 K for the melting of Bg at  
217 the CMB. We remind that the melting curve of MgSiO<sub>3</sub>-Bg should always plot at higher temperature  
218 than that of the (Fe,Al)-bearing composition, due to the incompatible character of Fe and Al. Thus,  
219 our experimental determination of the (Fe,Al)-bearing Bg melting curve implies that the melting  
220 temperature of MgSiO<sub>3</sub>-Bg at very high mantle pressures was underestimated by a couple hundred  
221 degrees in some previous studies (de Koker and Stixrude, 2009; Mosenfelder et al., 2009). Thus, for  
222 further discussions, we will choose the higher melting curve of MgSiO<sub>3</sub> Bg as determined from *ab*  
223 *initio* calculations (Stixrude and Karki, 2005). It can be modeled using a modified Simon and Glatzel  
224 equation [ $T=T_0 (P/a + 1)^{1/c}$ ] with parameters  $T_0=91$  K,  $a=0.00125$  GPa and  $c=2.83$  (Simon and  
225 Glatzel, 1929).

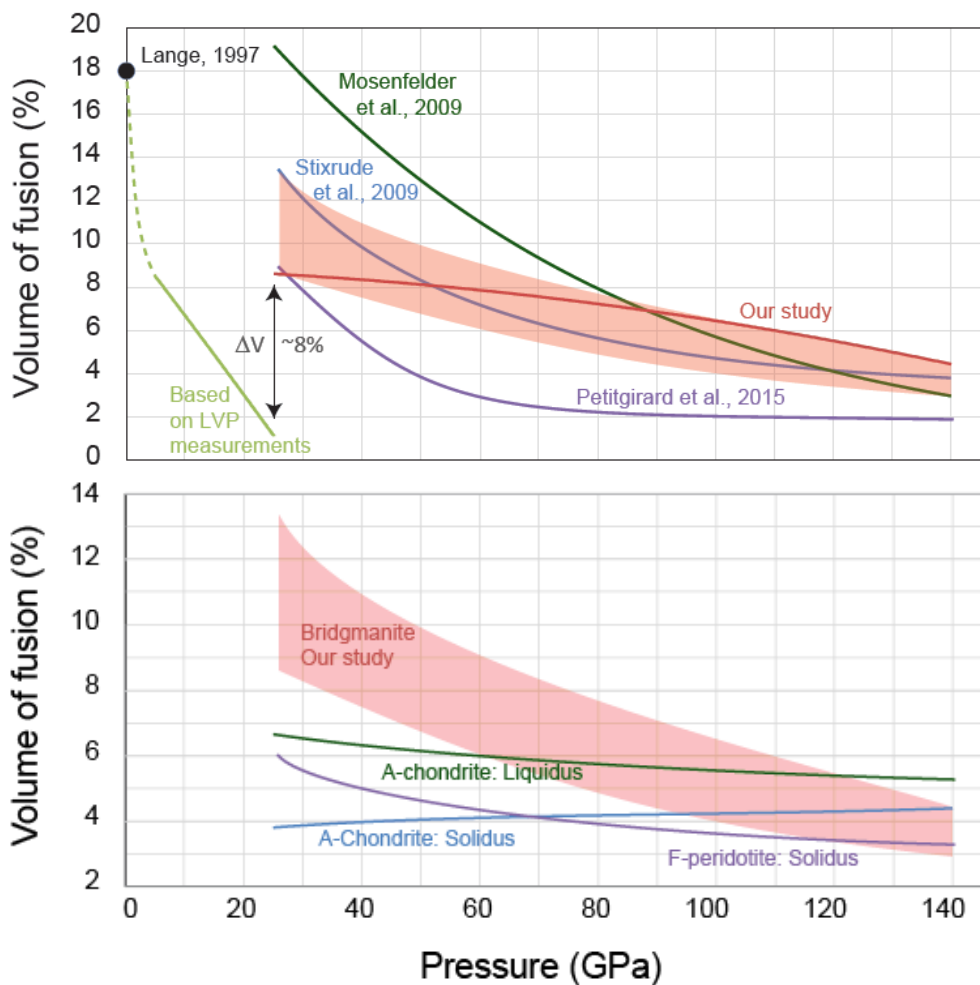
226 We note that the liquidus temperature profile reported previously for peridotite (Fiquet et al.,  
227 2010) appears superimposed with the melting curve of MgSiO<sub>3</sub>-Bg derived from *ab initio* calculations  
228 and shock experiments (Figure 1). This is unexpected because (i) the more complex chemical  
229 composition of the Bg phase itself, compared to MgSiO<sub>3</sub>, and (ii) additional Fp and CaSiO<sub>3</sub>-  
230 perovskite (CaPv) phases should both lower the peridotite liquidus below the melting temperature of  
231 pure MgSiO<sub>3</sub>. In their study, (Fiquet et al., 2010) observed large crystals of Bg at the center of the  
232 heated spot, where the melting behavior was monitored using *in situ* X-ray diffraction. Chemical  
233 composition of Bg grains measured at different locations on a sample synthesized at ~61 GPa show  
234 Fe/(Mg+Fe) and Al/Si ratios of ~2.5% and ~8%, respectively. It is possible that their reported  
235 measurements of the peridotite liquidus correspond in fact to the melting curve of these large grains  
236 of MgSiO<sub>3</sub>-bearing Bg.

### 237 3.4. VOLUME OF BRIDGMANITE MELTING

238 The dT/dP slope of the Bg melting curve is directly related to the volume ( $\Delta V_m$ ) and entropy  
239 ( $\Delta S_m$ ) of Bg melting through the classical Clapeyron relation  $dT/dP = \Delta V_m/\Delta S_m$ .  $\Delta S_m$  was reported  
240 to be 42.2 J/molK for MgSiO<sub>3</sub> at room pressure, based on calorimetric measurements (Stebbins et al.,  
241 1984). For melting of MgSiO<sub>3</sub> in the stability field of Bg, *ab initio* simulations suggest a  $\Delta S_m$  value  
242 1.5 times higher (Stixrude et al., 2009). Assuming then a constant  $\Delta S_m$  value of 63.3 J/molK for  
243 melting of (Fe,Al)-bearing Bg at all lower mantle conditions, we now calculate  $\Delta V_m$  values from the  
244 clapeyron slopes of the different melting curves available for Bg (Figure 2a). For the (Fe,Al)-bearing  
245 composition, we observe a progressive decrease of  $\Delta V_m/V_{Bg}$  ( $V_{Bg}$  being the Bg volume) from ~9%  
246 to ~5%, when pressure increases from 30 to 140 GPa, respectively. For comparison, earlier studies  
247 of the melting behavior of pure MgSiO<sub>3</sub> suggest a significantly larger effect of pressure, with  
248  $\Delta V_m/V_{Bg}$  varying from 13% at low pressures for some *ab initio* calculations (Stixrude et al., 2009) or  
249 even 19% for a shock-wave study (Mosenfelder et al., 2009), to 3-4% at pressures of 135 GPa. The  
250 flatter  $\Delta V_m$  found for the (Fe,Al)-bearing implied by our results is due to a more linear melting curve  
251 measured from 30-35 GPa to 135 GPa, compared to pure MgSiO<sub>3</sub> (Figure 1). We also show recent  
252 measurements of the MgSiO<sub>3</sub>-glass density performed in the DAC at 300 K up to the CMB pressure  
253 (Petitgirard et al., 2015). The  $\Delta V_m/V_{Bg}$  recalculated from the later study is significantly lower than  
254 all other calculations at high pressures, which should translate into a very flat melting curve. Based  
255 on the shadowed region in Figure 2a, we define a most probable range of  $\Delta V_m/V_{Bg}$  values decreasing  
256 from 11( $\pm 2$ )% to 4( $\pm 1$ )% when pressure is increased from 24 to 140 GPa, respectively.



257 We also calculated  $\Delta V_m$  at pressures below 24 GPa using  $\Delta S_m=42.2$  J/molK (Stebbins et al.,  
 258 1984) and using the Clapeyron of melting curves measured in large volume press (LVP) experiments.  
 259 We note that the final interpretation of  $\Delta V_m$  can be complicated by the occurrence of four different  
 260  $MgSiO_3$  polymorphs between 1 bar and 24 GPa (Presnall, 1995). In particular, the Clapeyron slope  
 261 of majorite melting remains largely uncertain, due to a limited pressure range available. For this  
 262 reason, we modeled the  $MgSiO_3$  melting line using a 2<sup>nd</sup> degree polynomial regression across the  
 263 whole pressure range from 0 to 24 GPa. The calculated  $\Delta V_m/V_{Bg}$  decreases strongly with increasing  
 264 pressure converging to 1% at ~24 GPa (Figure 2a). It makes a volume change of ~8% at the majorite  
 265 to Bg transition for the (Fe,Al)-bearing composition of our study, or ~10% in average for the most  
 266 probable range of  $\Delta V_m/V_{Bg}$  that we have defined above, both values agreeing well with the ~10%  
 267 suggested previously for  $MgSiO_3$  (Yu et al., 2011).



**Figure 2:** (a) Volume of melting ( $\Delta V_m = V_{melt} - V_{Solid} / V_{Bg}$ , where  $V_{Bg}$  is volume of Bridgmanite) derived from the melting curve of Bg (Figure 1) with various (Mg,Fe)(Si,Al) $O_3$  compositions. We also report the value of 18% measured for pure  $MgSiO_3$  at 1 bar (Lange, 1997) and  $\Delta V_m/V_{Bg}$  recalculated from density measurements of  $MgSiO_3$ -glass in a DAC (Petitgirard et al., 2015). Shaded pink region is the most probable range of mantle  $\Delta V_m/V_{Bg}$  values. (b)  $\Delta V_m$  derived from the solidus and/or liquidus profiles of the A-chondritic (Andraut et al., 2011) and F-peridotitic (Fiquet et al., 2010) models of mantle melting.  $\Delta V_m$  is calculated using the Clapeyron relation. Calculation of  $\Delta V_m/V_{Bg}$  along solidus and liquidus profiles assume an ideal mixing model to estimate the melt entropy (see text).

