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Joint inversion of geophysical (seismic and selenodetic) and geochemical data for internal structure and composition of the Moon

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Abstract. We investigate lunar internal structure models which are consistent with the seismic and the selenodetic data and thermodynamic constraints. The seismic travel time data constrain crustal and mantle structures and composition, while selenodetic data are expected to contribute to infer the structure below the deep moonquake region.

1. Introduction

In the recent paper [1] lunar interior models by complementing Apollo seismic travel time data with selenodetic data which have recently been improved by Gravity Recovery and Interior Laboratory (GRAIL) and Lunar Laser Ranging were explored. Important information on the thickness of the crust, Low-velocity/viscosity zone (LVZ), core structure and seismic velocities were obtained. But this problem statement retains lunar mantle composition to be uncertain. In [2, 3] mantle composition can be simulated based on thermodynamic approach and petrological evidence from seismic data, moment of inertia (MOI) and mass.

The goal of our investigation is to obtain geochemically and geophysically consistent information on the internal structure of the Moon. The first step was to use thermodynamic approach to calculate elastic properties (shear modulus μ , bulk modulus κ) and density ρ in the Moon's layers. But it lead to increasing number of model parameters, and it was impossible to obtain reasonable result. Here we modified the problem statement and included geochemical data (bulk Al and Fe composition) as observed data and used more constraints on the model (such as magma ocean condition) and fixed some model parameters.

2. Thermodynamic approach

Our general methodology is to combine the geophysical and geochemical constraints and thermodynamic approach, and to develop, on this joint basis, the self-consistent models of Moon, accounting for its chemical composition and internal structure. Thermodynamic modeling of phase relations and physical properties in the multicomponent mineral system (NaTiCFMAS) was used to develop a method for solving the inverse problem. The technique of Gibbs free energy minimization was used, and minerals equations of state and solid solutions were included in the database. While

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solving the inverse problem, we require a non-negative density gradient in the mantle and include additional geochemical and cosmochemical constraints. For the computation of elastic properties and density for a given chemical composition we have used the THERMOSEISM software [4].

3. Geochemical model of the Moon.

Current geochemical models for bulk FeO and Al₂O₃ concentrations in the Moon are shown in Fig. 1. Apparently there is a slight difference in FeO content and significant difference in refractory elements (Al₂O₃, CaO) content. In our study we consider only Al₂O₃ concentration presuming Ca/Al ratio to be chondritic. Models of the lunar composition can be conventionally divided into two groups: 1 - bulk Al₂O₃ content is close to Earth's value, 2 - bulk Al₂O₃ concentration is higher than 4,5 wt.%.

The analysis of majority of current Moon's composition models revealed the following Al₂O₃and FeO content with corresponding error bars for Group 1: $3,5 \le Al_2O_3 \le 4,5$ ("average" $Al_2O_3 = 4,05 \pm 0,35$ wt.%) and for Group 2: $4,5 \le Al_2O_3 \le 7,7$ ("average" $Al_2O_3 = 5,91 \pm 0,39$ wt.%). For both groups of models $10 \le FeO \le 14$ ("average" FeO = $12,25 \pm 1,33$ wt.%).



Figure 1. Geophysical and geochemical models of a bulk-Moon composition (crust + mantle) compared with that of the bulk silicate Earth [5].

The difference in concentrations of refractory elements can be interpreted by models of Moon's origin. Currently the hypothesis of giant impact is the prevalent theory of the Moon's origin. If we follow this theory, then the volatile loss occurred as a result of giant impact and further high-temperature processes but concentrations of refractory elements and there ratio must have remained equal to Earth's values, and it is assumed that isotope compositions of the Moon and colliding body were equal.

One of the possible arguments confirming giant impact hypothesis is possibility of modeling of Moon's composition with bulk Al_2O_3 content similar to models with Earth's bulk Al_2O_3 content. In the present study we consider geochemical models with smaller Al_2O_3 content (similar to Earth's value - Group 1).

4. Geophysical data

We employed the same data as [1]: six selenodetically observed data of the mean radius (R), mass (M), normalized mean solid moment of inertia (Is), and degree 2 potential tidal Love number k_2 reported by [6] who summarized recent results of selenodetic data analyses and monthly and annual quality factors (Qmand Qa) reported by [7]. These values are summarized in Table 1.The mean radius R constrains

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the size of the modeled Moon, and M, solid MOI, k_2 , Qm, and Qa are used, together with the seismic travel time data, to form the likelihood function (equation (2))

Parameter	Value
Mean radius (<i>R</i>)	1737.151 km
Mass (M)	$(7.34630 \pm 0.00088) \times 10^{22} \text{ kg}$
Normalized mean solid moment of inertia (Is)	0.393112 ± 0.000012
Degree 2 potential tidal Love number (k_2)	0.02422 ± 0.00022
Monthly quality factor (<i>Qm</i>)	38 ± 4
Annual quality factor (<i>Qa</i>)	41 ± 9

Table 1. Selenodetic Data Used to Constrain Internal Structure Models of the Moon

We used the seismic travel time data selected by [8], i.e., 318 data (183 P-wave and 135 S-wave) from 59 sources (24 deep quakes, 8 shallow quakes, 19 meteoroid impacts, and 8 artificial impacts). The error for *n*th travel time σ_m is given by

$$\sigma_{\tau n} = \sqrt{\sigma_{n,r}^2 + \sigma_{n,e}^2} \qquad (1)$$

where $\sigma_{n,r}$ and $\sigma_{n,e}$ are the read time error and the event time error of *n*th travel time data. In our model we considered $\sigma_{\tau n}$ increased by a factor of three, which resulted in better solution.

