Estimation of the probable size of the lunar core based on geophysical and geochemical data

E Kronrod 1, O Kuskov 1, K Matsumoto 2,3, V Kronrod 1

1Vernadsky Institute of Geochemistry and Analytical Chemistry (GEOKHI RAS), 19, Kosygin str., Moscow 119991, Russia
2RISE Project, National Astronomical Observatory of Japan, 2-12, Hoshigaoka, Mizusawa, Oshu 023-0861, Japan
3The Graduate University for Advanced Studies, SOKENDAI, Shonan Village, Hayama, Kanagawa 240-0193, Japan

E-mail: e.kronrod@gmail.com

Abstract. This study is devoted to estimations of the possible sizes of the lunar core, which were obtained with two independent approaches based on solving the inverse problem of determining the internal structure and composition of the Moon. For calculations Monte Carlo method was used taking into account geophysical and geochemical constraints on the models. In the first method, the inverse problem was solved for two different temperature models (“cold” and “hot”). In the second method, two different models of the bulk composition of the lunar mantle (Earth-like and enriched in Al2O3) were considered. Both approaches led to similar values for the radius of the lunar core. It was found that the radii of Fe-S core are in the range of 50–350 km with the most probable value of about 300 km (~ 1% of the mass of the Moon) and are rather weakly dependent on the thermal regime and chemical composition of the lunar mantle.

1. Introduction

The study of the central zone (core) and the region adjacent to the core at the boundary between the solid mantle and the liquid or partially molten core is of particular interest in the thermochemical evolution of the Moon. The average density of the Moon indicates a scarcity of metallic iron, but the question of the composition, properties and size of the lunar core remains unsolved. The composition of the cores of large satellites (Moon, Io, Europa, and Ganymede) is often considered as a model of iron-sulfide alloy, which is a liquid and/or solid Fe-Ni solution with an admixture of sulfur. According to cosmochemical data, the sulfur content varies from ~2% in ordinary chondrites and carbonaceous chondrites CO and CV to ~6 wt. % in enstatite and carbonaceous chondrites CI. The results of Apollo experiments and their mathematical processing led to the construction of a number of seismic models of the Moon, but did not give direct information about the presence of a core. Besides, there are not enough experimental data on the physical properties of Fe–S melts under P–T conditions of the lunar core. In the present study, the effect of the thermal state on the lunar core sizes in the Fe-S system was investigated using two independent methods. Both methods are based on the combined inversion of seismic and gravity data using the Monte Carlo method combined with the Gibbs free energy
minimization. The first method consists in converting of geophysical data into geochemical models of the inner structure of the mantle and core of the Moon. As the main boundary conditions, we used seismic velocity models of [1] constructed from Apollo experimental data, mass and moment of inertia from the data of the GRAIL mission. In the second approach Markov chain Monte Carlo method (MCMC) for inversion of selenodetic and seismic data together with thermodynamic approach was used. The main difference of the second approach was that, in contrast to the first approach, the inversion did not use seismic velocity models, but data on the seismic travel time (TT) data. In addition, selenodetic data (Love number \( k_2 \) and quality factors \( Q \)) were taken into account in the inversion. Modeling of the phase composition and physical properties of the mantle in both methods was carried out using the method of minimizing the Gibbs free energy.

2. The model of the Moon

A model of a spherically symmetric Moon, differentiated as a result of partial melting of an initially homogeneous body, is considered. The Moon consists of anorthosite crust, a three-layer (in Method 1) or four-layer (in Method 2) mantle, and an iron-sulfide core [2, 3, 4]. It is assumed from the lunar magma ocean (LMO) condition that the composition of the primary lower mantle, unaffected by magmatic differentiation processes, should be equal to the modern composition of uniformly mixed overlying shells (crust, upper and middle mantle) formed as a result of LMO differentiation up to the boundary with the lower mantle. LMO depth is assumed to be 750 km, which corresponds to the seismic boundary according to [1, 5].

When modeling the composition of the Moon, the following ranges of oxide concentrations in the upper, middle and lower mantle (wt%) were considered, covering a set of potentially possible compositions from the analysis of geochemical and geophysical data: \( 25 \leq \text{MGO} \leq 45\% \), \( 40 \leq \text{SiO}_2 \leq 55\% \), \( 5 \leq \text{FeO} \leq 15\% \), \( 0.1 \leq \text{CAO}, \text{Al}_2\text{O}_3 \leq 7\% \), and the concentrations of \( \text{Al}_2\text{O}_3 \) and \( \text{CaO} \) are related by the dependence \( \text{CaO} \sim 0.8\text{Al}_2\text{O}_3 \) [6].

