Assignment 03 ESS5031

12232660 Shuhao SONG

December 2022

1 Phase diagrams for Olivine to Wadsleyite phase transition and the 410 km boundary

1.1 Single component

The phase diagram of T-P plane for the Mg_2SiO_4 Olivine to Mg_2SiO_4 Wadsleyite is:

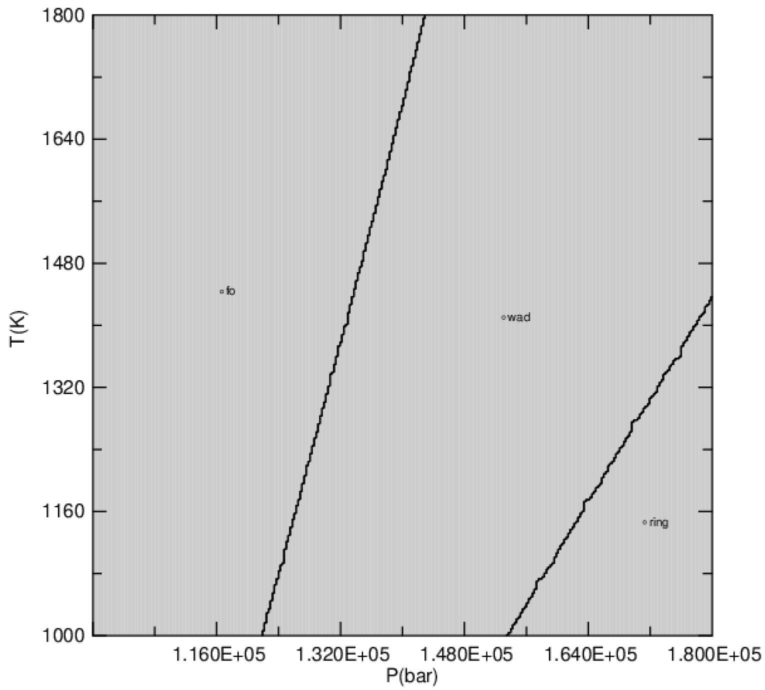

Figure 1: phase diagram of Mg_2SiO_4 Olivine to Mg_2SiO_4 Wadsleyite

At equilibrium state, we have

$$\Delta G(P,T) = \Delta H(P_0, 298K) - T\Delta S(P_0, 298K) + P\Delta V(P_0, 298K) = 0 \tag{1}$$

The Clapeyron slope correspoding to Mg_2SiO_4 Olivine to Mg_2SiO_4 Wadsleyite is calculated as:

$$k = (\frac{dP}{dT})_{eq} = \frac{\Delta S}{\Delta V} = \frac{-9.0\ J/mol \cdot K}{-3.16\ cm^3/mol} = 2.848\ J/K \cdot cm^3 \tag{2}$$

1.2 Solide solution

1.2.1 By PerpleX

The phase diagram of X-P for a solid-solution $(Mg, Fe)_2SiO_4$ at 1800K by Perple_X is shown in Figure 2 and Figure 3:

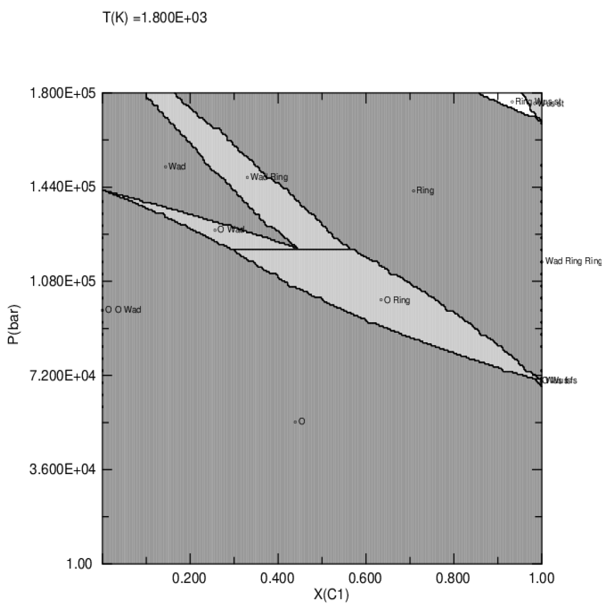

Figure 2: phase diagram of Olivine to Wadsleyite with mole fraction of Fe_2SiO_4 ,$X \in [0, 1]$