5. The model of the Moon:

We apply spherically symmetric viscoelastic hydrostatic model of the Moon (Fig.2). The Moon consists of nine layers: megaregolith, crust, four-layer mantle, low viscosity zone (LVZ), liquid outer core and fluid inner core. In each zone physical properties are assumed to be constant.

Crustal thickness was assumed to be 34 km [9] (including 1 km regolith layer). Composition of the crust was taken from [10].



Figure 2 (a) The model of the Moon considered in the present study; **(b)**The mantle structure of the Moon. The depth of boundaries between mantle layers was fixed at the depths of 250, 500, 750 km. The depth of mantle-LVZ boundary was estimated during calculation. Temperature (T1-T4) and main oxides (Al₂O₃, FeO, MgO) concentrations (C1, C2) were specified at the depth of the middle of each mantle layer. C1 - equal for three upper layers, C2 in fourth layer (mantle 4) was calculated from balance equations.

In the present work, in the modeling of the chemical composition of the Moon, we considered four intervals of oxides concentrations in four mantle layers. Division mantle into layers was performed according to [11] model. Concentrations of main oxides were equal in 1-3 upper mantle layers and we applied the model of magma ocean to calculate oxide concentrations in fourth lower mantle layer (which implies that concentrations of main oxides in the lower mantle is equal to average concentrations in upper mantle and crust and equal to bulk concentrations). The models of the magma ocean in such a formulation were considered in our previous work [3].

Temperature gradient in the mantle was assumed to be approximate constant down to a depth of 1000 km [12] with the upper mantle temperature of 550 (\pm 10) °C at the depth of 150 km and lower mantle temperature of 1150 (\pm 10) °C at the depth of 1000 km.

6. Inversion:

A Bayesian inversion approach is an effective method to solve for a nonlinear problem such as planetary internal structure modeling [2, 13]. This study utilizes Markov chain Monte Carlo (MCMC) algorithm to infer the parameters of the lunar internal structure. The solutions of the parameters and their uncertainties are obtained from the posterior distribution which is sampled by the MCMC algorithm. Then, the likelihood function L(m), which is a measure of misfit between the model predictions and the observations is written as (2):

$$LHF = \exp\left(-\frac{\left(d_{obs}^{mass} - d_{cal}^{mass}(m)\right)^{2}}{2\sigma_{mass}^{2}} - \frac{\left(d_{obs}^{MOI} - d_{cal}^{MOI}(m)\right)^{2}}{2\sigma_{MOI}^{2}} - \frac{\left(d_{obs}^{k2} - d_{cal}^{k2}(m)\right)^{2}}{2\sigma_{k2}^{2}} - \frac{\left(d_{obs}^{Qa} - d_{cal}^{Qa}(m)\right)^{2}}{2\sigma_{Qa}^{2}} - \frac{\left(d_{obs}^{Qa} - d_{cal}^{Qa$$

where d_{obs} , $d_{cal}(m)$, σ , τn , denote observed data, data calculated from the model *m*, uncertainty of the observed data, and *n*th seismic travel time, respectively (similar to [1]. In the present model bulk Al₂O₃ content and bulk FeO content are included into LHF (Al_{bulk} and Fe_{bulk}).

7. Results:

The results of the inversion are shown in Fig. 3 and Fig. 4. Probable bulk silicate Moon oxide concentrations is $Al_2O_{3bulk} \sim 4,1 (\pm 0,5)$ wt.% and FeO_{bulk} $\sim 12,5 (\pm 0,5)$ wt.%.

As a result of our investigation it turned out that the solution can be obtained only at short range of mantle temperatures. Even slight temperature variation as well as including additional variable parameters (such as crustal thickness and density) lead to geochemically unreasonable main oxides concentrations. The main reasons of this situation might be the following: 1. The model is overspecified. 2. Seismic and geochemical models possess narrow general solution region. 3. There might be errors in seismic model and travel time estimations.



Figure 3 Posterior probability density functions for bulk concentrations of Al₂O₃(a) and FeO (b).

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Figure 4 Posterior probability density functions in layers 1-4 of the lunar mantle for (a) Al₂O₃ concentration, (b) FeO concentration, (c) MgO concentration, (d) P-wave seismic velocity distribution, (e) S-wave seismic velocity distribution, (f) density distribution.

8. Conclusions:

We have studied lunar internal structure models which are consistent with the seismic data, the selenodetic (GRAIL and LLR) data and thermodynamic constraints. Our research revealed that the solution appears at short range of mantle temperatures and additional constraints on model parameters

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(constraints on bulk composition, magma ocean condition, fixed crustal parameters) are required. Probably this result substantially stems from paucity of observation data used or the problem is overspecified (too much model parameters), narrow solution space satisfying both the geophysical and geochemical constraints. In our future study we are going to investigate this problem.

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