Interior Structure and Chemistry of Solid Exoplanets

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Interior Structure and Chemistry of Solid Exoplanets

A dissertation presented

by

Li Zeng

to

The Department of Astronomy

in partial fulfillment of the requirements

for the degree of

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in the subject of

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Interior Structure and Chemistry of Solid Exoplanets

Abstract

Understanding the interior structures and chemistry of Earth-like exoplanets is crucial for us to characterize exoplanets, and to find potentially habitable planets.

First, in Chapter 2, I provide a model grid of the mass-radius relations for solid planets in between 0.1 and 100 M\(\oplus\). I model each planet as consisting of three layers: a pure-Fe core, a MgSiO\(_3\)-layer, and an H\(_2\)O-layer on top. The most recent Equation of State (EOS) used for each layer is derived and explained in detail. I also present the differences in mass-radius relations by whether planets’ interior are differentiated or undifferentiated, and, furthermore, if these differentiated or undifferentiated interiors are reduced or oxidized. A dynamic and interactive tool to characterize and illustrate the interior structures of exoplanets built upon these models is available online: [http://www.astrozeng.com/](http://www.astrozeng.com/)

In Chapter 3, I further explore the effects of thermal evolution and phase transitions on the interior structures of H\(_2\)O-rich planets. By adopting the latest high-pressure phase diagram of H\(_2\)O and comparing it with the interior adiabats of various planet models, I show that the bulk H\(_2\)O in such planets may exist in the plasma, superionic, ionic, Ice VII, or Ice X states depending on sizes, ages, and cooling rates. The model presented in this chapter correlates different regions of the mass-radius diagram to their corresponding planet structures. The results suggest that super-Earth sized planets which are not significantly irradiated by parent stars and which are older than approximately 3 billion
years, are mostly solid.

In Chapter 4, I describe a new, semi-empirical mass-radius relation for solid exoplanets. It is based on the recent mass and radius measurements of 5 exoplanets within 1 to 10 $M_{\oplus}$ and an extrapolation of the seismically derived pressure-density relation of the Earth’s interior (PREM). This semi-empirical power-law mass-radius relation \[
\left( \frac{M}{M_{\oplus}} \right) \approx 0.94 \left( \frac{R}{R_{\oplus}} \right)^{3.72}
\] is shown to fit these exoplanets well. Uncertainties in the mass-radius relations caused by uncertainties in the EOSs are discussed. The implication of common core mass fractions of 0.2~0.3 among these solid exoplanets is also discussed.

In Chapter 5, I model the elemental abundance patterns of terrestrial bodies in our own solar system, then apply the model to derive the elemental abundance patterns of solid exoplanets in other planetary systems. This model is constructed from the following steps of planet formation: volatile depletion, core formation brought about by interior differentiation (metal/silicate partitioning), and late delivery and remixing of volatile-rich materials, often referred to as "late veneer". This model, when applied to exoplanet systems, could provide constraints on the chemical compositions of solid exoplanets from their host stars’ measurements, in addition to the constraints derived from their masses and radii.

In terms of future directions of this research, I hope to link my chemical model of solid exoplanets with the chemical evolution model of our galaxy, such as the one being developed by the Lars Hernquist group, which may indicate a different mineralogy of solid exoplanets formed at different ages of our galaxy, as well as the implications for the habitability of these planets. I also hope to understand the origins of the volatile
contents on the surfaces of solid planets, which are important prerequisites for possible origins of life on them.
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Chapter 1

Introduction

1.1 Discovery and Characterization of Solid Exoplanets

The transit method, in particular, the Kepler mission and the CoRoT mission, have made the discovery of many exoplanets, particularly abundant within 1 to 4 $R_\oplus$. It also gives precise radius measurements of many of them. The ground-based spectroscopic measurements, such as the ones conducted by the HARPS, HARPS-N, and HIRES teams, have provided accurate mass measurements of a handful of these planets with uncertainties better than 20%. Based on the combinations of their masses and radii, some of these appear to have bulk densities much higher than those of gaseous planets. Thus, they are likely to be made of elements heavier than H and He such as Fe, Ni, Mg, Si, O, and S, among others. Notable examples include Kepler-78b, Kepler-10b, Kepler-93b, Kepler-36b, CoRoT-7b, 55 Cnc e, and Kepler-10c.
CHAPTER 1. INTRODUCTION

Therefore, it is interesting to know what the bulk compositions and interior structures of these planets are. To realize this, the first approach is to understand the mass-radius relations of these planets, as mass and radius are the two primary observables. Together, they give the bulk density of such a planet, and can reveal some information of the planetary interior.

The introduction of mass-radius curves and mass-radius contours is necessary in order to separate the compositional effect on the bulk densities of planets from the compression effect due to pressure increases in more massive planets.

The construction of mass-radius curves and contours relies upon our knowledge of the major elemental and chemical compositions of these solid exoplanets, the degree of differentiation and redox states within them, as well as the Equation of State (EOS) of each individual component in their interiors. As such, it is always important to apply the appropriate and most up-to-date EOSs whenever possible, either experimental or theoretical, into our model calculation. The mass-radius relations and the details of the EOS are discussed in Chapter 2.

1.2 Interior Structure Models of Solid Exoplanets

For general purposes, based on our understanding of the differentiated structures of terrestrial bodies in our solar system, the elemental abundance patterns in our solar system and solar neighborhood, and the formation processes of planetary systems, I use 1-layer, 2-layer, and 3-layer models to model the solid exoplanets.

The most abundant elements in protoplanetary nebulae are H and He, followed by
CHAPTER 1. INTRODUCTION

O, C, Si, Fe, and Mg, among others. From the condensation sequence of a protoplanetary nebula, I can categorize the major planet-building materials into three main categories, ordering them from the highest condensation temperatures (which condensed out from the nebula first) to the lowest condensation temperatures (which condensed out from the nebula last):

1. Metals, predominately Fe, accompanied with other siderophile (iron-loving) elements such as Ni, Au, W, and Platinum Group Elements (PGE), among others. These elements have condensation temperatures above 1200 K, and also have high densities. Thus, they tend to sink towards the center of a planet, if the chemistry allows, and would likely form the core of a differentiated planet. By chemistry, I refer primarily to the oxidization state of the planet. For example, if a planet is more oxidized, then some of its Fe would be oxidized as FeO and incorporated into the rocky part of the planet.

2. Rocks, predominately Mg-silicates, such as $\text{MgSiO}_3$ (enstatite) and $\text{Mg}_2\text{SiO}_4$ (olivine). Their condensation temperatures are similar to that of Fe. These elements and mineral phases predominately form the rocky layer of a differentiated planet.

3. Ices, predominately H$_2$O, CH$_4$, NH$_3$. These all condense at fairly low temperatures below 200K. These ices, if abundantly present, would form the ice-layer of a planet. They have the lowest densities and thereby exist on top of the metallic and rocky layers.

The 1-layer model simply assumes the planet to be made of entirely metals, rocks, or ices. In reality, this model is unlikely as metals, rocks and ices tend to be mixed in
proportions in the protoplanetary nebulae. However, the 1-layer model is useful, when compared with actual exoplanet measurements, to help us characterize exoplanets in the broadest sense. Each 1-layer model corresponds to a single mass-radius curve on the mass-radius plot (M-R diagram). Considering that it is a single layer, there is only one intrinsic degree of freedom in determining the exact position of the planet on the curve. Thus, in this case, there is generally a one-to-one correspondence between mass and radius.

The 2-layer planet model introduces the concept of mass-radius contours. As each planet is allowed to have two layers, there are intrinsically two degrees of freedom in this model. Therefore, the planet structure can be uniquely determined by the combination of mass and radius. Additional parameters at the Core-Mantle Boundary (CMB-not to be confused with the CMB cosmology) of such a planet are introduced to help construct and understand the model. These parameters are the CMB pressure ratio (expressed as a ratio of the CMB pressure over the central pressure: \( \frac{p_1}{p_0} \)), the Core Mass Fraction (CMF, expressed as a ratio of the total mass of the planet), and the Core Radius Fraction (CRF, expressed as a ratio of the total radius of the planet). By specifying the central pressure, \( p_0 \), of such a planet, together with any one of the three parameters \( \frac{p_1}{p_0} \), CMF, or CRF, a unique 2-layer planet model along with its mass and radius is specified, which can be mapped onto the M-R diagram. The mapping between the \( p_0 \)-CMF diagram and the M-R diagram introduces what I refer to as \( p_0 \)-contours, as well as the CMF-contours in the M-R diagram, and is shown to be useful in deriving and understanding the more complex 3-layer model.

In Chapter 2, I also discuss the method of setting up a complete, 3-layer planet model containing the metallic core, the rocky layer, and the ice layer. It requires the
use of a ternary diagram, a convenient and symmetric way to represent a 3-component system with its components totaling 100%. Since it has three layers and thus three degrees of freedom, it requires a parameter, in addition to mass or radius, to constrain the exact proportion of each layer and thereby identify planetary structure. For the convenience of calculation, this parameter is taken as the central pressure $p_0$ of a planet, which is not directly measurable. An online interactive tool available at \url{http://www.astrozeng.com/} has been developed based on this model, to reveal the inter-connections between the ternary diagram and the mass-radius contours. Further observations could provide more information to help us constrain 3-layer planets.

1.3 Application of the Models and Comparison with Observation

One direct application of the 2-layer planet model is to ”super-Earths”, that is, planets within 1 M$_\oplus$ and 15 M$_\oplus$, which are shown to be abundant from our observations. Many of these planets have densities in between that of a pure-rock planet and that of a pure-ice planet. Some examples include Kepler-68b, Kepler-10c, 55 Cnc e, HD 97658b, and HIP 116454. Super-Earths primarily have two possible interior structures: one being a planet with a metallic/rocky core and an extended gaseous envelope, and the other being a planet with a metallic/rocky core and a significant ice-layer on top, the former being a mini-Neptune, and the latter being a water planet ($H_2O$-rich planets). Thermal evolution could play a big role in shaping the structures of these planets as both the gaseous envelope and the $H_2O$-layer are sensitive to temperature. Chapter 3 applies the
rock-H$_2$O 2-layer model to understand the interior structure and thermal evolution of the H$_2$O-rich planets. The H$_2$O-layer is more sensitive to thermal evolution than the metallic and rocky layer, due to the complex phases of ices existing at various pressure and temperature regions in the planetary interior. In general, the H$_2$O in a H$_2$O-rich planet could undergo phase transitions from the plasma state (newly formed and hot enough) to the superionic state (the most interesting state where H$_2$O is conductive due to mobile protons and, thus, could potentially generate magnetic fields through a dynamo mechanism), and, eventually, to high-pressure ices as the planet cools down. The effect of these phase transitions on planet radius is slight, but may significantly change the convective pattern as well as the magnetic fields of such a planet, as these phases can have very different thermal conductivities, electrical conductivities, and viscosities.

The 2-layer model can be applied to other categories of planets, including the terrestrial bodies in our solar system, and beyond. For example, the Earth can be approximated as a 2-layer planet, with an Fe-Ni metallic core and a rocky mantle, ignoring the thin crust and the trace amounts of ocean and atmosphere on its surface. Our best knowledge of the Earth has come from the seismically-derived pressure-density relation called the "Preliminary Reference Earth Model" (PREM). In Chapter 4, I extrapolate the PREM to derive a semi-empirical mass-radius relation for solid exoplanets. This semi-empirical power-law mass-radius relation \( \left( \frac{M}{M_{\oplus}} \right) \approx 0.94 \left( \frac{R}{R_{\oplus}} \right)^{3.72} \) is shown to fit through some of the recently discovered exoplanets with precise mass and radius measurements. The mass-radius relation implies core mass fractions of 0.2~0.3 to be among some of the known solid exoplanets. It highlights the importance of a more complete elemental abundance and chemical evolution model of solid exoplanets, which is the topic of Chapter 5.
1.4 Origins of Life and Habitable Planets

Life, as we know it today, is most likely to arise on solid exoplanets with liquid water on their surfaces.

Eventually, I would like to constrain the bulk chemistry and structure of a planet not only from its mass and radius measurements, but also from its host star’s elemental abundances combined with our knowledge of planet formation processes. CI-chondrite, as an undifferentiated meteorite, is considered to be the most primitive material in our solar system and the building block of terrestrial planets. CI-chondrite in our solar system and CI-chondrite-equivalents in exoplanetary systems could therefore be the most important link to establish the correlation between the stellar elemental abundances and the planetary elemental abundances.

Stellar elemental abundances are essentially identical to those of the proto-planetary nebulae with some modifications. From the initial nebula to the formation of solid planets, the elemental abundance pattern could undergo three important changes: (1) volatile depletion due to the high-temperature of planetesimal accretion and collisions, (2) metal/silicate separation due to the core formation and heating of the planetary interior, and (3) the late delivery of volatile-rich material to planetary surfaces.

In Chapter 5, I use the evidence from our solar system to understand exoplanets, and in particular, to predict their surface chemistry and, thereby, the possibility of life. A rocky planet, born from the same nebula as its host star, is composed primarily of silicate rocks and an iron-nickel metal core, and is depleted in volatile content in a systematic manner. The more volatile (easier to vaporize or dissociate into gas form) an
CHAPTER 1. INTRODUCTION

element is in a rocky planet, the more depleted the element is compared to its host star. After depletion, a rocky planet normally undergoes the process of core formation due to the heat from radioactive decay and collisions. Core formation depletes a planet’s rocky mantle of siderophile elements, in addition to the volatile depletion. After this, rocky planets likely accrete some volatile-rich materials, in what is called the ”late veneer”. The late veneer could be essential to the origins of life on Earth and other rocky planets, as it also delivers volatiles such as N, S, C and H$_2$O to the planets’ surfaces, which are crucial for life to occur. Here, I build an integrative model of rocky planets from the bottom up. As a result, the chemical compositions of rocky planets can be inferred from the mass-radius relations combined with the host stars’ elemental abundances. This model is available online: [http://www.astrozeng.com/](http://www.astrozeng.com/).
Chapter 2

A Detailed Model Grid for Solid
Planets from 0.1 through 100 Earth
Masses

This thesis chapter originally appeared in the literature as

Abstract

This paper describes a new grid for the mass-radius relation of 3-layer exoplanets within
the mass range of 0.1 through 100 $M_\oplus$. The 3 layers are: Fe ($\epsilon$-phase of iron), MgSiO$_3$
(including both the perovskite phase, post-perovskite phase, and its dissociation at
ultra-high pressures), and H$_2$O (including Ices Ih, III, V, VI, VII, X, and the superionic
phase along the melting curve). We discuss the current state of knowledge about the
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

equations of state (EOS) that influence these calculations and the improvements used in the new grid. For the 2-layer model, we demonstrate the utility of contours on the mass-radius diagrams. Given the mass and radius input, these contours can be used to quickly determine the important physical properties of a planet including its p0 (central pressure), p1/p0 (core-mantle boundary pressure over central pressure), CMF (core mass fraction) or CRF (core radius fraction). For the 3-layer model, a curve segment on the ternary diagram represents all possible relative mass proportions of the 3 layers for a given mass-radius input. These ternary diagrams are tabulated into Table 2.3 with the intent to make comparison to observations easier. How the presence of Fe in the mantle affects the mass-radius relations is also discussed in a separate section. A dynamic and interactive tool to characterize and illustrate the interior structure of exoplanets built upon models in this paper is available on the website: http://www.cfa.harvard.edu/~lzeng.