3. Composition and density of the core

In [7], the molecular dynamics (MD) method was used to simulate the thermodynamic properties of solid and liquid Fe–S solutions (density, speed of sound, Grüneisen parameter, etc.). A comparison of the MD calculations of the density of liquid iron with experiment [8, 9] at normal pressure shows good agreement within 1%. In both calculations and experiments, the density of Fe–S melts noticeably decreases with an increase in the sulfur concentration. Table 1 shows the dependences of the density of Fe–S solutions on temperature at a pressure of 5 GPa (cells with liquid states are tinted).

| Temperature, K | 0 | 6 | 10 | 14 | 18 |
|---------------|---|---|----|----|----|
| 298           | 8.18 | 7.80 | 7.56 | 7.25 | 6.90 |
| 500           | 8.14 | 7.78 | 7.50 | 7.17 | 6.82 |
| 1000          | 8.02 | 7.64 | 7.38 | 6.99 | 6.61 |
| 1500          | 7.87 | 7.23 | 6.96 | 6.66 | 6.34 |
| 1800          | 7.47 | 7.08 | 6.81 | 6.51 | 6.18 |
| 2000          | 7.39 | 7.00 | 6.73 | 6.41 | 6.08 |
| 2200          | 7.31 | 6.90 | 6.62 | 6.31 | 5.98 |
| 2500          | 7.18 | 6.76 | 6.48 | 6.17 | 5.82 |

Note: Cells with liquid solutions are tinted
It follows from Table 1 that in the center of the Moon (~ 5 GPa) Fe–10 at.% S alloy is a solid phase at 1800 K and liquid at 2000 K, that is, the liquidus line is located between these boundaries. At 5 GPa /1800 K and sulfur content <14 at%, The Fe–S system is a solid solution. At 5 GPa and 1800–2000 K, pure iron has a density of 7.4–7.5 g/cm³, which corresponds to estimates [9, 10, etc.], but 0.5 g/cm³ lower than in the inner core [2]. With 10% nickel in the core, its density should increase by ~1%.

According to the models constructed from the GRAIL data, the radius of the fluid core is 200–380 km, and the radius of the solid inner core is estimated in the range of 0–280 km [4]. Geophysical data indicate inhomogeneities in the structure of the core, make it possible to set limits on the size of the outer and inner cores, but do not provide an opportunity to determine their density. Therefore, the density of the substance composing the core remains an unknown parameter and is determined from other assumptions.

4. Method 1

4.1 Method 1. Approach, Input Parameters

The input parameters of the Moon model are taken as follows: mass (7.3463×10²⁷ kg), average radius (1737.15 km) and dimensionless moment of inertia (Iₐ=(I/MR²) = 0.393112±0.000012) according to [Williams et al., 2014]; composition, average thickness (H_cr =34 km) and density of the crust (ρ_cr = 2.6 g/cm³) from [11] and [3]; average density of the Fe–S core (ρ = 7.1 g/cm³) [7]. The velocities of P-, S-waves (Vₚ, S) in the mantle are taken according to the seismic model [1]. The boundaries between the middle and lower mantle varied and were fixed at depths of 500, 625, and 750 km [1, 5, 12].

Reconstruction of the chemical composition of the mantle and the size of the core is carried out by the Monte Carlo method by joint inversion of gravity and seismic data, taking into account the mass-balance petrological relations. Modeling of the phase composition and physical properties of the mantle was carried out using the method of the Gibbs free energy minimization and equations of state for minerals in the Mie-Grüneisen-Debye approximation based on the THERMOSEISM software package and self-consistent database of thermodynamic constants of minerals, taking into account the interaction parameters for solid solution models [13]. The composition, average thickness and density of the anorthosite crust, and the average density of the Fe–S core are fixed. The chemical composition, mineralogy, and physical properties of each mantle zone are estimated by solving the inverse problem within the NaTiCFMAS software for a wide range of basic oxide concentrations [6, 14]. The results of determining the chemical composition of the mantle are presented in [15, 16].

Calculations were performed for two typical profiles for the "cold" (T₁₅₀km = 600°C, T₅₀₀km = 900°C, T₁₀₀₀km = 1100°C) and "hot" (T₁₅₀km = 700°C, T₅₀₀km = 1100°C, T₁₀₀₀km = 1300°C) models from the possible temperature range for the mantle, given in [15].