## 4. MELTING DIAGRAMS FOR TYPICAL LOWER MANTLE MATERIALS

### 4.1. EXPERIMENTAL DETERMINATION OF THE MELTING BEHAVIOR

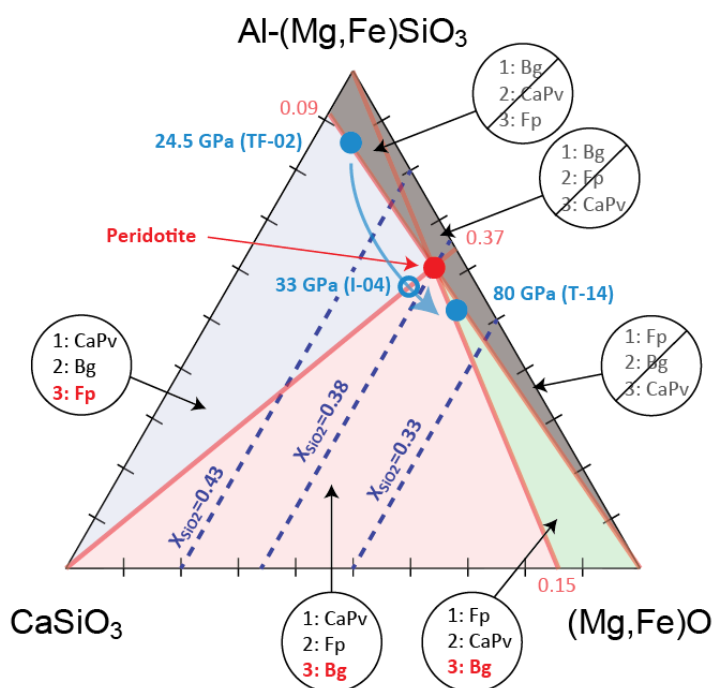
270 Studying experimentally phase relations in a partially molten geological material under P-T  
271 conditions of the Earth's interior remains a challenging task. The use of LVP facilitates largely the  
272 chemical analysis of coexisting phases in recovered samples, compared to LH-DAC. For example,  
273 melting behavior of fertile peridotite and CI chondritic mantle were documented up to ~35 GPa (Ito  
274 et al., 2004). It was demonstrated that the liquidus phase changes from Fp to Bg at about 33 GPa, a  
275 situation that was confirmed later by LH-DAC experiments (Andraut et al., 2011; Fiquet et al., 2010).  
276 However, LVP samples (and *a fortiori* LH-DAC samples) synthesized at lower mantle conditions  
277 always encounter relatively large temperature gradients, which yields heterogeneous microstructure  
278 and chemical zoning. In such cases, the sequence of phase disappearance from solidus to liquidus  
279 temperatures is usually retrieved from the position of phases relative to the temperature gradient. Still,  
280 this procedure prevents the precise determination of the equilibrium solid-liquid partition coefficients.

281 When coupled with *in situ* X-ray diffraction, LH-DAC is well suited to determine melting curves  
282 of various geological materials, because the available temperature range extends up to more than  
283 6000 K (Suppl. Figure 1). Melting criteria are generally based on the disappearance of diffraction  
284 peaks and phase(s), which corresponds in fact to the determination of a pseudo-eutectic temperature  
285 (PET). Recently, PET of peridotite (Fiquet et al., 2010), chondritic-mantle (Andraut et al., 2011) and  
286 pyrolite (Nomura et al., 2014) was reported with substantially different values. Disagreements cannot  
287 be reconciled based on the moderate compositional variations between starting materials, among  
288 which the major difference lies in the Bg/(Bg+CaPv+Fp) ratio from 0.59, 0.63 and 0.75 for peridotite,  
289 pyrolite and chondritic mantle, respectively. Studies using peridotitic (F-peridotitic model) and  
290 chondritic (A-chondritic model) starting materials show similar solidus evolution as a function of  
291 pressure, pointing out to a PET of  $4150 \pm 150$  K at the CMB. The lower value reported in the study  
292 using pyrolite could be due to a more precise determination of the solidus, thanks to the use of 3D X-  
293 ray tomography, but more likely because of the presence of 400 ppm H<sub>2</sub>O in their sample that triggers  
294 melting (Nomura et al., 2014).

### 4.2. PSEUDO-EUTECTIC TYPE MELTING IN THE DEEP MANTLE?

296 The melting diagram between the three lower mantle phases (Bg, CaPv and Fp) presents an  
297 eutectic behavior (e.g. (de Koker et al., 2013; Liebske et al., 2005; Liebske and Frost, 2012)), which  
298 implies (i) a PET and (ii) a melt composition at the PET located within the ternary diagram. The PET  
299 and the melt composition should be independent of the Bg, CaPv and Fp molar fractions in the bulk  
300 material, as long as the chemical compositions of these three phases do not vary significantly. A major  
301 issue for geological materials is that the onset of melting (the solidus) can possibly occur at a  
302 temperature lower than the PET. In such a case, a melt appears without disappearance of a phase from  
303 the mineral assemblage. This can happen when the solubility limit of an incompatible element is  
304 overpassed at a given condition of pressure and temperature. This behavior has not been reported yet  
305 for any mantle compositions under the P-T conditions typical of the lower mantle. In contrast,  
306 available LH-DAC experiments report disappearance of one phase at the onset of melting (see above).  
307 Also, chemical analyses of melts obtained after partial melting of peridotite at ~24 GPa show  
308 compositions close to the starting material (e.g. with a relatively lower MgO/SiO<sub>2</sub> ratio (Tronnes and  
309 Frost, 2002)), which is incompatible with incipient mantle melting.

311 Above the solidus temperature, partition coefficients between Bg or CaPv and the melt  
 312 ( $D_i^{\text{Solid/melt}}$ ) were investigated experimentally for many elements. Except for a very few of them (such  
 313 as Li and Ba),  $D_i^{\text{Solid/melt}}$  values are found to lie above  $3 \cdot 10^{-1}$ , which corresponds to a moderately  
 314 incompatible behavior (Corgne et al., 2005). These results suggests that the minor elements may not  
 315 reach their solubility limit easily. Of course, volatiles such as H<sub>2</sub>O (but also CO<sub>2</sub>) are well known to  
 316 depress the solidus and potentially favor incipient mantle melting. We note, however, that (i)  
 317 carbonate phases may be relatively refractory in the lower mantle (Thomson et al., 2014) and (ii)  
 318 a high water content in the lower mantle is unlikely, due to limited capability of the lower mantle  
 319 minerals to store water below the 660 km discontinuity (Bolfan-Casanova et al., 2003). Thus, even if  
 320 water has an effect of the solidus of the lower mantle it does not mean that water is actually present.  
 321 In summary, experimental evidences strongly suggest a moderate temperature difference between  
 322 solidus and PET, if any.



**Figure 3:** Ternary diagram between Bg, Fp and CaPv, the three major phases in the lower mantle. Due to its eutectic shape, melt compositions should always plot within this diagram. The Red dot and lines correspond to the peridotitic composition and its associated Fp/Bg, CaPv/Bg and CaPv/Fp ratios. Blue dots are melt compositions determined experimentally (Ito et al., 2004; Tateno et al., 2014; Tronnes and Frost, 2002). The blue arrow shows the change in melt composition with pressure. In each colored region of the ternary diagram, the expected sequence of phase disappearance upon melting are reported inside circles: 1, 2 and 3 are solidus, intermediate and liquidus phases, respectively.

### 323 4.3. SEQUENCE OF PHASE DISAPPEARANCE UPON MELTING

324 In the ternary diagram between Bg, CaPv and Fp, the difference in composition between the bulk  
 325 composition and the melt defines the sequence of phase disappearance upon melting. For example,  
 326 melting of peridotite would likely induce a melting sequence from CaPv (at solidus), Bg to Fp (at  
 327 liquidus), if the PE-melt would present significantly higher CaSiO<sub>3</sub>-content and lower (Mg,Fe)O-  
 328 content, compared to peridotite. Thus, the ternary diagram can be divided into six different regions  
 329 where the melting sequence should be different, depending on the PE-melt composition (Figure 3).

330 Composition of melts relevant to deep mantle partial melting were reported after experiments  
 331 performed at 24.5 GPa using LVP (Tronnes and Frost, 2002) and 80 GPa using LH-DAC (Tateno et  
 332 al., 2014). Despite the fact that these melts may differ from PE-melts, if experimental temperatures  
 333 have been higher than PET, they provide precious anchors for melt compositions in the ternary  
 334 diagram. Composition of these two melts (corresponding to 24.5 and 80 GPa) plot on each side of the  
 335 Fp/Bg ratio of 0.37, which corresponds to the peridotite composition. This observation is compatible  
 336 with a third experimental anchor point where the liquidus phase has changed from Fp to Bg at about

337 ~33 GPa for a fertile peridotite (Ito et al., 2004). Thus, the melt composition evolves toward higher  
338 (Mg,Fe)O-contents with increasing pressure.

339 Another important observation is the melt composition at 80 GPa, which presents a CaPv/Fp  
340 ratio very close to the peridotitic value of 0.15. It suggests that both phases, CaPv and Fp, disappear  
341 almost simultaneously at the PET upon partial melting of peridotite in the deep lower mantle. In this  
342 work, we make the assumption that CaPv and Fp disappear simultaneously at the PET at lower mantle  
343 pressures. This assumption is not severe. If Fp would disappear first, negligible amount of CaPv  
344 would remain. Indeed, the total amount of CaPv is below ~6 mol% for compositions relevant to the  
345 deep mantle. In the case where CaPv would disappear first, higher Fp content could theoretically  
346 remain after melting at the PET. Indeed, Fp is found at a level of 19, 32 or 35 mol%, for chondritic,  
347 pyrolitic or peridotitic compositions, respectively. However, the molar volume of Fp is twice less  
348 than those of Bg and CaPv. Also, it is likely that the melt dissolves a significant part of Fp at the PET  
349 (Tateno et al., 2014; Tronnes and Frost, 2002), which should yield to a low Fp-content in the residual  
350 solid.

