

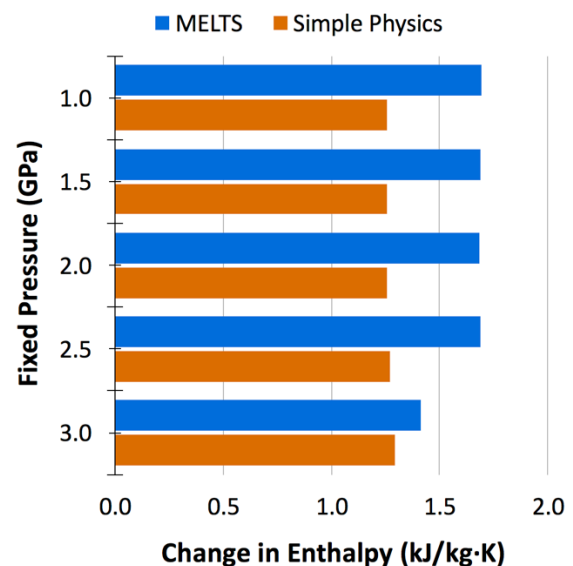
**DEVELOPING AN INTEGRATED THERMOCHEMICAL CODE FOR MODELING LUNAR MAGMA OCEAN EVOLUTION.** V. Perera<sup>1</sup>, S. Schwinger<sup>2</sup>, P. D. Asimow<sup>3</sup>, A. P. Jackson<sup>4</sup>, and C. R. Neal<sup>5</sup>, <sup>1</sup>Johns Hopkins University Applied Physics Laboratory (11100 Johns Hopkins Road, Laurel, MD 20723-6099, USA. Email: vi-ranga.perera@jhuapl.edu), <sup>2</sup>German Aerospace Center (DLR), <sup>3</sup>Division of Geological and Planetary Sciences, California Institute of Technology, <sup>4</sup>Centre for Planetary Sciences, University of Toronto, <sup>5</sup>Department of Civil and Environmental Engineering & Earth Sciences, University of Notre Dame.

**Introduction:** The Lunar Magma Ocean (LMO) model was first proposed nearly 50 years ago to explain ferroan anorthosite (FAN) rock fragments found in the Apollo 11 sample collection [1]. The LMO is fundamentally linked to the thermal evolution of the Moon [2], formation of the primordial lunar crust [3], and enrichments of incompatible “KREEP” elements (i.e., potassium [K], rare earth elements [REE], and phosphorus [P]) on the lunar surface [4]. While the LMO has been closely studied through geochemical analyses [e.g., 5] and computer models [e.g., 6], there remain several fundamental open questions. What was the initial composition of the LMO? How deep was the LMO? Where in phase space did plagioclase feldspar become stable and separate out of the LMO? When did the primordial anorthositic lunar crust acquire sufficient mechanical strength to function as a thermally conductive lid? What was the primordial crustal thickness and was the crustal dichotomy linked to LMO solidification? Why is there age overlap between FAN and Mg-suite anorthosite samples? While all these questions are related to this work, here we focus on the overall duration of the LMO solidification process to demonstrate the need for an integrated thermochemical code for LMO evolution.

**LMO Solidification Time:** According to radiometric age dating of lunar crust samples [e.g., 7], LMO solidification may have continued for ~100 Myr (or more) after the Moon formed. Thermal models, however, generally calculate much shorter solidification times of ~10 Myr [e.g., 2, 6]. As a result, previous studies have suggested that tidal heating of the Moon may have prolonged LMO solidification [e.g., 8]. Quantifying tidal heating is difficult, however, due to a number of large uncertainties, including the evolution of the Earth-Moon distance over time. Moreover, existing thermal models have their own significant uncertainties that would be fruitful to address before introducing additional external influences like tides. Existing models rely on simplified geochemistry that neglect the chemical evolution of a crystallizing magma ocean. In this work we consider how quantifying crystallization energy in detail could affect the timing of LMO solidification from the baseline duration of ~30 Myr [6].

**Integrated Thermochemical Code:** In previous studies, LMO solidification is modeled by assuming an

initial LMO composition, determining mineral assemblages as a function of depth a priori, calculating a temperature profile based on those assemblages, and then modeling heat loss through the lunar surface [e.g., 2]. This method has its limits since the entire analysis needs to be redone if the initial LMO composition were to be changed or if newer experimental phase equilibrium or calorimetry data become available. An improved method would combine a updated geochemical model that self-consistently calculates mineral assemblages and corresponding crystallization energies (i.e., secular cooling and heat of fusion) with a thermal model that calculates the time required to transfer energy to and through the surface. Such an integrated code would allow for a much wider exploration of the parameter space and help address the fundamental open questions mentioned earlier.



