EVOLUTION OF LUNAR MANTLE MINERALOGY DURING MAGMA OCEAN CRYSTALLIZATION AND MANTLE OVERTURN.
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Introduction: The mineralogy of the lunar mantle has been shaped by a sequence of several processes since the formation of the Moon, including lunar magma ocean (LMO) crystallization, cumulate overturn and partial melting during convection.

We investigated the mineralogical composition of cumulates crystallized from the lunar magma ocean and their changes during mantle overturn by applying different petrological models in order to identify possibilities to further constrain the properties of the lunar mantle and the conditions of its evolution.

LMO crystallization:

Model: Since the properties of the LMO, including its composition and dimensions, are largely unknown, the study of its thermochemical evolution and the compositions of LMO cumulates requires igneous crystallization models capable of exploring a large range of possible LMO properties.

However, the capability of such igneous crystallization programs to accurately model LMO solidification could not be sufficiently evaluated until recently when LMO crystallization was simulated in experimental studies that explicitly consider the progressive changes of pressure, temperature and composition during magma ocean differentiation [1, 2, 3]. Using the results of these experiments, we tested the ability of the igneous crystallization programs FXMOTR [4] and alphaMELTS [5] to reproduce experimental mineralogies and crystallization sequences as well as the thermal and compositional evolution of the liquid phase. We found that neither program succeeded in reproducing the experimental results due to their specific limitations. However, using a combined model using FXMOTR for early and alphaMELTS for late crystallization stages, we can reproduce the crystallization sequence, the temperatures of phase saturation, the mineral modal abundances, as well as the temperature change with the degree of solidification with sufficient accuracy [6].

Using this approach, we modeled LMO cumulate mineralogies, assuming fractional crystallization in a full mantle LMO with a bulk composition based on [7]. FeO/MgO ratios were varied (9.5-12.5 wt% FeO) to investigate the effect of the FeO content on cumulate densities and mineralogies. All crystals were assumed to sink and equilibrate with the liquid at the bottom of the magma ocean prior to fractionation, except for plagioclase which was assumed to float to the surface to form anorthositic crust.

Results: We found that increased bulk LMO FeO contents lead to increased densities of cumulate minerals but have only minor effects on the relative abundances of mineral phases in the bulk cumulate – except for increased abundances of the Fe-rich minerals appearing late in the crystallization sequence. As a consequence, the thickness of the dense, ilmenite bearing cumulate layer increases systematically with increasing FeO content of the bulk LMO.

Cumulate metamorphism during mantle overturn:

Model: As a consequence of the higher compatibility of Mg compared to Fe in olivine and pyroxene dominated layers that constitute the largest part of the LMO cumulate, the density of the produced cumulate increases with progressing LMO solidification. This results in a gravitationally unstable cumulate stratification that facilitates convective overturn. Overturn is typically considered to result only in spatial redistribution of magma ocean cumulate reservoirs. However, the overturn process may lead to changes in local cumulate composition by mixing of different primary reservoirs and involves the transport of cumulate layers to different depths, which is associated with changes in pressure and temperature. All of these changes have an effect on phase equilibria and hence may affect local cumulate mineralogies. Local equilibrium mineral assemblages can only be determined if pressure, temperature and composition during overturn are known, which requires coupling of phase equilibria models with models of convection dynamics. However, direct coupling of convection models with thermodynamic codes is computationally expensive, hence in this study we focused on some basic qualitative effects of cumulate mixing on mineralogy.

For this purpose we calculated equilibrium mineral parageneses of different cumulate layers using Perple_X [8]. For simplicity we considered six homogeneous cumulate reservoirs, whose compositions were derived from the results of the LMO crystallization model by averaging the compositions of cumulate layers in the respective depth ranges. The boundaries of the three lower layers are each defined by the appearance or disappearance of a new mineral phase in the cumulate assemblage (olivine, olivine+pyroxene, pyroxene). The overlying ilmenite bearing layer (IBC) is defined based on its higher bulk density compared to neighboring layers, the crust contains all plagioclase that crystallized from the LMO and the KREEP layer consists of light material that crystallized after IBC solidification.

The mineralogies and densities of each layer were calculated as a function of depth along the thermal profile proposed by [9] for the lunar Farside. To evaluate the effect of mixing, we made the same calculations for some compositional mixtures of the layers. The results of these calculations were used as input in a simple density structure model in order to to investigate the effect of mantle overturn on the bulk lunar density and moment of inertia.

Results: The main difference in the resulting mineral assemblages compared to the cumulate mineralogies resulting from the LMO crystallization model, is the appearance of garnet. According to crystallization experiments, garnet most likely did not crystallize from the magma ocean [10], but it can be formed by metamorphic reactions since the pressures and temperatures in the deeper lunar interior are in the range of eclogite facies conditions.

The amount of garnet forming in the cumulate strongly depends on the local composition and is hence influenced by the assumed degree of mixing of different cumulate reservoirs. The largest amount of garnet is produced in cumulates containing Al_2O_3 and CaO-rich pyroxene. The local concentration of garnet can be reduced by mixing with olivine and orthopyroxene layers. However, trapping of liquid or contemporaneously crystallizing plagioclase in the cumulate can lead to a local increase in Al_2O_3 and CaO concentrations and hence increase local garnet contents. These mechanisms illustrate the necessity for models that a) quantify the degree of chemical mixing during overturn and b) quantify the fraction of trapped plagioclase and trapped liquid in the bottom cumulate for a quantitative evaluation of the compositional evolution of the lunar mantle during mantle overturn.

Discussion:

Implications for the bulk LMO composition: In our model the bulk density of the lunar mantle is mainly controlled by its total FeO content and the amount of garnet. Since garnet and ilmenite are the densest minerals in the cumulate, their distribution has a significant influence on the bulk lunar moment of inertia. Dynamical models of the overturn of dense ilmenite bearing cumulates (IBC) suggest that after overturn most of the IBC is located either at the core mantle boundary or stuck in the lithosphere right beneath the crust [11]. These results indicate that the low seismic velocity zone at the core mantle boundary [12] might consist largely of IBC material. If the observed low seismic velocities are associated with IBC content, then the observed thickness of the low velocity zone could be used to constrain the fraction of overturned IBC material for a given LMO model.

Since the fraction of overturned IBC is limited by the bulk lunar moment of inertia, the thickness of the low velocity zone could then potentially be used as proxy for IBC thickness and hence for the FeO content of the bulk LMO.

Implications for overturn dynamics: The differences among the mantle source compositions of different lunar volcanic rocks indicate that the lunar mantle is heterogeneous, implying that mantle overturn did not lead to compositional homogenization of mantle cumulates. The presence of garnet in the cumulate leads both to a higher density and a higher rheological strength of the material [13]. A higher density facilitates faster sinking of the cumulate during mantle overturn, while a higher rheological strength might impede mixing with other cumulate reservoirs during sinking. Hence the presence or absence of garnet might play an important role for the degree of cumulate mixing during mantle overturn and help to explain the preservation of distinct compositional reservoirs during mantle overturn.

Conclusions: We applied a combination of petrological models to simulate the mineralogy of lunar magma ocean cumulates and the changes induced by cumulate overturn and mixing.

Our results suggest that a) our combination of petrological models with constraints by overturn dynamics and seismic observations could help constrain LMO properties and b) metamorphic changes of the lunar mantle mineralogy might have significant effects on the dynamics of mantle overturn due to the associated changes in cumulate density and rheology. The degree of chemical mixing during convection, the amount of trapped liquid and fraction of plagioclase in the cumulate are important quantities that should be considered in future models simulating the evolution of lunar mantle mineralogies.

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