Machine Learning Approaches in Lunar Mantle Heterogeneity Investigations

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November 21, 2022

Abstract

Lunar mare basalts are the products of their corresponding parent magma compositions, sourced from the lunar upper mantle. The lunar mantle has been repeatedly modeled through numeric simulations to reflect lunar magma ocean (LMO) crystallization, resulting in an early-stage anorthositic crust and immediately underlying, late-stage, KREEP-rich and ilmenite-rich layer. This negatively buoyant layer is expected to have induced mixing with the underlying mantle, potentially to the core-mantle boundary. The lunar mare basalts, in this context, reflect mantle sources that are variably mixed between pristine mantle compositions and the dense ilmenite-rich layer. In order to constrain the geometry of lunar mantle heterogeneity, we simultaneously examined multiple mare basalt characteristics to extract significant multivariate patterns that might lend insight into the nature of this mixing-induced heterogeneity. Using two fundamental machine learning approaches and a newly compiled database of Apollo basalt characteristics (ApolloBasaltDB), we conducted a preliminary investigation, holding the assumptions that 1) mare basalts are assumed to retain the majority of their original characteristics at the time of extrusion: texture, isotopic age, major element composition, mineral mode, and geographic occurrence; 2) negligible basalt alteration occurred due to the lack of an atmosphere; and 3) impact gardening did not have significant bearing on final geographic location of basalt samples based on our nearside spatial partitions. The results of cluster and principal component analyses over changing spatial basalt groupings suggest that lunar nearside changes in major element concentrations and mineral modes vary spatially. Al2O3 concentrations increase in diversity within the Procellarum KREEP Terrane (PKT) compared to older regions immediately exterior to the eastern PKT, while a general nearside trend appears to suggest that ilmenite (TiO2) diversity comes at the expense of plagioclase (Al2O3) diversity. Cluster analysis suggests PKT perimeter rifting may have tapped into increasingly Ti-rich sources as rifting proceeded SE to NW. By establishing such trends over varying spatial scales through multivariate processing, the changing strengths of these surface correlative patterns may indicate the changing conditions (including temporal) of the immediately underlying mantle at the time of extrusion.

Insights into Lunar Mantle Heterogeneity through Machine Learning

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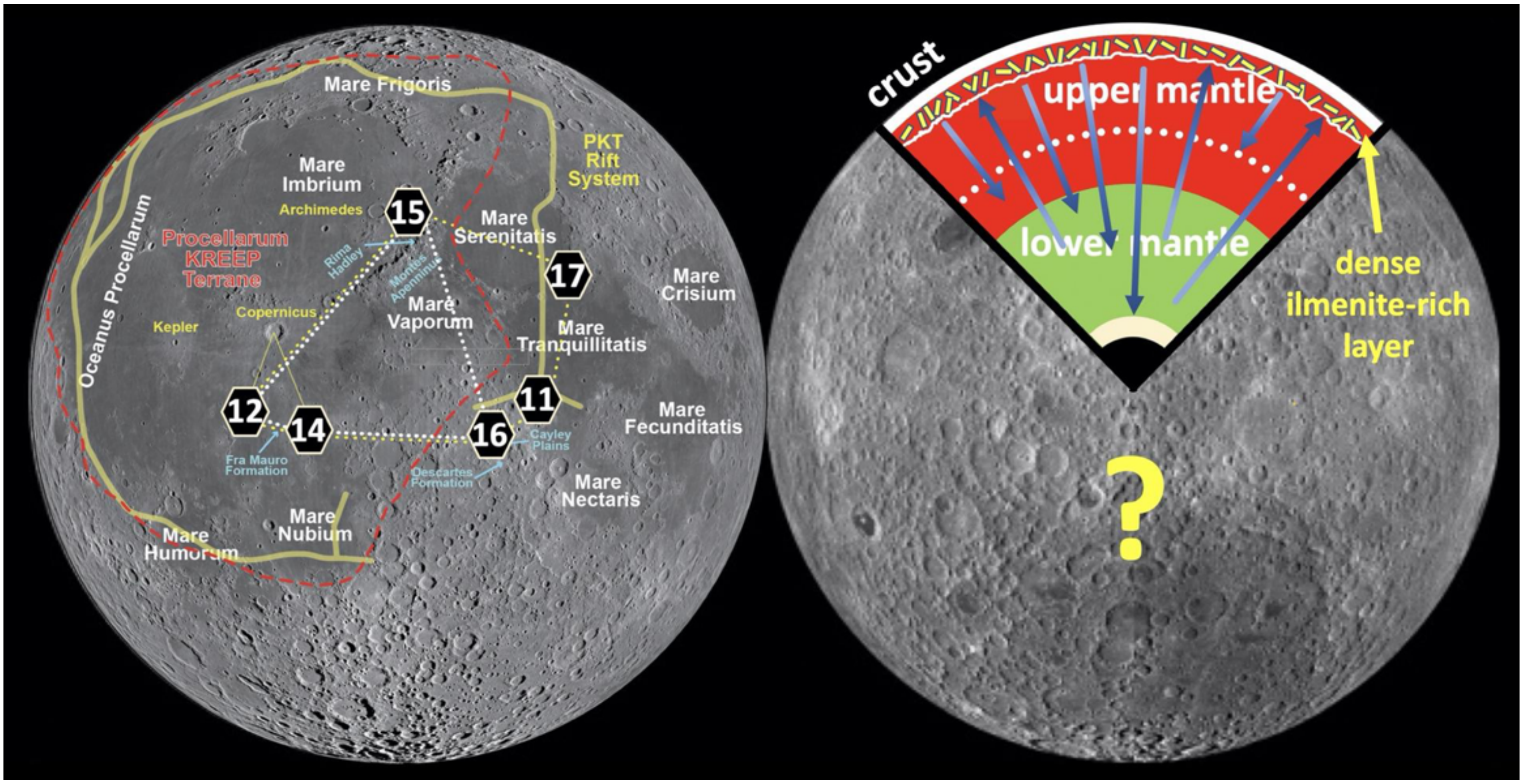
PRESENTED AT:

THE MOON'S COMPLEX EVOLUTIONARY HISTORY

The Moon is a small, but largely geologically inactive, terrestrial body that displays evidence of a complex crystallization history--when the global lunar magma ocean cooled and solidified soon after a Giant Impact, radiogenic and dense late-stage melts (rich in ilmenite and iron) that were trapped between the crust and mantle began to sink, mixing the mantle to an unknown depth (below figure; right). Geochemically, the most revealing evidence for this mixing exists through the compositional variety of nearside basalts returned by NASA's Apollo missions.



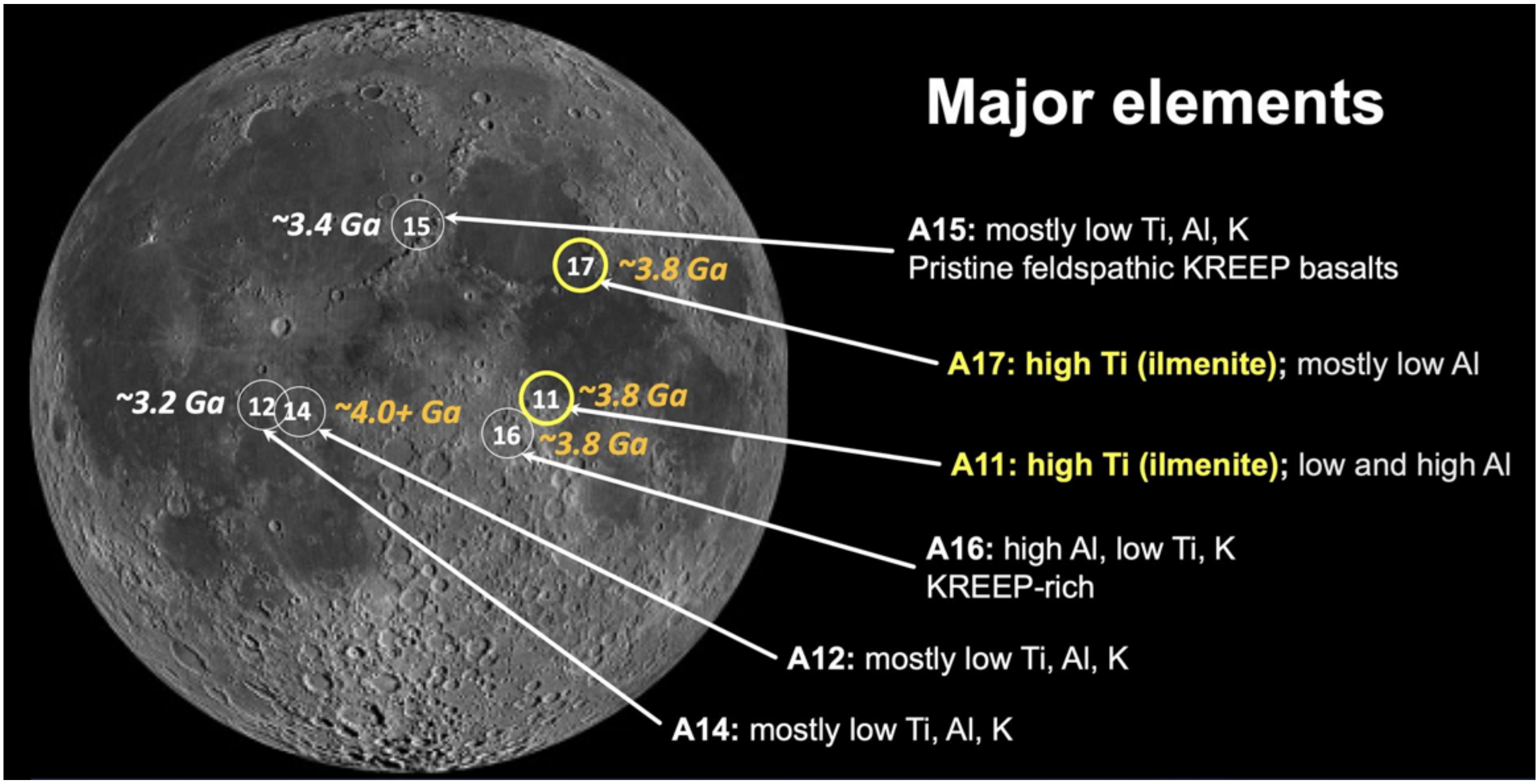
While the first-stage of lunar formation involved a bottom-up cooling of a ~1400-km deep lunar magma ocean produced a stratified mantle, a second-stage event induced top-down mixing of the mantle through the sinking of a dense, radiogenic layer (shown here as randomly-oriented yellow rectangles). Cone et al. (in prep).