4.2. Method 1. Results

The results of calculations are shown in fig. 1. Effect of the thermal state on the size of the lunar core is presented as frequency distributions, the average values of which correspond to solutions that satisfy the specified conditions for the thickness and density of the crust, mass and moment of inertia of the Moon, P-, S-waves velocities in the mantle [1, 3, 4], as well as constraints on the chemical composition of the three-layer mantle, its mineralogy, and density. A density of 6.73 g/cm³ was taken for the liquid component, and 7.47 g/cm³ for the solid component, which corresponds to an average density of the Fe–S core of 7.1 g/cm³ with an approximate sulfur content of 6–10 at.% (3.5–6 wt.%) (according to Table 1). As it can be seen from fig. 1, the sizes of the core are in the range of 50–350 km with the most probable value of about 300 km and are rather weakly dependent on the thermal regime. This is due to the fact that a change in temperature by 200 °C leads to a change in the density of the Fe–S melt within 1%. Testing has shown that variations in the thickness of the crust and the depths of the location of seismic boundaries do not significantly affect the calculated values of the core size.
Physical data are set of Tl as) and a solid inner core. SM/ncrnt concenct of the Bndance with the model (70x763)
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temperature (Is) and a shear modulus \( \mu = 0 \) Pa and a viscosity of 0 Pa s and a solid inner core [18]. The viscosity of all solid layers (except for the LVZ zone) was set at 10^{21} Pa s. The density of the inner core was taken as \( \rho = 7500 \) kg/m^3 [7], while the density of the liquid core was to be calculated.

For the inversion six basic geophysical data are set [18]: mean radius \( R \), mass \( M \), normalized moment of inertia \( I_s \), second-order Love number \( k_2 \) [4], quality factors \( Q_m \) and \( Q_a \) with a period of a month and a year and travel times of seismic waves. Travel times \( TT \) of seismic waves were set according to data from [5]. For the inversion, travel times were increased three times [19]. For Love number calculation we use program code developed by Kamata et al. [20].

5. Method 2

5.1 Method 2. Approach, Input Parameters
We consider a viscoelastic spherically symmetric model of the Moon (Maxwellian viscoelastic model), consisting of nine layers: megaregolith, crust, four mantle layers, low viscosity zone (LVZ), liquid outer core and solid inner core. The division of the mantle into layers from the crust–mantle boundary to LVZ was carried out in accordance with the model [1]: the first layer (Mantle 1) – 34–250 km, the second layer (Mantle 2) – 250–500 km, the third layer (Mantle 3) – 500–750 km, the fourth layer (Mantle 4) – 750 – ~ 1250 km (till the LVZ boundary, the thickness of which is calculated by solving the inverse problem). In each zone, the physical properties and concentrations of the main oxides are considered constant. When solving the inverse problem, conditions are imposed for the density in the mantle not to decrease with depth. The crust consists of a regolith layer 1 km thick and the crust itself with a total thickness of 34 km and an average density \( \rho_{\text{crust}} = 2590 \) kg/m^3 [3]. The composition of the crust is specified according to [11], wt%: \( \text{Al}_2\text{O}_3 = 27.3 \), \( \text{CaO} = 15.5 \), \( \text{MgO} = 6.8 \), \( \text{FeO} = 6.3 \), \( \text{SiO}_2 = 44.1 \). In the megaregolith layer, the average seismic velocities \( V_s \) and \( V_p \) are set at 1.0 km/s and 0.5 km/s, respectively [2]. The mantle is divided into layers according to the seismic model [1]: upper mantle (Mantle 1: 34–250 km), middle mantle "1" (Mantle 2: 250-500 km), middle mantle "2" (Mantle 3: 500-750 km), lower mantle (Mantle 4: 750 km – LVZ melting zone, the thickness of which is calculated from the inverse problem solution). Following [17], we apply uniform chemical composition in the three upper layers. The chemical composition and physical properties of each mantle zone \( i = 1 – 4 \) are modeled within the \( \text{Na}_2\text{O}-\text{TiO}_2-\text{CaO}-\text{FeO}-\text{MgO-Al}_2\text{O}_3-\text{SiO}_2 \) (NaTiCFMAS) system. The phase composition and physical properties of the mantle were modeled using the Gibbs free energy minimization method within NaTiCFMAS system and equations state of minerals in the Mie-Grunisen-Debye approximation based on the THERMOSEISM software package [13]. The lunar core is modeled as consisting of an outer liquid core (with a shear modulus \( \mu = 0 \) Pa and a viscosity of 0 Pa s) and a solid inner core [18]. The viscosity of all solid layers (except for the LVZ zone) was set at 10^{21} Pa s. The density of the inner core was taken as \( \rho = 7500 \) kg/m^3 [7], while the density of the liquid core was to be calculated.

For the inversion six basic geophysical data are set [18]: mean radius \( R \), mass \( M \), normalized moment of inertia \( I_s \), second-order Love number \( k_2 \) [4], quality factors \( Q_m \) and \( Q_a \) with a period of a month and a year and travel times of seismic waves. Travel times \( TT \) of seismic waves were set according to data from [5]. For the inversion, travel times were increased three times [19]. For Love number calculation we use program code developed by Kamata et al. [20].