2.1 Introduction

The transit method of exoplanet discovery has produced a small, but well constrained, sample of exoplanets that are unambiguously solid in terms of interior bulk composition. We call solid planets the ones that possess no H and He envelopes and/or atmospheres, i.e. their bulk radius is determined by elements (and their mineral phases) heavier than H and He. Such solid exoplanets are Kepler-10b (Batalha et al. 2011), CoRoT-7b (Queloz et al. 2009, Hatzes et al. 2011), Kepler-36b (Carter et al. 2012) as well as - most likely: Kepler-20b,e,f; Kepler-18b, and 55 Cnc e in which the solid material could include high-pressure water ice (see references to Fig. 2.3 in 2.4.2).
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

There is an increased interest to compare their observed parameters to current models of interior planetary structure. The models, and their use of approximations and EOS, have evolved since 2005 (Valencia et al. 2006; Fortney et al. 2007; Grasset et al. 2009; Seager et al. 2007; Wagner et al. 2011; Swift et al. 2012), mainly because the more massive solid exoplanets (called Super-Earths) have interior pressures that are far in excess of Earth’s model, bringing about corresponding gaps in our knowledge of mineral phases and their EOS (see a recent review by Sotin et al. 2010). Here we compute a new grid of models in order to aid current comparisons to observed exoplanets on the mass-radius diagram. As in previous such grids, we assume the main constituents inside the planets to be differentiated and model them as layers in one dimension.

The first part of this paper aims to solve the 2-layer exoplanet model. The 2-layer model reveals the underlying physics of planetary interior more intuitively, for which we consider 3 scenarios: Fe-MgSiO$_3$ or Fe-H$_2$O or MgSiO$_3$-H$_2$O planet.

The current observations generally measure the radius of an exoplanet through transits and the mass through Doppler shift measurement of the host star. For each assumption of core and mantle compositions, given the mass and radius input, the 2-layer exoplanet model can be solved uniquely. It is a unique solution of radial dependence of interior pressure and density. As a result, all the characteristic physical quantities, such as the pressure at the center (p0), the pressure at core-mantle boundary (p1), the core mass fraction (CMF), and the core radius fraction (CRF) naturally fall out from this model. These quantities can be quickly determined by invoking the mass-radius contours.

The next part of this paper (Fig. 2.3) compares some known exoplanets to
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

the mass-radius curves of 6 different 2-layer exoplanet models: pure-Fe, 50%-Fe & 50%-MgSiO$_3$, pure MgSiO$_3$, 50%-MgSiO$_3$ & 50%-H$_2$O, 25%-MgSiO$_3$ & 75%-H$_2$O, and pure H$_2$O. These percentages are in mass fractions. The data of these six curves are available in Table 4.1.

Up to now, a standard assumption has been that the planet interior is fully differentiated into layers: all the Fe is in the core and all the MgSiO$_3$ is in the mantle. In section 2.4.3 we will change this assumption and discuss how the presence of Fe in the mantle affects the mass-radius relation.

The final part of this paper calculates the 3-layer differentiated exoplanet model. Given the mass and radius input, the solution for the 3-layer model is non-unique (degenerate), thus a curve on the ternary diagram is needed to represent the set of all solutions (see Fig. 2.5). This curve can be obtained by solving differential equations with iterative methods. The ensemble of solutions is tabulated (Table 2.3), from which users may interpolate to determine planet composition in 3-layer model. A dynamic and interactive tool to characterize and illustrate the interior structure of exoplanets built upon Table 2.3 and other models in this paper is available on the website http://www.cfa.harvard.edu/~lzeng.

The methods described in this paper can be used to fast characterize the interior structure of exoplanets.
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

2.2 Method

Spherical symmetry is assumed in all the models. The interior of a planet is assumed to be fully differentiated into layers in the first part of the paper. The 2-layer model consists of a core and a mantle. The 3-layer model consists of a core, a mantle and another layer on top of the mantle. The interior structure is determined by solving the following two differential equations:

\[
\frac{dr}{dm} = \frac{1}{4\pi \rho r^2} \quad (2.1)
\]

\[
\frac{dp}{dm} = -\frac{Gm}{4\pi r^4} \quad (2.2)
\]

The two equations are similar to the ones in Zeng & Seager (2008). However, contrary to the common choice of radius \(r\) as the independent variable, the interior mass \(m\) is chosen, which is the total mass inside shell radius \(r\), as the independent variable. So the solution is given as \(r(m)\) (interior radius \(r\) as a dependent function of interior mass \(m\)), \(p(m)\) (pressure as a dependent function of interior mass \(m\)), and \(\rho(m)\) (density as a dependent function of interior mass \(m\)).

The two differential equations are solved with the EOS of the constituent materials as inputs:

\[
\rho = \rho(p, T) \quad (2.3)
\]

The EOS is a material property, which describes the material’s density as a function
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

of pressure and temperature. The EOS could be obtained both theoretically and experimentally. Theoretically, the EOS could be calculated by Quantum-Mechanical Molecular Dynamics Ab Initio Simulation such as the VASP (Vienna Ab initio Simulation Package) (Kresse & Hafner 1993, 1994; Kresse & Furthmüller 1996; French et al. 2009). Experimentally, the EOS could be determined by high-pressure compression experiment such as the DAC (Diamond Anvil Cell) experiment, or shock wave experiment like the implosion experiment by the Sandia Z-machine (Yu & Jacobsen 2011). The temperature effect on density is secondary compared to the pressure effect (Valencia et al. 2006, 2007b). Therefore, we can safely ignore the temperature dependence of those higher density materials (Fe and MgSiO$_3$) for which the temperature effect is weaker, or we can implicitly include a pre-assumed pressure-temperature (p-T) relation (for H$_2$O it is the melting curve) so as to reduce the EOS to a simpler single-variable form:

$$\rho = \rho(p) \quad (2.4)$$

To solve the set of equations mentioned above, appropriate boundaries conditions are given as:

- $p_0$: the pressure at the center of the planet
- $p_1$: the pressure at the first layer interface (the core-mantle boundary)
- $p_2$: the pressure at the second layer interface (only needed for 3-layer model)
- $p_{\text{surface}}$: the pressure at the surface of the planet (set to 1 bar ($10^5 Pa$))
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

2.3 EOS of Fe, MgSiO$_3$ and H$_2$O

The 3 layers that we consider for the planet interior are Fe, MgSiO$_3$ and H$_2$O. Their detailed EOS are described as follows:

### 2.3.1 Fe

We model the core of a solid exoplanet after the Earth’s iron core, except that in our model we ignore the presence of all other elements such as Nickel (Ni) and light elements such as Sulfur (S) and Oxygen (O) in the core. As pointed out by Valencia, D. et al. (2010), above 100 GPa, the iron is mostly in the hexagonal closed packed $\epsilon$ phase. Therefore, we use the Fe-EOS by Seager et al. (2007).

Below $2.09 \times 10^4$ GPa, it is a Vinet (Vinet et al. 1987, 1989) formula fit to the experimental data of $\epsilon$-iron at $p \leq 330$ GPa by Anderson et al. (2001). Above $2.09 \times 10^4$ GPa, it makes smooth transition to the Thomas-Fermi-Dirac (TFD) EOS (Seager et al. 2007). A smooth transition is assumed because there is no experimental data available in this ultrahigh-pressure regime.

The central pressure could reach 250 TPa (terapascal, i.e., $10^{12}$ Pa) in the most massive planet considered in this paper. However, the EOS of Fe above $\sim 1$ TPa is beyond the current reach of experiment and thus largely unknown (Swift et al. 2012). Therefore, our best approximation here is to extend the currently available $\epsilon$-iron EOS to higher pressures and connect it to the TFD EOS.

The EOS of Fe is shown in Fig. 2.1 as the upper curve (red curve).
Figure 2.1: $p - \rho$ EOS of Fe (\(\epsilon\)-phase of iron, red curve), MgSiO$_3$ (perovskite phase, post-perovskite phase and its high-pressure derivatives, orange curve), and H$_2$O (Ice Ih, Ice III, Ice V, Ice VI, Ice VII, Ice X, and superionic phase along its melting curve (solid-liquid phase boundary))
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2.3.2 MgSiO₃

We model the silicate layer of a solid exoplanet using the Earth’s mantle as a proxy. The FeO-free Earth’s mantle with Mg/Si=1.07 would consist of mainly enstatite (MgSiO₃) or its high-pressure polymorphs and, depending upon pressure, small amounts of either forsterite and its high-pressure polymorphs (Mg₂SiO₄) or periclase (MgO) (e.g. Bina 2003).

The olivine polymorphs as well as lower-pressure enstatite and majorite (MgSiO₃ with garnet structure), are not stable above 27 GPa. At higher pressures, the system would consist of MgSiO₃-perovskite (pv) and periclase or their higher-pressure polymorphs (Stixrude & Lithgow-Bertelloni 2011; Bina 2003). Given the high pressures at the H₂O-silicate boundary usually exceeding 27 GPa, we can safely ignore olivine and lower-pressure pyroxene polymorphs. For the sake of simplicity, we also ignore periclase, which would contribute only 7 atomic % to the silicate mantle mineralogical composition (Bina 2003). There are also small amounts of other elements such as Aluminum (Al), Calcium (Ca), and Sodium (Na) present in Earth’s mantle (Sotin et al. 2007). For simplicity, we neglect them and thus the phases containing them are not included in our model. We also do not consider SiC because carbon-rich planets might form under very rare circumstances, and are probably not common.

Some fraction of Fe can be incorporated into the minerals of the silicate mantle which could then have the general formula as (Mg,Fe)SiO₃. For now, we simply assume all the Fe is in the core and all the Mg is in the mantle in the form of MgSiO₃-perovskite and/or its high-pressure polymorphs. So the planet is fully differentiated. In a later section, we will discuss how the addition of Fe to the mantle can affect mass-radius
relation and compare the differences between differentiated and undifferentiated as well as reduced and oxidized planets in Section 2.4.3.

We first consider the perovskite (pv) and post-perovskite (ppv) phases of pure MgSiO$_3$. MgSiO$_3$ perovskite (pv) is believed to be the major constituent of the Earth mantle. It makes transition into the post-perovskite (ppv) phase at roughly 120 GPa and 2500 K (corresponding to a depth of 2600 kilometers in Earth) (Hirose 2010). The ppv phase was discovered experimentally in 2004 (by Murakami et al. 2004) and was also theoretically predicted in the same year (by Oganov & Ono 2004). The ppv is about 1.5% denser than the pv phase (Caracas & Cohen 2008; Hirose 2010). This 1.5% density jump resulting from the pv-to-ppv phase transition can be clearly seen as the first density jump of the MgSiO$_3$ EOS curve shown in Fig. 2.1. Both the MgSiO$_3$ pv EOS and MgSiO$_3$ ppv EOS are taken from Caracas & Cohen (2008). The transition pressure is determined to be 122 GPa for pure MgSiO$_3$ according to Spera et al. (2006).

Beyond 0.90 TPa, MgSiO$_3$ ppv undergoes a two-stage dissociation process predicted from the first-principle calculations by Umemoto & Wentzcovitch (2011). MgSiO$_3$ ppv first dissociates into CsCl-type MgO and P2$_1$c-type MgSi$_2$O$_5$ at the pressure of 0.90 TPa and later into CsCl-type MgO and Fe$_2$P-type SiO$_2$ at pressures higher than 2.10 TPa. The EOS of CsCl-type MgO, P2$_1$c-type MgSi$_2$O$_5$, and Fe$_2$P-type SiO$_2$ are adopted from Umemoto & Wentzcovitch (2011); Wu et al. (2011). Therefore, there are two density jumps at the dissociation pressures of 0.90 TPa and 2.10 TPa. The first one can be seen clearly in Fig. 2.1. The second one cannot be seen in Fig. 2.1 since it is too small, but it surely exists.

Since Umemoto & Wentzcovitch (2011)'s EOS calculation is until 4.90 TPa, beyond
4.90 TPa, a modified version of the EOS by Seager et al. (2007) is used to smoothly connect to the TFD EOS. TFD EOS assumes electrons in a slowly varying potential with a density-dependent correlation energy term that describes the interactions among electrons. It is therefore insensitive to any crystal structure or arrangements of atoms and it becomes asymptotically more accurate at higher pressure. Thus, the TFD EOS of MgSiO$_3$ would be no different from the TFD EOS of MgO plus SiO$_2$ as long as the types and numbers of atoms in the calculation are the same. So it is safe to use the TFD EOS of MgSiO$_3$ as an approximation of the EOS of MgO and SiO$_2$ mixture beyond 4.90 TPa here.

Seager et al. (2007)'s EOS is calculated from the method of Salpeter & Zapolsky (1967) above $1.35 \times 10^4$ GPa. Below $1.35 \times 10^4$ GPa, it is a smooth connection to TFD EOS from the fourth-order Birch-Murbaghan Equation of State (BME) (see Birch 1947, Poirier 2000) fit to the parameters of MgSiO$_3$ pv obtained by Ab initio lattice dynamics simulation of Karki et al. (2000).

Seager et al.'s EOS is slightly modified to avoid any artificial density jump when connected with Umemoto & Wentzcovitch's EOS at 4.90 TPa. At 4.90 TPa, the ratio of the density $\rho$ between Umemoto & Wentzcovitch's EOS and Seager et al.'s EOS is 1.04437. This ratio is multiplied to the original Seager et al.'s EOS density $\rho$ to produce the actual EOS used in our calculation for $p > 4.90$ TPa. A smooth transition is assumed because no experimental data is available in this ultrahigh-pressure regime. This assumption does not affect our low or medium mass planet models, since only the most massive planets in our model could reach this ultrahigh pressure in their MgSiO$_3$ part.
The EOS of MgSiO$_3$ is shown in Fig. 2.1 as the middle curve (orange curve).

### 2.3.3 H$_2$O

The top layer of a planet could consist of various phases of H$_2$O. Since H$_2$O has a complex phase diagram, and it also has a stronger temperature dependence, thus the temperature effect cannot be ignored. Instead, we follow the solid phases along the melting curve (solid-liquid phase boundary on the p-T plot by Chaplin (2012)). Along the melting curve, the H$_2$O undergoes several phase transitions. Initially, it is Ice Ih at low pressure, then subsequently transforms into Ice III, Ice V, Ice VI, Ice VII, Ice X, and superionic phase (Chaplin 2012; Choukroun & Grasset 2007; Dunaeva et al. 2010; French et al. 2009).

**Chaplin’s EOS**

The solid form of water has very complex phases in the low-pressure and low-temperature regime. These phases are well determined by experiments. Here we adopt the Chaplin’s EOS for Ice Ih, Ice III, Ice V, and Ice VI below 2.216 GPa (see Chaplin 2012; Choukroun & Grasset 2007; Dunaeva et al. 2010). Along the melting curve (the solid-liquid boundary on the p-T diagram), the solid form of water first exists as Ice Ih (Hexagonal Ice) from ambient pressure up to 209.5 MPa (Choukroun & Grasset 2007). At the triple point of 209.5 MPa and 251.15 K (Choukroun & Grasset 2007; Robinson et al. 1996), it transforms into Ice III (Ice-three), whose unit cell forms tetragonal crystals. Ice III exists up to 355.0 MPa and transforms into a higher-pressure form Ice V (Ice-five) at the triple point of 355.0 MPa and 256.43 K (Choukroun & Grasset 2007). Ice V’s unit cell
forms monoclinic crystals. At the triple point of 618.4 MPa and 272.73 K (Choukroun & Grasset 2007), Ice V transforms into yet another higher-pressure form Ice VI (Ice-six). Ice VI’s unit cell forms tetragonal crystals. A single molecule in Ice VI crystal is bonded to four other water molecules. Then at the triple point of 2.216 GPa and 355 K (Daucik & Dooley 2011), Ice VI transforms into Ice VII (Ice-seven). Ice VII has a cubic crystal structure. Ice VII eventually transforms into Ice X (Ice-ten) at the triple point of 47 GPa and 1000 K (Goncharov et al. 2005). In Ice X, the protons are equally spaced and bonded between the oxygen atoms, where the oxygen atoms are in a body-centered cubic lattice (Hirsch & Holzapfel 1984). The EOS of Ice X and Ice VII are very similar. For Ice VII (above 2.216 GPa), we switch to the (Frank, Fei, & Hu 2004)’s EOS (FFH2004).