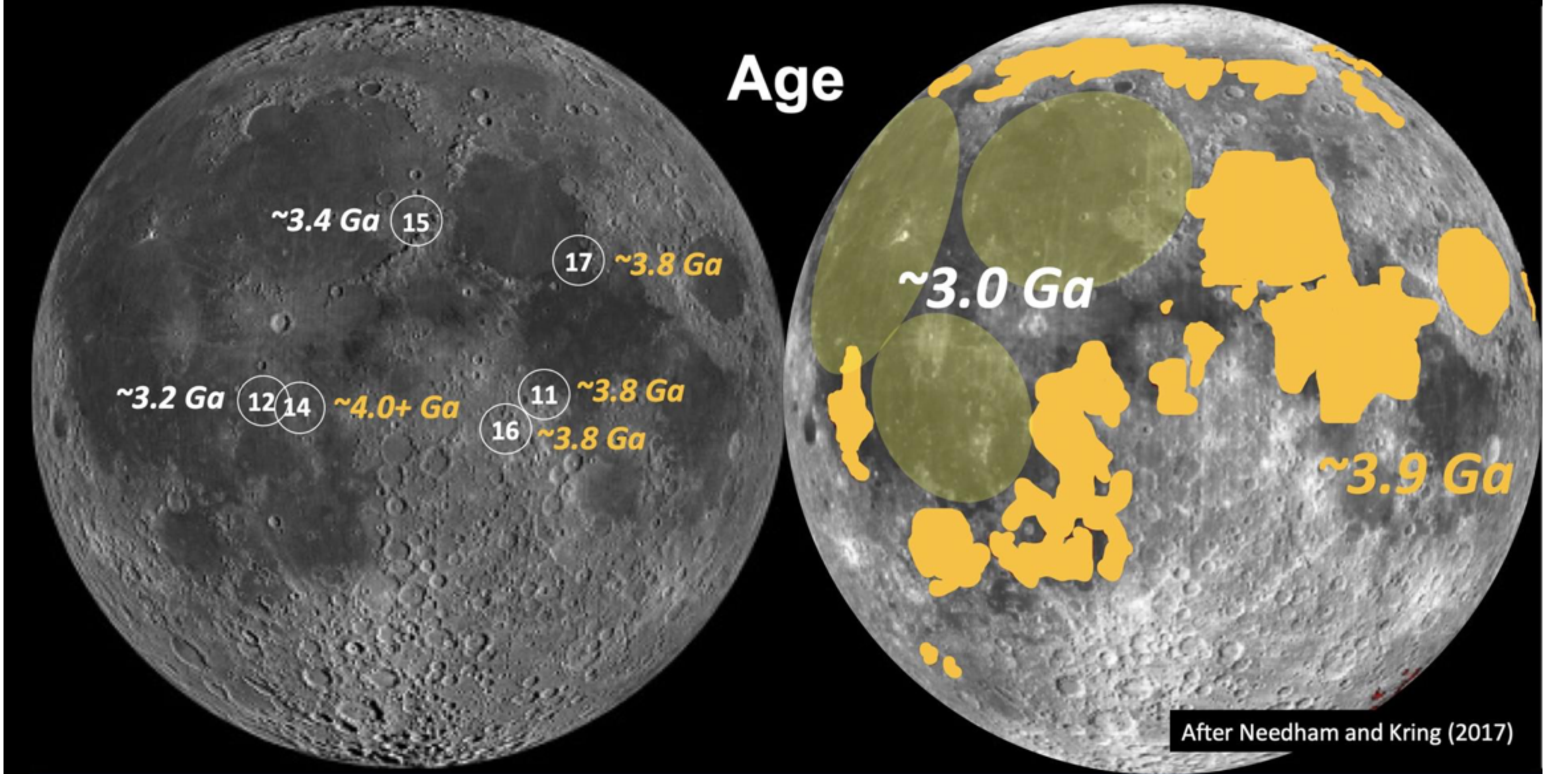
Current research suggests that at the end of the bulk cooling of an initially fully molten Moon (a lunar magma ocean (LMO) that reached near-solidification up to ~150 million years after inital formation), that dense ilmenite-rich layer began to sink, possibly as far down as the core-mantle boundary.

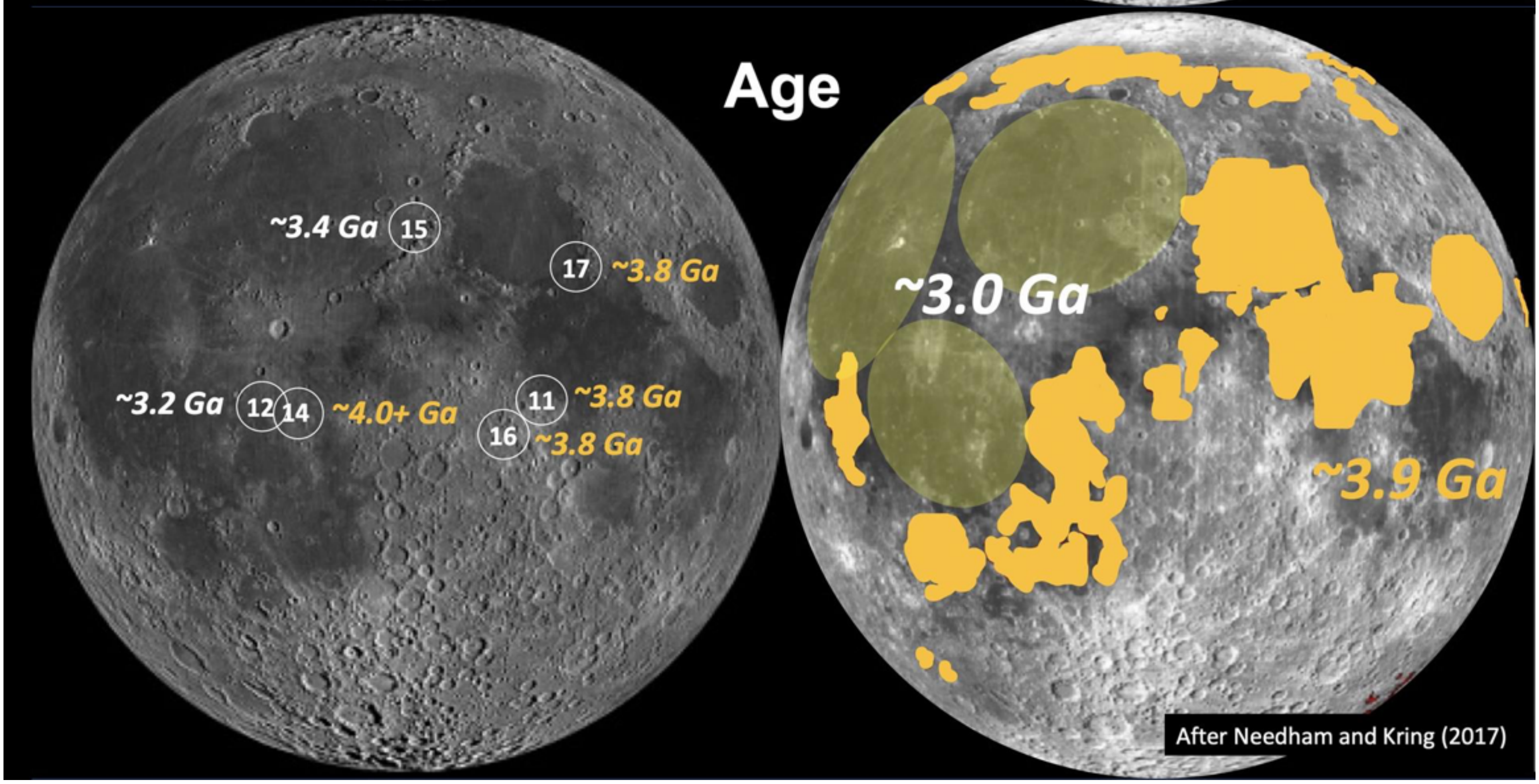
This sinking event is understood to be the key driver for the mixing of an already layered lunar mantle (the result of early crystal fractionation). What is not thoroughly understood is the depth to which this dense layer sank and how thoroughly mixed the mantle became as a result. Was this mantle overturn a global event or just confined to the nearside?