#### 351 **4.4. LIQUIDUS TEMPERATURES AND BG-CONTENT IN MELTS**

352 The melting behavior can be modeled at various mantle pressures (for example 40 GPa, 80 GPa  
353 and 135 GPa) using (pseudo) binary phase diagrams, where one end-member is Bg, the liquidus phase,  
354 and the other is the sum of all the other chemical components (Figure 4). We prefer to use Fe-free Bg  
355 as an end-member, instead of (Fe,Al)-bearing Bg, due to the preferential partition of Fe to the melt  
356 (this matter is discussed later in the article). Still, we consider an Al-bearing Bg end-member, because  
357 the Al-behavior upon partial melting remains poorly constrained. Compositional axis of such binary  
358 diagram is thus the molar fraction of Fe-free Bg. Melts include Fp, CaPv, (virtual) FeSiO<sub>3</sub>-Bg and a  
359 fraction of Fe-free Bg end-members. Peridotitic and chondritic mantle, as well as our (Fe,Al)-bearing  
360 Bg composition plot at 59, 75 and 88 mol% of Fe-free Bg, respectively. For the PET, the A-chondritic  
361 model indicate “solidus” temperatures of 2690, 3340 and 4130 K at pressures of 40, 80 and 135 GPa,  
362 respectively (Andrault et al., 2011). For the Fe-free Bg end-member, we use ab initio calculations for  
363 MgSiO<sub>3</sub>-Bg (Stixrude and Karki, 2005), as discussed above. Two LH-DAC studies report liquidus  
364 temperatures of A-chondritic and F-peridotitic models (Andrault et al., 2011; Fiquet et al., 2010).  
365 Finally, the independent reports of the Bg-content in melts (i) measured after partial melting of  
366 pyrolite (Tateno et al., 2014) and (ii) calculated in the MgSiO<sub>3</sub>-MgO system (de Koker et al., 2013;  
367 Liebske and Frost, 2012) are also shown. We note that the two later studies did not included the CaPv  
368 component, which could numerically yield an overestimation of the Bg-content in the melt.

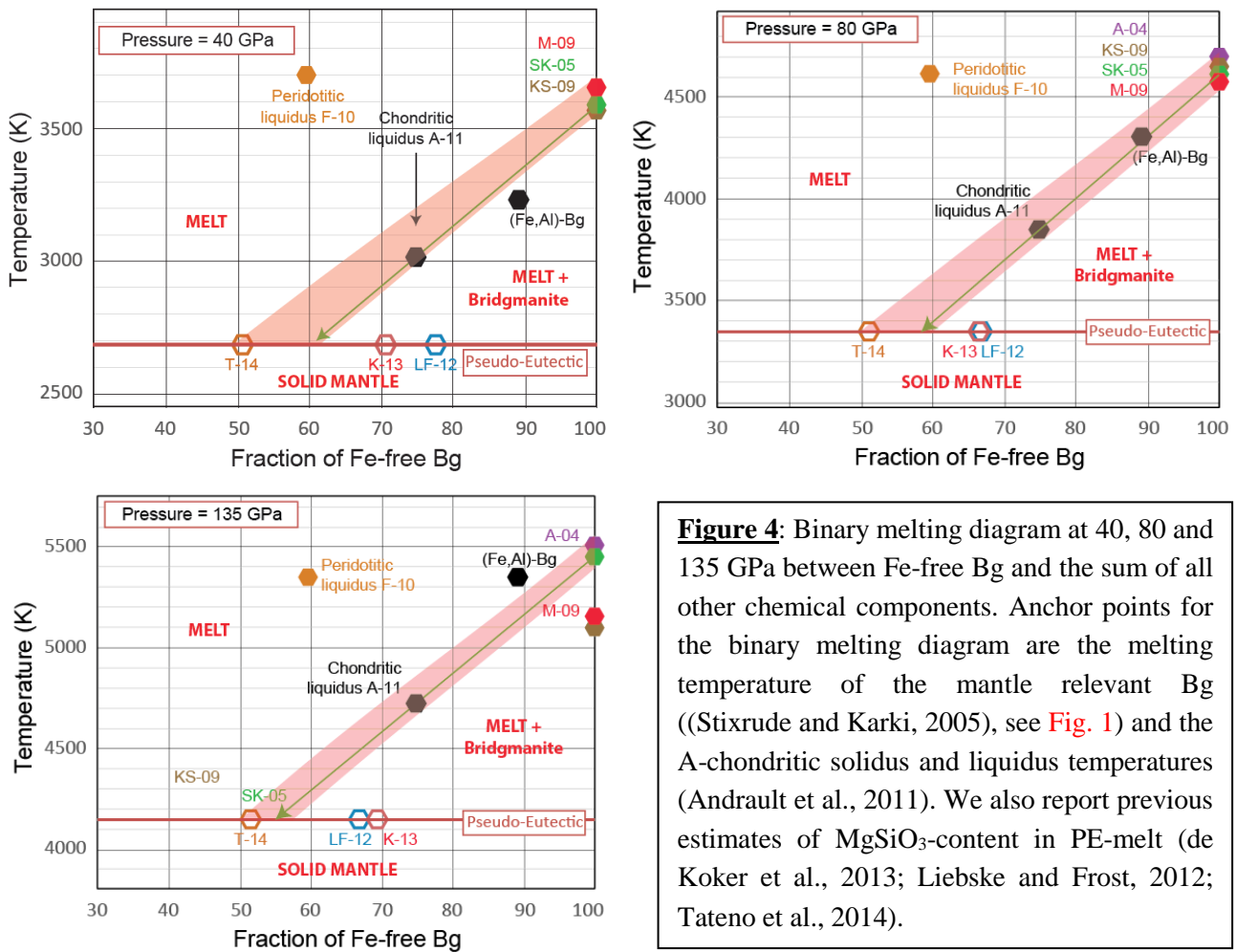
369 At each selected mantle pressure, we draw lines from the melting temperature of the Bg end-  
370 member, through the liquidus temperature of the A-chondritic model, toward the PET (Figure 4).  
371 These lines provide estimates of liquidus temperatures as a function of the bulk mantle composition.  
372 In addition, intersections between these lines and PET provide estimates of the Bg-content in PE-  
373 melts, as a function of pressure. Uncertainties arise from (i) controversial reports of the Bg melting  
374 temperature as a function of pressure (Figure 1) and (ii) unknown curvature of the liquidus profile in  
375 these diagrams. Consequently, we colored in pink regions where the presence of liquidus is the most  
376 probable. We excluded from colored regions (i) PE-melts with a fraction of Fe-free Bg higher than  
377 peridotite, because it would be contradictory with Bg becoming the liquidus phase above ~33 GPa  
378 (Ito et al., 2004), (ii) a previous study reporting inaccurate Bg melting curve at low pressures (Akins  
379 et al., 2004) and (iii) trends extrapolated from (de Koker and Stixrude, 2009; Mosenfelder et al., 2009)  
380 as they may have underestimated the Bg melting temperature by a couple hundred degrees in the

381 lowermost mantle (see text associated to [Figure 1](#)). We note that our method is not appropriate to  
 382 pressures lower than ~33 GPa, when Bg is not the liquidus phase.

383 Based on the width of the regions of confidence, the liquidus temperatures appears to be  
 384 constrained within  $\pm 150$  K at all mantle pressure, temperature and compositions. An uncertainty to  
 385 which we should still add a similar value associated to the experimental error in the determination of  
 386 PET and Bg melting temperature. On the other hand, uncertainty in Bg-content in PE-melt and along  
 387 liquidus lines is about  $\pm 5\%$ . The Bg-content in the PE-melt appears almost independent of lower  
 388 mantle pressure at  $55(\pm 5)$  mol%. With increasing temperature above PET, the Bg-content in melt  
 389 should logically increase until it reaches the bulk mantle composition. Altogether, these binary  
 390 melting diagrams can be numerically constrained by three parameters: (i) a constant Bg-content of  
 391  $55(\pm 5)$  mol% in PE-melt, and two modified Simon and Glatzel (SG) equations  $[T(P)=T_0 (P/a+1)^{1/c}]$   
 392 with parameters (ii)  $T_0=2045$  K,  $a=92$  GPa and  $c=1.3$  for the PET (Andrault et al., 2011) and (iii)  
 393  $T_0=91$  K,  $a=0.00125$  GPa and  $c=2.83$  for the Bg end-member ((Stixrude and Karki, 2005), see above).  
 394 Then, liquidus temperatures between PE-melt and Bg can be defined as a function of pressure and  
 395 mantle composition using:

$$396 T_{\text{Mantle}}^{\text{Liq}}(P, X_{\text{Bg}}^{\text{Mantle}}) = \text{SG}(\text{Bg}) - [(\text{SG}(\text{Bg}) - \text{SG}(\text{PEM})) * (1 - X_{\text{Bg}}^{\text{Mantle}}) / (1 - X_{\text{Bg}}^{\text{PEM}})]$$

397 where  $\text{SG}(\text{PEM})$  and  $\text{SG}(\text{Bg})$  are PE-melt and Bg melting temperatures, respectively, calculated at a  
 398 target mantle pressure (P) using SG equations.  $X_{\text{Bg}}^{\text{PEM}}$  and  $X_{\text{Bg}}^{\text{Mantle}}$  are Bg mole fractions in the PE-  
 399 melt (fixed at 55 mol%) and the bulk mantle, respectively.



**Figure 4:** Binary melting diagram at 40, 80 and 135 GPa between Fe-free Bg and the sum of all other chemical components. Anchor points for the binary melting diagram are the melting temperature of the mantle relevant Bg ((Stixrude and Karki, 2005), see [Fig. 1](#)) and the A-chondritic solidus and liquidus temperatures (Andrault et al., 2011). We also report previous estimates of  $\text{MgSiO}_3$ -content in PE-melt (de Koker et al., 2013; Liebske and Frost, 2012; Tateno et al., 2014).

