Composition of the lunar mantle for lower mantle high-velocity seismic model

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Abstract. We investigated models of the internal structure of initially homogeneous Moon differentiated as a result of partial melting, using data on seismic velocities according to the seismic models assume the zonal structure of the lunar mantle is a model of the Moon which was obtained with using the array processing methods of high velocities in the lower mantle. As a result of inversion of gravity (mass, moment of inertia), seismic (P- and S-waves velocities) and petrological (balance ratios) data, the Monte Carlo method was used to reconstruct the chemical composition and internal structure of the Moon. The phase composition and physical properties of the mantle were obtained with Gibbs free energy minimization method and equations of state in the five-component system CaO-FeO-MgO-Al₂O₃-SiO₂. For all models, possible values of seismic velocities and concentrations of the main oxides in three zones of the mantle were obtained, satisfying the geochemical and geophysical constraints and the possible sizes of the Fe-10%S core were determined. It was found that the lunar mantle chemical composition (concentration of FeO, Al₂O₃ and CaO) differs depending on the mantle zone. Constraints on the values of seismic velocities in the lower mantle and the most probable size of the lunar core were determined: \( V_P \leq 8.45 \text{ km/s; Fe-10\%S core radius is } \sim 360 \text{ km} \).

1. Introduction

Seismic data is one of the most important data in determining the internal structure of the Moon. From 1969 to 1977, the Apollo seismic experiment was carried out, during which four seismic stations on the lunar surface recorded seismic events. The processing of the data obtained by Apollo made it possible to obtain information about the structure of the lunar interior. Seismic models of the Moon were proposed in [1, 2, 3, 4, 5]. Most seismic models assume the zonal structure of the lunar mantle [3, 4, 6] Weber et al. (2011) ([6]) proposed a model of the Moon obtained using the array processing methods. The model [6] at depth less than 740 km is similar to earlier models proposed by groups of French scientists [3,4]; at greater depths, \( V_P \) velocity is significantly higher compared to previous models (up to 8.5 km/s), while in the model [4] \( V_P = 8.15 \pm 0.23 \text{ km/s} \).

In this study, the problem of determining the chemical composition and internal structure of the Moon is solved by Monte Carlo method using gravity (mass and moment of inertia), seismic (\( P \)- and \( S \)- wave velocities), and petrological data [7]. The internal structure of the Moon and the composition of the silicate mantle were obtained using the data of a high-velocity in the lower mantle seismic
2. Petrological and geophysical constraints

According to the existing hypothesis of the lunar magma ocean (LMO), it is assumed that the Moon was partially or completely melted as a result of meteorite bombardments. The depth of melting according to different authors is taken from about 200 km to complete melting. But there is no reason to believe that the Moon was ever completely melted (the lack of complete melting is confirmed by petrological, geochemical and geophysical data). We assume a melting depth of 500–600 km, which is in good agreement with experimental data (crystallization of lunar basalts, green and picrite glasses) [8, 9, 10, 11]. Interpretation of seismic data [2, 3, 4, 12] confirm the presence of boundaries at 500–750 km, which leads to the same conclusion.

In [13], a compilation of estimates of the thickness of the lunar crust obtained on the basis of seismic, gravity and topographic observations is presented. According to [13] the most probable crustal thickness is 49 + 16 km. The Al2O3 content was taken in accordance with the model [14]: 28.5–32% for the upper crust, 25–29% for the lower crust, and 18–25% for the bottom portions of the mafic crust (which is close to 25% Al2O3 in the entire crust). In this work, the inhomogeneous anorthosite lunar crust is replaced by spherical shell with uniform chemical composition, density, and thickness. The thickness of the crust is 45 km.

The lunar mantle temperature is probably below the solidus temperature. This is evidenced by the high-quality factor and recorded deep seismic events. In this work, the temperature was set in accordance with the models [15, 16]: 600 °C at the depth of 150 km, 900 °C at 500 km and 1200 °C at 1000 km. The distribution of pressure in the interior of the Moon over depth is determined by the equation for a model with constant density. Following [16, 17, 18], we assume that the core of the Moon consists of iron sulfide containing 10 wt% sulfur (Fe-10 wt% S, Fe0.84S0.16), core density ρ = 5.7 g/cm3 (at a pressure of 50 kbar and a temperature of 1500 °C).