Most research that investigates the nature of lunar mantle compostion will rely on aspects of exterior-based and/or interior-based data. The most revealing interior-based data is geophysical, in the form of seismic density profiles. However, these seismic profiles have little meaning unless coupled with a geochemical profile. That geochemical profile can be approximated through thermodynamic phase equilibria modeling but must involve two steps: 1) forward modeling of whole-Moon bulk compositions representing the initial LMO, and 2) forward modeling of the late-stage mixing event. These two steps combined are responsible for the bulk of the Moon's ***current*** internal structure; it is only after the effects of these two steps that reverse modeling using the nearside basalts to constrain upper mantle compositions (the source of the Apollo basalt samples) acquire improved context.

Indeed, the Apollo basalt samples are compostionally diverse and suggest upper mantle heterogeneity. Compositional and age trends exist by site (below).

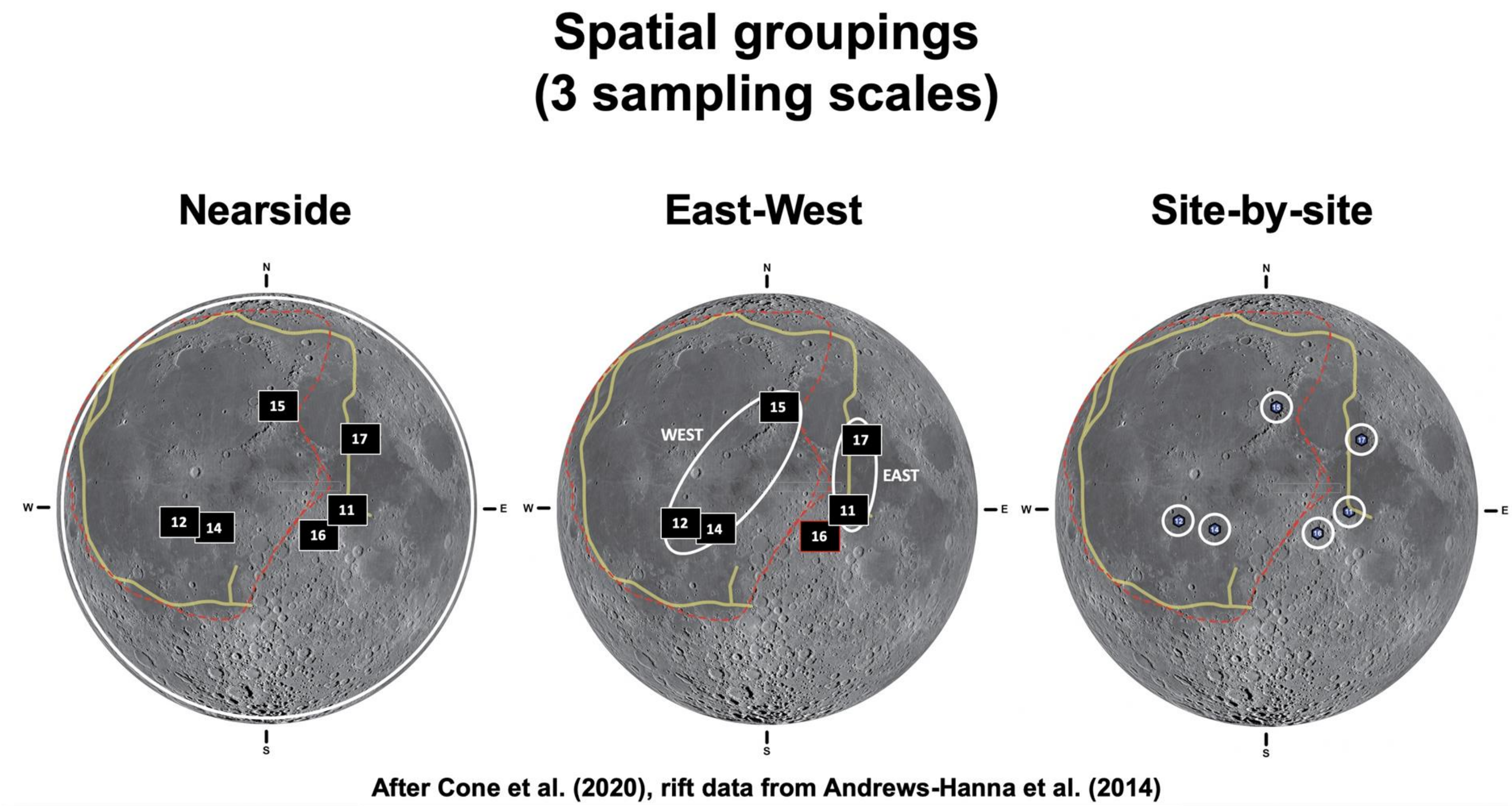






Geochemical and age trends per Apollo site. Cone et al. (in prep).

Most lunar basalt investigations focus on specific geochemical groupings (like those with high-Ti content). We try something different here--instead of focusing on lunar basalts with a specific compositional character, we examine the lunar nearside as a vast field site where spatial scales for sampling sites are varied. Changing the areal sizes of field sampling sites (what we call here "spatial groupings", see below figure) produces related changes in the correlational strengths of major element and mineral concentrations.



Lunar nearside field sampling groups. The areal extent of sampling is reduced from left to right. The yellow solid line is the approximate location of a rift boundary that encircles the Procellarum KREEP Terrane region. Cone et al. (in prep).

By applying a more planetary-scale approach, we expected to gain insight into global-scale mantle composition and structure (the interior) through changing trends in basalt characteristics (the exterior). This approach does not render previous analyses of compositionally-similar lunar basalts myopic in scope; on the contrary, these analyses serve as complementary in that we can use the source mantle characteristics assigned to specific basalt sample groups to refine mantle characteristics at specific nearside locales.

MACHINE LEARNING: WHAT, HOW, AND WHY?

Why machine learning?

Geochemists and petrologists typically employ traditional two-variable plots (sometimes called biplots; Harker diagrams, for example) to establish geochemical and/or petrological trends. While these types of biplots (and ternary diagrams) remain a valuable analytical tool, they are not efficient for establishing multivariable trends. Here, we examine multiple variables ***simultaneously*** to gain insight into nearside lunar mantle behavior.

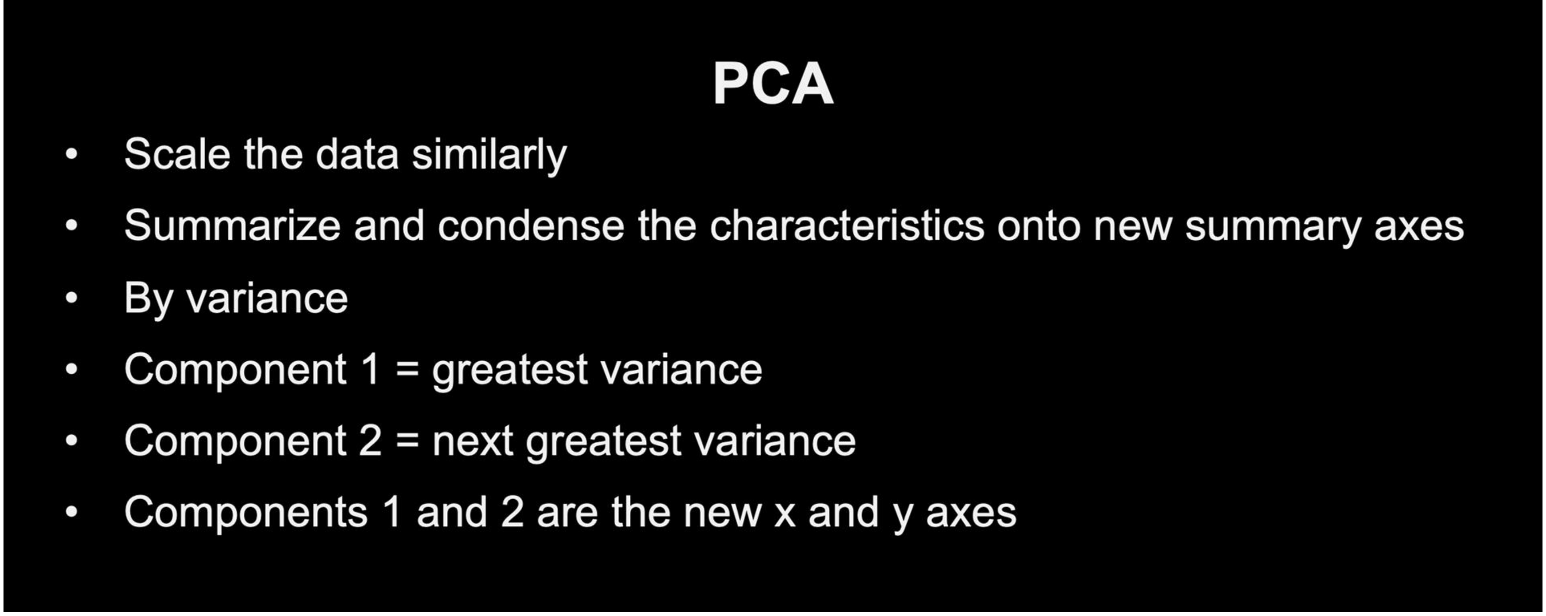
Current programming platforms like Python and Matlab offer low-cost, yet powerful capabilities for executing various machine learning algorithms. There are two basic types of machine learning **(ML)**: **supervised (SML)** and **unsupervised (UML)**. **SML** make assumptions about the desired outputs through algorithms that are created with training data (sometimes a subset of the actual data to be analyzed is used), while **UML** makes no assumptions about data behavior and classification in establishing data trends or patterns. ***UML is highly exploratory and is the method we use here.*** Caveat: exploratory methods rely heavily on the user to make sense of the patterns and trends, and any pattern established by UML does not necessarily convey meaningful significance. UML unsurprisingly and often creates more questions than solid answers, providing insight for new questions about a system being investigated.