**Figure 1:** Comparison of enthalpy released as magma cools under isobaric conditions from 1700 to 1690 °C using MELTS and simple physics.

**Geochemical Models:** Here we use the MELTS thermodynamic models of silicate systems, which have been calibrated with a variety of thermodynamic and phase equilibrium constraints [9]. We use alphaMELTS (v2.0) [10] as an interface that calls pMELTS (v5.6.1),

the preferred calibration for pressures between 1 to 3 GPa [11], although the initial LMO depth is estimated to be 1,000 km [2], which modestly exceeds the presently recommended pressure range for pMELTS. MELTS-family models, however, are actively being updated and extended and their accuracy and range of applicability will improve with time. An alternative to pMELTS is SPICEs [12]. While recent work has shown SPICEs to better match experimental data for certain crystallization stages [13], SPICEs does not have an internally consistent energy budget. Since the focus here is LMO solidification time, we use pMELTS because it provides more accurate crystallization energies.

**Initial Results:** In incremental thermal models of LMO solidification [e.g., 2, 6], total enthalpy released at each step is the sum of enthalpy released due to secular cooling of the LMO and enthalpy released by solidifying an incremental portion of the LMO. Typically, a fixed specific heat capacity (e.g., 1256.1 J/kg·K) and a fixed heat of fusion (e.g., 418.7 kJ/kg) are used for calculations. This simplification can be improved by incorporating a geochemical model such as pMELTS.

Preliminary calculations have compared crystallization enthalpies calculated using pMELTS to ones calculated using a fixed specific heat capacity and a fixed heat of fusion (Fig. 1). As an example, we use the Taylor Whole Moon (TWM) initial LMO composition from [14] and model isobaric equilibrium (batch) crystallization from 1700 to 1690 °C at given pressures (i.e., 1 to 3 GPa). Oxygen fugacity is set to one log-unit below the iron-wüstite (IW) buffer.

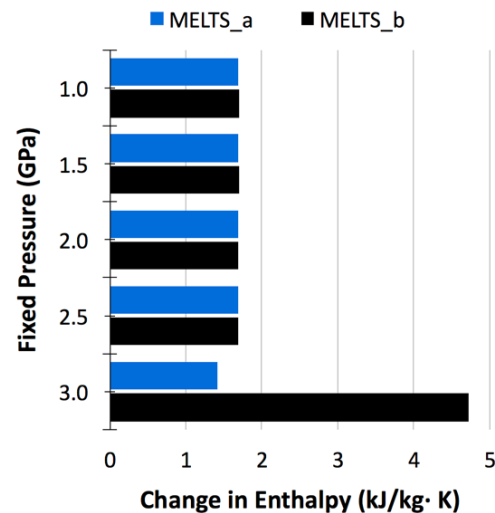
Enthalpy changes calculated using pMELTS are generally ~20% higher than the fixed estimates, since pMELTS incorporates calorimetric data for heat capacities of silicate liquids, which are larger than those of solids due to configurational degrees of freedom. In Figure 2 we compare energies calculated by pMELTS for two different initial LMO compositions: (a) the same TWM composition as above and (b) the initial composition from [15] as modified in [13]. Energies are only noticeably different at 3 GPa, because the latter bulk composition (only) encounters multiple saturation and undergoes a large increment of crystallization over the selected temperature range at this pressure.

**Outlook:** Calculations shown here are preliminary and have not yet been fully integrated into a thermal model, but they are sufficient to demonstrate the power and promise of this approach:

*Proper Energy Budget of the LMO.* Enthalpy changes returned by MELTS have more appropriate absolute values than previous fixed estimates and vary self-consistently with crystallizing assemblage and evolving liquid composition, affecting both the overall rate and the pattern of heat loss from the LMO.

*Initial Parameters of LMO.* Since pMELTS, unlike many phase equilibrium parameterizations, is not tied to a particular bulk composition, it can readily vary the composition and other parameters and investigate effects of such variation.

*Open Source and modular code.* alphaMELTS functions can now be integrated with Python or other coding environments to make flexible, modular, fully documented, open source tools for LMO modeling, available to the entire lunar science community.



**Figure 2:** Comparison of enthalpy released as magma cools under isobaric conditions from 1700 to 1690 °C using pMELTS with two different initial compositions. At 3 GPa, the latter composition undergoes a large increment of crystallization in this temperature range.

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