3. Calculation method

The approach used in this work allows the density and isotropic velocities VP and VS to be calculated for phase association, which depend on the chemical and phase composition of the lunar material. THERMOSEISM software package was used to calculate the equilibrium phase associations and physical properties (seismic velocities and density) in the lunar mantle [17, 19]. The THERMOSEISM database includes thermodynamic parameters (enthalpy, entropy, heat capacity, Grüneisen parameter, thermal expansion, bulk modulus and shear modulus for minerals) as well as mixing parameters of solid solutions. Using the Gibbs free energy minimization method, the chemical composition of the individual phases and the ratio between the phases were determined. The solution of the equation of state (EOS) of minerals is carried out in the quasi-harmonic Mie-Grüneisen-Debye approximation [20].

When constructing models of the internal structure of the Moon, based on seismic data, we assume a model of the Moon, which consists of five spherical shells: crust, three-layer (upper, middle and lower) mantle and iron-sulfide core. The core size is calculated during the inversion process. The thickness of the lunar crust is assumed to be 50 km, the upper mantle is located at depths from 50 to 250 km, the middle mantle is from 250 to 625 km, the lower mantle extends from 625 km to the mantle-core boundary. It is assumed that within each mantle layer, the composition (concentrations of MgO, FeO, Al2O3, CaO, SiO2) and density are almost constant. It is also assumed that there is no density inversion with depth. The composition of the outer mantle layers of the mantle region is determined from the condition of maintaining a balance in the system of oxides CaO-FeO-MgO-Al2O3-SiO2, taking into account geophysical constraints [21].

A detailed description of the inverse problem of determining the chemical and mineral composition and radius of the lunar core from geophysical constraints can be found in [15, 19, 22]. This paper uses the Monte Carlo method for a uniform distribution [23]. The applied approach makes it possible to determine the probable distributions of the concentration of rock-forming oxides and seismic
velocities in each of the three considered mantle layers. From the obtained distributions, we can estimate the mean values for concentrations and seismic velocities and the deviation of the obtained distributions from the mean values.

4. Results
The values of the parameters calculated as a result of solving the problem (bulk composition, concentration of rock-forming oxides, core size) depend on the constraints that were imposed on the model of the Moon. The models of the Moon considered are shown below. The models under consideration differ in the constraints imposed on seismic velocities and oxide concentrations in the lunar mantle. The main input parameters of the considered models are given in Table 1 and the constraints on the model parameters are given in Table 2.

### Table 1. Input model parameters.

| Parameter | Description | Value | Notes |
|-----------|-------------|-------|-------|
| $R_{\text{Moon}}$ | radius of the Moon | 1738 km | Set based on [24] |
| $I_{\text{Moon}}$ | normalized moment of inertia (MOI) | 0,3931±0,0002 | Set based on [24] |
| $\rho_{\text{Moon}}$ | Average density | 3,3437±0,0016 g/cm$^3$ | Set based on [24] (excluding errors for the mass of the Moon) |
| $H_{\text{crust}}$ | crustal thickness | $H_{\text{crust}}$: 0–50 km | |
| $H_{\text{upper}}$ | thickness of the upper mantle | $H_{\text{upper}}$: 50–250 km | Set based on the analysis of seismic models [1, 2, 3, 4, 25], model of the crust [13] and preliminary performed calculations |
| $H_{\text{middle}}$ | thickness of the middle mantle | $H_{\text{middle}}$: 250–650 km | |
| $H_{\text{lower}}$ | thickness of the lower mantle | $H_{\text{lower}}$: 650–$(R_{\text{Moon}}-R_{\text{core}})$ km | |
| $\rho_{\text{crust}}$ | density of the crust | 2.9 g/cm$^3$ | |
| The composition of the crust | System CFMAS, wt% | FeO = 6.5%, MgO = 7%, Al$_2$O$_3$ = 25%, CaO = 16.5%, SiO$_2$ = 45.5% | Set based on [14] |
| $T_{\text{layer}}$ | Temperature in mantle layers | $T_{\text{upper}}$ = 600 °C, $T_{\text{middle}}$ = 900 °C, $T_{\text{lower}}$ = 1200 °C | Set based on [15, 18] |

### Table 2. Constraints on the model parameters.

| Model | MOI | Mass | Balance for oxides (6) | Seismic velocities in the upper and middle mantle | Proximity of concentrations in the upper and middle mantle |
|-------|-----|------|------------------------|--------------------------------|--------------------------------------------------|
| MI    | +   | +    | +                      | -                               | -                                               |
| MIS   | +   | +    | +                      | +                               | -                                               |

Notes:
1. Seismic velocities are taken from the figures in [2] (there are no specific numbers in the text of [2]).
2. Model MI – constraints on the mass and moment of inertia of the Moon.
3. MIS model – constraints on mass, moment of inertia and seismic velocities in the upper and
middle mantle. The upper values are constraints according to the model [4], the lower ones are according to [3].