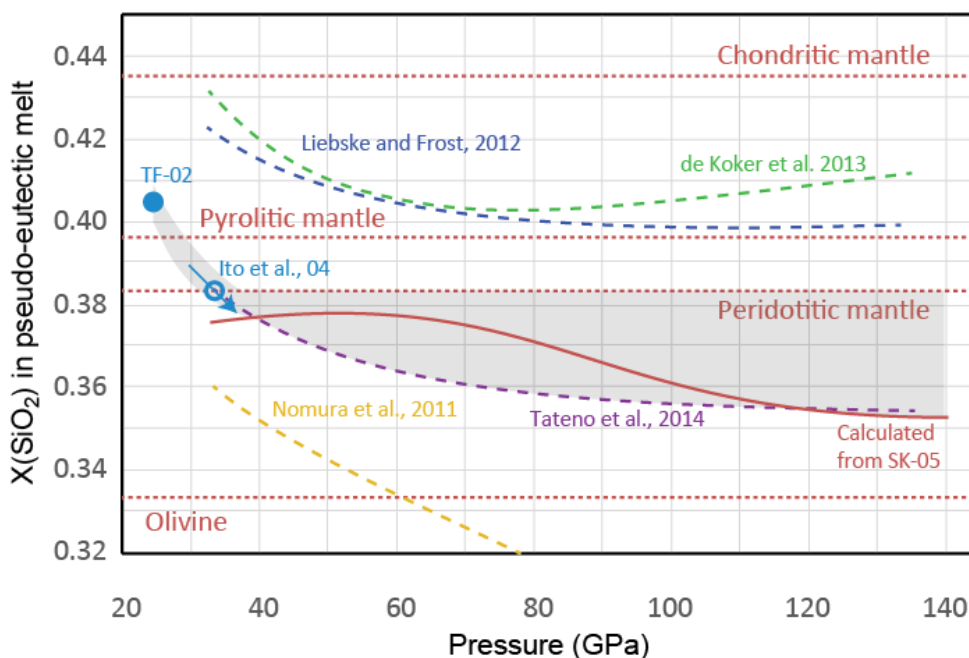
400 For a peridotitic mantle composition, binary phase diagrams suggest a difference of less than 300  
 401 K between PET and liquidus at all lower mantle pressures. This is in very good agreement with the  
 402 value of 250 K proposed based on a thermodynamic melting model (Liebske and Frost, 2012). The



403 difference between the PET and the liquidus increases for larger fractions of Bg in the bulk material,  
 404 and in a primitive chondritic mantle it can reach up to 500 degrees. This confirms the wide range of  
 405 mantle depths where partial melting should have occurred in the framework of an early magma ocean  
 406 (e.g. (Kojitani and Akaogi, 1997; Miller et al., 1991)).

#### 407 4.5. SiO<sub>2</sub> CONTENT IN PSEUDO-EUTECTIC MELTS

408 Another parameter controlling the melt properties is its SiO<sub>2</sub>-content (X(SiO<sub>2</sub>)). It can be derived  
 409 directly from Figure 4, by converting the amount of Fe-free Bg in the melt into its SiO<sub>2</sub> contribution.  
 410 Based on our primary assumption that Fp and CaPv dissolve concomitantly in the melt at the PET,  
 411 the SiO<sub>2</sub>-content of the CaPv component is also added to the melt composition. This calculation can  
 412 be performed for all types of melt along liquidii, as long as pressure is above ~33 GPa. Still, we only  
 413 discuss here the composition of PE-melts. We actually translate into X(SiO<sub>2</sub>) the regions of  
 414 confidence defined above for Bg-contents in PE-melts (Figure 5). Independent values of X(SiO<sub>2</sub>) in  
 415 lower mantle melts were reported previously based on *ab initio* calculations (de Koker et al., 2013),  
 416 thermodynamic modeling of LVP experiments (Liebske and Frost, 2012) and chemical analyses of  
 417 LH-DAC samples (Nomura et al., 2011; Tateno et al., 2014). At about ~33 GPa, the change of liquidus  
 418 phase from Fp to Bg reported upon peridotite melting suggests that X(SiO<sub>2</sub>) in the melt crosses the  
 419 peridotitic value of 38.3% (Ito et al., 2004).



**Figure 5:** Pressure change of the SiO<sub>2</sub>-content in pseudo-eutectic melt. Horizontal dotted lines are X(SiO<sub>2</sub>) typical of olivine, peridotite, pyrolite and chondritic-mantle. The red line is derived from the Bg melting curve (Stixrude and Karki, 2005) associated with the thermodynamical treatment elaborated for the discussion of Figure 4. Dashed lines represent previous calculations (de Koker et al., 2013; Liebske and Frost, 2012) or the experimental determination (Tateno et al., 2014) of X(SiO<sub>2</sub>) in melts. The shaded gray area corresponds to the most likely X(SiO<sub>2</sub>) of lower mantle melts.

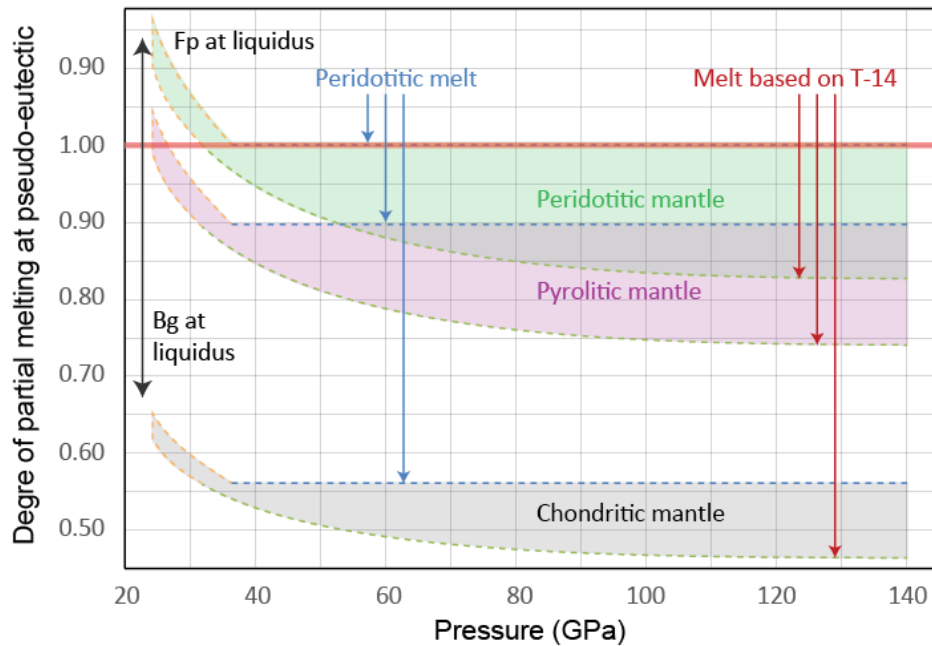
420 The melt X(SiO<sub>2</sub>) likely remains significantly lower than 0.40 at higher pressures in the lower  
 421 mantle, because Bg was broadly reported to be at the liquidus for pyrolite (Nomura et al., 2014) and  
 422 peridotite (Fiquet et al., 2010). The fact that two models (de Koker et al., 2013; Liebske and Frost,  
 423 2012) propose higher X(SiO<sub>2</sub>) could be related to calculations restricted to the MgSiO<sub>3</sub>-MgO system.  
 424 The difference between the simple MgO-SiO<sub>2</sub> system and the mantle-related compositions suggests  
 425 that Ca and Fe should enter the melt preferentially as CaO and FeO, rather than CaSiO<sub>3</sub> and FeSiO<sub>3</sub>,



426 thus lowering  $X(\text{SiO}_2)$ . Such behavior translates into a significantly stronger incompatible character  
 427 of Ca and Fe, compared to Mg and Si (Liebske et al., 2005), which is already well known for low-  
 428 pressure melting. The range of possible melt  $X(\text{SiO}_2)$  appears to extend between the peridotite and  
 429 chemical analyses performed on LH-DAC samples (Tateno et al., 2014). It corresponds to an almost  
 430 fixed  $X(\text{SiO}_2)$  value of 37.0% ( $\pm 1.5\%$ ). This most probable range of  $X(\text{SiO}_2)$  plots in good continuity  
 431 with data reported at lower pressure based on LVP experiments (Ito et al., 2004; Tronnes and Frost,  
 432 2002). In summary, deep PE-melts appear to adopt a composition only slightly enriched in Fp  
 433 compared to peridotite, if any.

#### 434 4.6. DEGREE OF PARTIAL MELTING AT PSEUDO-EUTECTIC TEMPERATURES

435 We can now calculate the expected degree of partial melting ( $F$ ) at the PET for peridotitic,



**Figure 6:** Degrees of mantle partial melting (vol%) expected at pseudo-eutectic temperature (PET) in the lower mantle under the assumptions that CaPv and Fp phases disappear jointly upon melting. Degrees of partial melting are calculated for typical chondritic, pyrolitic and peridotitic mantle compositions, based on the possible range of PE-melt composition refined in Figure 5. T-14 stands for (Tateno et al., 2014).

436 pyrolitic and chondritic mantle compositions, based on our estimation of deep-mantle melt  
 437 compositions (Figures 4 and 5).  $F$  (in vol%) at PET can be estimated using the molar volumes for Bg,  
 438 Fp and CaPv (Equations of state needed to take into account the effect of pressure and temperature on  
 439 volumes are described below). Logically, the calculated  $F$  value at PET varies with the difference in  
 440 composition between the PE-melt and the bulk material. The closest the mantle composition is from  
 441 the melt, the highest  $F$  value is expected at the PET. Calculated ranges of possible  $F$  values at PET  
 442 appear to be more than 83, 74 and 46 vol%, for peridotitic, pyrolitic and chondritic mantle  
 443 compositions, respectively (Figure 6).

