ESS 5031 Physics of Earth and Planetary Interiors Fall 2022

Homework Problem Set 2 (Due on 11/16/2022 in class)

1. Thermodynamics relations

- a) The isothermal and adiabatic bulk moduli are defined as $K_T = -V \left(\frac{\partial P}{\partial V}\right)_T$ and $K_S = -V \left(\frac{\partial P}{\partial V}\right)_S$, respectively. Show that $K_S = K_T (1 + \alpha \gamma T)$, where $\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P$ is the coefficient of thermal expansion and $\gamma = \frac{\alpha K_T V}{C_V}$ is Grüneisen parameter, and $C_V = T \left(\frac{\partial S}{\partial T}\right)_V$ is the heat capacity at constant volume.
- b) The pressure derivative of bulk modulus and the Anderson-Grüneisen parameter are defined as $K_T' = \left(\frac{\partial K_T}{\partial P}\right)_T$ and $\delta_T = \left(\frac{\partial \ln \alpha}{\partial \ln V}\right)_T$. Show that both K_T' and δ_T are related to the volume derivative of K_T as $K_T' = -\left(\frac{\partial \ln K_T}{\partial \ln V}\right)_T$ and $\delta_T = -\left(\frac{\partial \ln K_T}{\partial \ln V}\right)_P$. (Note: $\left(\frac{\partial \ln X}{\partial \ln Y}\right)_Z = \frac{Y}{X}\left(\frac{\partial X}{\partial Y}\right)_Z$).

2. Adiabatic temperature gradient of Earth's mantle

The Earth's mantle is convecting vigorously over the geological time scale. A consequence of that is the temperature of the majority of the mantle follows the adiabatic temperature gradient except for the top and bottom boundary layers. That is, the temperature of the mantle increases due to self-compression under adiabatic conditions (entropy is constant assuming the process is reversible).

- a) Show that the temperature gradient in the mantle is given by $\frac{dT}{dz} = \frac{g\alpha T}{c_P}$, where z is depth, g is gravity, α is thermal expansion coefficient, and c_P is specific hear at constant pressure. Note that c_P has a dimension of J kg⁻¹K⁻¹, whereas $C_P = T\left(\frac{\partial S}{\partial T}\right)_P$ has a dimension of J mol⁻¹K⁻¹, assuming S is the molar entropy. Therefore they are related by $C_P = \rho V c_P$. (Hint: You will utilize the hydrostatic equilibrium equation $\frac{dP}{dz} = \rho g$, where P is pressure and ρ is density.)
- b) Calculate $\frac{dT}{dz}$ in the Earth's mantle given $g=10\text{m/s}^2$ (assuming g is constant in the mantle), $\alpha=3\times10^{-5}\text{K}^{-1}$, $c_P=1\text{kJ kg}^{-1}\text{K}^{-1}$, and T=1600K.

3. Composition of the Earth's mantle

Density of the Earth's interior from seismological observations is often compared with densities of candidate Earth materials from laboratory measurements to infer the composition of Earth. In this homework, you will use the physical properties of typical mantle minerals given in the attached Table to calculate the density of olivine

((Mg_{0.9}Fe_{0.1})₂SiO₄) and wadsleyite (or β-phase, (Mg_{0.9}Fe_{0.1})₂SiO₄) at 355 km, 400 km, 450 km depths and compare these densities with the seismological model, the PREM (also attached). (1) Discuss which is the likely mantle mineral phase of (Mg,Fe)₂SiO₄ at depth of 355 km and 450 km, respectively. (2) Calculated the density contrast at the upper mantle and transition zone boundary (400 km depth) if the mantle is composed of (Mg_{0.9}Fe_{0.1})₂SiO₄.

To perform these calculations, you need to know the pressure (P) and temperature (T) at these depths. The values of pressure can be found in the PREM model. Assuming the temperature distribution in the mantle is adiabatic and assuming that the temperature at 660 km is 1900 K, estimate the temperatures at 355 km, 400 km, and 450 km using an adiabatic temperature gradient of 0.45 K/km.