How does it work?

Foundational machine learning algorithms commonly involve types of cluster analyses, where data are grouped by proximity-of-characteristics in multi-dimensional space (this may be linear or non-linear; the choices are up to the user), the latter often defined by Euclidean distances. ***We used two sets of clustering algorithms: 1) k-means clustering (KCA), and 2) independent componenet analysis (ICA)*** to assess correlative patterns among variables encompassing mineral modes, major element oxide percents, textures, and ages for lunar nearside basalts. All the data used for UML may be found in a freely available database called ApolloBasaltDB (ABDB). (http://people.mines.edu/kcone)

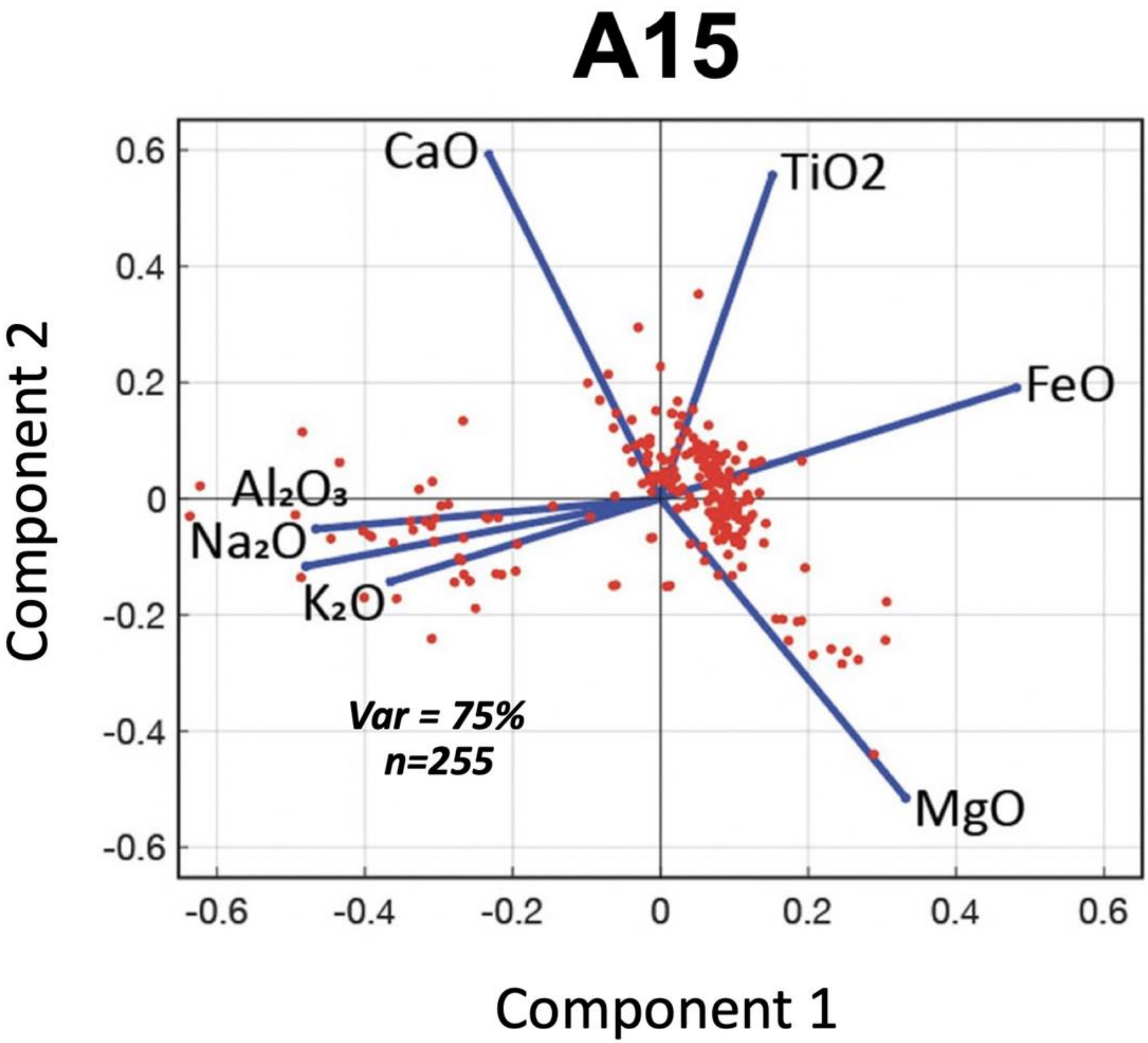
KCA

- Random cluster centers are assigned
- Data points are assigned to the nearest cluster center
- The cluster center is recalculated
- The data are then reassigned to the the (new) closest center
- Repeat until centers become stable



The basics of how to read PCA biplots

Here is an example of how PCA plots (we show only two variables here for ease of reading; these are called PCA biplots). Below is a PCA biplot for seven major element oxides from all unique basalt samples at Apollo site 15. The red dots indicate the scaled samples and the blue lines represent the amount of variance contributed to Component 1 (the new x-axis) and Component 2 (the new y-axis). The more the blue line is vertically oriented, the greater the contribution to Component 1, while a perfectly horizontal orientation indicates the maximum contribution in variance to Component 2 (and none to Component 1). The longer the line, the stronger that variable's effect on determining that Component's current orientation.



A major element oxide biplot for Apollo site 15 basalt samples. Components 1 and 2 together account for 75% of the total variance. Cone et al. (2020).

We observe that Al, Na, and K oxides are generally correlated; that is, as one increases, so do the others. In this way, as any of these three oxides increase, FeO decreases; such behavior shows an anti-correlation. Another anti-correlation is the CaO/MgO pair. In terms of Component 1 (representing the new x-axis that is oriented to reflect the greatest amount of variance in the scaled data), FeO has the greatest contribution while MgO contributes somewhat equally to both Components 1 and 2 (but slightly more to Component 2 and the variance bound to it).