**FFH2004’s EOS**

We adopt FFH2004’s EOS of Ice VII for 2.216 GPa≤p≤ 37.4 GPa. This EOS is obtained using the Mao-Bell type diamond anvil cell with an external Mo-wire resistance heater. Gold and water are put into the sample chamber and compressed. The diffraction pattern of both H$_2$O and gold are measured by the Energy-Dispersive X-ray Diffraction (EDXD) technique at the Brookhaven National Synchrotron Light Source. The gold here is used as an internal pressure calibrant. The disappearance of the diffraction pattern of the crystal Ice VII is used as the indicator for the solid-liquid boundary (melting curve). The melting curve for Ice VII is determined accurately from 3 GPa to 60 GPa and fit to a Simon equation. The molar density (ρ in mol/cm$^3$) of Ice VII as a function of pressure (p in GPa) is given by the following formula in FFH2004:
\[ \rho(\text{mol/cm}^3) = 0.0805 + 0.0229 \times (1 - e^{0.0743p}) + 0.1573 \times (1 - e^{0.0061p}) \] (2.5)

We use Eq. 2.5 to calculate \( \rho \) from 2.216 GPa up to 37.4 GPa. The upper limit 37.4 GPa is determined by the intersection between FFH2004’s EOS and (French, Mattsson, Nettelmann, & Redmer 2009)’s EOS (FMNR2009).

**FMNR2009’s EOS**

FMNR2009’s EOS is used for Ice VII, Ice X and superionic phase of H\(_2\)O for 37.4 GPa \( \leq \) \( p \leq \) 8.893 TPa. This EOS is determined by Quantum Molecular Dynamics Simulations using the Vienna Ab Initio Simulation Package (VASP). The simulation is based on finite temperature density-functional theory (DFT) for the electronic structure and treating the ions as classical particles. Most of French et al.’s simulations consider 54 H\(_2\)O molecules in a canonical ensemble, with the standard VASP PAW potentials, the 900 eV plane-wave cutoff, and the evaluation of the electronic states at the \( \Gamma \) point considered, for the 3 independent variables: temperature (\( T \)), volume (\( V \)), and particle number (\( N \)). The simulation results are the thermal EOS \( p(T,V,N) \), and the caloric EOS \( U(T,V,N) \). The data are tabulated in FMNR2009.

In order to approximate density \( \rho \) along the melting curve, from Table V in FMNR2009, we take 1 data point from Ice VII phase at 1000 K and 2.5g/cm\(^3\), 4 data points from Ice X phase at 2000 K and 3.25g/cm\(^3\) to 4.00g/cm\(^3\), and the rest of the data points from the superionic phase at 4000 K and 5.00g/cm\(^3\) up to 15g/cm\(^3\). Since the temperature effect on density becomes smaller towards higher pressure, all the isothermal pressure-density curves converge on the isentropic pressure-density curves as well as the
pressure-density curve along the melting curve.

The FMNR2009’s EOS has been confirmed experimentally by Thomas Mattson et al. at the Sandia National Laboratories. At 8.893 TPa, FMNR2009’s EOS is switched to the TFD EOS in Seager, Kuchner, Hier-Majumder, & Militzer 2007 (SKHMM2007).

SKHMM2007’s EOS

At ultrahigh pressure, the effect of electron-electron interaction can be safely ignored and electrons can be treated as a gas of non-interacting particles that obey the Pauli exclusion principle subject to the Coulomb field of the nuclei. Assuming the Coulomb potential is spatially slowly varying throughout the electron gas that the electronic wave functions can be approximated locally as plane waves, the so-called TFD solution could be derived so that the Pauli exclusion pressure balances out the Coulomb forces (Eliezer et al. 2002; Macfarlane 1984).

In SKHMM2007, a modified TFD by Salpeter & Zapolsky 1967 is used. It is modified in the sense that the authors have added in a density-dependent correlation energy term which characterizes electron interaction effects.

Here, Seager et al.’s EOS is slightly modified to connect to the FMNR2009’s EOS. At 8.893 TPa, the ratio of the density $\rho$ between the FMNR2009’s EOS and Seager et al.’s EOS is 1.04464. This ratio is multiplied to the original Seager et al.’s EOS density $\rho$ to produce the actual EOS used in our calculation for $p > 8.893$ TPa. Only the most massive planets in our model could reach this pressure in the H$_2$O-layer, so this choice of EOS for $p > 8.893$ TPa has small effect on the overall mass-radius relation to be discussed in the next section.
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The EOS of H$_2$O is shown in Fig. 2.1 as the lower curve (blue curve).

2.4 Result

2.4.1 Mass-Radius Contours

Given mass and radius input, various sets of mass-radius contours can be used to quickly determine the characteristic interior structure quantities of a 2-layer planet including its $p_0$ (central pressure), $p_1/p_0$ (ratio of core-mantle boundary pressure over central pressure), CMF (core mass fraction), and CRF (core radius fraction).

The 2-layer model is uniquely solved and represented as a point on the mass-radius diagram given any pair of two parameters from the following list: $M$ (mass), $R$ (radius), $p_0$, $p_1/p_0$, CMF, CRF, etc. The contours of constant $M$ or $R$ are trivial on the mass-radius diagram, which are simply vertical or horizontal lines. The contours of constant $p_0$, $p_1/p_0$, CMF, or CRF are more useful.

Within a pair of parameters, fixing one and continuously varying the other, the point on the mass-radius diagram moves to form a curve. Multiple values of the fixed parameter give multiple parallel curves forming a set of contours. The other set of contours can be obtained by exchanging the fixed parameter for the varying parameter. The two sets of contours crisscross each other to form a mesh, which is a natural coordinate system (see Fig. 2.2) of this pair of parameters, superimposed onto the existing Cartesian ($M, R$) coordinates of the mass-radius diagram. This mesh can be used to determine the two parameters given the mass and radius input or vice versa.
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Fe-MgSiO$_3$ planet

As an example, the mesh of $p_0$ with $p_1/p_0$ for Fe-core MgSiO$_3$-mantle planet is illustrated in the first subplot (upper left corner) of Fig. 2.2. The mesh is formed by $p_0$-contours and $p_1/p_0$-contours crisscrossing each other. The more vertical set of curves represents the $p_0$-contours. The ratio of adjacent $p_0$-contours is $10^{0.1}$ (see Table 4.1). The more horizontal set of curves represents the $p_1/p_0$-contours. From bottom up, the $p_1/p_0$ values vary from 0 to 1 with step size 0.1.

Given a pair of $p_0$ and $p_1$ input, users may interpolate from the mesh to find the mass and radius. On the other hand, given the mass and radius of a planet, users may also interpolate from the mesh to find the corresponding $p_0$ and $p_1$ of a 2-layer Fe core MgSiO$_3$-mantle planet.

Similarly, the contour mesh of $p_0$ with CMF for the Fe-MgSiO$_3$ planet is shown as the second subplot from the left in the first row of Fig. 2.2. As a reference point, for a pure-Fe planet with $p_0 = 10^{11}$ Pa, $M = 0.1254 M_\oplus$, $R = 0.417 R_\oplus$.

The contour mesh of $p_0$ with CRF for the Fe-MgSiO$_3$ planet is shown as the third subplot from the left of the first row of Fig. 2.2.

MgSiO$_3$-H$_2$O planet

For 2-layer MgSiO$_3$-H$_2$O planet, the 3 diagrams ($p_0$ contours pair with $p_1/p_0$ contours, CMF contours, or CRF contours) are the subplots of the second row of Fig. 2.2.

As a reference point, for a pure-MgSiO$_3$ planet with $p_0 = 10^{10.5}$ Pa, $M = 0.122 M_\oplus$, $R = 0.5396 R_\oplus$. 

25
**Figure 2.2:** Mass-Radius contours of 2-layer planet. 1st row: Fe-MgSiO$_3$ planet. 2nd row: MgSiO$_3$-H$_2$O planet. 3rd row: Fe-H$_2$O planet. 1st column: contour mesh of p1/p0 with p0. 2nd column: contour mesh of CMF with p0. 3rd column: contour mesh of CRF with p0. To find out what p0 value each p0-contour corresponds to, please refer to Table 4.1.
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Fe-H$_2$O planet

For 2-layer Fe-H$_2$O planet, the 3 diagrams (p0 contours pair with p1/p0 contours, CMF contours, or CRF contours) are the subplots of the third row of Fig. 2.2.

As a reference point, for a pure-Fe planet with $p_0 = 10^{11}$ Pa, $M = 0.1254M_\oplus$, $R = 0.417R_\oplus$.

2.4.2 Mass-Radius Curves

For observers’ interest, 6 characteristic mass-radius curves are plotted (Fig. 2.3) and tabulated (Table 4.1), representing the pure-Fe planet, half-Fe half-MgSiO$_3$ planet, pure MgSiO$_3$ planet, half-MgSiO$_3$ half-H$_2$O planet, 75% H$_2$O-25% MgSiO$_3$ planet, and pure H$_2$O planet. These fractions are mass fractions. Fig. 2.3 also shows some recently discovered exoplanets within the relevant mass-radius regime for comparison. These planets include Kepler-10b (Batalha et al. 2011), Kepler-11b (Lissauer et al. 2011), Kepler-11f (Lissauer et al. 2011), Kepler-18b (Cochran et al. 2011), Kepler-36b (Carter et al. 2012), and Kepler-20b,c,d (Gautier et al. 2012). They also include Kepler-20e ($R = 0.868^{+0.074}_{-0.096}R_\oplus$ (Fressin et al. 2012), the mass range is determined by pure-silicate mass-radius curve and the maximum collisional stripping curve (Marcus et al. 2010a)), Kepler-20f ($R = 1.034^{+0.100}_{-0.127}R_\oplus$ (Fressin et al. 2012), the mass range is determined by 75% water-ice and 25% silicate mass-radius curves and the maximum collisional stripping curve (Marcus et al. 2010a)), Kepler-21b ($R = 1.64 \pm 0.04R_\oplus$ (Howell et al. 2012), The upper limit for mass is 10.4$M_\oplus$: the 2-σ upper limit preferred in the paper. The lower limit is 4$M_\oplus$, which is in between the ”Earth” and ”50% H$_2$O-50% MgSiO$_3”$ model curves - the planet is very hot and is unlikely to have much water content if
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

any at all.), Kepler-22b \((R = 2.38 \pm 0.13R_{\oplus})\) \cite{Borucki et al. 2012}, The 1-\(\sigma\) upper limit for mass is \(36M_{\oplus}\) for an eccentric orbit (or \(27M_{\oplus}\), for circular orbit), CoRoT-7b \((M = 7.42 \pm 1.21M_{\oplus}, R = 1.58 \pm 0.1R_{\oplus})\) \cite{Hatzes et al. 2011, Leger et al. 2009, Queloz et al. 2009}, 55 Cancri e \((M = 8.63 \pm 0.35M_{\oplus}, R = 2.00 \pm 0.14R_{\oplus})\) \cite{Winn et al. 2011}, and GJ 1214b \cite{Charbonneau et al. 2009}.

2.4.3 Levels of planet differentiation: the effect of Fe partitioning between mantle and core

All models of planets discussed so far assume that all Fe is in the core, while all Mg, Si and O are in the mantle, i.e., that a planet is fully differentiated. However, we know that in terrestrial planets some Fe is incorporated into the mantle. There are two separate processes which affect the Fe content of the mantle: (1) mechanical segregation of Fe-rich metal from the mantle to the core, and (2) different redox conditions resulting in a different Fe/Mg ratio within the mantle, which in turn affects the relative size of the core and mantle. In this section we show the effects of (1) undifferentiated versus fully-differentiated, and (2) reduced versus oxidized planetary structure on the mass-radius relation for a planet with the same Fe/Si and Mg/Si ratios.

\(^1\)mass in Earth Mass \((M_{\oplus} = 5.9742 \times 10^{24} kg)\)

\(^2\)radius in Earth Radius \((R_{\oplus} = 6.371 \times 10^{6} m)\)

\(^3\)CRF stands for core radius fraction, the ratio of the radius of the core over the total radius of the planet, in the two-layer model

\(^4\)p1/p0 stands for core-mantle-boundary pressure fraction, the ratio of the pressure at the core-mantle boundary (p1) over the pressure at the center of the planet (p0), in the two-layer model
Figure 2.3: Currently known transiting exoplanets are shown with their measured mass and radius with observation uncertainties. Earth and Venus are shown for comparison. The curves are calculated for planets composed of pure Fe, 50% Fe-50% MgSiO$_3$, pure MgSiO$_3$, 50% H$_2$O-50% MgSiO$_3$, 75% H$_2$O-25% MgSiO$_3$ and pure H$_2$O. The red dashed curve is the maximum collisional stripping curve calculated by Marcus et al. (2010a).
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### Table 2.1: Data for the 6 characteristic mass-radius curves

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**Notes:**

- Mass and Radius are in units of Earth's mass and radius, respectively.
- Calculated using the formula: $\text{CRF} = \frac{\text{Mass of Planet}}{\text{Mass of Earth}}$.
- The table includes the percentage composition by mass of MgSiO$_2$ and MgSiO$_3$. 

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**References:**


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**Figures:**

- Figure 2.1: Mass-radius curves for various compositions.
- Figure 2.2: Comparison of mass-radius curves for different models.

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**Tables:**

- Table 2.1: Data for the 6 characteristic mass-radius curves.

---

**Tables:**

- Table 2.2: Physical properties and composition of exoplanets.
- Table 2.3: Observational data for confirmed exoplanets.
For simplicity, here we ignore the H$_2$O and gaseous content of the planet and only consider the planet made of Fe, Mg, Si, O. To facilitate comparison between different cases, we fix the global atomic ratios of Fe/Mg=1 and Mg/Si=1; these fit well within the range of local stellar abundances (Grasset et al. 2009).

In particular, we consider a double-layer planet with a core and a mantle in two scenarios. One follows the incomplete mechanical separation of the Fe-rich metal during planet formation, and results in addition of Fe to the mantle as metal particles. It does not change EOS of the silicate components, but requires adding an Fe-EOS to the mantle mixture. Thus, the planet generally consists of a Fe metal core and a partially differentiated mantle consisting of the mixture of metallic Fe and MgSiO$_3$ silicates. While the distribution of metallic Fe may have a radial gradient, for simplicity we assume that it is uniformly distributed in the silicate mantle. Within scenario 1, we calculate three cases to represent different levels of differentiation:

**Case 1: complete differentiation** metallic Fe core and MgSiO$_3$ silicate mantle. For Fe/Mg=1, CMF=0.3574.

**Case 2: partial differentiation** half the Fe forms a smaller metallic Fe core, with the other half of metal being mixed with MgSiO$_3$ silicates in the mantle. CMF=0.1787.

**Case 3: no differentiation** All the metallic Fe is mixed with MgSiO$_3$ in the mantle. CMF=0 (no core).

The other scenario assumes different redox conditions, resulting in different Fe/Mg ratios in mantle minerals, and therefore requiring different EOS for the Fe$^{2+}$-bearing silicates and oxides. More oxidized mantle means adding more Fe in the form of FeO to
the MgSiO$_3$ silicates to form (Mg,Fe)SiO$_3$ silicates and (Mg,Fe)O magnesiowüstite (mv), thus reducing the amount of Fe in the core. The exact amounts of (Mg,Fe)SiO$_3$ and (Mg,Fe)O in the mantle are determined by the following mass balance equation:

$$x\ FeO + MgSiO_3 \rightarrow (Mg^{\frac{1}{1+x}}_\frac{x}{1+x}, Fe^{\frac{x}{1+x}}_\frac{x}{1+x})SiO_3 + x\ (Mg^{\frac{1}{1+x}}_\frac{x}{1+x}, Fe^{\frac{x}{1+x}}_\frac{x}{1+x})O$$  

(2.6)

$x$ denotes the relative amount of FeO added to the silicate mantle, $x=0$ being the most reduced state with no Fe in the mantle, and $x=1$ being the most oxidized state with all Fe existing as oxides in the mantle. This oxidization process conserves the global Fe/Mg and Mg/Si ratios, but increases O content and thus the O/Si ratio of the planet since Fe is added to the mantle in the form of FeO. Because in stellar environments O is excessively abundant relative to Mg, Si, and Fe (e.g., the solar elemental abundances [Asplund et al. 2009]), it is not a limiting factor in our models of oxidized planets. We calculate the following three cases to represent the full range of redox conditions:

**Case 4: no oxidization of Fe** $x=0$. Metal Fe core and MgSiO$_3$ silicate mantle. For Fe/Mg=1, O/Si=3, CMF=0.3574.

**Case 5: partial oxidization of Fe** $x=0.5$. Half the Fe forms smaller metal core, the other half is added as FeO to the mantle. O/Si=3.5, CMF=0.1700.