The density can be calculated using the 3^{rd} order Birch-Murnaghan equation of state (EoS), which is given as

$$P = \frac{3}{2} K_{T0} \left[\left(\frac{V_0}{V} \right)^{7/3} - \left(\frac{V_0}{V} \right)^{5/3} \right] \left\{ 1 + \frac{3}{4} \left(K_T' - 4 \right) \left[\left(\frac{V_0}{V} \right)^{2/3} - 1 \right] \right\}$$
 (1)

where V is molar volume, V_0 , K_{T0} , and K'_T are the molar volume, isothermal bulk modulus, and the pressure derivative of bulk modulus at ambient pressure. V_0 , K_{T0} , and K'_T at $T_0 = 298$ K are given in the attached Table. To calculate the density at high pressure and high temperature conditions, you can first calculate V_0 and K_{T0} at high T (assuming K'_T is independent of T) and ambient P from

$$V_0(T) = V_0(T_0) \exp\left(\int_{T_0}^T \alpha(T') dT'\right)$$
 (2)

and

$$K_{T0}(T) = K_{T0}(T_0) + \left(\frac{\partial K_T}{\partial T}\right)_{P} (T - T_0), \quad (3)$$

and then use the Birch-Murnaghan EoS to calculate the density at the desired P-T conditions. All required parameters are given in the attached Table. Be careful that the thermal expansion coefficient (α) is temperature dependent, so you should integrate equation (2) to get V₀ at T. Also pay attention to the units in the Table, especially those for thermal expansion coefficients (thermal expansion coefficients for mantle minerals should be on the order of 10⁻⁵ K⁻¹). To calculate the density from Birch-Murnaghan EoS, you need to solve a nonlinear equation. This can be accomplished by a nonlinear solver in *Excel*, *Matlab* or *Python*. To calculate densities for mineral compositions with an Fe₂SiO₄ mole fraction of Fe/(Fe+Mg)=0.1, you need first to calculate the densities for the Mg₂SiO₄ and Fe₂SiO₄ end members and then use the following ideal mixing model,

$$\rho = \frac{M}{V} = \frac{X_{Mg} M_{Mg} + X_{Fe} M_{Fe}}{X_{Mo} V_{Mo} + X_{Fe} V_{Fe}}$$

where X and M are the mole fraction and atomic weight for the Mg (Mg₂SiO₄) and Fe (Fe₂SiO₄) end members, respectively.

Table 3
Parameters used for density profile calculations

Phases	V^0_{298}	$\alpha(T) = \alpha_0$	$+\alpha_1T+\alpha_2T^{-2}$		K_0	$K_{\mathrm{T}}{}'$	$(\partial K_{\mathrm{T}}/\partial T)_{\mathrm{P}}$
	(cm ³ /mol)	α_0 (10 ⁴)	$\alpha_1 (10^8)$	α_2	(GPa)		(GPa/K)
Olivine							
Mg2SiO4	43.60	0.3034	0.7422	-0.5381	129.0	5.37	-0.0224
Fe ₂ SiO ₄	46.29	0.2386	1.1530	-0.0518	137.9	4.00	-0.0258
β-Phase							
Mg ₂ SiO ₄	40.52	0.2893	0.5772	-0.8903	174.0	4.00	-0.0323
Fe ₂ SiO ₄	43.15	0.2319	0.7117	-0.2430	166.0	4.00	-0.0215
Spinel							
Mg ₂ SiO ₄	39.49	0.2497	0.3639	-0.6531	183.0	4.30	-0.0348
Fe ₂ SiO ₄	42.03	0.2697	0.0000	-0.0000	197.0	4.00	-0.0375
Pyroxene							
Mg ₂ Si ₂ O ₆ (ortho-)	62.67	0.2947	0.2694	-0.5588	107.0	4.20	-0.0200
Fe ₂ Si ₂ O ₆ (ortho-)	65.94	0.3930	0.0000	-0.0000	101.0	4.20	-0.0200
Mg ₂ Si ₂ O ₆ (clino-)	62.99	0.2947	0.2694	-0.5588	107.0	4.20	0.0200
Fe ₂ Si ₂ O ₆ (clino-)	65.89	0.3930	0.0000	0.0000	101.0	4.20	-0.0200
CaMgSi ₂ O ₆ (clino-)	66.04	0.3330	0.0000	-0.0000	113.0	4.80	-0.0200
CaFeSi ₂ O ₆ (clino-)	67.87	0.2980	0.0000	-0.0000	119.0	4.00	-0.0200
Garnet-majorite							
$Mg_3Al_2Si_3O_{12}$	113.08	0.2311	0.5956	-0.4538	179.0	4.00	-0.0220
Fe ₃ Al ₂ Si ₃ O ₁₂	115.43	0.1776	1.2140	-0.5071	175.0	4.00	-0.0220
Ca ₃ Al ₂ Si ₃ O ₁₂	125.12	0.1951	0.8089	-0.4972	168.0	6.20	-0.0220
$Mg_4Si_4O_{12}$	114.32	0.2311	0.5956	-0.4538	161.0	4.00	-0.0220
Perovskite							
MgSiO ₃	24.45	0.3156	0.9421	-0.3271	262.0	4.00	-0.0550
FeSiO ₃	25.60	0.3156	0.9421	-0.3271	287.2	4.00	-0.0596
CaSiO ₃	27.32	0.3156	0.9421	-0.3271	281.0	4.00	-0.0220
Magnesiowüstite							
MgO	11.25	0.3768	0.7404	-0.7446	160.3	4.13	-0.0272
FeO	12.25	0.3203	0.6293	0.0000	146.0	4.00	-0.0200
Iron-iron sulfide							
Fe (fcc)	7.09	0.7700	0.0000	-0.0000	170.0	4.00	-0.0200
FeS(IV) at 800 K	17.79	0.6852	0.0000	-0.0000	54.0	4.00	-0.0200

