ESS 5031 Physics of Earth and Planetary Interiors
Fall 2022

Homework Problem Set 3
(Due on 12/14/2022 in class)

1. Phase diagrams for olivine to wadsleyite phase transition and the 410 km boundary

The table below shows the thermodynamic data for Mg_2SiO_4 and Fe_2SiO_4 during the olivine to wadsleyite phase transformation at 298 K and 1 atm.

(1) Draw the phase boundary for the Mg_2SiO_4 olivine to Mg_2SiO_4 wadsleyite phase transition on the T-P plane (T=1000-1800 K, P=10-18 GPa) and calculate the Clapeyron slope.

(2) Consider a solid-solution $(Mg,Fe)_2SiO_4$. Assuming that the Mg_2SiO_4 and Fe_2SiO_4 components mix ideally (ideal solution), draw a phase diagram on the X-P plane (X is the mole fraction of the Fe_2SiO_4 component in the system) for T = 1800 K, P in the range of 0-18 GPa, and $0.0 \leq X \leq 0.3$.

(3) Calculate the width (the depth interval) of the olivine to wadsleyite transition (that is the thickness of the 410 km boundary) at T=1800 K and X=0.1, assuming the gravity acceleration is 10 m/s^2 in the mantle.

(Hint: You do not need to consider the effect of temperature on ΔH, ΔS, and ΔV, only the pressure effect. That is,

$$\Delta G°(P,T) = \Delta H°(P_0, 298K) - T\Delta S°(P_0, 298K) + P\Delta V°(P_0, 298K).$$

You will need a plotting software package/programming language to make the diagrams.)

Olivine to wadsleyite phase transformation	$\Delta H°$ (kJ/mol)	$\Delta S°$ (J/mol·K)	$\Delta V°$ (cm^3/mol)
Mg_2SiO_4	27.1	-9.0	-3.16
Fe_2SiO_4	9.6	-10.9	-3.20

2. Oxygen fugacity of the early Earth

It is widely believed that the Earth's core formed during the early accretion stage, when Earth experienced a range of impact events, including possibly a Moon-forming giant impact. These impacts converted a large amount of gravitational energy to kinetic energy, and eventually to heat that would warm up the early Earth to a temperature higher than the melting temperatures of silicate rocks and the iron metal, resulting in a deep magma ocean. The molten Fe and silicate magma were immiscible (do not mix chemically) in the magma ocean and thus were separated under gravity due to their density difference. The Fe droplets sank to the center of Earth, along with Ni and other siderophile elements, to form the core, while lithophile elements such as Mg, Si, Ca, Al, and some Fe remained oxidized in silicate minerals and formed the proto-mantle before mantle convection and plate tectonics started to operate. Due to the very high temperature of the core-formation process, and the highly mobile nature of the Fe and silicate liquids, it is often thought that the core and the magma ocean had achieved chemical equilibrium before the magma ocean solidified to the solid mantle. Once the mantle solidified, the mantle and core would evolve independently, without achieving a global chemical equilibrium again. Given these assumptions, we can estimate the oxygen fugacity of Earth during core formation by examining the bulk compositions of the core and mantle after the core formation process.

The table below shows the likely compositions for the present mantle and core. (Note there are other compositions models, but they should not affect our results significantly.) Assuming the silicate melt and Fe melt in the early magma ocean had similar compositions as the present mantle and core, respectively, and considering the chemical reaction as

$$\text{Fe (in core)} + 1/2\ O_2 = \text{FeO (in mantle)},$$

calculate the oxygen fugacity (fO_2) of the early Earth, relative to the IW (iron-wüstite) oxygen buffer $f_{O_2}^{IW}$. Use the ideal solution model for calculating activities of Fe in metal and FeO in the mantle. (**Hint**: When fO_2 of the IW buffer is used as a reference fO_2, then you will not need to calculate ΔG^0 from thermodynamic properties, but can express ΔG^0 in terms of $f_{O_2}^{IW}$.)

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	1.7
CaO	3.5		