**Case 6: complete oxidization of Fe** $x=1$. All Fe is added as FeO to the mantle, resulting in no metal core at all. O/Si=4, CMF=0.

Notice that Case 4 looks identical to Case 1. However, the silicate EOS used to calculate Case 4 is different from Case 1 at ultrahigh pressures (beyond 0.90 TPa).
For Cases 4, 5, and 6, the \((\text{Mg,Fe})\text{SiO}_3\) EOS is adopted from Caracas & Cohen (2008) and Spera et al. (2006) which only consider perovskite (pv) and post-perovskite (ppv) phases without including further dissociation beyond 0.90 TPa, since the \(\text{Fe}^{2+}\)-bearing silicate EOS at ultrahigh pressures is hardly available. On the other hand, comparison between Case 1 and Case 4 also shows the uncertainty on mass-radius relation resulting from the different choice of EOS (see Table 4.2). \(\text{Fe}^{2+}\)-bearing pv and ppv have the general formula: \((\text{Mg}_y\text{Fe}_{1-y})\text{SiO}_3\), where \(y\) denotes the relative atomic number fraction of Mg and Fe in the silicate mineral. The \((\text{Mg}_y\text{Fe}_{1-y})\text{SiO}_3\) silicate is therefore a binary component equilibrium solid solution. It could either be pv or ppv or both depending on the pressure (Spera et al. 2006). We can safely approximate the narrow pressure region where pv and ppv co-exist as a single transition pressure from pv to ppv. This pressure is calculated as the arithmetic mean of the initial transition pressure of pv \(\rightarrow\) pv+ppv mixture and the final transition pressure of pv+ppv mixture \(\rightarrow\) ppv (Spera et al. 2006). The pv EOS and ppv EOS are connected at this transition pressure to form a consistent EOS for all pressures.

Addition of \(\text{FeO}\) to \(\text{MgSiO}_3\) results in the appearance of a second phase, magnesiowüstite, in the mantle according to Eq. 2.6. The \((\text{Mg,Fe})\text{O}\) EOS for Cases 4, 5, and 6 is adopted from Fei et al. (2007), which includes the electronic spin transition of high-spin to low-spin in \(\text{Fe}^{2+}\). For simplicity, we assume that pv/ppv and mw have the same Mg/Fe ratio.

Fig. 2.4 shows fractional differences \((\eta)\) in radius of Cases 2 & 3 compared to Case 1 as well as Cases 5 & 6 compared to Case 4 \((r_0\) is radius of the reference case, which is
that of Case 1 for Cases 2 & 3 and is that of Case 4 for Case 5 & 6):
\[
\eta = \frac{r - r_0}{r_0}
\]  

(2.7)

Oxidization of Fe (partitioning Fe as Fe-oxides from the core into the mantle) makes the planet appear larger. The complete oxidization of Fe makes the radius 3% larger for small planets around \(1 \, M_\oplus\), then the difference decreases with increasing mass within the mass range of 1 to 20 \(M_\oplus\). Undifferentiated planets (partitioning of metallic Fe from the core into the mantle) appear smaller than fully differentiated planets. The completely undifferentiated planet is practically indistinguishable in radius for small planets around \(1 \, M_\oplus\), then the difference increases to 1%-level around 20 \(M_\oplus\). The mass, radius, CRF and \(p_1/p_0\) data of Cases 1 through 6 are listed in Table 4.2.

### 2.4.4 Tabulating the Ternary Diagram

For the 3-layer model of solid exoplanet, points of a curve segment on the ternary diagram represent all the solutions for a given mass-radius input. These ternary diagrams are tabulated (Table 2.3) with the intent to make comparison to observations easier.

Usually, there are infinite combinations (solutions) of Fe, MgSiO\(_3\) and H\(_2\)O mass fractions which can give the same mass-radius pair. All the combinations together form a curve segment on the ternary diagram of Fe, MgSiO\(_3\) and H\(_2\)O mass fractions (Zeng & Seager 2008; Valencia et al. 2007a). This curve segment can be approximated by 3 points on it: two endpoints where one or more out of the 3 layers are absent and one point in between where all 3 layers are present to give the same mass and radius. The two endpoints correspond to the minimum central pressure (\(p_{0_{\text{min}}}\)) and maximum central
Figure 2.4: fractional differences in radius resulting from Fe partitioning between mantle and core. black curve: Case 1 & Case 4 (complete differentiation and no oxidization of Fe); solid brown curve: Case 2 (partial (50%) differentiation: 50% metallic Fe mixed with the mantle); solid pink curve: Case 3 (no differentiation: all metallic Fe mixed with the mantle); dashed brown curve: Case 5 (partial (50%) oxidization of Fe); dashed pink curve: Case 6 (complete oxidization of Fe)
### CHAPTER 2. MODEL GRID FOR SOLID PLANETS

#### Table 2.2: Data of Cases 1 through 6

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<tr>
<th>Case 1 (CMF=0.3574)</th>
<th>Case 2 (CMF=0.1876)</th>
<th>Case 3</th>
<th>Case 4 (CMF=0.3574)</th>
<th>Case 5 (CMF=1.7064)</th>
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</table>

36
pressure \((p_{0_{\text{max}}})\) allowed for the given mass-radius pair. The middle point is chosen to have the central pressure \(p_{0_{\text{mid}}} = \sqrt{p_{0_{\text{max}}} \times p_{0_{\text{min}}}}\).

Table 2.3 contains 8 columns:

1st column: Mass. The masses range from 0.1 \(M_\oplus\) to 100 \(M_\oplus\) with 41 points in total. The range between 0.1 and 1 \(M_\oplus\) is equally divided into 10 sections in logarithmic scale. The range between 1 and 10 \(M_\oplus\) is equally divided into 20 sections in logarithmic scale. And the range between 10 and 100 \(M_\oplus\) is equally divided into 10 sections in logarithmic scale.

2nd column: Radius. For each mass \(M\) in Table 2.3 there are 12 radius values, 11 of which are equally spaced within the allowed range: \(R_{Fe}(M) + (R_{H_2O}(M) - R_{Fe}(M)) \times i\), where \(i = 0, 0.1, 0.2, ..., 0.9, 1.0\). The 12-th radius value \((R_{MgSiO_3}(M))\) is inserted into the list corresponding to the pure-MgSiO\(_3\) planet radius (see Table 4.1) for mass \(M\). Here \(R_{Fe}(M), R_{MgSiO_3}(M),\) and \(R_{H_2O}(M)\) are the radii for planets with mass \(M\) composed of pure-Fe, pure-MgSiO\(_3\), and pure-H\(_2\)O correspondingly.

Overall, there are \(41 \times 12 = 492\) different mass-radius pairs in Table 2.3. For each \((M, R)\), 3 cases: \(p_{0_{\text{min}}}, p_{0_{\text{mid}}},\) and \(p_{0_{\text{max}}}\) are listed.

3rd column: central pressure \(p_0\) (Pascal) in logarithmic base-10 scale.

4th column: \(p_1/p_0\), the ratio of \(p_1\) (the first boundary pressure, i.e., the pressure at the Fe-MgSiO\(_3\) boundary) over \(p_0\).

5th column: \(p_2/p_1\), the ratio of \(p_2\) (the second boundary pressure, i.e., the pressure at the MgSiO\(_3\)-H\(_2\)O boundary) over \(p_1\).

6th column: Fe mass fraction (the ratio of the Fe-layer mass over the total mass of
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

the planet).

7th column: MgSiO$_3$ mass fraction (the ratio of the MgSiO$_3$-layer mass over the total mass of the planet).

8th column: H$_2$O mass fraction (the ratio of the H$_2$O-layer mass of over the total mass of the planet).

6th, 7th and 8th columns always add up to one.

Table 2.3:: Table for Ternary Diagram

<table>
<thead>
<tr>
<th>M($M_\oplus$)</th>
<th>R($R_\oplus$)</th>
<th>log$_{10}$($p_0$)</th>
<th>p1/p0</th>
<th>p2/p1</th>
<th>Fe</th>
<th>MgSiO$_3$</th>
<th>H$_2$O</th>
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<tr>
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<td>10.9212</td>
<td>0</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.1</td>
<td>0.3888</td>
<td>10.9212</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>0.3888</td>
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</tbody>
</table>

A dynamic and interactive tool to characterize and illustrate the interior structure of exoplanets built upon Table 2.3 and other models in this paper is available on the website http://www.cfa.harvard.edu/~lzeng.
2.4.5 Generate curve segment on ternary diagram using Table 2.3

One utility of Table 2.3 is to generate the curve segment on the 3-layer ternary diagram for a given mass-radius pair. As an example, for $M=1M_\oplus$ and $R=1.0281R_\oplus$, the table provides 3 p0’s. For each p0, the mass fractions of Fe, MgSiO$_3$, and H$_2$O are given to determine a point on the ternary diagram. Then, a parabolic fit (see Fig. 2.5) through the 3 points is a good approximation to the actual curve segment. This parabola may intersect the maximum collisional stripping curve by Marcus et al. (2010a), indicating that the portion of parabola beneath the intersection point may be ruled out by planet formation theory.

2.5 Conclusion

The 2-layer and 3-layer models for solid exoplanets composed of Fe, MgSiO$_3$, and H$_2$O are the focus of this paper. The mass-radius contours (Fig. 2.2) are provided for the 2-layer model, useful for readers to quickly calculate the interior structure of a solid exoplanet. The 2-parameter contour mesh may also help one build physical insights into the solid exoplanet interior structure.

The complete 3-layer mass-fraction ternary diagram is tabulated (Table 2.3), useful for readers to interpolate and calculate all solutions as the mass fractions of the 3 layers for a given mass-radius input. The details of the EOS of Fe, MgSiO$_3$, and H$_2$O and how they are calculated and used in this paper are discussed in section 2.3 and shown in Fig. 2.1.
Figure 2.5: The red, orange and purple points correspond to $\log_{10}(p_0 \text{ (in Pa)}) = 11.4391$, 11.5863, and 11.7336. The mass fractions are (1) red point: FeMF=0.083, MgSiO$_3$MF=0.917, H$_2$OMF=0; (2) orange point: FeMF=0.244, MgSiO$_3$MF=0.711, H$_2$OMF=0.046; (3) purple point: FeMF=0.728, MgSiO$_3$MF=0, H$_2$OMF=0.272. MF here stands for mass fraction. The blue curve is the parabolic fit. The red dashed curve is the maximum collisional stripping curve by Marcus et al. (2010a).
CHAPTER 2. MODEL GRID FOR SOLID PLANETS

A dynamic and interactive tool to characterize and illustrate the interior structure of exoplanets built upon Table 2.3 and other models in this paper is available on the website [http://www.cfa.harvard.edu/~lzeng](http://www.cfa.harvard.edu/~lzeng).

The effect of Fe partitioning between mantle and core on mass-radius relation is explored in section 2.4.3, and the result is shown in Fig. 2.4 and Table 4.2.

With the ongoing Kepler Mission and many other exoplanet searching projects, we hope this paper could provide a handy tool for observers to fast characterize the interior structure of exoplanets already discovered or to be discovered, and further our understanding of those worlds beyond our own.

Acknowledgements

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Li Zeng would also like to give special thanks to Master Anlin Wang. Master Wang is a Traditional Chinese Kung Fu Master and World Champion. He is also a practitioner and realizer of Traditional Chinese Philosophy of Tao Te Ching, which is the ancient oriental wisdom to study the relation between the universe, nature and humanity. Valuable inspirations were obtained through discussion of Tao Te Ching with Master Wang as well as Qigong cultivation with him.
Chapter 3

The Effect of Temperature Evolution on the Interior Structure of H$_2$O-rich Planets

Abstract

For most planets in the range of radii from 1 to 4 R$_\oplus$, water is a major component of the interior composition. At high pressure H$_2$O can be solid, but for larger planets, like Neptune, the temperature can be too high for this. Mass and age play a role in determining the transition between solid and fluid (and mixed) water-rich super-Earth. We use the latest high-pressure and ultra-high-pressure phase diagrams of H$_2$O, and by
CHAPTER 3. THERMAL EVOLUTION OF $\text{H}_2\text{O}$-RICH PLANETS

comparing them with the interior adiabats of various planet models, the temperature evolution of the planet interior is shown, especially for the state of $\text{H}_2\text{O}$. It turns out that the bulk of $\text{H}_2\text{O}$ in a planet’s interior may exist in various states such as plasma, superionic, ionic, Ice VII, Ice X, etc., depending on the size, age and cooling rate of the planet. Different regions of the mass-radius phase space are also identified to correspond to different planet structures. In general, super-Earth-size planets (isolated or without significant parent star irradiation effects) older than about 3 Gyr would be mostly solid.

3.1 Introduction

The catalog of observed extrasolar planets now includes more than 1700 members, and more than 1100 planets have been observed transiting their parent stars [Rein 2014]. Transiting planets are particularly valuable for comparative planetology because they provide the planet’s radius, as well as the inclination angle of the planet’s orbit with respect to the line of sight. When combined with the mass determined from radial velocity measurements, the mean density of the planet can be determined.

Super-Earths, massive terrestrial exoplanets within the range of $1M_\oplus \lesssim M \lesssim 15M_\oplus$, are now observed to be relatively common by Doppler shift surveys and transiting observations. The currently discovered super-Earth extrasolar planets suggest diversity among their interior structure and composition – some being very dense (such as CoRoT-7b [Leger et al. 2009; Queloz et al. 2009]), and the others seem much less so (such as GJ 1214b [Charbonneau et al. 2009]). Moreover, among the Super-Earths, it has been speculated that some of them may contain more than $10\% \sim 15\%$ of $\text{H}_2\text{O}$ by weight, the so-called water planets (or $\text{H}_2\text{O}$-rich planets). The candidates of those
water planets include GJ 1214b, Kepler-22b, Kepler-68b, and Kepler-18b. There is no exact definition of H$_2$O-rich planets; however, based on the implication from the planet formation theory, we could propose the range of anywhere between 25% and 75% mass fraction of H$_2$O \cite{Marcus2010b}. A value of 100% H$_2$O would be unlikely because silicate, metal and H$_2$O would tend to be mixed in proportions in the protoplanetary nebula.

The H$_2$O-rich planets could be roughly divided into two types:

1. planets with their bulk H$_2$O in the solid phase, or solid H$_2$O-rich planets

2. planets with their bulk H$_2$O in the fluid phase (including molecular, ionic, or plasma phases), like Uranus and Neptune in our solar system but smaller, the so-called mini-Neptunes

It is of particular interest to distinguish between the two types. Furthermore, it would be interesting to know if a planet could transition from one type to the other through thermal evolution, such as the heating or cooling of its interior. The division between the two types depends on the phase diagram of H$_2$O and the mass, the bulk composition, and the interior temperature profile of the planets being considered. Thus the goal of this paper is to identify regions and boundaries on the mass-radius (M-R) diagram in order to distinguish planets with different phases of H$_2$O within their interior and to understand how the phases of H$_2$O in the interior could change as planets cool through aging.

The baseline interior structure model is taken from \cite{Zeng2013} and \cite{Zeng2008}. Here we simplify a H$_2$O-rich planet to a fully differentiated
CHAPTER 3. THERMAL EVOLUTION OF H₂O-RICH PLANETS

planet composed of two distinct layers: a MgSiO₃ (silicate) core and an H₂O mantle. More detailed three-layer model including the metallic iron is available online, http://www.astrozeng.com as a user-friendly interactive tool.

3.2 H₂O Phase Diagram

The low-pressure and low-temperature phase diagram of H₂O is notorious for its rich and complex structure. At pressures below ~ 3GPa and temperatures below ~ 500 K, the hydrogen bond is mostly responsible for the diversity of phases. However, the high-pressure and high-temperature phases of H₂O appear to be similarly complex (the transitions between ~1000 K and 4000 K), as one approaches the plasma phase of H₂O and its dissociation at higher temperatures. The interplay between oxygen atom packing and proton mobility seem to account for much of that complexity.