Data sources: Smyth and McCormick [33]; Fei et al. [34], Mao et al. [35], Boehler et al. [36], Fei et al. [37], Fei [38], and Knittle [39].

of γ -spinel at 13.5 GPa, is γ -spinel plus majorite. The lower mantle assemblage is Mg–Fe silicate perovskite, magnesiowüstite, and majorite. The mineral compositions and modal abundances of the MB high-pressure assemblages are given in Ref. [11]. These assemblages are used to calculate the density of the MB model mantle as a function of pressure and temperature with a Birch–Murnaghan equation of state. A detailed description of the calculations is given in Fei et al. [13]. The database for the end-member phases used in these calculations is given in Table 3.

The calculated mantle density profile is shown in Fig. 1.

The mantle density profile shown in Fig. 1 assumes a crustal density of 3.0 g/cm^3 and a crust thickness of 50 km. Uncertainties in Martian crust density and thickness are discussed below. The density increase marking the beginning of the transition zone at 13.5 GPa is shown in Fig. 1, as is an increase in density at 17 GPa that is produced by the complete replacement of clinopyroxene by majorite and β -phase by γ -spinel. The density increase at 22.5

TABLE II Earth model PREM and its functionals evaluated at a reference period of 1 s. Above 220 km the mantle is transversely isotropic; the parameters given are "equivalent" isotropic moduli and velocities. See Table IV for complete elastic constants in this region.