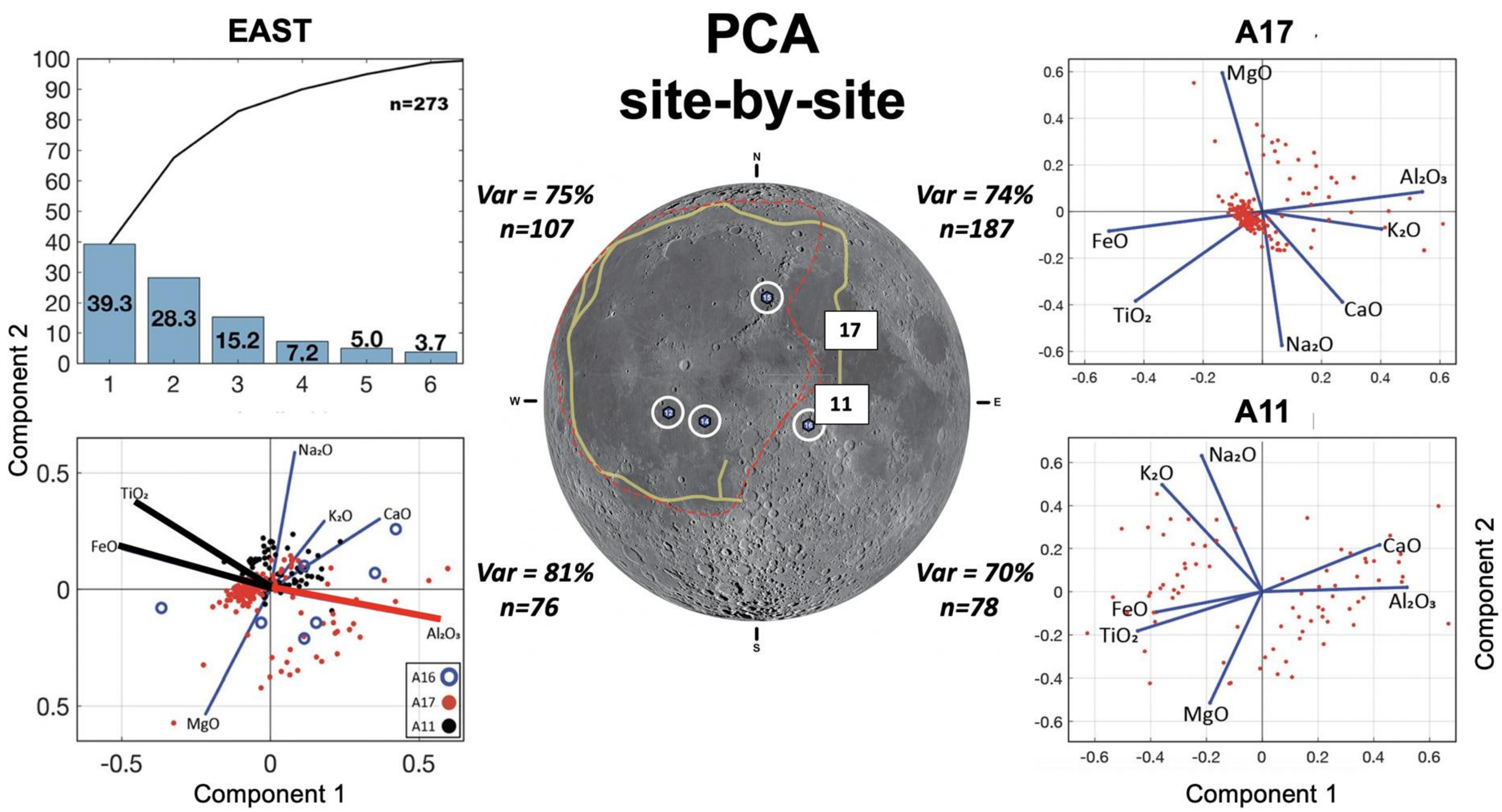
RESULTS: HIGHLIGHTS FROM MACHINE LEARNING

Expected results

The results from PCA and KCA do show some expected behaviors in the data patterns (for example, when olivine increases, Mg also increases). In general, the seven major element oxides do trend with the four main minerals that contain them (plagioclase, ilmenite, olivine, and pyroxene), although slight deviations for FeO-based correlations are expected, as ilmenite and pyroxene both contain FeO as well.

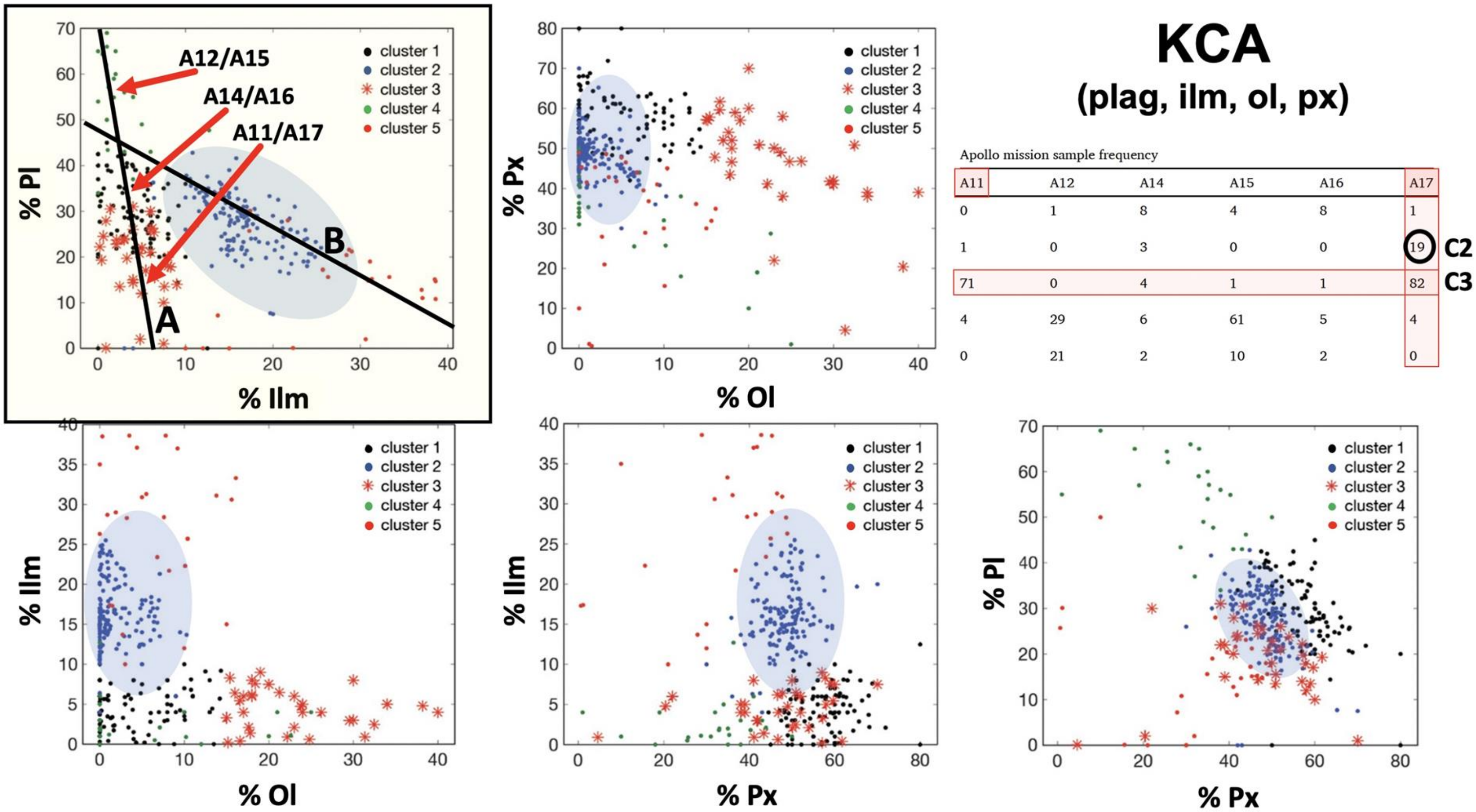
Notable results

Sites 11 and17 are geochemcially similar through PCA analysis, and both sites show increases in modal ilmenite with decreases in modal plagioclase (a pl/ilm anti-correlative pair; see below).



East grouping (which includes Apollo sites 11 and 17) versus sites 11 and 17 separately. Modified from Cone et al. (2020).

More interesting, however, are the cluster patterns through KCA that establish a global nearside trend of ilmenite-to-plagioclase ratios based on site locations, moving NW to SE. ***We observe the correlative ilm/pl pair not just at individual sites but as a global trend across the lunar nearside*** (below, upper-left). Plagioclase increases with decreasing ilmenite, but cluster 2 (below, blue dots) which is almost exclusively defined by site 17, now stands apart from site 11, their geochemical similarity now standing in added constrast.