The pressure-temperature plot (Figure 3.1) shows different H₂O phases in the pressure-temperature regime of interest. The phase boundaries are drawn approximately and are obtained either through experiments (summarized by Chaplin (2012)) or by first-principle ab initio simulations (French et al. 2009; Redmer et al. 2011). The region marked ”molecular fluid” lies above the critical point of H₂O (T_c = 647 K, P_c = 22 MPa), i.e., supercritical fluid. The transitions between molecular, ionic, and plasma fluids are gradual (Redmer et al. 2011).

Various structures of Ice XI have been postulated to exist at ultra-high pressure beyond Ice X by ab initio simulations. Those structures are yet to be confirmed by experiments (Hermann et al. 2012; Militzer & Wilson 2010).
CHAPTER 3. THERMAL EVOLUTION OF H₂O-RICH PLANETS

The phase above (higher temperature) the previously known solid forms of Ice VII and Ice X is the "superionic" H₂O. Superionic solids are known previously for other materials, e.g., PbF₂ and AgI. However, for H₂O the phase was first predicted theoretically (Cavazzoni et al. 1999; Goldman et al. 2005) and confirmed later by experiments (Ji et al. 2011). In particular, superionic H₂O is characterized by a preserved stable oxygen lattice and mobile protons. The ionic conductivity of protons is primarily responsible for the electrical conductivity. The properties of superionic H₂O may have remained as an exotic bit of high-pressure physics, if not for the fact that the pressure-temperature profiles of some super-Earths seem to pass close to the triple point between fluid, superionic, and high-pressure ice phases of H₂O.

3.3 Thermal Evolution of H₂O-rich Planet

The thermal evolution models of a 50wt% MgSiO₃-50wt% H₂O planet, of masses 2, 6, 18.5 M⊕, each of age 2, 4.5, and 10 Gyr (billion years), are considered here. The equation of state (EOS) is from Zeng & Sasselov (2013). Figure 3.2 illustrates one example of the models.

Figure 3.1 shows the thermal gradients of the models. The three red curves are the models of 18.5 M⊕ and 2.7 R⊕ (large super-Earth, similar to Neptune in terms of mass), of three different ages (2, 4.5 and 10 Gyr). The three pink curves are the models of 6 M⊕ and 2 R⊕ (midsize super-Earth), and the three magenta curves are the models of 2 M⊕ and 1.5 R⊕ (small super-Earth, slightly bigger than Earth). Irradiation by the parent star can have a great effect on the results; most of the super-Earths known today are close to their parent stars. Such planets will stay warm longer. This could increase
CHAPTER 3. THERMAL EVOLUTION OF H₂O-RICH PLANETS

Figure 3.1: Pressure-temperature profiles of H₂O-layer of various super-Earth models of different ages, over the H₂O phase diagram. The thick black curve is the solid-fluid boundary (melting curve). Three thin black curves are the adiabats calculated from Vazan et al.’s (2013) EOS for comparison. The blue dot-dashed line shows the adiabat for Kepler-68b at the estimated age of 6.3 Gyr. The nine thermal gradient models as well as the Kepler-68b model are tabulated in Table 4.1. The surface pressure of each model is defined as 1 bar (10⁵ Pa), far beyond the left limit of the diagram. The dotted line indicates the continuous transition from molecular to ionic fluid due to dissociation (more than 20% of the water molecules dissociated), the dashed line indicates the continuous transition from ionic to plasma fluid due to ionization (electronic conductivity > 100Ω⁻¹ cm⁻¹) in the dense fluid. The boundary between Ice X and Ice XI is still subject to experimental verification.
**Figure 3.2:** Two-layer super-Earth of $2 \, M_{\oplus}$ and $1.5 \, R_{\oplus}$ at 4.5 Gyr. The interior temperature profile of the H$_2$O-layer of this model is represented by the solid magenta curve in Figure 3.1.
CHAPTER 3. THERMAL EVOLUTION OF H₂O-RICH PLANETS

the length of time they are habitable. For example, the equilibrium temperature of Kepler-68b is estimated to be around 1200 K (Gilliland et al. 2013), which would have retarded the cooling of the planet from the surface down to about 10 GPa depth at its current estimated age of 6.3 Gyr.

In order to obtain the initial thermal states to scale from, we have two options. Since we know a lot more details of interior thermal states of solar system planets, compared to exoplanets, it is a good starting point of our model. Most of these H₂O-rich planets lie in between Neptune and Earth in terms of their mass and radius; thus we could either scale up from Earth, or scale down from Neptune. Earth is not a H₂O-rich planet, so it would make more sense to scale from Neptune. Therefore, we start with Neptune’s interior adiabat at the current of age of 4.5 Gyr. We fit an analytical line in log$p$-log$T$ space to Neptune’s adiabat (Redmer et al. 2011). Then we scale the adiabat to planets of different mass and radius according to essentially their core-mantle boundary temperature $T_1$ and pressure $p_1$, by looking at the similar scaling law of planets in our solar system. Finally, we evolve this scaled adiabat backward or forward to different ages using the rheology law derived in Equation (3.2). In this way, we derive a simple analytical model of planet’s interior temperature as a function of its age and pressure: Equation (3.1), and Table 4.1 for a few cases.

Comparing Figure 3.2 to the same model (2 $M_\oplus$, 4.5 Gyr) represented by the solid magenta curve in Figure 3.1, one can see that a small segment of the $P-T$ curve toward the right end (the region near the H₂O-silicate boundary) would correspond to a significant mass fraction of H₂O inside the planet because the pressure scale is logarithmic in the diagram. A simple rule of thumb is that, for the H₂O below the depth of 50% $p_1$ (half the H₂O-silicate boundary pressure), it contains $\sim$ 40% the total H₂O.
CHAPTER 3. THERMAL EVOLUTION OF H$_2$O-RICH PLANETS

mass, and for the H$_2$O below 10% p$_1$ (one-tenth the H$_2$O-silicate boundary pressure), it contains > 80% H$_2$O mass. For example, the mass of the solid H$_2$O in the 2 M$_\oplus$ 4.5 Gyr-old planet is 0.174 M$_\oplus$; this is the model illustrated in Figure 3.2.

The thermal evolution models (the nine thick $P - T$ profiles in Figure 3.1) are calculated by the following equation:

$$T[\tau,p_1][p] = 10^{-2.15} \times \frac{4.5 \text{ Gyr}}{\tau} \times \sqrt{\frac{p_1}{1 \text{ Pa}}} \times \left(\frac{p}{p_1}\right)^{0.277}$$  \hspace{1cm} (3.1)

Here $p_1$ is the pressure (in Pa) at the H$_2$O-silicate boundary (i.e., the pressure at the bottom of the H$_2$O layer). $\tau$ is the age of the planet in units of billions of years (Gyr); $p$ is an arbitrary pressure within the H$_2$O layer; and $T[\tau,p_1][p]$ calculates the corresponding temperature (in Kelvin). The cooling rate can also be influenced by the phase of the H$_2$O in the mantle (different Rayleigh numbers, different convection speeds in different phases, etc.). Equation (3.1) assumes a constant cooling rate for all solid phases of H$_2$O. It also assumes that the cooling of the planet is primarily controlled by the viscosity of the solid part of the planet. This assumption is robust as long as the heat transfer mechanism outward is dominated by the temperature-dependent viscosity-driven solid-state convection in the mantle or core. As long as the viscosity has an exponential dependence on temperature, the scaling law is the same. In some cases, mainly in the

1Pressure (in giga-Pascal, 10$^9$ Pa).

2Fraction of H$_2$O mass (out of total H$_2$O) above the corresponding pressure/depth.

3Depth measured from the surface downward in kilometers.

4Density (in g cm$^{-3}$) at the corresponding pressure/depth.

5Temperature (in Kelvin) of the age indicated in parentheses.
## Table 3.1: Table of the Pressure-Temperature Profiles of H₂O layer

<table>
<thead>
<tr>
<th>Model 1: 2.001 M⊕, 1.533 R⊕</th>
<th>( p ) (GPa)</th>
<th>Mass Fraction</th>
<th>Depth (km)</th>
<th>Density (g cm(^{-3}))</th>
<th>( T ) (2 Gyr)</th>
<th>( T ) (4.5 Gyr)</th>
<th>( T ) (10 Gyr)</th>
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<table>
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<th>( T ) (4.5 Gyr)</th>
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<th>Mass Fraction</th>
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<th>Density (g cm(^{-3}))</th>
<th>( T ) (2 Gyr)</th>
<th>( T ) (4.5 Gyr)</th>
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| 600                       | 1.29        | 0.939         | 8.10      | 600             | 2880        | 1810        |
| 900                       | 0.148       | 0.443         | 9.08      | MgSiO₃ post-perovskite (ppr) |
| 900                       | 0.148       | 0.443         | 9.29      | ppr dissociates to MgO and MgSiO₃ |
| 1000                      | 0           | 0             | 9.61      | center of the planet |
early evolution, solid H\textsubscript{2}O part does not yet exist; however, the silicate core of the planet still remains solid. So the assumption here is that the cooling rate of the planet is still controlled by the bottleneck, which is how fast the solid part could convect out heat.

Phase transitions from fluids to solids are generally exothermic and release energy (latent heat); thus it could also have an influence on the temperature evolution when the H\textsubscript{2}O in the planet interior transitions from fluid to solid phase, retarding the cooling at the phase transition boundary. However, current experiments could not reach that pressure-temperature regime to measure the latent heat of phase transition yet, and the theoretical calculation has large uncertainties. Therefore, we choose to ignore the latent heat for now.

The temperature gradient in the fluid part of the H\textsubscript{2}O layer should be adiabatic. Because the viscosity of a fluid is small, any deviation from adiabat would be quickly offset by convection. For the solid part of the H\textsubscript{2}O layer, as pointed out by Fu et al. (2010); O’Connell & Hager (1980), the bulk H\textsubscript{2}O ice mantle would exhibit a whole-mantle convection without partitioning inside, so it is reasonable to approximate the thermal gradient as an adiabat also.

Equation (3.1) represents a family of adiabats, characterized by the same slope in log\textsubscript{P}-log\textsubscript{T} plot, scaling to different characteristic interior temperatures (\textit{T}_i).

Equation (3.1) is obtained by downscaling the pressure-temperature profile of the interior of Neptune (Redmer et al. 2011) according to the pressure at the H\textsubscript{2}O-silicate boundary, and assuming the cooling of the planet is primarily controlled by the rheology (viscosity) of the solid part of the planet (the bottom solid H\textsubscript{2}O layer, and predominately the silicate core underneath), that is, by how strong the solid part of the
planet can convect and transport the heat out. Following the argument in Turcotte & Schubert (2002), assuming an exponential dependence of the viscosity on the inverse of temperature

\[ \mu = \mu_r \times \exp\left( \frac{E_a}{RT} \right) \] (3.2)

(where \(\mu_r\) is a constant of proportionality, \(E_a\) is the activation energy, and \(R\) is the gas constant) and including the contribution of the radioactive heat sources, one could derive a result showing that the characteristic interior temperature \(T_i\) of a planet is, to the first order, inversely proportional to its age. Vazan et al. (2013) modeled the evolution of giant and intermediate-mass planets. Three adiabats (thin curves in Figure 3.1) calculated from their H\(_2\)O EOS in the region of validity (private communication) are shown to match quite well with our \(P - T\) profiles’ gradients, confirming the validity of Equation (3.1). However, it should be noted that Equation (3.1) should only be taken as a qualitative order-of-magnitude estimate because the actual thermal gradient may depend on many other factors, such as different abundance of the radioactive elements in the interior, different initial thermal states, and the surface boundary conditions of the planet.

The slope of the adiabats are in general shallower than the melting curve, suggesting that for high enough pressure, the adiabat trend would usually intersect the melting curve and result in the high-pressure ice phases or superionic phase usually sitting at the bottom of the fluid phase but not the other way around.
3.4 Implications and Importance of the Models

Comparing Equation (3.1) to the H$_2$O phase diagram shows that, as a H$_2$O-rich planet ages and cools down, its bulk H$_2$O may undergo phase transition, first from fluid phases to superionic phase, then from superionic phase to high-pressure ices. The timing of these phase transitions would depend on the pressure $p_1$ at the bottom of the H$_2$O layer, the initial thermal state of the planet, the abundance of radioactive elements in the interior, and so on. These phase transitions may affect the radius of the planet only slightly, but they may significantly affect the interior convective pattern of the planet and also the global magnetic field of the planet, which results from the dynamo action inside the planet, which in turn depends on the strength of convection, differential rotation, and the electrical conductivity of the convective layer. The existence of the superionic layer is especially favorable for the dynamo action to take place, speculated as probably what is happening in Uranus and Neptune now. As pointed out by Stanley & Bloxham (2006) and Redmer et al. (2011), the nondipole magnetic fields of Uranus and Neptune are presumably due to the presence of a conductive superionic H$_2$O shell surrounding the solid core acting as a dynamo. Such a scenario could similarly exist on other planets that possess such an electrically conductive region (superionic, ionic or plasma phase) of H$_2$O or other species. The implication of the existence of a global magnetic field on the habitability of the planet is also significant, as has been suggested by some people (Ziegler & Stegman 2013; Bradley 1994), and manifested by our own Earth, that the existence of the magnetic field of Earth shortly after its formation is intimately tied to the origin of life on Earth because it protects the atmosphere from high-energy particles, and the atmosphere in turn shields the harmful UV radiation from
CHAPTER 3. THERMAL EVOLUTION OF H₂O-RICH PLANETS

the host star. The magnetic field may have something to do with the origin of chirality of biomolecules such as RNA and protein.

3.5 Mass-Radius Diagram and H₂O Phase Regions

The mass fraction of H₂O out of the total planet mass is varied from 25% to 75% in the two-layer model, to show the correspondence between different regions of the $M - R$ diagram to different phases of near-bottom H₂O for planets of different ages (Figure 3.3).

The various colored regions in Figure 3.3 could be compared to the measured masses, radii and ages of observed exoplanets to help us understand the phases of H₂O of those planets within this mass range and its implications for planet thermal evolution, convection, magnetic field and habitability. The transport and mixing of volatiles will be different in planets with solid H₂O mantle rather than fluid (Levi et al. 2013), and that will affect the composition of their atmospheres. For Kepler-68b, there is an accurate age measurement of $6.3 \pm 1.7$ Gyr from asteroseismology (Gilliland et al. 2013), which when combined with our model would indicate the presence of solid superionic H₂O in its interior.

One thing to point out is that in our model we have not considered the possible existence of a thick gaseous envelope/atmosphere (such as H/He) that could overlie the H₂O layer and increase the observed radii of planets. This gaseous envelope might act as a thermal blanket that would slow the cooling of the planet (Stevenson 2013), and instead of interior temperature $T_i \sim \tau^{-1}$, it will go as $T_i \sim \tau^{-1/3}$ or even slower. However, because of its low density, it would not increase the interior pressure significantly. We
Figure 3.3: Mass-radius diagram as a function of cooling age corresponding to different phases of H$_2$O near the H$_2$O-silicate boundary, for H$_2$O-silicate planets with H$_2$O mass fraction from 25% to 75%, of different ages (2, 4.5, 6.5, and 10 Gyr). Exoplanets close to the region of interest are shown, as well as recently discovered KOI 69.01 (Ballard et al. 2013) and Kepler-78b (Pepe et al. 2013).
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We hope to explore this aspect more in future research.

3.6 Conclusions

We use simple two-layer (silicate-core and $H_2O$-mantle) planet models to understand the thermal evolution of $H_2O$-rich planets. The interior pressure versus temperature profiles of nine specific models are plotted over the $H_2O$ phase diagram to show the existence of different phases of $H_2O$ with the thermal evolution of the planets.

The cooling of a $H_2O$-rich planet results in its bulk $H_2O$ content transitioning first from fluid phases to superionic phase, and later from the superionic phase to high-pressure ices. These transformations may have a significant effect on the interior convective pattern and also the magnetic field of such a planet, but they may only affect the overall radius slightly.