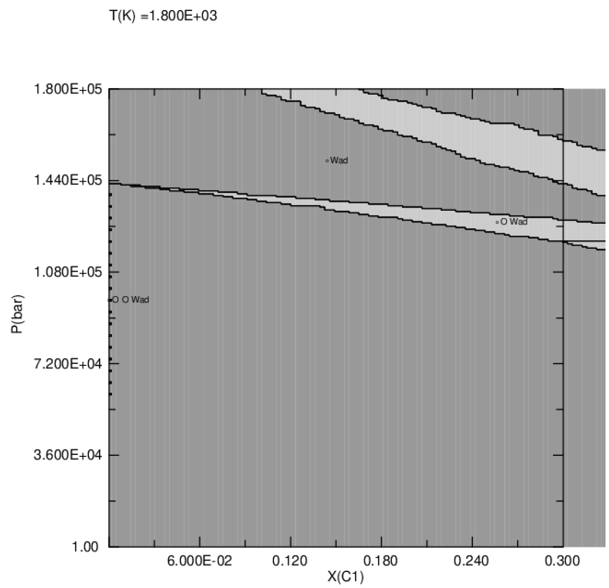

Figure 3: phase diagram of Olivine to Wadsleyite with mole fraction of Fe_2SiO_4 ,$X \in [0, 3]$

where, the x axis stands for the mole fraction of the Fe_2SiO_4 component in the system; the y axis stands for the pressure.

1.2.2 By equation

When given mole fraction X_{Fe} of Fe_2SiO_4, the transition boundaries of total Olivine and total Wadsleytie can be expressed as:

$$\begin{cases} x_{Fe}^{Oli} = \dfrac{1-\lambda_{Mg}}{\lambda_{Fe}-\lambda_{Mg}} \\ x_{Fe}^{Wad} = \dfrac{\lambda_{Fe}\cdot(1-\lambda_{Mg})}{\lambda_{Fe}-\lambda_{Mg}} \end{cases} \tag{3}$$

$$\begin{cases} \lambda_{Fe} = e^{\frac{-\Delta G_m^{Fe}}{RT}} \\ \lambda_{Mg} = e^{\frac{-\Delta G_m^{Mg}}{RT}} \end{cases} \tag{4}$$

$$\begin{cases} \Delta G_{Mg}(P,T) = \Delta H_{Mg}(P_0, 298K) - T\Delta S_{Mg}(P_0, 298K) + P\Delta V_{Mg}(P_0, 298K) \\ \Delta G_{Fe}(P,T) = \Delta H_{Fe}(P_0, 298K) - T\Delta S_{Fe}(P_0, 298K) + P\Delta V_{Fe}(P_0, 298K) \end{cases} \tag{5}$$

So, the phase diagram is:

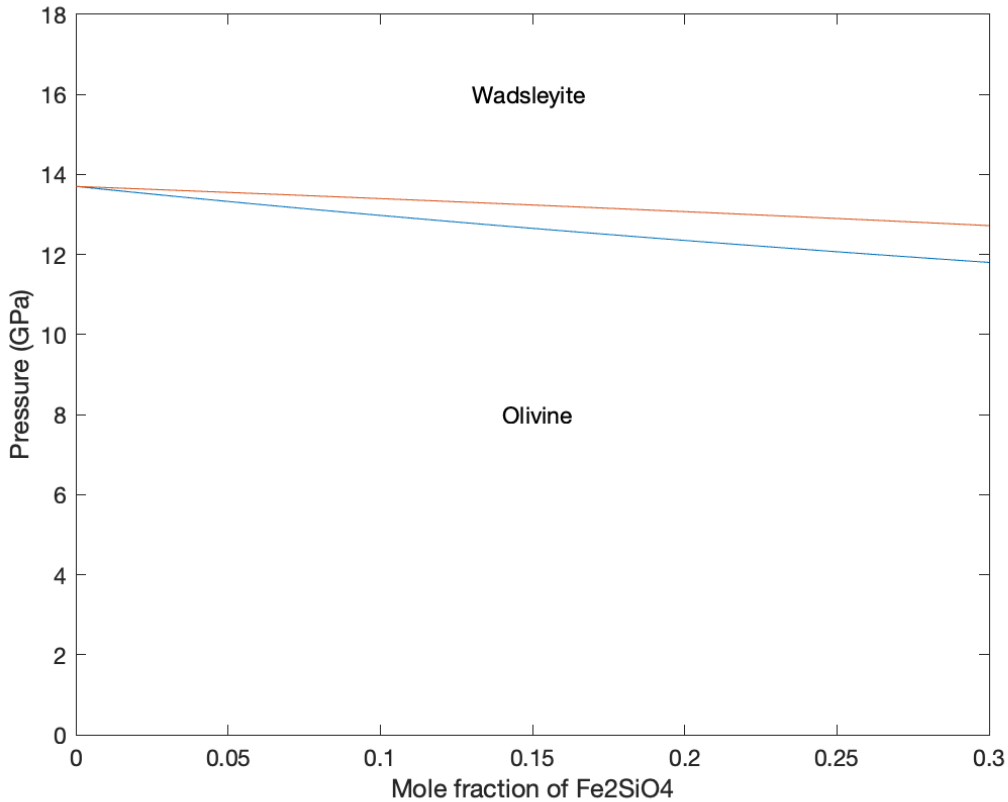

Figure 4: phase diagram of Olivine to Wadsleyite with mole fraction of Fe_2SiO_4 ,$X \in [0, 0.3]$

1.3 Width of transition zone

For T=1800K, X = 0.1, the density variation with pressure is:

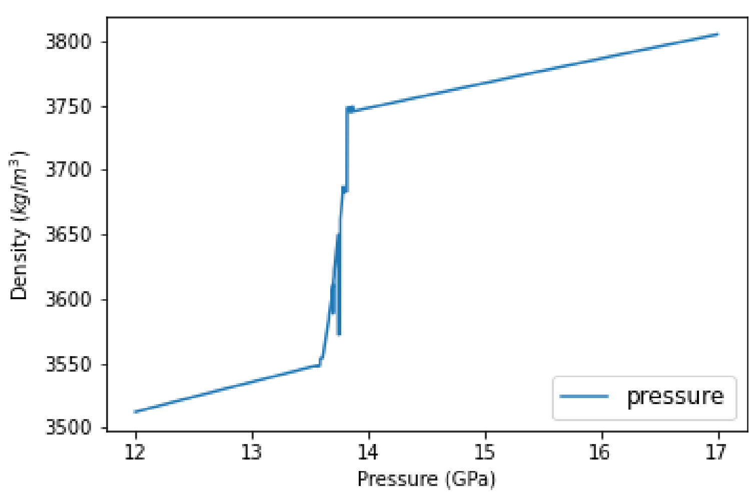

Figure 5: Density variation with pressure between (12,17) GPa

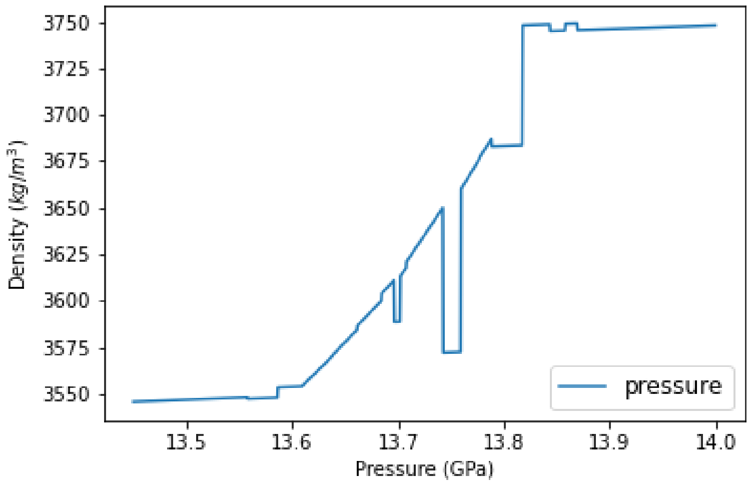

Figure 6: Density variation with pressure between (13.5,14) GPa

From Figure 5 and Figure 6, the phase transition should occur at pressure from 13.59 to 13.82 GPa in this background. And the mean density at this range is around $\bar{\rho} = 3650\ kg/m^3$.

Based on the gravity acceleration g in the mantle, the pressure gradient is:

$$\frac{dP}{dr} = \bar{\rho} \cdot g = 36500\ Pa/m \tag{6}$$

The width of the Olivine to Wadsleyite transition is:

$$h = \frac{P_{end} - P_{start}}{\frac{dP}{dr}} = \frac{(13.82 - 13.59)GPa}{36500\ Pa/m} = 6301\ m \tag{7}$$

2 Oxygen fugacity of the early Earth

The mass fraction of mantle and core is:

Mantle composition	wt.%	Core composition	wt.%
SiO_2	45.5	Fe	86.0
MgO	38.3	Ni	5.5
FeO	8.2	Si	6.8
Al_2O_3	4.5	O	17
CaO	3.5		

Table 1: Mass composition ω of core and mantle

The mole fraction in core and mantle given each components mass fraction ω can be calculated as:

$$x_{FeO} = \frac{\frac{\omega_{FeO}}{M_{FeO}}}{\frac{\omega_{SiO_2}}{M_{SiO_2}} + \frac{\omega_{MgO}}{M_{MgO}} + \frac{\omega_{FeO}}{M_{FeO}} + \frac{\omega_{Al_2O_3}}{M_{Al_2O_3}} + \frac{\omega_{CaO}}{M_{CaO}}} = 5.88\% \tag{8}$$

$$x_{Fe} = \frac{\frac{\omega_{Fe}}{M_{Fe}}}{\frac{\omega_{Fe}}{M_{Fe}} + \frac{\omega_{Ni}}{M_{Ni}} + \frac{\omega_{Si}}{M_{Si}} + \frac{\omega_{O}}{M_{O}}} = 77.64\% \tag{9}$$

The chemical reaction of Iron to Wustite is:

$$Fe + \frac{1}{2}O_2 \rightleftharpoons FeO \tag{10}$$

The oxygen fugacity of IW buffer can be calculated as:

$$K_{eq} = \frac{1}{1 \cdot (\frac{f_{O_2}^{IW}}{P_0})^{\frac{1}{2}}} = \left(\frac{P_0}{f_{O_2}^{IW}}\right)^{\frac{1}{2}} \tag{11}$$

Assume the core and the magma ocean had achieved chemical equilibrium and while the silica melt and Fe melt in the early magma ocean had similar compositions as the present mantle and core, respectively. The equilibrium of the early earth using ideal solution model can be expressed as:

$$K_{eq} = \frac{a_{FeO}}{a_{Fe} \cdot a_{O_2}} = \frac{x_{FeO}}{x_{Fe} \cdot (\frac{f_{O_2}}{P_0})^{\frac{1}{2}}} = \frac{x_{FeO}}{x_{Fe}} \cdot \left(\frac{P_0}{f_{O_2}}\right)^{\frac{1}{2}} \tag{12}$$

So,using (8) and (9), the oxygen fugacity of the early earth related to the IW oxygen buffer is:

$$\left(\frac{f_{O_2}}{f_{O_2}^{IW}}\right)^{\frac{1}{2}} = \frac{x_{FeO}}{x_{Fe}} \tag{13}$$

$$log_{10}^{f_{O_2}} = log_{10}^{f_{O_2}^{IW}} + 2 \cdot log_{10}^{\frac{x_{FeO}}{x_{Fe}}} = log_{10}^{f_{O_2}^{IW}} - 2.241 \tag{14}$$