1-3. The seismic velocities and associated uncertainties in these models represent mean values and standard deviations (assuming normal distribution).

4. $V_P$ in the lower mantle is $4.5\pm0.05$; there are no restrictions for $V_S$.
5. $V_P$ in the lower mantle is $4.45\pm0.05$; there are no restrictions for $V_S$.

| Model, reference | Depth, km | $V_P$, km/s | $V_S$, km/s |
|------------------|-----------|-------------|-------------|
| [3, 12]          | 30–300    | 7.75±0.15   | 4.53±0.15   |
|                  | 300–500   | 7.75±0.15   | 4.50±0.15   |
|                  | 500–750   | 7.50±0.30   | 4.35±0.30   |
|                  | 750–1000  | 7.90±0.30   | 4.20±0.30   |
| [4]              | 40–240    | 7.65±0.06   | 4.44±0.04   |
|                  | 240–500   | 7.79±0.12   | 4.37±0.07   |
|                  | 500–750   | 7.62±0.22   | 4.40±0.11   |
|                  | 750–1000  | 8.15±0.23   | 4.50±0.10   |
| [15]             | 60–300    | 7.67–7.80   | 4.45–4.51   |
|                  | 400       | 7.53–7.60   | 4.29–4.30   |
|                  | 800       | 8.17–8.20   | 4.50–4.51   |
| [22]             | 60–300    | 7.81±0.40   | 4.51±0.18   |
|                  | 300–500   | 7.85±0.40   | 4.42±0.19   |
|                  | 500–1000  | 8.01±0.38   | 4.44±0.20   |
| [7], model MI.   | 50–250    | 7.76±0.06   | 4.51±0.03   |
|                  | 250–625   | 8.03±0.01   | 4.49±0.05   |
|                  | 625–1000  | 8.073±0.07  | 4.49±0.03   |
| [7], model MIS.  | 50–250    | 7.67±0.029  | 4.46±0.01   |
|                  | 250–625   | 7.8±0.06    | 4.51±0.03   |
|                  | 625–1000  | 7.84±0.044  | 4.41±0.18   |
|                  |           | 7.81±0.06   | 4.45±0.02   |
|                  |           | 7.91±0.025  | 4.42±0.14   |
|                  |           | 7.97±0.045  | 4.51±0.03   |
| Present study^4, | 50–250    | 7.68±0.015  | 4.42±0.012  |
| Model 1          | 250–625   | 7.76±0.03   | 4.42±0.01   |
|                  | 625–1000  | 8.48        | 4.67        |
| Present study^5, | 50–250    | 7.68±0.015  | 4.42±0.012  |
| Model 2          | 250–625   | 7.76±0.03   | 4.42±0.01   |
|                  | 625–1000  | 8.43        | 4.62        |

Notes:
1. Model MI – constraints on the mass and moment of inertia of the Moon.
2. MIS model – restrictions are imposed on mass, moment of inertia and seismic velocities in the upper and middle mantle. The highest values for seismic velocities were taken according to the model [4], the lowest ones are according to [3].
3. The seismic velocities and associated uncertainties in these models represent mean values and standard deviations (assuming normal distribution).

Due to the formulation of the problem, the concentrations of the main rock-forming oxides in the lower mantle correspond to the bulk composition of the silicate Moon with an error not exceeding 0.3-0.5 wt% (Table 3). The lower mantle is enriched in Al$_2$O$_3$ and CaO in comparison with the upper and middle ones, which is reflected in the increased content of garnet and clinopyroxene. The middle
mantle is enriched in FeO compared to the lower mantle, which qualitatively agrees with our previous estimates [15, 21]. For model 1 ($V_p = 4.5\pm0.05$ km/s), paradoxically small values of SiO$_2$ (34 wt%) and very large values of Al$_2$O$_3$ (12 wt%) are observed. But for model 2 ($V_p = 4.45\pm0.05$ km/s), the bulk values are SiO$_2 = 40.4$ wt%, Al$_2$O$_3 = 6.2$ wt%. According to the results of our calculations, the velocities in the lower mantle can reach values $V_p = 8.43$ km/s, $V_s = 4.62$ km/s.