otropie	ic moduli	isotropic moduli and velocities. See	E	able IV for complete clastic constants in this region	plete elasti	CODIN	stants in	this reg	ion.			•		1			
LEVEL	RACIUS KM	DEP TH KM	DENSITY 6/CCM	VP KM/S	VS KM/S	₽	ğ	OAL	PHI KM2/S2	KAPPA KBAR	KBAR	SIGNA	PRESSURE KBAR	0K / 0P	F. P.	GRAVITY CM/S2	
	•	6371.0	13.0884	11.26220	3.66780	85	1328	431	108	14253	1761	0.4407	3638.524	2.3360	0.99	•	
~	00	6271.0	13.08	7	.6667	85	1328	431	-	14248	1759	0.4407	3636.131	2.3363	0.0	36.56	
n 4	200.0	6171.0	13.0588	11 -25593	3.65342	ב ני	1328	437	108.	14203	1749	0.44.0	3617.011	2.3369	0.99	. 9	
- 10	3 8	5971.0	13.0536	• •	. 4	. 6	1328	432	108	14164	1739		3600.315	.337	0.99	. •	
9	38	5871.0	13.0340	11.22301	.640	85	1328	433		14114	1727	*	578.	338	0.99	2.3	
~	9	5771.0	13.0100	11.20576	3.62835	80	1328	434	108	14053	1713	0.4414	552.78	.33	0.99	18.6	
æ	8	5671.0	12.9817	11-18538	•614	œ	1328	436	107	13981	1696	ŧ	22.02	340	0.99	·.	
Б.	800.0	5571.0	12.9491	11.16186	3.59767	∞ •	1328	437	107	13898	1676	0.4420	9 1	341	66.0	9.	
0 T	1000.0	5371.0	12.9121	11-13521	3.55823	ສຸດ	1328	4 6 9		2 6	1630	•	2 2	2.3443	0.99	362-03	
12	100	5271.0	12,8250	11.07249	מיי	8 2	1328	4	105	13586	1603		3353.596	2.3460	1.00	397.39	
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14	221	5149.5	12.7636	O.	r.	85	-	445	•	13434	1567		÷	8	1.00	440.02	
12	221	5149.5	12.1663	10.35568	•	0	-	57822	_	13047	.	0.5000	3288.502	\$ 1	1.03	0.0	
9:	300	5071.0	12-1250	10.30971	•	- •	57822	57822		9 7	0 9	•	3243.423	3.6559	1.02	465.68	
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9 6	909	4771.0		10.12291	•	•	57822	57822	102.47	12242		0.5000	3061.461	: *	1.00	•	
2	700	4671.0	11.8799	10.05572		0	57822	57822	101.12	12013	•		2993.457	3.3552	1.00	5.1	
=	800	4571.0	11.8090	9.98554		0	_	57822	99.71	11775	0	ĸ.	2922.221	3,3230	1.00	9	
	1900.0	4471.0	11.7340	9.91206	•	0	∞	57822	98.25	11529	0	• 500		30	1.00	•	
	2000-0	4371.0	11.6547	9.83496	•	-	∞ '	57822	96.73	11273	0			3.2927	1.00	677.15	
	0.0002	42/1.0	11.55/11	24.0343	•	-	57876	57975	1000	11009	-		2690.033	3.2911	3 6	710 07	
	2300.0	4071.0	11.3904	9.57881	•		57822	57822	91.75	10451	• •	500	2520.942	80	1.00	Ñ	
	2400.0	3971.0	11.2929	9.48409	•	•	. ~	57822	89.95	10158	0	.500	2432.484	3.3242	1.00	N	
	2500.0	3871.0	11.1906	9.38418	•	0	57822	57822	98.06	9855	•	ີ	2341.603	344	1.00	*	
	2600.0	3771.0	11.0833	9.27876		0	57822	57822	86.10	9542	0	500	2248.453	67	1.00	850.23	
	2800.0	3571.0	100	9-16/32	•		57822	57822	84.04	9220	-	000	2155.189	3.4180	1.00	914.140	
	2900.0	3471.0	10.7301	8-92632		, 0	57822	57822	79.68	8550	• •		. 5	3.4448	1.00	~	
	3000.0	3371.0	10.6015	8.79573		0	57822	57822	77.36	8202	0	•	856.40	3.4714	1.00	5.7	
	3100.0	3271.0	10.4672	8 • 65805	•	0	∞ .	57822	74.96	7846	0	0.5000	1754.418	3.4972	1.00	ຜູ່	
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	3400.0	2971.0	10-0294	8.19939	• •	-	57822	7822	67.03	6743	-	0.5000	44	3,5629	0.99	1050.65	
36	8	2891.0	9.9034	8.06482		•	57822	7822	5.0	644	•		357.51	3.5769	0.98	3	
39	8	2891.0	5.5664	13.71660	7.26466	312	57822	826	117.78		2938	5	2	•	0.99	8.2	