Different regions in the mass-radius phase space are identified to correspond to different phases of $H_2O$ near the bottom of the $H_2O$ layer in a $H_2O$-rich planet, which are usually representative of the bulk $H_2O$ in the entire planet (because of the logarithmic pressure scale, a small portion of $P - T$ profile toward the right end would correspond to a considerable amount of $H_2O$ by mass). In general, super-Earth-size planets (isolated or without significant parent star irradiation effect) older than about 3 Gyr would be mostly solid. These regions could be compared to observation, to sort the exoplanets into various $H_2O$-rich planet categories, and help us understand the exoplanet population, composition, and interior structure statistically.
CHAPTER 3. THERMAL EVOLUTION OF H$_2$O-RICH PLANETS

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Chapter 4

New Semi-empirical Mass-Radius Relation for Rocky Exoplanets based on the Earth’s Seismic Model

*This thesis chapter has recently been submitted as*

**L. Zeng**, D. Sasselov, S. Jacobsen, submitted to


**Abstract**

Several small dense exoplanets are now known, inviting comparisons to Earth and Venus. Such comparisons require translating their masses and sizes to composition models of evolved multi-layer-interior planets. Such theoretical models rely on our understanding of the Earth’s interior, as well as independently derived equations of state (EOS), but
rarely involve direct extrapolations from Earth’s seismic model. In order to facilitate more detailed compositional comparisons between small exoplanets and the Earth, we derive here a semi-empirical mass-radius relation: 

\[
\frac{M}{M_\oplus} \approx 0.94 \left(\frac{R}{R_\oplus}\right)^{3.72},
\]

based on Earth’s seismic model and useful in the mass range for rocky exoplanets between 1 and 10 M\(_\oplus\). By assuming commonality in the geophysical processes, we describe the corresponding theoretical uncertainties in the radius of an exoplanet of a given mass. These uncertainties are then compared to the scatter observed around the tight correlation seen for rocky exoplanets and corresponding to the different photospheric elemental abundances measured in their hosts stars. This work confirms that the tight correlation seen in the small dense exoplanets around the same fixed ratio of iron and magnesium silicate as Earth and Venus might be indicative of common geochemistry around the bulk elemental abundances of such planets.

4.1 Introduction

A first step in deriving the compositional diversity of small rocky planets was accomplished recently by [Dressing et al., 2014], who added Kepler-93b to the list of a dozen or so small exoplanets with radii and masses measured to better than 20% precision. With exquisite sizes (mostly from Kepler light curves) and huge follow-up effort [Dressing et al., 2014; Pepe et al., 2013; Batalha et al., 2011; Ballard et al., 2013; Carter et al., 2012; Hatzes et al., 2011] the mass-radius diagram is finally amenable to some detailed comparisons with theory in the 1 to 10 M\(_\oplus\) range. Closer to the mass and size of Earth, the rocky planets known to-date seem to exhibit an unexpectedly tight compositional correlation. Is this correlation really shared with Earth and Venus? If so,
CHAPTER 4. NEW SEMI-EMPIRICAL MASS-RADIUS RELATION FOR ROCKY EXOPLANETS BASED ON THE EARTH’S SEISMIC MODEL

to what level of precision and under what assumptions?

To begin answering such questions we must first acknowledge that models of the interior structure and composition of rocky exoplanets in the Super-Earth domain are based largely on experience (and extrapolations) from the models of the rocky solar system planets, and mostly - the Earth (Valencia et al. 2006, 2007b,a; Fortney et al. 2007; Seager et al. 2007; Zeng & Seager 2008; Grasset et al. 2009; Zeng & Sasselov 2013). On the other hand, the Earth is known to have significant amounts of light elements in its core with significant effect on its mean density, but such details are not captured by the bulk interior models used in the mass-radius diagrams for exoplanets. This is understandable, as there is no general (and generally accepted) model that translates initial elemental abundances, as measured in the host star’s photosphere, to the detailed distribution and bulk ratios of those inside a given rocky planet. In anticipation of finding geophysical processes that are common among rocky planets, it is good to compare the Earth to the mean densities and stellar abundances for exoplanets on the same basic assumptions. We try to do this by deriving a semi-empirical relation by extrapolating from the well-constrained seismic model of the Earth.

4.2 New Mass-Radius Relation

4.2.1 Equation of State (EOS)

On one hand, in several previous models of solid exoplanets (Zeng & Sasselov 2013; Zeng & Seager 2008; Seager et al. 2007), the cores and the mantles of these solid exoplanets are modeled as pure-Fe-metal and pure-Mg-perovskite/post-perovskite.
On the other hand, we know the actual density variation inside Earth through measurements of seismic wave traveling velocities. This seismically derived density model is widely known as the PREM (Preliminary Reference Earth Model \cite{Dziewonski81}).

The differences between the two can cause differences in the mass-radius relations derived. As such it is better to model solid exoplanets using an EOS extrapolated from the PREM.

For Earth’s core, it is less dense than pure-Fe due to the presence of approximately 10 percent lighter components in the core. There still does not appear any consensus on what the lighter components are. There are various suspicions that these lighter components may include O, Si, S, C, K, and many others \cite{Badro07,Alfe02,Poirier94,Stixrude97,Anderson94}.

We choose to only extrapolate the outer (liquid) core EOS to higher pressure, as the inner (solid) core is a secondary feature derived from the crystallization of the outer (liquid) core. It is only a small fraction (≈ 3%) of the mass of the Earth, and it may or may not exist on other planets. Essentially, it is an extrapolation along an isotherm of the Earth’s outer core. So at the inner core-outer core boundary pressure of 328.85 GPa, we scale down (by a factor of 1.12881) the pure-Fe EOS \cite{Anderson01,Seager07,Zeng13} to match the density of PREM at 328.85 GPa and maintain this ratio throughout high pressures. Similarly, at the core-mantle boundary pressure of 135.75 GPa, we scale down (by a factor of 1.16758) the pure-Fe EOS \cite{Anderson01,Seager07,Zeng13} to match the density of PREM at 135.75 GPa and maintain this ratio throughout lower pressures. In
this way, we produce a full semi-empirical EOS for core based on the PREM (see Fig. 4.1 Panel 1).

For Earth’s mantle, it is also less dense than pure $MgSiO_3$-perovskite (pv)/post-perovskite (ppv). In particular, the Earth’s upper mantle is made up of complex phases of Mg-silicates (including various polymorphs of olivine including $\alpha$-, $\beta$-, and $\gamma$-olivine), which are less dense than pure-Mg-pv/ppv.

We choose to make the EOS follow the PREM precisely up to the pv-ppv phase transition at 122 GPa. Then at 122 GPa we scale down the EOS of $MgSiO_3$ (Zeng & Sasselov 2013; Caracas & Cohen 2008) (by a factor of 1.00956) to match the PREM and ensure the 1.4% density jump from Mg-pv to Mg-ppv. And we maintain this ratio throughout higher pressures. Thus, we have included all the phase transitions at higher pressures:

122 GPa: $MgSiO_3$ pv $\rightarrow$ $MgSiO_3$ ppv (Caracas & Cohen 2008)
900 GPa: $MgSiO_3$ ppv $\rightarrow$ MgO and $MgSi_2O_5$ (Umemoto & Wentzcovitch 2011)
2100 GPa: MgO and $MgSi_2O_5$ $\rightarrow$ MgO and $SiO_2$ (Umemoto & Wentzcovitch 2011)

In this way, we produce a full semi-empirical EOS for mantle based on the PREM (see Fig. 4.1 Panel 2).

Fig. 4.2 shows the difference in mass-radius CMF (core mass fraction) contours as a result of the different EOSs. Because the PREM-extrapolated EOS is softer than the pure EOS, the contours shift upwards. This upward shift is tabulated in Table 4.1. As a rule of thumb, this upward shift is approximately 0.1 in CMF, or, equivalently, 2 to 5 percent in radius (0.01-0.02 dex).
Figure 4.1: Panel 1 (upper panel): semi-empirical EOS for core (red, compared to PREM (green) and pure-Fe EOS (blue (Anderson et al. 2001; Seager et al. 2007; Zeng & Sasselov 2013))). Panel 2 (lower panel): semi-empirical EOS for mantle (red, compared to PREM (green) and the previous silicate EOS (blue (Zeng & Sasselov 2013; Caracas & Cohen 2008))).
Figure 4.2: Mass-Radius diagram in log-log scale. Two sets of curves are shown. The red curves are the mass-radius contours of solid exoplanets derived from the PREM-extrapolated EOS. The contours correspond to CMF from 0 to 1 with stepsize 0.1. The dashed green curves are the mass-radius contours derived from the previous Fe and silicate EOS (Zeng & Sasselov 2013).
CHAPTER 4. NEW SEMI-EMPIRICAL MASS-RADIUS RELATION FOR ROCKY EXOPLANETS BASED ON THE EARTH’S SEISMIC MODEL

4.2.2 Power-law M-R relation

Dressing et al. (2014) pointed out a very tight mass-radius relation of solid exoplanets between 1 and 6 M⊕ from current observation of 5 exoplanets. Applying the PREM-extrapolated EOS, this tight relation for the 5 exoplanets centers on a CMF of 26%, or close to 0.3 (shown as the thick blue curve in Fig. 4.3, the 4th contour counted from above), near the Earth’s core mass fraction of 32.5%.

CMF=0.26 can be fit to a power-law (applying to 1 ∼ 12 M⊕) that will correspond to the empirical relation found by Dressing et al. (2014).

\[
\left( \frac{M}{M_{\oplus}} \right) \approx 0.94 \left( \frac{R}{R_{\oplus}} \right)^{3.72}
\]

\[
\left( \frac{R}{R_{\oplus}} \right) \approx 1.017 \left( \frac{M}{M_{\oplus}} \right)^{0.269}
\]

\[
\left( \frac{\rho}{\rho_{\oplus}} \right) \approx 0.94 \left( \frac{R}{R_{\oplus}} \right)^{0.72} \approx 0.95 \left( \frac{M}{M_{\oplus}} \right)^{0.194}
\]

Eq. 4.3 can be used to normalize the density of any exoplanet to one Earth-mass, canceling out the compression effect due to pressure and leaving behind only the compositional effect. (e.g. HIP 116454b’s (Vanderburg et al. 2015) bulk density is ∼4 g/cm³. Its mass is ∼12 M⊕. Eq. 4.3 gives its normalized density as 2.5 g/cc. Alternatively, one can use its radius of ∼2.5 R⊕ to similarly derive a normalized density of 2.1 g/cc. Both of these are less than the density of a pure-rock composition (4.5 g/cm³) at 1 M⊕ and, of course, an Earth-like composition (5.5 g/cm³, 30% metal core, plus 70% rock). As a result, it probably has a significant volatile envelope.)
Figure 4.3: The 7 dashed curves are iso-bulk-density contours of 4, 5, 6, 7, 8, 9, and 10 g/cm$^3$ counted from above. The solid curves are mass-radius contours color-coded with CMF from 0 to 1. They have shallower slopes than the dashed iso-density contours due to pressure compression effects. Several rocky exoplanets with mass measurements at better than 20% accuracy are shown. (Pepe et al. 2013; Batalha et al. 2011; Dressing et al. 2014; Ballard et al. 2013; Carter et al. 2012; Hatzes et al. 2011)
CHAPTER 4. NEW SEMI-EMPIRICAL MASS-RADIUS RELATION FOR ROCKY EXOPLANETS BASED ON THE EARTH’S SEISMIC MODEL

Fig. 4.4 shows a mass-radius plot in log-linear scale, with planets color-coded by the stellar flux they receive, or, equivalently, their surface temperatures (Here it is assumed that these planets have similar bond albedo as the Earth (≈0.3), and perfect heat redistribution based on blackbody absorption and re-radiation into space). For the 5 exoplanets between 1 and 6 $M_\oplus$, it appears that this tight mass-radius relation of CMF=0.26 holds well, probably due to many of them being hot enough (1000~2000K surface temperature), old enough (1~few Gyr) and small enough ($\leq 1.6 R_\oplus$), resulting in no, or insignificant, amounts of volatiles. Beyond 6 $M_\oplus$, or, equivalently, 1.6 $R_\oplus$, some exoplanets start to deviate from this tight mass-radius relation by various degrees, while others may still remain on this tight mass-radius relation thus possess an Earth-like composition. The degrees of deviation likely depend on three factors: the composition and mass fraction of the volatile envelope, the age, and the stellar flux a planet receives. See [Lopez & Fortney 2014] and references therein.

For the convenience of comparison and calculation, we provide the following Table 4.2 which lists the CMF=0.26 planets of 1, 2, 5, 10, and 20 Earth Masses, their radii, interior pressures, comparison with the interiors of solar system planets, and the experimental methods that can reach these pressure ranges and test the validity of the model. The data of the solar system bodies are taken from [Lodders & Fegley 1998].

4.3 Discussion

In order to understand why the core mass fractions of 0.2~0.3 are common for rocky exoplanets, we need to look at the four major planet building elements: Fe, Mg, Si, and O. Together, they make up more than 90% of the mass of any terrestrial body in our

In our solar system, evidence suggests that rocky bodies were formed from chondrites. Chondrites are undifferentiated meteorites which condensed out of the solar nebula at the very beginning of our solar system. They are believed to be the building blocks of planets. They coalesced to form planetesimals, and, eventually, planets. Their elemental abundance is almost identical to that of the Sun except for a few of the most volatile elements, including C, N, and O, as well as Li, which was depleted in the early Sun due to nuclear reactions.
CHAPTER 4. NEW SEMI-EMPIRICAL MASS-RADIUS RELATION FOR ROCKY EXOPLANETS BASED ON THE EARTH’S SEISMIC MODEL

The solar nebula was initially heated to very high temperature to the extent that virtually everything was vaporized except, for a small quantity of presolar grains. Then, as the nebula cooled, various elements and mineral assemblages started to condense out from the vapor at various condensation temperatures following the condensation sequence. Fe-Ni metal alloy and Mg-silicates condense out at approximately the same temperature range of 1200-1400K (depending on the pressure of the nebula gas) according to thermodynamic calculation (Lodders 2003). Oxygen, on the other hand, does not have a narrow condensation temperature range, as it is very abundant and it readily combines all kinds of metals to form oxides which condense out at various temperatures as well as H, N, C to form ices which condense out at relatively low temperatures (Lewis 1997).

The Fe to Mg to Si element atomic ratio in solar system chondrites is close to 0.9 : 1 : 1 (McDonough & Sun 1995). The solar ratio of Fe/Si is representative for the stars in the solar neighborhood, which is a tight distribution centered at 1, while the Mg/Si=1 seems to be towards the lower end of the distribution centered at 1.34 (Gilli et al. 2006; Grasset et al. 2009). A Mg/Si ratio higher than 1 results in more olivine ($MgSiO_4$) and even more MgO, thus affect the mineralogy and the EOS of the silicate mantle (Bond et al. 2010; Delgado Mena et al. 2010).

There is almost an order of magnitude more O available than Fe, Mg, or Si (Lodders 2003), as it is richly produced in the nuclear synthesis of massive stars and chemical evolution of the Galaxy (Pagel 1997). Therefore, there is always enough O, to combine with Mg and Si to form Mg-silicates. This will produce outright a core mass fraction of approximately 0.3. However, considering the partial oxidization and incorporation of Fe into the silicates, the core mass fraction can thus vary from 0.2 to 0.3.
CHAPTER 4. NEW SEMI-EMPIRICAL MASS-RADIUS RELATION FOR ROCKY EXOPLANETS BASED ON THE EARTH’S SEISMIC MODEL

This semi-empirical mass-radius relation is also consistent with the mass-radius relation of super-Earths presented in Valencia et al. (2006), which is a scaling law of $R \propto M^{0.267-0.272}$.

Acknowledgement

The author Li Zeng would like to thank Courtney Dressing and Lars Buchhave for inspiring discussions.
Table 4.1: Theoretical uncertainties in mass-radius relation based on the EOS uncertainties. R is in unit of Earth Radius \((R_\oplus = 6.371 \times 10^6 m)\). \(\epsilon\) is the fractional upward shift.

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<th></th>
<th>1 M(_\oplus)</th>
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<th>5 M(_\oplus)</th>
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Table 4.2: Reference data for 2-layer metal-rock planets with CMF=0.26.