**Table 4.** Models of the silicate part composition (crust and mantle) of the Earth and the Moon

| Reference | FeO   | MgO   | SiO$_2$ | CaO | Al$_2$O$_3$ | MG# |
|-----------|-------|-------|---------|-----|-------------|-----|
| The Earth (wt%) [26] | 8.1   | 38.8  | 45.9    | 3.2 | 4.0         | 89.5|
| The Earth (wt%) [14] | 8.0   | 35.3  | 50.1    | 2.9 | 3.7         | 88.8|
| The Earth (wt%) [27] | 8.2   | 38.2  | 45.5    | 3.6 | 4.5         | 89.3|
| The Moon (wt%) [26]  | 14.1  | 32.9  | 45.1    | 3.7 | 4.2         | 80.6|
| The Moon (wt%) [28]  | 12.6  | 35.0  | 46.1    | 2.8 | 3.5         | 83  |
| The Moon (wt%) [29]  | 12.5  | 35.3  | 44.9    | 3.3 | 4.0         | 83  |
| The Moon (wt%) [30]  | 13.1  | 32.6  | 45.9    | 3.8 | 4.6         | 81.6|
| The Moon (wt%) [14]  | 13.1  | 32.3  | 43.9    | 4.6 | 6.1         | 81.5|
| The Moon (wt%) [31]  | 13 + Fe in the core | 32 | 43.4 | 10.8 ($\Sigma$ CaO + Al$_2$O$_3$) | 81.5|
| The Moon (wt%) [12]  | 13.3  | 21.9  | 53.5    | 4.9 | 6.4         | 74.6|
| The Moon (wt%) [2]   | 12.2  | 34.6  | 46.1    | 3.6 | 4.1         | 82  |
| The Moon (wt%) [19]  | 10.8  | 27.5  | 49.9    | 4.9 | 6.9         | 82  |
| The Moon (wt%) [15] Model 1 | 10.4 | 28.5 | 50.0    | 4.8 | 6.3         | 83  |
| Model 2              | 11.7  | 29.6  | 48.5    | 4.3 | 5.9         | 82  |
| The Moon (wt%) [7] Model MI' | 9.9±1.1 | 30.6±1.2 | 49±1.5 | 4.7±0.8 | 5.8±1 | 84.5|
| The Moon (wt%) [7] Model MIS' | 12.1±0.5 | 29.5±0.9 | 50.9±0.6 | 3.4±0.4 | 4.1±0.5 | 81.3|
| Present study, Model 1 | 11.3 | 34.2 | 32.8 | 9.6 | 12.1 | 84  |
| Present study, Model 2 | 11.4 | 40.4 | 38 | 5.0 | 6.2 | 86  |

The results of our study confirm the previously obtained conclusions on the qualitative difference between the bulk composition of the silicate Moon and the composition of the Earth's mantle [15, 21] (Table 4). The entire spectrum of the considered models lies in the FeO range of 9.9–12.1%, which are higher than in pyrolite (8.2%) [27]. The value of one of the most important geochemical parameters – the magnesium number (MG# 84) is close to geochemical and geophysical models [2, 14, 15, 21, 30]. This value is less than the accepted values for the Earth's mantle (MG# 89.3) [27], but higher than in [12] (MG# 74.6).

5. Conclusions

Models of the internal structure of differentiated as a result of partial melting of the initially homogeneous Moon for a high-velocity seismic model [6] were investigated by the method of numerical simulation. Reconstruction of the chemical composition and physical properties in the lunar mantle was carried out using the Monte Carlo method with gravity and seismic constraints. Possible
distributions of seismic velocities and concentrations of rock-forming oxides in three zones of the mantle, as well as the size of the core, have been obtained (calculated values satisfy geophysical and geochemical constraints).

The values of the seismic velocities at the depths of the lower mantle according to our estimations must satisfy the conditions: $V_p \leq 8.45 \text{ km/s}$, $V_s \leq 4.67 \text{ km/s}$. The radius of the Fe-FeS core is ~360 km.

The lunar mantle is chemically stratified with different concentrations of rock-forming oxides FeO, Al$_2$O$_3$ and CaO in different zones of the mantle.

Acknowledgments

This work was partially supported by Russian Science Foundation, grants no. 20-12-00105 (according to the grant, the method for data analysis was created and the numerical calculations were carried out). This work is performed according to the Kazan Federal University Strategic Academic Leadership Program. This work was partially supported by the state assignment of Vernadsky Institute of Geochemistry and Analytical Chemistry № 0137-2021-0004.

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