444 We note that a similar conclusion was reached previously (e.g. (Herzberg and Zhang, 1998))  
 445 based on the residual harzburgite signature of most komatiites with Cretaceous and late-Archaean  
 446 ages, which can be interpreted to have formed by about 25 to 60% anhydrous melting of mantle  
 447 peridotite in hot plumes.

448 The melting relations discussed above have implications for our understanding of the melting in  
 449 the deep mantle today. For example, in the ultra-low velocity zones (ULVZ) just above the CMB, the

450 high F values determined for PET imply that the ULVZ cannot correspond to partial melting of the  
451 average mantle, because the degree of partial melting in the ULVZ as inferred by seismology is much  
452 lower than the threshold value of 46%. But a lower F-value could be achieved (i) for a locally high  
453 concentration in volatile elements, which would favor incipient mantle melting below the PET or (ii)  
454 for another type of geological material, such as subducted basalts (Andrault et al., 2014).  
455

## 5. MELT BUOYANCY IN THE DEEP MANTLE

### 5.1. MAJOR PARAMETERS CONTROLLING THE MELT BUOYANCY

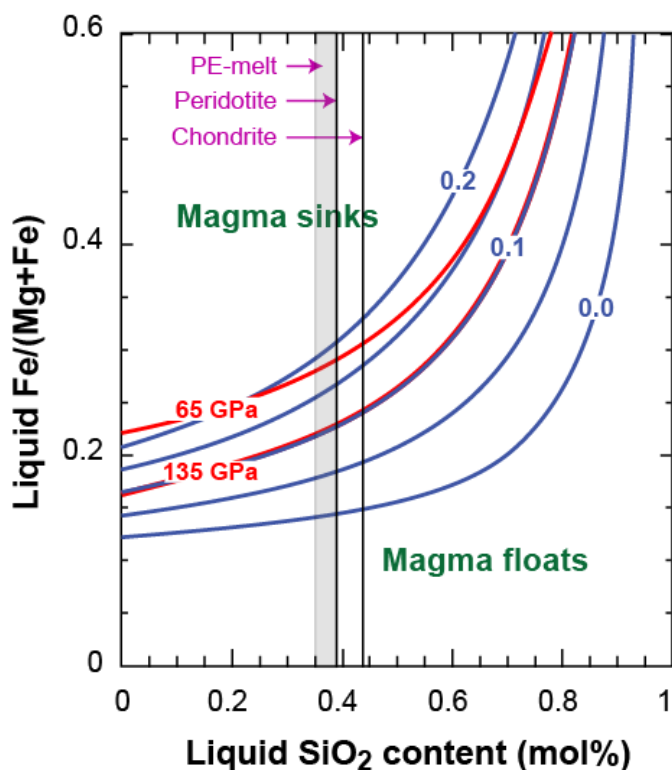
Dynamical behavior of a partially molten mantle is largely affected by the density contrast between the melt and the solid fractions ( $\Delta\rho_{m-s}=(\rho_m-\rho_s)/\rho_s$ ). While melt buoyancy plays a major role in chemical segregation and planetary differentiation, the fact that its sign is positive or negative produces two different geodynamical situations. Melt buoyancy can also vary with mantle depth, due to (i) a possible change of the melt composition and (ii) different PVT equations of state for the melt and the mantle residue. In the present-day mantle, ascent, or descent, of some melts could contribute to surface volcanism, or accumulation of melts in the lowermost mantle, respectively. In a crystallizing magma ocean, it is classically accepted that crystals would settle, compact and reject the melt toward the Earth's surface (Boukare et al., 2015; Solomatov, 2007). However, this question became much debated after it was proposed that an early basal magma ocean could be produced by dense melts stored above the CMB (Labrosse et al., 2007; Nomura et al., 2011). Solid-liquid density inversions are not unusual. Many years ago, it was already proposed that basaltic and komatiitic magmas would become denser than olivine and garnet at depths of 245-500 km (Agee, 1998).

Major parameters controlling the buoyancy of deep-mantle melts are (i) changes in atomic packing between solid and liquid phases, which most generally produces a positive volume of melting ( $\Delta V_m$ ), (ii) Fe partition coefficient between the solid residue and the melt ( $D_{Fe}^{Bg/melt}$ ), because Fe is the heaviest major element, and (iii) MgO/SiO<sub>2</sub> ratio in the melt, because SiO<sub>2</sub>-based atomic packing presents a relatively high bulk modulus. We chose to use  $D_{Fe}^{Bg/melt}$  ( $D=X_{Fe}^{Bg}/X_{Fe}^{melt}$ , with X being the molar fraction), rather than the distribution coefficient  $K_{Fe}^{Bg/melt}$  ( $K=(X_{Fe}/X_{Mg})^{Bg}/(X_{Fe}/X_{Mg})^{melt}$ ), because  $X_{Mg}^{melt}$  can vary with pressure, temperature and bulk composition independently from  $X_{Fe}^{melt}$ . Nothing prevents  $X_{Mg}^{melt}$  and  $X_{Fe}^{melt}$  to vary in a correlated way, which would contradict the proper definition of K.

Concerning the volume difference between solids and melts, both phases undergo (i) volume changes upon P and T according to their respective equation of state and (ii) a number of structural transformations with increasing mantle depth. In the solid state, equation of states of major mantle minerals are relatively well constrained (Matas et al., 2007). Structural transformations in the melt are much more progressive than in the solid, but can still contribute to a net increase of the melt density with increasing mantle depths. Due to the disordered and time-dependent nature of the melt structure, each structural entity has a finite lifetime. And when pressure is applied, structural entities can progressively evolve. In polymerized liquids, polyhedral chains can bend, eventually break and recombine differently (Stolper and Ahrens, 1987; Wang et al., 2014). All major cations progressively change their coordination shell (Bajgain et al., 2015) to allow compaction of the oxygen sub-lattice (Zeidler et al., 2014). The major change is probably Si, which progressively changes coordination number from four-fold to six-fold between ~20 to ~40 GPa (Benmore et al., 2010; Guillot and Sator, 2007; Sanloup et al., 2013; Sato and Funamori, 2010). These progressive transformations yield a room pressure bulk modulus significantly lower for the melt than for the crystalline counterpart. However, the pressure derivative of the bulk modulus is generally much higher, due to the progressive loss of some compaction mechanisms, after major voids have disappeared from the melt structure at moderate pressures.

497 At shallow mantle depths, while the melt structure has already undergone significant compaction,  
 498 major mantle minerals, in particular olivine, have not yet transformed to a denser polymorph. For this  
 499 reason, there could be a neutral melt buoyancy, or even a positive  $\Delta\rho_{m-s}$  (i.e. a sinking melt), at mantle  
 500 depths just above the 410 km discontinuity (Matsukage et al., 2005; Sakamaki et al., 2006). It could  
 501 produce a kind of density trap, where melts produced above and below would accumulate and remain  
 502 gravitationally stable in this mantle region (e.g. (Lee et al., 2010)). At lower mantle pressures, a  
 503 previous study tentatively addresses  $\Delta\rho_{m-s}$  for a number of melt and solid compositions (Figure 7;  
 504 (Funamori and Sato, 2010), see also (Thomas et al., 2012)). Reporting in this diagram our estimates  
 505 of  $X(\text{SiO}_2)$  in PE-melt retrieved from Figure 5 narrows down the range of possible silica contents  
 506 between  $\sim 35.2$  to  $\sim 38.3$  mol%. We note that the  $\text{SiO}_2$ -content in the melt should increase with  
 507 increasing temperature above the PET, because the PE-melt is relatively depleted in  $\text{SiO}_2$  compared  
 508 to the mantle composition. Ultimately, the melt and the bulk mantle become similar at the liquidus  
 509 temperature, when the solid residue disappears completely. Altogether, the rather limited range of  
 510 possible  $\text{SiO}_2$ -content in mantle melts points out to the fact that the less constrained parameters needed  
 511 to address melt buoyancy at mantle depths are  $\Delta V_m$ , the volume of melting, and  $D_{\text{Fe}}^{\text{Bg/melt}}$ , the Fe solid-  
 512 liquid partitioning.

**Figure 7:** Relative buoyancy between mantle melts of various compositions and (i) the  $(\text{Mg,Fe})\text{SiO}_3$  Bg with Fe-contents of 0, 10, or 20% (blue lines) and (ii) the lower mantle at pressures of 65 and 135 GPa (red lines). Along each blue or red lines, the melt and the given solid phase (Bg or lower mantle) have the same density. Higher  $\text{SiO}_2$ -content or lower  $\text{Fe}/(\text{Mg}+\text{Fe})$  ratio, compared to a given line, yield melts buoyant compared to the solid phase considered. The gray region corresponds to the likely  $\text{SiO}_2$ -content in PET-melts in the mantle (see Figure 5).  $\text{SiO}_2$ -content values for chondritic and peridotitic mantle are also reported. This Figure is modified from (Funamori and Sato, 2010).



## 513 5.2. VOLUME OF MANTLE MELTING

514 While the  $\Delta V_m$  corresponding to the melting of a pure phase, such as Bg, can be estimated based  
 515 on its melting curve (Figure 2a), the volume of melting becomes more difficult to address in the case  
 516 of the partial melting of the mantle between its solidus and liquidus. In addition, the equation of state  
 517 of the melt changes significantly with its composition (de Koker et al., 2013; Thomas and Asimow,  
 518 2013). For example,  $\text{Mg}_2\text{SiO}_4$ -liquid becomes denser than lower mantle phases at pressures above  
 519  $\sim 40$  GPa, while  $\text{MgSiO}_3$ -liquid remains buoyant at all mantle pressures (Thomas and Asimow, 2013).  
 520 Thus, assuming a simplified melt composition, such as  $\text{MgSiO}_3$ , may not be much relevant for  
 521 discussing the buoyancy of natural melts in the deep mantle. A more realistic exercise is to estimate  
 522 the real density difference between the solid residue and a melt of relevant composition in the Bg-  
 523 CaPv-Fp system. The solid residue can be a simple phase (Bg, or Fp below  $\sim 33$  GPa), or a typical

524 mantle composition (e.g. pyrolite), which would be relevant to model melt buoyancy in the context  
525 of an early crystallizing magma ocean (high F), or partial melting in the present-day lower mantle  
526 (low F), respectively. The melt composition at various P and T can be derived from melting diagrams  
527 (Figure 4).