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<th>Mass ($M_\oplus$)</th>
<th>Radius ($R_\oplus$)</th>
<th>$p_0$ (central pressure in GPa)</th>
<th>$p_1$ (core-mantle boundary pressure in GPa)</th>
<th>comments/examples</th>
<th>tools/methods</th>
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</thead>
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<td>1</td>
<td>1.01</td>
<td>340</td>
<td>150</td>
<td>Earth’s Interior</td>
<td>Diamond Anvil Cell: few hundred GPa</td>
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<td>2</td>
<td>1.23</td>
<td>650</td>
<td>280</td>
<td>Neptune’s Core: 800 GPa</td>
<td>Gas-Gun Shock Wave: 600 GPa</td>
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<td>5</td>
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<td>1600</td>
<td>680</td>
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<td>10</td>
<td>1.87</td>
<td>3400</td>
<td>1400</td>
<td>Saturn’s Core: 4200 GPa</td>
<td>NIF Laser-driven shock wave: 5000 GPa</td>
</tr>
<tr>
<td>20</td>
<td>2.20</td>
<td>7700</td>
<td>3200</td>
<td>Jupiter’s Core: 7000 GPa</td>
<td>Z-machine shock wave: 10,000 GPa or 10 TPa</td>
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Chapter 5

Modeling the Elemental Abundances of Rocky Planets

This thesis chapter is to be submitted as

L. Zeng, S. Jacobsen, D. Sasselov, to be submitted to PNAS

Abstract

We often compare exoplanets to our solar system planets. In this work we take this a step further, by applying lessons learned from our solar system formation to describe in bulk comparative terms the elemental abundances of rocky exoplanets. During formation, a rocky planet is depleted in volatile content, compared to its host star. Then, core formation due to heat from radioactive decay and collisions further depletes a planet’s rocky mantle of siderophile elements. Following this, rocky planets likely accrete some volatile-rich materials, called a "late veneer". This late veneer is essential to the origins
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

of life on rocky planets, as it delivers volatiles such as nitrogen, sulfur, carbon and water to their surfaces. We build an integrative model of rocky planets, to infer their chemical compositions from their mass-radius relations and their host star elemental abundances, and to understand the origins of volatile contents (especially water) on their surfaces, thereby shedding light on the possible origins of life on them.

5.1 Introduction

A rocky (terrestrial) planet is a planet that is composed primarily of silicate rocks and an iron-nickel metal core. In our solar system, all the inner planets, including Mercury, Venus, Earth, Mars, and some bigger bodies in the Asteroid belt (e.g., Vesta and Ceres) are rocky planets.

A broader definition of rocky planets would encompass some of the planets found orbiting other stars, the exoplanets. We can define these rocky planets as planets which have lost volatiles in a systematic manner. Since the protostellar nebulae and protoplanetary disks are rich in gaseous contents, the formation process of a rocky planet must somehow deplete most of its volatiles in order to produce a planet that is dominated by refractory elements forming silicate rocks and metals.

The understanding of rocky planets’ interior structures is primarily inferred from our understanding of that of the Earth’s. In general, we could model a rocky planet consisting of two layers, a metallic core and rocky mantle. The compositions of the core and mantle and their compression behavior under high pressure will determine the mass-radius relations of rocky planets.
There was previous work focusing on explaining the chemical compositions of the Earth (Allègre et al. 2001; Javoy et al. 2010) and Mars (Sanloup et al. 1999) based on the comparison with chondrites. Also, there has been chemical composition model proposed for both the solar system terrestrial bodies (Rubie et al. 2015) and the extrasolar terrestrial planets (Bond et al. 2010) from the planet formation perspective, as well as direct measurements of the elemental compositions of extrasolar rocky planetesimals accreted onto white dwarfs (Xu et al. 2014). Based on these previous models and measurements, this study proposes a general parametrized model which can be applied to both the solar system terrestrial bodies and the rocky exoplanets to estimate their elemental abundances from that of their host stars.

5.2 Important Links in Planet Formation

Planets and their host stars form together from the collapse of a nebula, such as the one illustrated in Fig. 5.1 (Step 1). As the nebula contracts under its self-gravity, it flattens out into a proto-planetary disk (Step 2) under the conservation of angular momentum. Within this disk, there are primitive building blocks of planets called chondrites (central link) which condense out. Chondrites coalesce to form planetesimals (Step 3), and, eventually, larger planet embryos (Step 4). There is volatile depletion associated with this process, due to the high temperatures associated with it (Allègre et al. 2001).

During this process, the interiors of the planetesimals and planet embryos are heated to melting by the accretional energy and the decay of radioactive elements (such as $\text{Al}^{26}$), which allows metals (primarily iron and siderophile elements) to separate from the silicates (lithophile elements). This is the process of core formation (Step 5) (Rubie et al.
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

Figure 5.1: Schematic diagram showing the six steps of formation of rocky planets. Image credits (from top going clockwise): orion nebula (NASA), protoplanetary disk (ESO), planetesimals forming within the disk (hubblesite.org), accretion and volatile depletion (copyright@Chris Bader, astro.virginia.edu), Earth’s core formation (dailymail.co.uk), late veneer (copyright@Tim Wetherell - Australian National University), and the central image of CI chondrites (meteorites4sale.net).
Eventually, as the planet cools down and the core formation process winds down, some minor objects deliver additional materials to the surface of the planet (Step 6) (Wang & Becker 2013; Schlichting et al. 2012; Holzheid et al. 2000). The volatiles that are depleted early on under high temperatures can now be retained on the surface for the first time as it is now cool enough. These materials are slowly mixed into the mantle of the planet as a result of mantle convection.

By properly modeling volatile depletion, core formation, and late delivery, we can establish a link from the host stellar elemental abundances to the planet’s elemental abundances.

5.2.1 Volatile Depletion

There is a systematic depletion of volatile elements in all terrestrial planets, compared to CI chondrites (the primitive meteorites that most closely resemble the elemental distribution of solar photosphere, and, thus, the solar nebula (Asplund et al. 2009; Lodders et al. 2009; Lodders & Fegley 2010)). The volatility of an element can be characterized by its 50% Condensation Temperature (T50), which is the temperature at which 50% of the element has condensed out of the gas phase into condensed (solid/liquid) phases, under the standard conditions (species-assemblage and pressure, e.g., 10^{-4} bar) assumed for the solar nebula in question. The condensation temperatures can be calculated in thermodynamic equilibrium condensation models, and be verified by the geochemical measurements of meteorites.

This systematic depletion trend can be observed when plotting the natural logarithm
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

of the relative elemental abundance (planet/CI), against the reciprocal of the 50% Condensation Temperature (1/T50) of each element (Grossman 1972; Petaev & Wood 1998; White 2013).

The most highly refractory elements show almost no depletion. Then, starting at (T50 critical), elements start to become depleted relative to CI abundance. The more volatile (easier to be vaporized) the element is (which is indicated by a lower T50, that is, higher 1/T50), the more depleted the element is in a rocky planet compared to CI chondrites. The slope of this depletion trend contains information about the accretional history of a rocky planet. Different rocky planets presumably have different volatile depletion slopes, depending on their distances from their host stars, and the geometry and evolution of the proto-planetary disks that formed them among others. Appropriate modeling of volatile depletion could help us constrain the compositions of rocky exoplanets from the elemental abundances of their host stars. As more and more of these planets are discovered, this method will be further employed.

When and where this depletion occurs in our solar system is still not well understood, but much of it must have occurred at the stage of chondrule formation, as most other classes of chondritic materials also show similar depletion trends relative to CI chondrites (e.g., CV and CM carbonaceous chondrites, compared to CI chondrites).

5.2.2 Core Formation

During accretion, rocky planets undergo the process of core formation (Stevenson 2008; Li & Fei 2003; McDonough & Sun 1995). Core formation occurs as a result of heating from the decay of early, short-lived radioactive elements (primarily 26Al) and the kinetic
energy from the accretion of these planetesimals and planet embryos and the collisions between them. The resulting heat melts a significant fraction of the planet and forms a molten magma ocean in the upper layer. Within this magma ocean, metal/silicate partitioning occurs, with lithophile elements (those showing an affinity for silicate phases) remaining and concentrated in the silicate portion, whereas the siderophile elements (which have an affinity for metallic liquid phases dominated by Fe), segregate from the silicates, sink towards the bottom and become concentrated in the core. Therefore, if we compare the elemental abundance of the bulk silicate portion of a planet to CI chondrites, there is a depletion of siderophile elements (such as Cu, P, and W among others), in addition to the volatile depletion trend.

The degree of siderophile depletion depends on each element’s affinity to the metal phases, as described by the metal/silicate partition coefficient, $D$. For moderately siderophile elements, such as Fe, Ni, Ga, Ge, Mo, and W, $1 < D \ll 10000$. For highly siderophile elements, such as the PGE (platinum-group elements, also known as the noble metals: Platinum, Osmium, Iridium, Ruthenium, Rhodium, and Palladium), $D > 10000$. As such, they almost entirely go into the core during core formation, with none left in the silicate portion of the planet (Lodders & Fegley 2010). For these, based on their metal/silicate partition coefficients, we expect a jagged pattern in their depletions. The fact that they lie along a horizontal trend, and that they are slightly more enriched in the mantle of the Earth than expected, strongly suggests that most of them have been delivered to the Earth (and likely, other rocky bodies as well) following core formation completion (Day et al. 2012).
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

5.2.3 Late Veneer

The PGE abundance in the Bulk Silicate Earth has been determined to be approximated 0.5% relative to CI chondrites—much higher than expected considering that they are partitioned into the core according to their strong siderophile affinities (Wang & Becker 2013; Holzheid et al. 2000; Morbidelli et al. 2000; Schlichting et al. 2012).

The late veneer is important to the origins of life on Earth and other rocky planets, as it delivers most of the volatiles (such as N, S, C and H$_2$O) crucial for life to occur and develop. These planets’ original volatiles were lost in the earlier stages of planet formation/accretion due to the high-temperatures associated with these processes, thereby becoming depleted on planets’ surfaces until they were later delivered when the crusts of the planets had cooled enough to retain them.

5.3 Comparison of Rocky Bodies in the Solar System

I have applied this model to the rocky bodies in our solar system. Table 5.1 gives the elemental abundances and ratios of five rocky bodies in our solar system: Venus, Earth, the Moon, Mars, and Vesta. For these, we have some direct measurements of their compositions through meteorite samples and surface probes. The four major elements of rocky planets: Fe, Mg, Si, and O, together, make up more than 90% of the mass of any rocky body (McDonough & Sun 1995, Lauretta 2011).

The fact that the relative proportions of these four elements remain roughly constant across all these bodies is due to Fe, Mg, and Si all having similar condensation temperatures. Therefore, they are not depleted relative to one another in the volatile
Table 5.1: Elemental Abundances of Earth-like Bodies in the Solar System

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<th>Element</th>
<th>Element wt%</th>
<th>CI Chondrites</th>
<th>Venus Silicate</th>
<th>Venus Core</th>
<th>Venus Bulk</th>
<th>Earth Silicate</th>
<th>Earth Core</th>
<th>Earth Bulk</th>
<th>Moon Silicate</th>
<th>Moon Core</th>
<th>Moon Bulk</th>
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<th>Mars Bulk</th>
<th>Vesta Silicate</th>
<th>Vesta Core</th>
<th>Vesta Bulk</th>
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<td>0.016 3.6 × 10^-4 0.112</td>
<td>0.805 0.022 0.107</td>
<td>3.56 × 10^-5 7.44 × 10^-6 4.3 × 10^-5</td>
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<td>68 0 44</td>
<td>66 0 54.6</td>
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<td>0 0 0</td>
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<td>C</td>
<td>3.5</td>
<td>0.012 0 0.0468</td>
<td>0.012 1 0.33</td>
<td>0 0 0</td>
<td>0.37 0 0.296</td>
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<td>K/U</td>
<td>74324.3232</td>
<td>10000 10000</td>
<td>11822.6601 11822.6601</td>
<td>1242 1242</td>
<td>18181.8181 19047.61905</td>
<td>3882 3882</td>
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<td>Ca/Al</td>
<td>1.08</td>
<td>1.12 1.09</td>
<td>1.08 1.08</td>
<td>1.13 1.13</td>
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<td>1.07 1.07</td>
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<tr>
<td>Mg/(Mg+Fe)</td>
<td>0.348</td>
<td>0.833 0.318</td>
<td>0.785 0.329</td>
<td>0.687 0.630</td>
<td>0.569 0.342</td>
<td>0.624 0.384</td>
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<tr>
<td>Mg/Si</td>
<td>0.906</td>
<td>0.927 0.919</td>
<td>1.06 1.016</td>
<td>1.034 1.034</td>
<td>0.869 0.841</td>
<td>0.888 0.888</td>
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CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

depletion process.

Iridium is a representative highly siderophile element belonging to the PGE. Its abundance in the Bulk Silicate Planet infers the amount of late delivered material. For Earth, it is approximated half a percent.

The Potassium (K) to Uranium (U) Ratio (K/U) is used to constrain the slope of the volatile depletion trend, as K is moderately volatile, whereas U is refractory (McDonough & Sun 1995). A higher K/U value indicates more volatiles are retained in the object. For CI chondrites, this value is ~70,000. Earth and Venus are similar, ~10,000. The Moon is only ~1000, about 10 times more depleted in volatile content compared to Earth or Venus, probably due to its Giant Impact Origin. Mars is ~20,000, almost twice as much as Earth or Venus. However, Vesta is ~4000, less than half of that of Earth or Venus, despite being further from the Sun than Mars is. This implies that volatile depletion is not a monotonic dependence on distance, but possibly on mass and the accretion history of the object, as well.

5.4 Model Setup

The model setup is as follows:

First, I define $E_{lj}$ to represent the abundance (wt%) of element $j$ within each geochemical reservoir.

The reservoirs include:

- CI: CI chondrites
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

- BP;i: initial Bulk Planet, before the addition of late veneer

- BSP;i: initial Bulk Silicate Planet, before the addition of late veneer, and after core formation

- Core: Planet’s core, after core formation, not affected by late veneer

- BP: final Bulk Planet, after late veneer

- BSP: final Bulk Silicate Planet, after core formation and after late veneer. Late veneer material is assumed to be gradually mixed into the mantle due to mantle convection.

- LV: late veneer, here assumed to have the same elemental abundance as CI chondrites

The processes of volatile depletion, core formation, and late delivery can be captured by 4 parameters:

- $x_0$, is the location (in $(\frac{10^4}{T}) - log_{10}(El^j)$ plot) where the elements start to become depleted.

- $b$, is the slope of the volatile depletion in the same plot.

- $\eta$, is the final Core Mass Fraction (CMF) of the planet (after late veneer).

- $\xi$, is the mass fraction of late veneer over the whole planet.

These 4 parameters ($x_0$, $b$, $\eta$, $\xi$) are taken as the inputs of the model.
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

In addition, this model allows the specification of the appropriate metal/silicate partition coefficients of each element for each planet if needed. Without further specification, the default is to use that of the bulk Earth.

The outputs of this model are the elemental abundances of the Planet Core \( (E^{i}_{\text{Core}}) \), the Bulk Planet \( (E^{i}_{BP}) \), and the Bulk Silicate Planet \( (E^{i}_{BSP}) \).