Apollo mission sample frequency

A11	A12	A14	A15	A16	A17	
0	1	8	4	8	1	
1	0	3	0	0	19	C2
71	0	4	1	1	82	C3
4	29	6	61	5	4	
0	21	2	10	2	0	

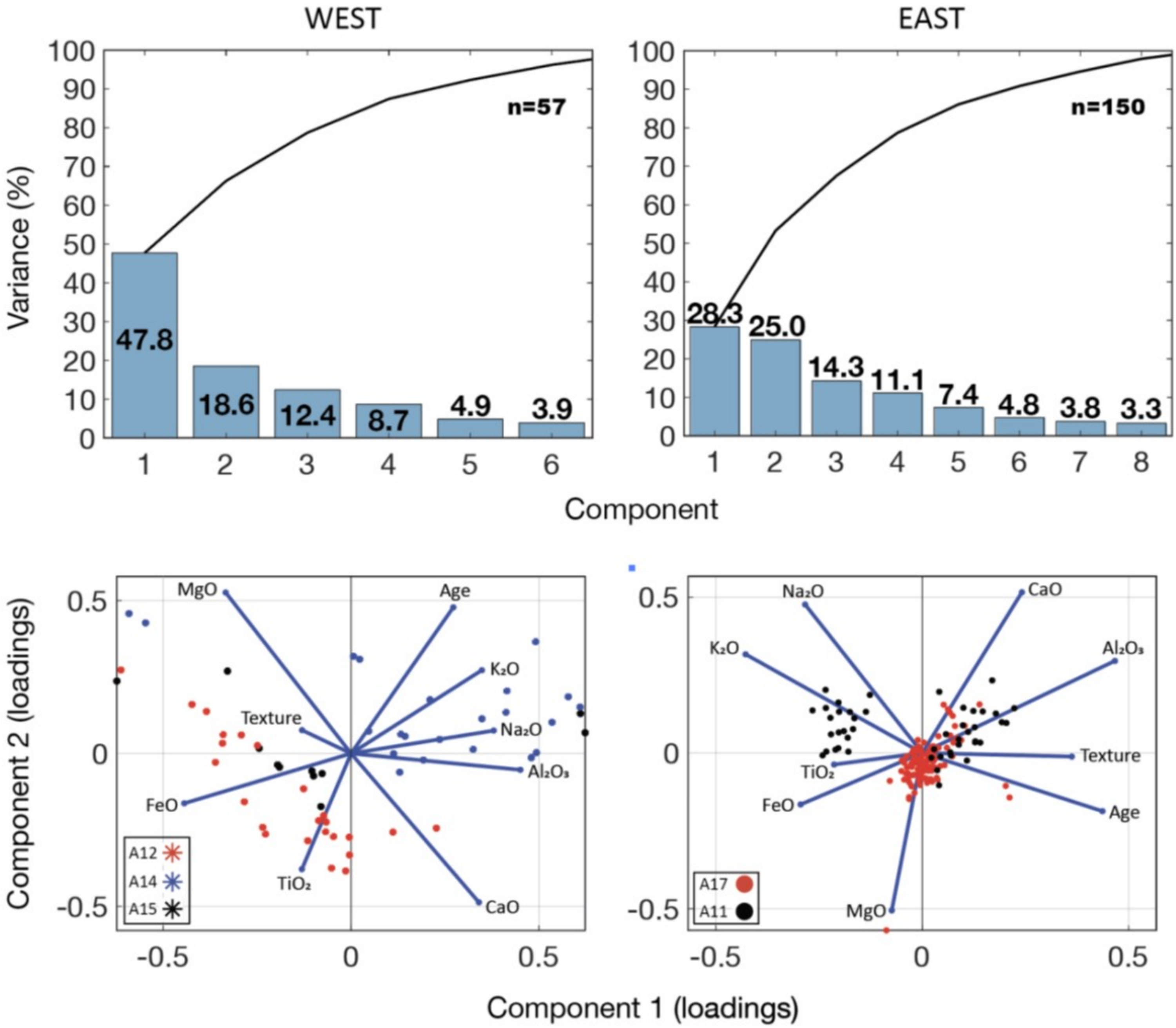
Modal mineralogy patterns through k-means clustering (Cone et al., in prep).

Other notable results

For the Nearside spatial grouping, we observed a moderate signal for coarsening/lower Ti content.

In the East spatial grouping, we observed textural fining with younger samples as well as reductions in Al (plagioclase) with increasing Fe/Ti (below, right column).

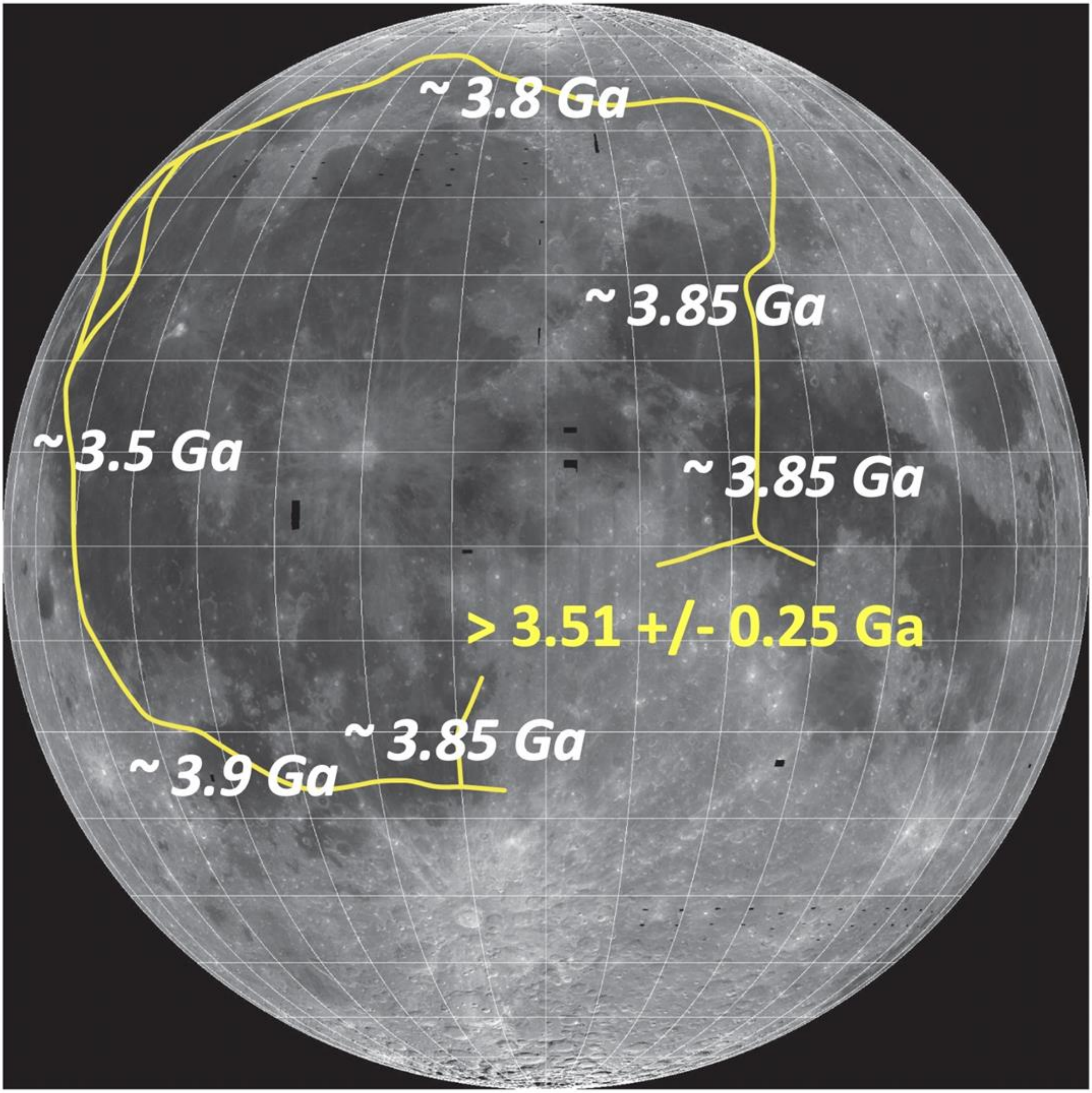
In the West spatial grouping, a moderate signal for increasing Ti for more recent volcanism appeared (below, left column).



Comparison of major element oxides in West and East groups. Cone et al. (2020).

POTENTIAL SIGNATURES OF MANTLE DYNAMICS?

A brief discussion: A potential link to early rifting and mantle source characteristics



Approximate ages of regions along the PKT rift boundary (solid yellow line). Cone et al. (in prep).