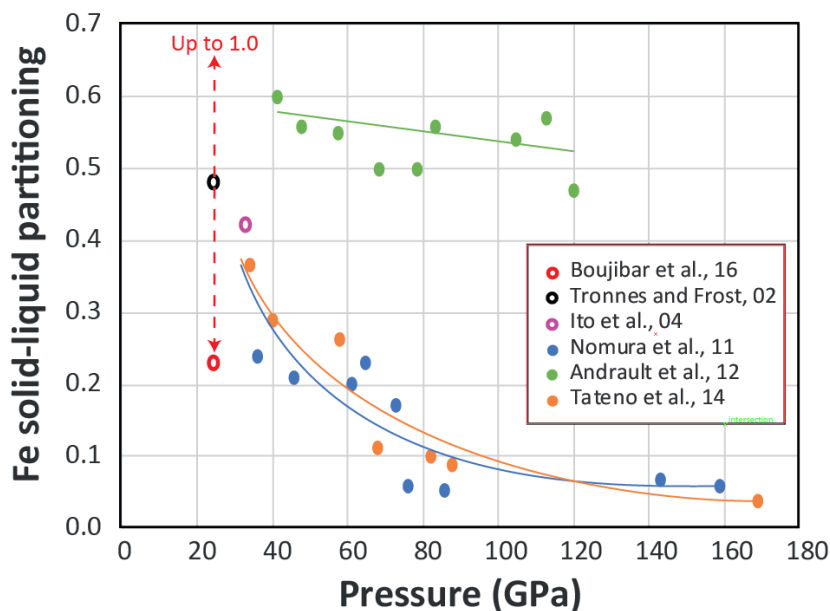
528 In Figures 2b, we intend to use the slopes of solidus and liquidus reported for mantle melting  
529 from LH-DAC experiments (Andraut et al., 2011; Fiquet et al., 2010) to retrieve thermodynamical  
530 information relevant to melts. We compare the solidus, or liquidus, profile to a Clapeyron slope which  
531 would record melting of the first fraction of solid mantle, or the last fraction of Bg, respectively. At  
532 the solidus temperature, the entropy of melting ( $\Delta S_m$ ) can be estimated from the sum of melting  
533 entropies of each phase present in the melt, plus a mixing entropy. We used  $\Delta S_m^i$  values of 63.3, 63.3  
534 and 13.0 J/molK for the melting entropy of Bg (Stixrude et al., 2009), CaPv (similar to Bg) and Fp,  
535 respectively. We note that the room pressure value of  $\Delta S_m^{MgO}$  was reported to be significantly larger  
536 than that of Fp, at  $\sim 35$  J/molK, however, it decreases rapidly with increasing pressure to 25 GPa  
537 (Vocadlo and Price, 1996). Composition of the PE-melt is considered to be 60% Bg, 30% Fp and  
538 10% CaPv, in agreement with Figures 3 and 4. However, changing the phase contents does not affect  
539 greatly the calculated  $\Delta S_m$  value of  $\sim 55$  J/molK. At the liquidus temperature, we assume that the  $\Delta S_m$   
540 of the bulk rock is similar to that of Bg, neglecting the fact that the melt in which last grains of Bg  
541 get dissolved has a composition slightly different from Bg. Based on these assumptions, we calculate  
542 volumes of melting at solidus and liquidus, using the Clapeyron equation (Figure 2b).

543 For the A-chondritic model, the values of  $\Delta V_m/V_{Bg}$  at the solidus and at the liquidus appear  
544 almost independent of mantle pressure, at values of  $4(\pm 1)\%$  and  $6(\pm 1)\%$ , respectively. The  $\Delta V_m/V_{Bg}$   
545 at the solidus of the F-peridotitic model plots at similar values, however, due to a larger curvature in  
546 the melting curve, its associated  $\Delta V_m/V_{Bg}$  varies more with pressure. We note that if we would have  
547 included a supplementary non-ideal mixing contribution to  $\Delta S_m$  (de Koker et al., 2013), the  $\Delta V_m/V_{Bg}$   
548 values would have been  $\sim 0.5\%$  higher. Calculations appear compatible with a small variation of the  
549 volume of melting with temperature increasing from the solidus to the liquidus and a small decrease  
550 with pressure from  $\sim 6\%$  to  $\sim 4\%$  from 30 to 130 GPa, respectively. This significantly positive value  
551 of  $\Delta V_m/V_{Bg}$  should contribute to a positive melt buoyancy for all types of melts.

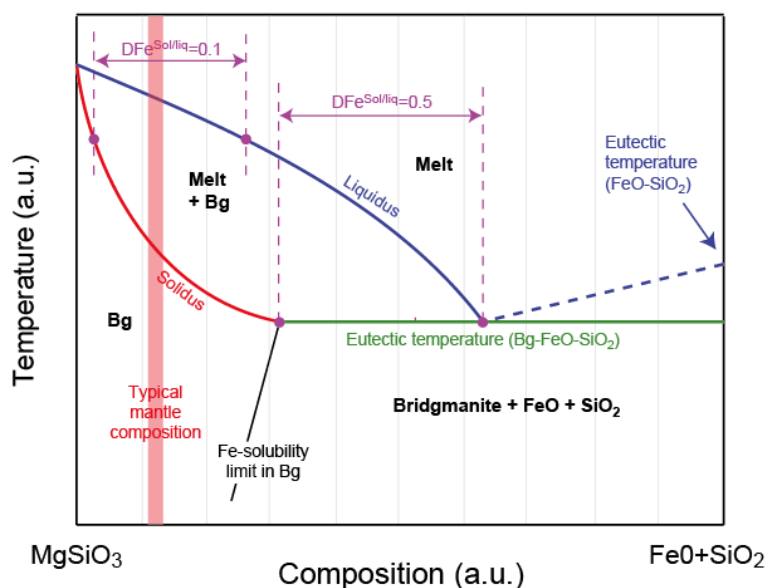
### 552 5.3. LIQUID-SOLID FE PARTITIONING

553 Based on LVP experiments performed up to  $\sim 35$  GPa, Fe is recognized as an incompatible  
554 element, with a concentration  $\sim 1.5$  to  $\sim 3$  times higher in the melt compared to the solid mantle (e.g.  
555 (Ito et al., 2004; Liebske et al., 2005)). For samples recovered from LH-DAC experiments, Fe was  
556 reported to become extremely incompatible with the Bg structure at pressures above  $\sim 70$  GPa, with  
557 a Fe concentration more than 10 times higher in the melt, compared to Bg (Nomura et al., 2011)  
558 (Figure 8). Such an enrichment of iron in melts (associated to a very low Fe-concentration in the  
559 residual Bg) favors their higher density relative to the solid residue, facilitating their sinking towards  
560 the CMB. In this previous study, olivine was used as a starting material and the absence of Al could  
561 have favored a relatively low  $D_{Fe}^{Bg/melt}$  value (Wood and Rubie, 1996). Still, another study performed  
562 on an Al-bearing peridotitic composition using the same experimental methodology confirms the very  
563 low Fe-content in the residual Bg (Tateno et al., 2014). We note that the Al partition coefficient  
564 between Bg and melt ( $D_{Al}^{Bg/melt}$ ), which was also reported to decrease significantly from 1.8 to 0.64  
565 with increasing pressure from 34 to 88 GPa in the same study. On the other hand, much higher  
566  $D_{Fe}^{Bg/melt}$  values of 0.5-0.6 were reported for a chondritic-mantle starting material using *in situ* X-ray  
567 fluorescence spectroscopy (Andraut et al., 2012). These last results favor denser Bg grains and

568 buoyant melts. The controversy cannot arise from slight compositional differences between starting  
 569 materials, especially between peridotitic and chondritic mantle compositions used in (Tateno et al.,  
 570 2014) and (Andraut et al., 2012), respectively. It should be related to differences in experimental  
 571 and/or analytical techniques.



**Figure 8:** Change in Fe partitioning ( $D_{\text{Fe}}^{\text{Bg/melt}}$ ) between the Bg and a coexisting melt. Starting materials for LH-DAC experiments were olivine (bleu, (Nomura et al., 2011)), chondritic-type mantle (green, (Andraut et al., 2012)) and peridotite (red, (Tateno et al., 2014)). Open circles correspond to previous multi-anvil experiments (Boujibar et al., 2016; Ito et al., 2004; Tronnes and Frost, 2002). The red arrow corresponds to the range of  $D_{\text{Fe}}^{\text{Bg/melt}}$  measured in a same study at varying F values.



**Figure 9:** A possible, schematic, melting diagram between  $\text{MgSiO}_3$  and  $\text{FeSiO}_3$  in the lower mantle. We plot  $\text{FeO}+\text{SiO}_2$  as the Fe-bearing end-member because  $\text{FeSiO}_3\text{-Bg}$  is unstable, except maybe at very high pressures. Vertical purple dashed lines are compositions of coexisting Bg and melt. Strong curvatures of solidus and liquidus lines can yield a decrease of  $D_{\text{Fe}}^{\text{Bg/melt}}$  with increasing temperature between the eutectic and the liquidus temperature, in agreement with a previous study (Boujibar et al., 2016).