Figure 1 Histograms of the calculated radii of the Fe-S core of the Moon with an average density of 7.1 g/cm^3 and a sulfur content of 3.5-6 wt% for two models of the thermal state for the cold (left) and hot (right) models.
The inverse problem of determining the parameters of the internal structure of the Moon is solved using the Bayesian method; Markov chain Monte Carlo (MCMC) was applied \[17, 18, 19,\] etc. The solution for the required parameters was determined from their posterior distribution. Then the likelihood function \( L (m) \) was calculated, which shows the measure of the deviation of the model calculated values from the observed ones. The model is described by 22 parameters (layer thickness \( t \), density \( \rho \), shear modulus \( \mu \), modulus of all-round compression \( \kappa \) (in the mantle layers, the parameters were the concentrations of the main oxides \( \text{Al}_2\text{O}_3, \text{FeO}, \text{MgO} \) in the upper mantle and the temperature \( T \) in each layer, from which \( \rho, \mu \) and \( \kappa \), as well as viscosity \( \eta \) in each layer were calculated). Some of the parameters were fixed: the thickness of the mantle layers, except for the LVZ layer, the thickness and density of the crust, seismic properties of the crust, the density of the inner core, the viscosity of the solid layers (crust, mantle except for the LVZ and the solid inner core). The temperature, physical properties and chemical composition in each zone of the mantle, the size and viscosity of the LVZ, the dimensions of the outer and inner core, and the density of the outer core were calculated. Geophysical data for \( R, M, MOI, k_2, Q_m \) and \( Q_a, TT \); and bulk concentrations of \( \text{Al}_2\text{O}_3 \) and \( \text{FeO} \) are included in the LHF as observed data.

Temperature distribution was fixed and it was considered as intermediate between the “cold” and “hot” models of the thermal state of the Moon considered by \[16\]:

\[
\begin{align*}
T_{150 \text{ km}} &= 595–605 ^\circ \text{C}, \\
T_{375 \text{ km}} &= 755–765 ^\circ \text{C}, \\
T_{625 \text{ km}} &= 930–940 ^\circ \text{C}, \\
T_{1000 \text{ km}} &= 1195–1205 ^\circ \text{C}
\end{align*}
\]

\section{5.2. Method 2. Results}

The inversion was carried out for two models of the mantle chemical composition in accordance with \[15, 16\]: terrestrial bulk alumina content \( (C(\text{Al}_2\text{O}_3)) \) models with \( 3.5 \leq C_E(\text{Al}_2\text{O}_3) \leq 4.5 \) wt\% (Models E, \( \text{Al}_2\text{O}_3 \sim 1 \times \text{BSE} \)) and models substantially enriched in refractory oxides \( 4.5 \leq C_M(\text{Al}_2\text{O}_3) \leq 7.7 \) wt\% (Models M, \( \text{Al}_2\text{O}_3 \sim 1.2 – 1.7 \times \text{BSE} \)) compared to terrestrial values. For both models, Mg\# values are 80–83, and bulk FeO content in the silicate Moon is in the range \( 11 \leq C_{E,M}(\text{FeO}) \leq 14 \) wt\%. The simulation results are shown in Fig. 2. For both models E and M, the probable radii of the and the outer core \((\sim 300–350 \text{ km})\), which is in good agreement with previous estimates. For calculated inner core there is a significantly larger variation in values, but it can be concluded that probable inner core size is in the range of \( \sim 50–250 \text{ km} \).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Posterior probability density functions of the inversion for the radii of the fluid outer core and solid inner core. \( a, b \) – models E; \( a', b' \) – models M}
\end{figure}
6. Conclusions
The radii of the Fe–S core with an average density of 7.1 g/cm³ and a sulfur content of 3.5–6 wt% are in the range of 50–350 km with the most probable value of about 300 km (~ 1% of the mass of the Moon). The calculation results obtained with two independent methods show similar values of possible lunar core size. The relative sizes of the lunar core (inner and outer) significantly depend on the concentration of sulfur, but weakly depend on the thermal regime and the total contents of main oxides. The density of Fe–6–10 at% S (3.5–6 wt% sulfur) melts is 20–30% higher than the density of the liquid core of the Moon, applied in seismic models. The revision of the density values of the Fe–S core leads to a revision of its size and mass, since, taking into account the implementation of the restrictions on the mass and moment of inertia of the Moon, an increase in the core density should lead to a decrease in its radius.

In conclusion, we note that the fully crystallized core does not satisfy the analysis of data on laser ranging of the Moon, seismic and gravity models [2, 4, 18, etc.]. The presence of a relatively small dense, electrically conductive and partially molten Fe–S core of the Moon is consistent with geochemical observations[21], and are compatible with model of the lunar dynamo generation ~ 3–4 billion years ago, caused by interaction between the solid silicate mantle and the liquid core or crystallization of the inner core [22].

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