

THERMO-CHEMICAL CONSTRAINTS ON THE LUNAR BULK COMPOSITION AND THE STRUCTURE OF THE THREE-LAYER MANTLE.

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Introduction: The chemical composition of the Moon should be considered as a fundamental geochemical constraint when testing cosmogonic models of its origin. One of the most important problems of lunar geochemistry is the determination of its bulk composition - mainly the concentrations of rock-forming oxides SiO₂, Al₂O₃, CaO, FeO and the MG# affecting mineralogy and physical properties (density (ρ), bulk (K_S) and shear (G) moduli, V_P and V_S) of the mantle. The purpose of this work is to evaluate these geochemical parameters and to construct a model of chemical composition of the Moon based on a joint inversion of lunar mass and moment of inertia, the mantle P-, S-velocity profiles and petrological models by the Monte Carlo and Gibbs free energy minimization methods. Within this general problem, we consider two tasks: 1) to study the effect of the thermal state on the chemical composition and mineralogy of the three-layer mantle; 2) to reveal whether mantle is homogeneous or it is stratified by chemical composition. The solution of both problems will allow us to compare the composition of silicate fractions of the Moon and the Earth and to reveal their geochemical similarity and / or difference.

Data and method: We investigate the thermal state and chemical composition of the silicate portion of the Moon (crust + mantle; BSM) for the magma ocean model (which implies that modern composition of uniformly mixed overlying shells is identical with the bulk composition of the magma ocean, and reflect the bulk composition of the silicate Moon). We consider a five-layer model of the internal structure of the Moon including the crust, three zones of the mantle (the upper (39-240 km), the middle (240-750 km) and the lower mantle (750 km - core)) and Fe-S core. The input parameters of the model are the lunar mass and moment of inertia [1], the composition, the mean density and thickness of the crust, the seismic P- and S-wave velocities in the mantle [2,3], the oxide concentration interval in the NaTiCFMAS system, the average density of the Fe-S core.

The modeling of the composition and physical properties of the Moon was performed in the NaTiCFMAS system using Monte Carlo method and Gibbs free energy minimization combined with a Mie-Grüneisen equation of state of minerals described in detail in our previous publications [4,5]. The following ranges of oxide concentrations in the mantle (wt.%) were considered: $25 \leq \text{MgO} \leq 45\%$, $40 \leq \text{SiO}_2 \leq 55\%$, $5 \leq \text{FeO} \leq 15\%$, $0.1 \leq \text{CaO}, \text{Al}_2\text{O}_3 \leq 7\%$, where the concentrations of Al₂O₃ and CaO are related by the dependence of CaO/Al₂O₃ ~ 0.8 [6].

Since the temperature at different depths is not exactly known [5,7], the mean volume mantle temperature T_{mean} , controlling the mantle mineral composition and physical properties, is chosen as an integral characteristic of the thermal state of the Moon, which for our model is calculated from the expression: $T_{\text{mean}} = (T_u V_u + T_m V_m + T_l V_l) / (V_u + V_m + V_l)$, where T_u, T_m, T_l is the mean temperature (°C) in the three zones of the mantle, V_u, V_m, V_l are the volumes of the upper, middle and lower mantle. In terms of T_{mean} , all thermal models can be conditionally divided into "cold" ones with $T_{\text{mean}} \sim 690\text{-}860^\circ\text{C}$ and "hot" ones with $T_{\text{mean}} \sim 925\text{-}1075^\circ\text{C}$.

Results and conclusions: Regardless of the thermal state, BSM is characterized by almost constant bulk FeO $\sim 12\text{-}13$ wt.% and MG# 80-81.5, which significantly differs from those for the bulk-silicate Earth (BSE). The FeO content of 11-14 wt.% and MG# 80-83 are approximately identical in the upper and lower mantle. The abundance of SiO₂ slightly depends on the thermal state and is 50-55% in the upper mantle and 45-50% in the lower mantle. On the contrary, there are two different groups for the lunar abundance of alumina depending on the thermal state: 1) Cold models of BSM (3-4.6 wt.% Al₂O₃) are comparable to the Al₂O₃ content for the BSE; 2) Hot models – bulk Al₂O₃ is $1.2 - 1.7 \times$ BSE. The results indicate a gradual increase in the alumina content from the upper mantle (1-2%) to the lower one up to 4-7 wt.% Al₂O₃ with a garnet amount up to ~ 20 wt.%. The simulation results suggest that the lunar mantle is stratified by chemical composition. However, the question of the similarity and / or difference in their composition with regard to the abundance of refractory elements remains unresolved and requires further research.

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