572 A recent study addresses the value of  $D_{\text{Fe}}^{\text{Bg/melt}}$  as a function of F, the degree of partial melting,  
 573 based on LVP experiments performed at ~25 GPa (Boujibar et al., 2016).  $D_{\text{Fe}}^{\text{Bg/melt}}$  was found to vary  
 574 from ~1 to a constant value of ~0.3, for F values below ~5 wt% or above 10 wt%, respectively. It  
 575 suggests a  $D_{\text{Fe}}^{\text{Bg/melt}}$  negatively correlated with temperature between the solidus and the liquidus, in  
 576 agreement with a typical binary melting diagram (Figure 9). Thus, controversial results between  
 577 previous LH-DAC experiments could arise from different heating conditions. Experiments reporting  
 578 very low  $D_{\text{Fe}}^{\text{Bg/melt}}$  values were performed using a very thin insulating material (hardly detectable  
 579 using X-ray diffraction). A clear advantage is to facilitate the recovery of relatively thick samples,  
 580 which can be cut after the experiment in order to obtain relatively large and homogeneous sample  
 581 regions for chemical analyses using the electron microprobe. However, such experimental procedure  
 582 implies strong axial temperature gradient between the two diamonds. The center part of the recovered  
 583 samples is likely to correspond to relatively high temperatures, potentially close to the liquidus (high  
 584 F possibly inducing low  $D_{\text{Fe}}^{\text{Bg/melt}}$ , Figure 9). Alternatively, experiments reporting higher  $D_{\text{Fe}}^{\text{Bg/melt}}$



585 values used very thin samples well embedded in the insulating material (producing major diffraction  
586 peaks). While this type of loading minimizes axial temperature gradients in the sample, it makes the  
587 sample recovery much more difficult. In a previous study, X-ray diffraction was used to monitor  
588 carefully the onset of melting at the solidus temperature (Andrault et al., 2011) (low F possibly  
589 inducing high  $D_{\text{Fe}}^{\text{Bg/melt}}$ ). Differences in heating procedure and thus in melting temperature between  
590 previous works could have induce significantly different values of  $D_{\text{Fe}}^{\text{Bg/melt}}$ . We note that the Fe  
591 behavior could be complicated by other factors: (i) the role of Al, which is not well constrained at  
592 high pressures; Due to the strong Al-Fe coupling in the Bg structure, an Al-depletion from the Bg  
593 structure would contribute to lower  $D_{\text{Fe}}^{\text{Bg/melt}}$ ; (ii) the variable  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  fractions, because each  
594 one could partition differently between Bg and the melt, etc. Needless to say that a full quantitative  
595 model of  $D_{\text{Fe}}^{\text{Bg/melt}}$  at lower mantle conditions requires additional experimental and theoretical studies.

#### 596 **5.4. SOLID-LIQUID DENSITY CONTRAST**

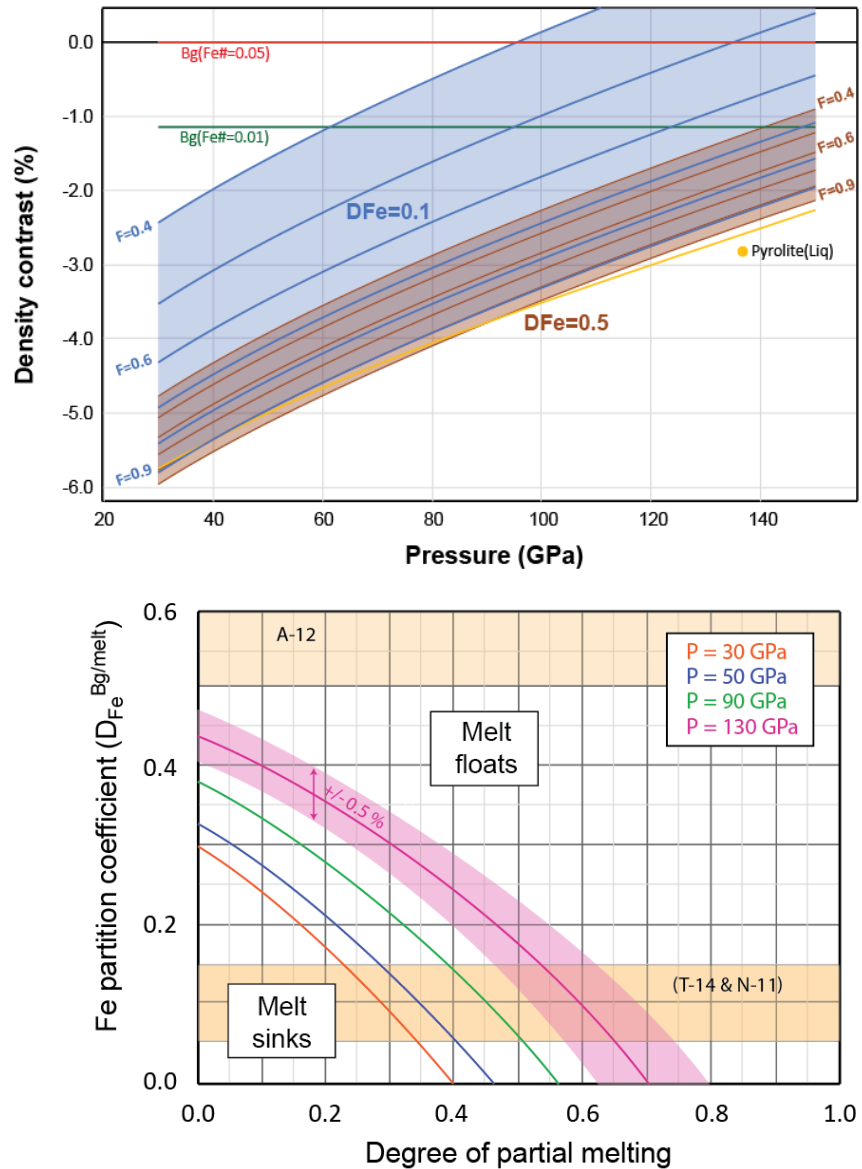
597 The  $\Delta\rho_{\text{m-s}}$  can be evaluated based on the density of both phases. All calculations were performed  
598 for a bulk mantle of pyrolitic composition. We consider a bulk Fe/(Mg+Fe) ratio (Fe#) of 0.1. We  
599 adjust the Fe-contents in the solid and the melt in order to reproduce the bulk mantle Fe-content, for  
600 various values of  $D_{\text{Fe}}^{\text{Bg/melt}}$ , which remains an adjustable parameter in the calculation. For the  
601 coexisting solid and melt compositions, we first calculate the densities in the solid state, before we  
602 apply a correction to the melt density of 6% to 4% for pressures between 30 and 130 GPa,  
603 respectively, to take into account the volume of melting (Figure 2). Composition of the solid can  
604 correspond either to (i) pure Bg, as expected for the residual solid from solidus to liquidus  
605 temperatures in our pseudo-binary melting diagrams (Figure 4), or to (ii) the mineral assemblage  
606 typical of pyrolite, which would correspond to the mantle composition in case of incipient melting.  
607 On the other hand, composition of the melt is approximated by a mixture of 55% Bg, 6.2 % CaPv and  
608 38.8 % Fp, which represents well the PE-melt at all lower mantle pressures (Figure 4). We neglect  
609 the P-T dependence of melt composition, because the  $X(\text{SiO}_2)$  value of the PET is not very different  
610 from the bulk pyrolitic mantle. Densities at high P and T of each phases are calculated based on their  
611 respective molar fractions of the following five different end-members: Al-bearing  $\text{MgSiO}_3$ ,  $\text{FeSiO}_3$ ,  
612  $\text{MgO}$ ,  $\text{FeO}$ ,  $\text{CaPv}$ , using the PVT equation of state of each of them. We used the Mie-Grüneisen  
613 formalism with an auto-coherent set of elastic parameters (Matas et al., 2007).

614 Our calculation shows that the degree of partial melting has a major effect on melting properties  
615 (Figure 10). It affects (i) the Bg-content (and thus  $X(\text{SiO}_2)$ ) in the melt, which increases moderately  
616 with temperature from PET to the liquidus (Figure 4), (ii) potentially the  $D_{\text{Fe}}^{\text{Bg/melt}}$  value ((Boujibar  
617 et al., 2016); Figure 9) and (iii) Fe-contents in coexisting solid and melt, which vary with F  
618 independently from  $D_{\text{Fe}}^{\text{Bg/melt}}$ . In the context of mantle partial melting, two end-member situations  
619 arise:

620 A) During the first stages of magma ocean crystallization, F values are expected to be large. They  
621 could range between ~0.6 to 1, which corresponds to temperatures between the PET and the liquidus  
622 (Figure 6). We also note the threshold F value of ~0.4 corresponding to point when the magma ocean  
623 becomes more viscous (Abe, 1997). The situation corresponds to a variable fraction of Bg grains  
624 entrained in a major amount of melt. Close to the liquidus (F~1), Fe# in Bg could vary from ~0.05 to  
625 ~0.01, depending on the controversial values of  $D_{\text{Fe}}^{\text{Bg/Melt}}$  from 0.5 to 0.1, respectively, because the  
626 Fe# in the melt is ~0.1, similar to the bulk mantle. Using the procedure described above, we calculate  
627  $\Delta\rho_{\text{m-s}}$  between coexisting Bg and pyrolitic melt along melting curves and obtain mostly negative  
628 values, meaning a relatively denser Bg grains (Figure 10). The value of  $\Delta\rho_{\text{m-s}}$  increases with pressure,

629 due to a smaller volume of fusion at higher pressures but remains negative at all pressures from 30 to  
 630 135 GPa.  $\Delta\rho_{m-s}$  also increases with decreasing the melt fraction, because the melt Fe# increases faster  
 631 than the solid Fe#. We find no solid-melt density crossover for  $D_{Fe}^{Bg/Melt} = 0.5$ , at least for F values  
 632 higher than 0.4. For  $D_{Fe}^{Bg/Melt} = 0.1$ , Bg can become less dense than the melt for F values below  $\sim 0.7$ .  
 633 B) At the latest stages of magma ocean crystallization, as well as in the context of partial melting  
 634 in the present-day lower mantle, the situation corresponds to a minor amount of melt trapped in the

**Figure 10:** Density contrast for various couples of coexisting melt and Bg, in the context of a crystallizing magma ocean (F higher than 0.4). All values are normalized to the density of a same Bg having an Fe# of 5% (red). Negative values correspond to buoyant melt. We report relative densities of Bg with Fe# of 1% (green), fully molten pyrolite (yellow) and partial melts calculated for F values from 0.9 to 0.4. We perform the calculation for  $D_{Fe}^{Bg/melt}$  values of 0.1 (blue area, corresponding to (Nomura et al., 2011; Tateno et al., 2014)) and 0.5 (brown area, corresponding to



**Figure 11:** Domains of positive or negative melt buoyancy for varying degrees of mantle partial melting and various possible values of the solid-liquid Fe partition coefficient. We report boundaries between “sink” and “float” domains at pressures of 30, 50, 90 and 130 GPa. The pink shaded region corresponds to a density contrast within 0.5%. Horizontal orange shaded regions correspond to ranges of  $D_{Fe}^{Bg/melt}$  reported around 0.1 (T-14 & N-11; (Nomura et al., 2011; Tateno et al., 2014)) and 0.5 (A-12; (Andrault et al., 2012)) at high mantle depths (Figure 8).