•	200	2871.0	5.5564	_	• 56	312	57822	826	117.64	653	2933	7		•	1.00	65.	
-	909	2771.0	5.5064	•	•	312	57822	823	116.96	644	2907	'n.	2:	642	1.01	~	
7 -	20000	2741.0	5.4914	•	7.26597	5	57822	822	•	7	2899	თ •		1.6420	10.1	1048-44	
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PRESSURE KBAR	1010.363	905-646	854.332	803.660	753.598	704.119	655.202	606.830	558.991	511.676	464.882	418.606	372.852	327.623	282.928	282.927	260.783	238.342	238.334	224.364	210.426	210-425	190.703	171.311	152.251	133.527	133.520	117.702	102.027	86.497	71-115	71.108	07.466	36.183	24.546	24.539	17.891	11.239	6.043	6.040	3.370	3.364	0.303	0.299	000-0-
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PHI KM2/S2	106.04	101.73	99.59	97.43	95.26	93.06	90.81	88.52	86.17	83.76	81.28	78.72	76.08	73.34	70.52	70.52	69.51	68.47	64.03	63.32	62.61	62.61	59.60	56.65	53.78	50.99	48.97	47.83	46.71	45.60	44.50	37.80	100	38.41	38.60	38.60	38.71	38.81	38.89	25.96	25.96	19.99	19.99	2.10	2.10
OAL	803	795	792	788	784	119	175	170	166	761	755	150	743	137	730	730	144	159	362	362	362	362	363	364	365	366	372	370	367	365	362	195	2 2 2	195	195	1447	1447	1446	1446	1350	1350	•	1456	57822	57822
š	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57822	57875	57833	57822	57822	57822	57822		87	B)	57822	57822	57822	57822	57822
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VS KM/S	7.05525	5653	.91	.8728	6.82512	6.77606	9	9	6.6189	ġ	9	ō	6.37		. 5	6.24046	6.09418	5.94508	5.57020	5.54311	5.51602	5.51600	5.37014	5.22428	5.07842	4.93259	4.76989	4.73840	4.70690	4.67540	4.64391	4.41885	4.43100	4-45643	4.46953	9	•	4848	•	.98	•90	ē	-20	•	:
VP KM/S	13,13055	12.90045	12.78389	12-66550	12.54466	12.42075	12.29316	12.16126	12.02445	11.88209	11.73357	11.57828	11.41560	11.24490	•	11.06556	10.91005	10.75131	10.26622	10.21203	10.15782	10.15782	9.90185	9.64588	9.38990	9.13397	8.90522	8.81867	8.73209	8 - 64552	8.55896	0.489.7	001100	8 - 8 - 8 - 8 - 8 - 8 - 8 - 8 - 8 - 8 -	8.07688	8.07689	8.08907	8.10119	8.11061	. 8000	6-80000	5.80000	-800	1.45000	1.45000
DENSITY G/CCM	5.25729	5-15669	5.10590	5.05469	5.00299	4.95073	4.89783	4.84422	4.78983	4.73460	4.67844	•6212	4.56307	-5037	19491	.4431	4.41241	.3807	3.99214	3.98399	3.97584	3.97584	3.91282	3.84980	_	.7237	.5432	3.51639	4895	.4626	4357	3.55950	36.75	3.37091	3747	.3747	.3768	ã	3.38076	.99	ç	•	2.60000	9	1.02000
DEPTH KM	2271.0		971.	•	1771.0	1671.0	1571.0	1471.0	1371.0	1271.0	1171.0	1071.0	971.0	871.0	771.0	771.0	721.0	670.0	670.0	635.0	0.009	600.0	550.0	500.0	450.0	400.0	400.0	355.0	310.0	265.0	220.0	220-0		115.0	80.0	80.0	60.0	40.0	24.4	24.4	15.0	15.0	3.0	0°0	ċ
RACIUS	4100.0	300.	4400.0	9	4600.0	4700.0	4800.0	4900.0	5000.0	5100.0	5200.0	5300.0	5400.0	5500.0	2600.0	2600.0	5650.0	5701.0	5701.0	5736.0	5771.0	5771.0	5821.0	5871.0	5921.0	5971.0	5971.0	6016.0	6061.0	6106.0	6151.0	0.1014	6.0010	6256.0	6291.0	6291.0	6311.0	6331.0	6346.6	6346.6	6356.0	6356.0	6368.0	•	6371.0
LEVEL	8 9	20	51	25	5	*	35	26	2	200	59	9	5	9	9	•	9	99	67	9	69	7	7	72	73	٤	2	16	7	28	6 3	D .		9 90	8	80	98	87	88	6	96	91	92	93	ž