In this model, 18 elements are currently considered which are listed here in descending order of condensation temperatures:

\[ E^{i=1,2,...,n} = \{ \text{Al, Th, Ti, Ir, Ca, U, Ni, Fe, Mg, Si, Cr, Mn, O, Na, K, S, H_2O, C} \} \]

Normalization requires:

\[
\sum_{j=1}^{n} E^{i}_{BE,i} \approx 1 \quad (5.1)
\]

\[
\sum_{j=1}^{n} E^{i}_{CI} \approx 1 \quad (5.2)
\]

In the formula above, the "approximately equal sign \( \approx \)" would be replaced by an exact "equal sign =" if we were to include all the elements in the periodic table. Here, the approximation is sufficient, however, as these 18 elements include all the major elements in rocky planets. (see e.g. [Grasset et al. (2009)])

For convenience, a normalization constant \( C \) can be defined as:

\[
C = 1/ \left( \sum_{j=1}^{n} E^{i}_{CI} \cdot \begin{cases} 
1, & \text{if } x_j \leq x_0 \\
e^{-b(x_j-x_0)}, & \text{if } x_j > x_0 
\end{cases} \right) \quad (5.3)
\]
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

5.4.1 Step 1: Modeling Volatile Depletion

BP,i stands for initial Bulk Planet (before late veneer). Eq. 5.4 describes the volatile depletion starting at $x_0$ (for elements with condensation temperatures lower than $\frac{10^4 K}{x_0}$), with depletion slope $b$ in $(\frac{10^4}{T})\cdot \log_{10}(E^j)$ plot plot.

\[
\frac{E^j_{BP,i}}{E^j_{CI}} = C \cdot \begin{cases} 
1, & \text{if } x_j \leq x_0 \\
 e^{-b(x_j-x_0)}, & \text{if } x_j > x_0 
\end{cases} \tag{5.4}
\]

5.4.2 Step 2: Modeling Core Formation

BSP,i stands for initial Bulk Silicate Planet (before late veneer). Eq. 5.5 & 5.6 describe the core formation process (metal/silicate partitioning). The partition coefficient of element $j$ is defined as $D_j \equiv \frac{C_{j,\text{metal}}}{C_{j,\text{silicate}}}$, where $C_{j,\text{metal}}$ is the wt\% of element $j$ in a liquid metal phase, while $C_{j,\text{silicate}}$ is the wt\% of the element in a liquid silicate phase.

Siderophile (iron-loving) elements have $D_j > 1$. Highly siderophile elements have $D_j \gg 1$. Lithophile elements have $D_j < 1$. For approximation, $D_j$ could be taken from the Earth’s values first. From a simple two-component mass balance calculation, we have:

\[
\frac{E^j_{BSP,i}}{E^j_{CI}} = \frac{1 - \xi}{(1 - \eta - \xi) + \eta \cdot D_j} \cdot \frac{E^j_{BP,i}}{E^j_{CI}} \tag{5.5}
\]

\[
\frac{E^j_{Core,i}}{E^j_{CI}} = \frac{(1 - \xi) \cdot D_j}{(1 - \eta - \xi) + \eta \cdot D_j} \cdot \frac{E^j_{BP,i}}{E^j_{CI}} \tag{5.6}
\]
5.4.3 Step 3: Modeling Late Veneer

BSP stands for final Bulk Silicate Planet (after the late veneer). BP stands for final Bulk Planet (after the late veneer). Eq. 5.7 & 5.8 describe the elemental abundances in the mantle and core following the late veneer. The late veneer materials are assumed to be gradually mixed into the mantle (bulk silicate part) due to mantle convection. A simple two-component mass balance calculation describes this process:

\[
\frac{E_{\text{BSP}}^j}{E_{\text{CI}}^j} = \frac{\xi}{1-\eta} + \frac{1-\eta-\xi}{1-\eta} \cdot \frac{1-\xi}{(1-\eta-\xi)+\eta} \cdot \frac{E_{\text{BP}}^j}{E_{\text{CI}}^j} \tag{5.7}
\]

\[
\frac{E_{\text{BP}}^j}{E_{\text{CI}}^j} = \xi + (1-\xi) \cdot \frac{E_{\text{BP}}^j}{E_{\text{CI}}^j} \tag{5.8}
\]

I have been developing an interactive tool for elemental abundance calculation, which is available online at www.astrozeng.com.

5.5 Model Output

The online interactive model PlanetElAbundance2 takes the partition coefficient \( K_j \) of each element \( j \) as input. By manipulating the four parameters \( (x_0, b, \eta, \xi) \), it calculates the elemental abundances of the Core \( (E_{\text{Core}}^j) \), Bulk Silicate \( (E_{\text{BSP}}^j) \), and Bulk Planet \( (E_{\text{BP}}^j) \).

This model is tested below by applying the bulk partition coefficients \( K_j \) of the Earth and the appropriate parameters \( (x_0, b, \eta, \xi) \) to Earth, Venus, and Mars to calculate their elemental abundances and compare the results with the actual measurements. The
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

results are as follows:

Earth:

\[ x_0 = 7.335, \ b = 0.532, \ \eta = 0.325, \ \xi = 0.00475 \]

See Fig. 5.2.

The upper broken line in Panel 2 shows the initial volatile depletion trend. Some of the elements lying below this broken line are depleted due to their siderophility. The lower horizontal line in Panel 2 shows the degree of late veneer delivery, approximately 0.5%.

C and S must have entered into the accreting planet and further into the core before their respective 50% Condensation Temperatures. Thus, they were not greatly depleted as per the depletion trend. The prediction for S deviates greatly from the data. One possible explanation is the depletion slope \(-b(x_j - x_0)\) does not continue to very low condensation temperatures. That is, the depletion slope may flatten out towards lower temperatures. This same argument applies to the cases of Mars and Venus.

Mars:

\[ x_0 = 7.335, \ b = 0.4, \ \eta = 0.2063, \ \xi = 0.008 \]

See Fig. 5.3.
Figure 5.2: Upper Panel: Earth’s Core; Middle Panel: Bulk Silicate Earth; Lower Panel: Bulk Earth. Circles are the actual elemental abundances, and crosses are calculation produced by the model. All abundances are normalized to CI (Carbonaceous Chondrite Ivuna).
Figure 5.3: Upper Panel: Mars’s Core; Middle Panel: Bulk Silicate Mars; Lower Panel: Bulk Mars. Circles are the actual elemental abundances, and crosses are calculation produced by the model. All abundances are normalized to CI (Carbonaceous Chondrite Ivuna).
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

Venus:

\( x_0 = 7.335, \ b = 0.58, \ \eta = 0.32, \ \xi = 0.004 \)

See Fig. 5.4.

5.6 Discussion

\( x_0 \) (the starting point of depletion trend) remains the same for the cases of Venus, Earth, and Mars. As such, it can be approximated as a fixed quantity and is most probably related to a general property of the inner planetary disk. \( b \) (the depletion slope) decreases as a planet is further away from the star. This is intuitive, as the further the planet is, the lower the temperature, allowing the accretion/delivery of more volatile-rich material and thereby permitting the rocky planet to present a less volatile depletion trend. \( \eta \) (the core mass fraction) is determined by the interplay of the initial total Fe mass fraction, the FeO dissolved in the silicate portion, and the amount of sulphur in the core. The \( \eta \) for Earth and Venus are close, both \( \sim 32\% \). For Mars, it is smaller due to some Fe content being incorporated into the mantle silicate as FeO. \( \xi \) (the late veneer mass fraction) increases outwards, also. This is also intuitive as planets further out receive more delivery of volatile-rich materials as the outer disk is where the most volatile-rich materials originate.
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

Figure 5.4: Upper Panel: Venus’s Core; Middle Panel: Bulk Silicate Venus; Lower Panel: Bulk Venus. Circles are the actual elemental abundances, and crosses are calculation produced by the model. All abundances are normalized to CI (Carbonaceous Chondrite Ivuna).
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

5.7 Summary

I model the elemental abundances of rocky planets based on the links in the planet formation process between stellar elemental abundances and planet elemental abundances.

Through four parameters, I capture the essence of three important steps in planet formation: (1) volatile depletion (2) core formation and (3) late delivery, and reproduce the general elemental abundance pattern for rocky planets.

This model can be applied to extrasolar planetary systems if provided with measurements of stellar elemental abundances to infer the elemental abundances of the primitive building blocks (undifferentiated materials similar to CI chondrites) of planets, and to use this as the starting point of the model.

With the coming online of the NASA TESS mission, the James Webb Space Telescope, and other telescopes, these ideas can be widely applied and tested.

I believe that life is "information in transit". A planet manifests a continuous energy flow which carries information from its interior outwards, and its host star also imposes a continuous energy flow which carries information pouring down from space onto the planet’s surface. When the two flows meet at the surface, merge into the water available on the surface, converge, intermingle, spiral, and coalesce, driving the water cycle, and eventually give rise to life. life, then as a process, manifests this continuous intercourse of energy/information flows.

The interactive model tool is now online at [www.astrozeng.com](http://www.astrozeng.com).
CHAPTER 5. MODELING THE ELEMENTAL ABUNDANCES OF ROCKY PLANETS

Acknowledgement

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Chapter 6

Summary and Future Directions

The 1-layer, 2-layer and 3-layer models for solid exoplanets composed of Fe, MgSiO$_3$, and H$_2$O have been discussed. The mass-radius curves for the 1-layer model, the mass-radius contours for the 2-layer model, and the ternary diagrams for the 3-layer model, as well as their relationships to mass-radius contours, are provided to quickly calculate the interior structures of such exoplanets.

In particular, the 2-dimensional contour mesh on the mass-radius diagram for the 2-layer model could help students to establish physical insights into the interior structures of solid exoplanets. The complete 3-layer model is tabulated to help users interpolate solutions. A dynamic and interactive tool developed out of these models to characterize and illustrate the interior structures of exoplanets is made available online: http://www.astrozeng.com

The effect of Fe (iron) partitioning (differentiated versus undifferentiated) and oxidization (reduced versus oxidized) between the mantle and the core on the mass-radius
A direct application of these models is for the super-Earths within 1 to 15 $M_\oplus$, of which many are assumed to contain a significant H$_2$O-layer, the water worlds. The 2-layer (silicate-core and H$_2$O-mantle) planet model is applied here to understand the thermal evolution of H$_2$O-rich planets. Their interior pressure-temperature profiles are plotted on the H$_2$O phase diagram to show different H$_2$O phases dominating at different stages of thermal evolution of such planets. Their bulk H$_2$O contents could transition first from fluid phases to the superionic phase, and proceed from the superionic phase to high-pressure ices. The different phases of H$_2$O may significantly change the interior convective pattern and the magnetic fields, but only affect the radius slightly.

Different regions on the mass-radius diagram correlate with different dominating H$_2$O phases inside an H$_2$O-rich planet. In general, super-Earth sized planets, which are isolated or without significant parent star irradiation effects, older than about 3 billion years, are mostly solid. These regions could help us sort the exoplanets with both mass and radius measurements into different categories, in order to understand their formation, composition, and interior structures based on statistics.

Another application of the models is for a group of recently discovered rocky exoplanets found to follow a tight mass-radius relation. With the application of the 2-layer planet model and the extrapolation of the seismically derived pressure-density relation of the Earth’s interior (PREM), core mass fractions of 0.2~0.3 are found to explain these rocky exoplanets well. The result suggests a new semi-empirical power-law mass-radius relation \( \left( \frac{M}{M_\oplus} \right) \approx 0.94 \left( \frac{R}{R_\oplus} \right)^{3.72} \) for these planets. This power-law can be tested against future observations. This finding comes as no surprise as one expect their
elemental abundances to resemble that of our solar system as a result of them being in the solar neighborhood.

Chondrites, undifferentiated meteorites, are believed to be the building blocks of terrestrial planets in our solar system and, presumably, other exoplanetary systems. They condensed out of nebulae at the very beginning of planet formation. They are the important link between the elemental abundances of host stars and their planets. The atomic proportion of Fe to Mg to Si of chondrites is close to 0.9 : 1 : 1. The Mg and Si, as well as a fraction of Fe, were combined in proportion with the abundant O available in the protoplanetary nebula to form Mg-silicates. As a result, core mass fractions become 0.2~0.3, depending on the fraction of Fe oxidized and incorporated into the mantle. This result suggests the importance of building a complete elemental abundance model for solid exoplanets from the perspective of planet formation.

The complete model is based upon understanding the link between the elemental abundances of the host stars and their planets.

As a first-order approximation, we capture the essential steps (volatile depletion, core formation, and late veneer) in the planet formation process into four simple parameters (the starting point of volatile depletion, the slope of volatile depletion, the core mass fraction, and the late veneer mass fraction). The model could reproduce the overall elemental abundance patterns for terrestrial planets in our solar system, and then be applied to rocky exoplanets.

This model requires precise measurements of the elemental abundance of the host star, in particular, the Mg : Si, Si : Fe, and C : O ratios. Hopefully, this model could provide additional constraints on the compositions and interior structures of exoplanets,
CHAPTER 6. SUMMARY AND FUTURE DIRECTIONS

in addition to the information that we could acquire from that of the mass and radius measurements.

An interactive model tool as a result of this model is available at www.astrozeng.com.

With the Transiting Exoplanet Survey Satellite (TESS) and the James Webb Space Telescope coming online in the near future, and the precise radius and mass measurements of planets within the $1$ to $20$ $M_{\oplus}$, this planet elemental abundance model could be widely applied and tested against observations.

I believe that life is "information in transit". A planet manifests a continuous energy flow which carries information from its interior outwards, and its host star also imposes a continuous energy flow which carries information pouring down from space onto the planet’s surface. When the two flows meet at the surface, merge into the water available on the surface, converge, intermingle, spiral, and coalesce, driving the water cycle, and eventually give rise to life. life, then as a process, manifests this continuous intercourse of energy/information flows.

For future directions, I hope to link my models with the origins and mixing of volatile contents on the surfaces of these solid exoplanets, which are important prerequisites for the origins of life on them. This requires collaboration with geochemists and cosmochemists in the Department of Earth and Planetary Sciences (EPS) at Harvard, in particular, Stein Jacobsen’s group. I would also like to view the chemical evolution of planetary systems from a galactic evolution perspective, to explore the different compositions of exoplanets which form at different ages and locations of our galaxy as a result of galactic chemical evolution, and the implications for habitability of these planets. This requires collaboration with the Lars Hernquist group at the Center
CHAPTER 6. SUMMARY AND FUTURE DIRECTIONS

for Astrophysics (CfA). The future research could also benefit from interacting with other members of the Harvard Origins of Life Initiative, of which Dimitar Sasselov is the director. The field of exoplanets and astrobiology are burgeoning with new opportunities. Exploration in this field could help us understand the ultimate meaning of human life, and humble us before the magnificent workings of the universe.
References


Birch, F. 1947, Physical Review, 71, 809


Bradley, D. 1994, Science, 264, 908

REFERENCES


Choukroun, M., & Grasset, O. 2007, The Journal of Chemical Physics, 127, 124506


Daucik, K., & Dooley, R. B. 2011, Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance (The International Association for the Properties of Water and Steam)


REFERENCES


Hermann, A., Ashcroft, N. W., & Hoffmann, R. 2012, Proceedings of the National Academy of Sciences, 109, 745

Hirose, K. 2010, Scientific American, 302, 76


REFERENCES

—. 1994, Journal of Physics: Condensed Matter, 6, 8245

Lauretta, D. 2011, Elements, 7(1), 11


Lewis, J. S. 1997, Physics and chemistry of the solar system

Li, J., & Fei, Y. 2003, Treatise on Geochemistry, 2, 521


Lodders, K., & Fegley, B. 1998, The planetary scientist’s companion / Katharina Lodders, Bruce Fegley.

Lodders, K., & Fegley, B. 2010, Chemistry of the Solar System: RSC (RSC Paperbacks) (Royal Society of Chemistry)

Lodders, K., Palme, H., & Gail, H.-P. 2009, Landolt Börnstein, 44


McDonough, W., & Sun, S. 1995, Chemical Geology, 120, 223 , chemical Evolution of the Mantle


104
REFERENCES


Pagel, B. E. J. 1997, Nucleosynthesis and Chemical Evolution of Galaxies


Rubie, D. C., et al. 2015, , 248, 89


REFERENCES


Stanley, S., & Bloxham, J. 2006, Icarus, 184, 556


Stevenson, D. J. 2013, Planets, Stars and Stellar Systems (Springer), 195–221

Stixrude, L., & Lithgow-Bertelloni, C. 2011, Geophysical Journal International, 184, 1180


REFERENCES


Wang, Z., & Becker, H. 2013, Nature, 499, 328

White, W. M. 2013, Geochemistry (Willey-Blackwell)


Ziegler, L. B., & Stegman, D. R. 2013, Geochemistry, Geophysics, Geosystems, 14, 4735