635 solid mantle. The solid phase can be Bg or pyrolite, depending on the melting degree, F. Here, we  
 636 report  $\Delta\rho_{m-s}$  values corresponding to a solid phase made of pure Bg, however, results are not very  
 637 different for pyrolite. Due to the lack of constraints, we assume a melt with  $X(SiO_2)$  equal to that of  
 638 the PE-melt, even if the situation could correspond to incipient mantle melting below the PET (low

639 F). Under these assumptions, the major change in melt composition with decreasing F is a higher Fe#.  
640 Calculations show that a denser melt, compared to a bridgmanitic mantle, is favored for (i) lower  
641  $D_{\text{Fe}}^{\text{Bg/Melt}}$ , (ii) lower F and (iii) higher pressures (Figure 11). There is a significant range of parameters,  
642 for values of F below 0.7 and  $D_{\text{Fe}}^{\text{Bg/Melt}}$  below 0.45, where melts could sink in the solid mantle toward  
643 the CMB. We remind here that the possible increase of  $D_{\text{Fe}}^{\text{Bg/Melt}}$  at low F values (Boujibar et al.,  
644 2016) would favor buoyant melts.  
645

## 646 **6. IMPLICATIONS FOR CRYSTALLIZATION OF THE MAGMA OCEAN**

### 647 **6.1. DYNAMICS OF THE MAGMA OCEAN CRYSTALLIZATION**

648 The crystallization of the early magma ocean is the primary mechanism invoked to produce a  
649 chemical stratification of the mantle (Boyet and Carlson, 2005; Caro et al., 2005). Concerning the  
650 mantle depth at which the crystallization began, our model suggests a mantle liquidus increasing  
651 smoothly with pressure up to the CMB pressure of 135 GPa (i.e. the A-chondritic model in **Figure 1**).  
652 Thus, the adiabatic temperature profile of the cooling magma ocean, which also presents a relatively  
653 constant slope, would likely cross the liquidus starting from the CMB upwards (e.g. **Figure 7a** in  
654 (Thomas and Asimow, 2013)). Magma ocean solidification should therefore occur from bottom up.  
655 We note that major changes in the dynamics of the magma ocean should occur at  $F$  values lower than  
656  $\sim 40\%$ , the critical melt fraction when the mantle becomes more viscous (Abe, 1997), rather than when  
657 the adiabatic profile crosses the liquidus (Monteux et al., 2016).

658 It has been proposed that Bg grains could settle in the magma ocean, inducing rejection of melts  
659 toward the Earth's surface (Boukare et al., 2015; Solomatov, 2007). Our calculations confirm a Bg  
660 denser than the coexisting melt at  $F$  values higher than 0.7 (**Figure 11**). Still, the effective gravitational  
661 segregation of Bg grains in a crystallizing magma ocean is not obvious. Highly turbulent flows have  
662 certainly dominated in the molten mantle.  $\Delta\rho_{m-s}$  may not have been sufficiently high to  
663 counterbalance mixing forces, especially in the lowermost mantle where  $\Delta\rho_{m-s}$  decreases. This could  
664 have prevented major chemical segregation until late stages of the magma ocean crystallization. On  
665 the other hand, while an abrupt change in rheological behavior at  $F\sim 40\%$  should disable turbulent  
666 mixing flows, it should also slow down chemical segregation by inhibiting the atomic diffusion. Thus,  
667 the two side-effects of crystallization, turbulent flow followed by high mantle viscosity, are not in  
668 favor of large scale chemical heterogeneities early in the crystallizing Earth's mantle.

669 Following the assumption that Bg grains have efficiently segregated from the crystallizing  
670 magma ocean, the melt composition should drift toward higher Fe#, because Fe enters preferentially  
671 into the melt (e.g. (Boukare et al., 2015)) and also to a slightly higher SiO<sub>2</sub>-content (due to the  
672 composition of the PET melt, **Figure 5**). Increasing the Fe# in melt favors higher  $\Delta\rho_{m-s}$  and sinking  
673 melts. This effect could have contributed to produce an early BMO (Labrosse et al., 2007) and/or  
674 overturns (Elkins-Tanton, 2008). However, our melting model suggests that the Fe-enrichment of the  
675 melt could remain moderate. If we consider the most extreme case of (i) full gravitational segregation  
676 of the crystallizing Bg grains, (ii) a  $D_{Fe}^{Sol/liq}$  value close to 0 and (iii) a bulk fractional crystallization  
677 of 60% (thus  $F=0.4$ ), we find that the melt would reach Fe# of  $\sim 0.25$  (for a bulk pyrolitic mantle with  
678 Fe# of  $\sim 0.1$ ). For more reasonable sets of parameters, a high degree of Fe-enrichment can only occur  
679 at the very final stages of the magma ocean crystallization.

### 680 **6.2. CHEMICAL SIMILARITIES BETWEEN THE PSEUDO EUTECTIC-MELT AND PERIDOTITE**

681 Major consequences arise from the very high  $F$  values found at the PET (**Figure 6**). Brutal  
682 solidification of the magma ocean could occur when the degree of partial melting becomes lower than  
683 83% (for peridotite), 74% (for pyrolite) or 56% (for chondritic mantle) at a given mantle depth. Such  
684  $F$  values are significantly higher than the threshold value of 40% necessary to produce a relatively  
685 viscous mantle (Abe, 1997). Therefore, final mantle crystallization could be achieved at the same time  
686 as the mantle became viscous. It would disable chemical segregation by melt gravitation in a mushy  
687 mantle and favor instead a homogeneous mantle after bulk magma ocean crystallization. Mantle

688 overturn would also be unlikely, because the magma ocean would crystallize before a too significant  
689 Fe-enrichment of the melt.

690 Our model shows that the peridotite composition is close to the PE-melt at high pressure (Figures  
691 3 to 6). This compositional similarity was already discussed a long time ago (e.g. (Zhang and  
692 Herzberg, 1994)). This situation could result from a large scale chemical differentiation during magma  
693 ocean crystallization, where the upper part of the mantle would correspond to the last melt that  
694 solidified, and the residual solid, Bg, would be concentrated in the deep mantle. A floating layer of  
695 peridotitic melt of several hundred kilometers thickness (possibly even more than 1000 km) would  
696 have crystallized as a bulk, in agreement with our high F values at the PET. A highly bridgmanitic  
697 deep lower mantle would agree with previous studies (Matas et al., 2007; Murakami et al., 2012;  
698 Samuel et al., 2005).

699 Today, presence of volatile elements could induce incipient partial melting in the deep mantle.  
700 The melt could be denser than the mantle and sink, in the case the value of  $D_{\text{Fe}}^{\text{Bg/melt}}$  would indeed be  
701 as low as 0.4, as suggested by some previous studies (Nomura et al., 2011; Tateno et al., 2014).  
702 Sinking melts could produce the ULVZ in the lowermost mantle, independently from the temperature  
703 prevailing in the lowermost mantle early in Earth's history. This scenario contrasts with another one  
704 suggesting that the ULVZ are the relic of an ancient BMO (Labrosse et al., 2007).

### 705 **6.3. MAXIMUM CORE TEMPERATURE AFTER MAGMA OCEAN CRYSTALLIZATION**

706 After the Moon forming giant impact, the Earth has been largely molten. Subsequent cooling of  
707 the magma ocean could have been relatively fast, within 100 ky (Abe, 1997; Monteux et al., 2016;  
708 Solomatov, 2007). It was proposed that a BMO could have persisted in the lowermost mantle for a  
709 much longer time, due to a large amount of heat stored in the core (Labrosse et al., 2007). Still, the  
710 early temperature of the CMB (a good proxy for the core temperature), as well as the lifetime of the  
711 BMO remain highly debated. To keep a hot BMO thermally stable, there must be a layer of solid  
712 material just above it producing an efficient thermal blanketing between the molten BMO in contact  
713 with the hot core and the solid mantle. This solid shell would hamper escape of the core heat. This  
714 solid material could only be Bg, the liquidus phase in the deep mantle. Consequently, the Bg melting  
715 point of ~5400 K at a pressure of 135 GPa (Figure 1) corresponds formally to the highest possible  
716 CMB temperature after crystallization of the magma ocean. It is ~1300 K above the current CMB  
717 temperature.

718 However, a temperature of ~5400 K represents an improbable upper limit for the early CMB  
719 temperature. Indeed, the physical contact between the BMO and the overlaying Bg layer can react  
720 chemically. The further away from Bg is the chemical composition of the BMO, the lower should be  
721 the equilibrium temperature, in agreement with binary phase diagrams (Figure 4). And the more likely  
722 the CMB temperature after magma ocean crystallization could correspond to the first occurrence of  
723 a more viscous mantle at the CMB (Monteux et al., 2016). This temperature is estimated to ~4400 K,  
724 only ~300 K higher than the CMB temperature today (Andraut et al., 2016).

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