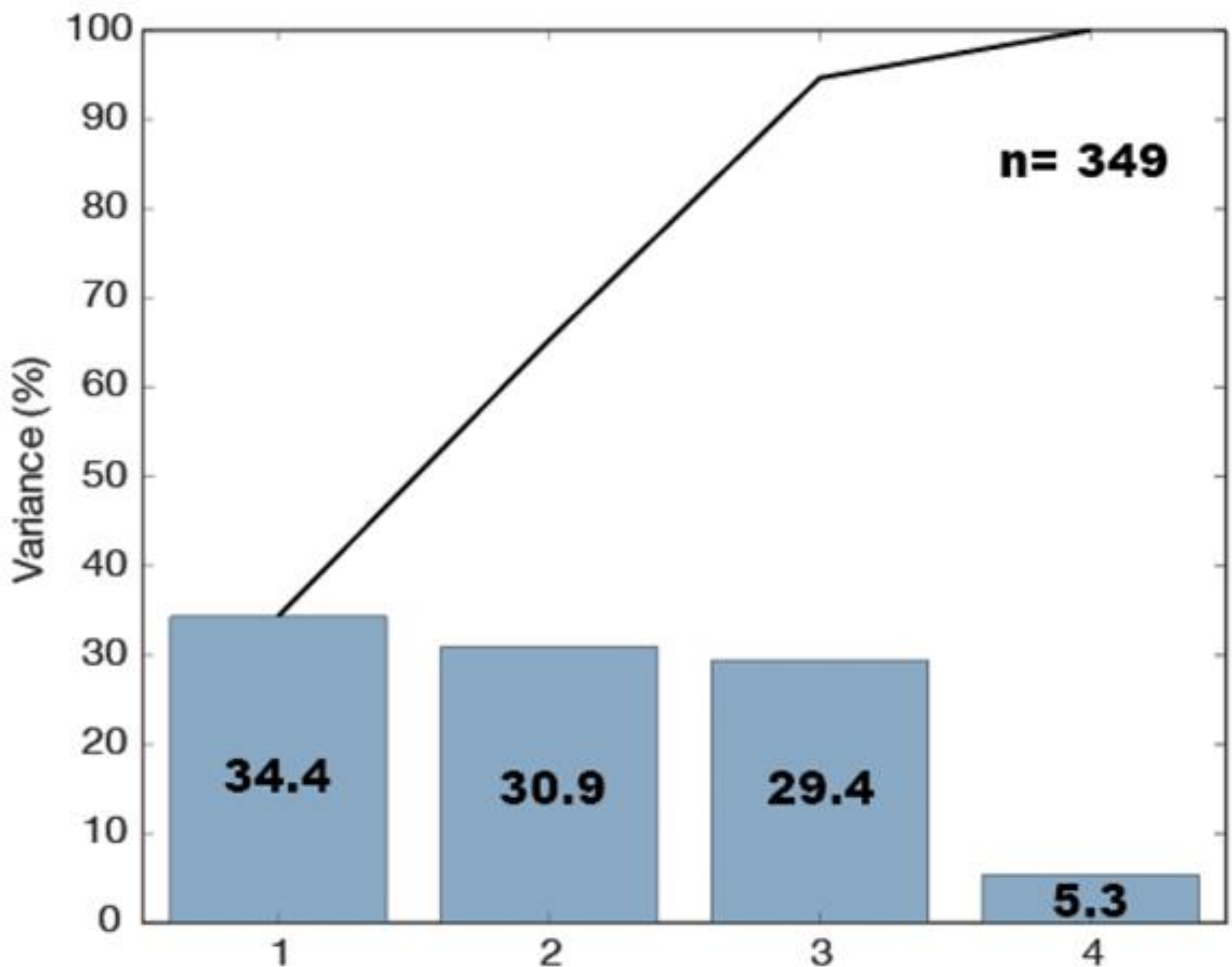
GRAIL gravity data, as interpreted by Andrews-Hanna et al. (2014), suggest that a large rift perimeter (the yellow line in the figure above, with corresponding crater ages in yellow text; white text indicates basalt ages) exists around the Procellarum KREEP Terrane (PKT). The ages that appear are based in part on crater size frequency distributions (CSFDs) baselined against Apollo basalt sample ages. Although it was beyond the scope of this work to include hyperspectral and spectral data, using just the Apollo basalt sample data suggest that the PKT rift boundary may have rifted from the SE to the NW, with volcanism tapping into increasingly rich sources of Ti over time. What does this mean? Higher concentrations of Ti (i.e. ilmenite) in younger basalts suggest that more Ti may exist in the source regions of the upper mantle to the NW; a "pocket" or "downwelling plume" of Ti-rich melt may have served as the source melts for that region. There are other possible interpretations, but at this point, the original samples require revisiting for KREEP content.

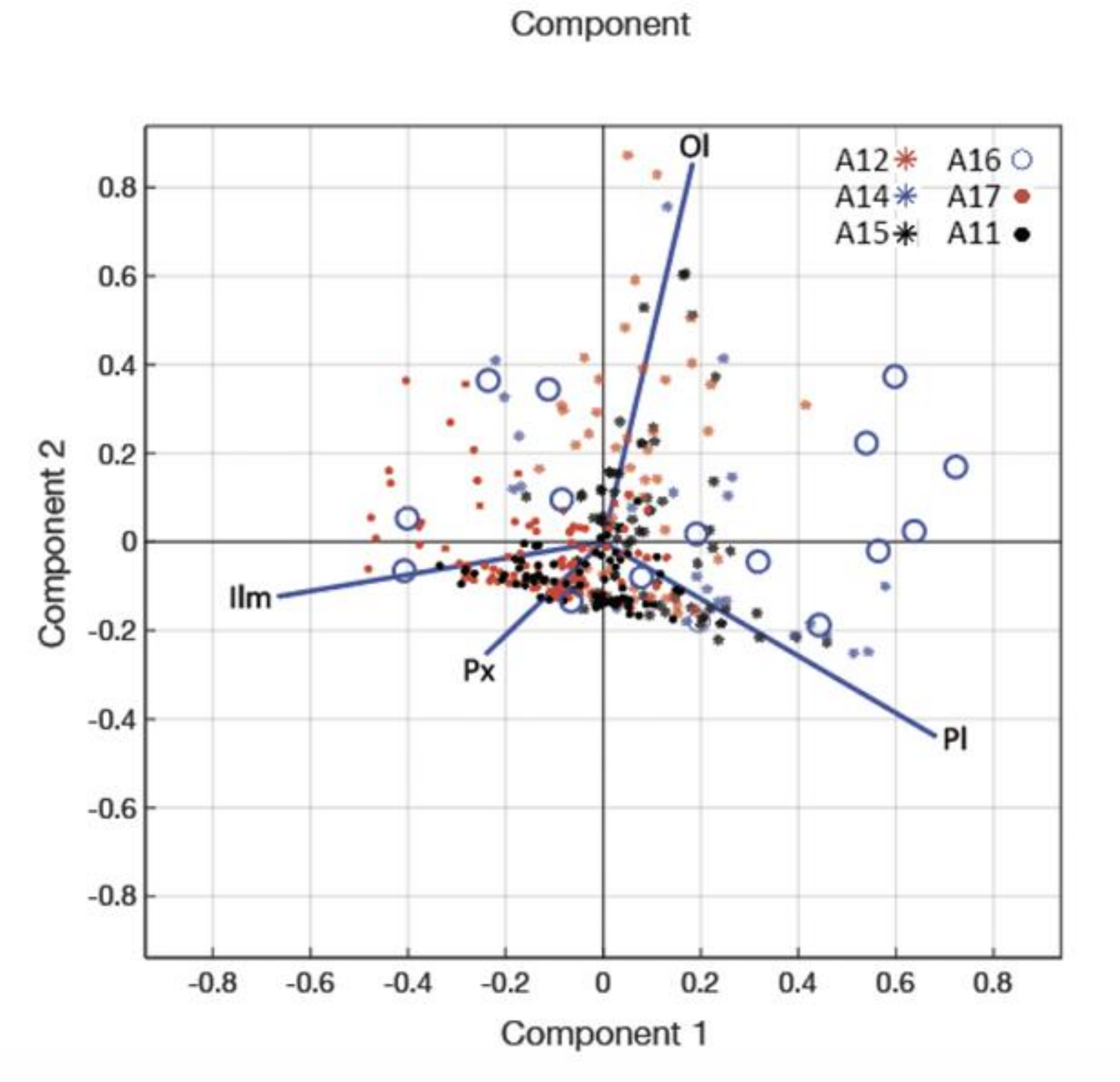
Following the Ti: Changing Ti gradients based on surface locales

The style of volcanism teased from the above observations may have initially reflected a high-Al, crystal-rich extrusion with a low-Ti magma source. Using this information, we can begin to trace the ***compositional geometry*** of the lunar upper mantle, the source of the Apollo basalt samples. This should yield clues to the late-stage ilmenite-driven mixing event.

Complementary uses of PCA and KCA

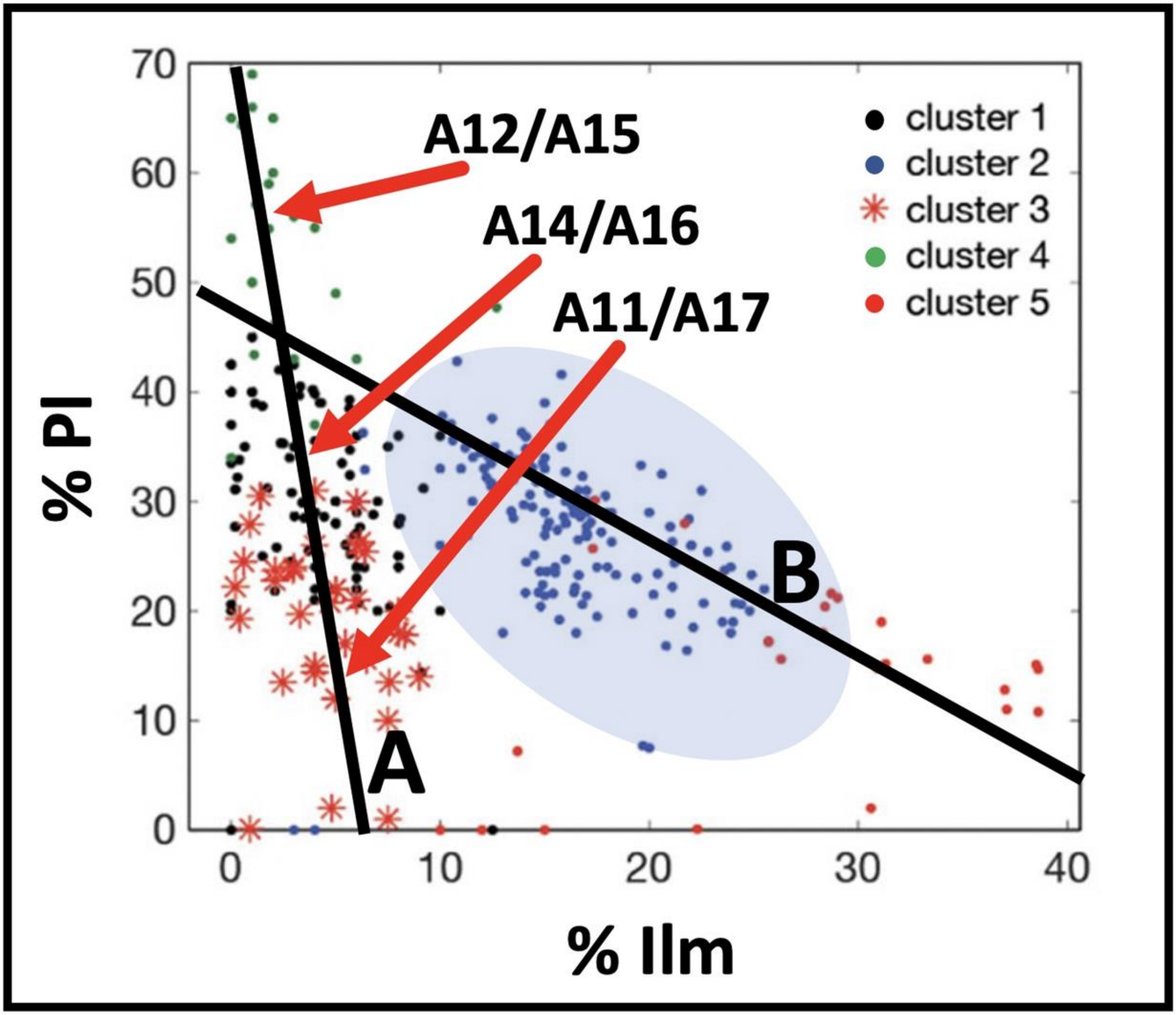
Both PCA and KCA can establish first-order multivariate trends more apparently than conventional biplots and ternary diagrams. PCA focuses on variance-based pronouncements, which may also be viewed as a type of signal attenuation across groupings in this study. For example, PCA biplots for the Nearside spatial grouping showed the following:





Modal mineralogy PCA biplot for the Nearside rgoup. Note that ilmenite and plagioclase above define most of the variance within the data. Cone et al. (2020).

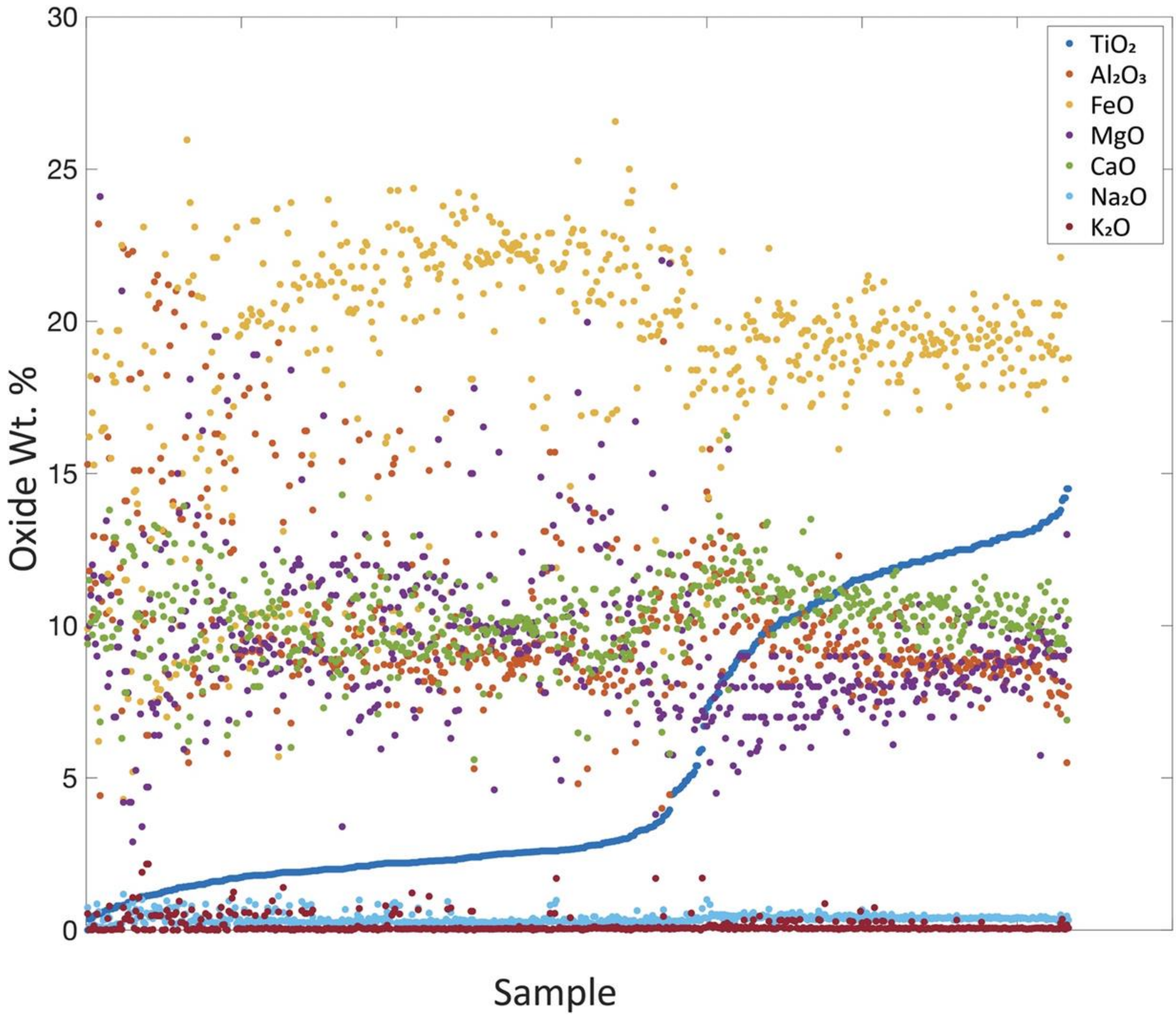
However, KCA analyses of the same data (below) places futher constraints on the general PCA pattern, showing two distinct ilm-pl clusters. The blue cluster below is dominated by site 17 samples, with higher ilmenite content. Although sites 11 and 17 are physically close to each other, these patterns suggest that they do not share the same eruptive histories.



Plagioclase and ilmenite modes across the lunar nearside (Cone et al., in prep).

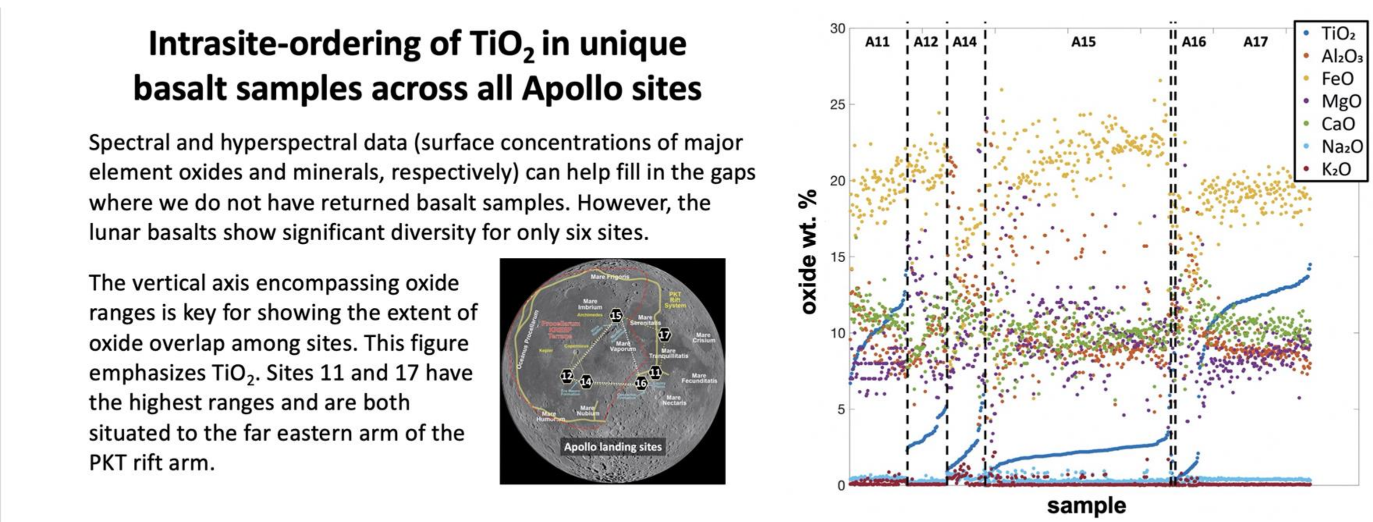
THE SIGNIFICANCE OF TITANIUM IN LUNAR MANTLE EVOLUTION

What's so special about titanium in the lunar mantle?



A plot showing all unique Apollo basalt samples in order of increasing Ti concentration (the blue curve). In general, higher Ti signatures are associated with lower Fe and Mg concentrations. TiO_2 is almost continuously represented from 1 wt.% to ~16 wt.%**.** (Cone et al., in prep).

Titanium (Ti), primarily bound to ilmenite, is modeled to have formed as a concentrated phase at the end stages of lunar cooling. After ~80% of the initially molten Moon crystallized, plagioclase began to float to the surface, creating the primary anorthositic crust. After about 95% of LMO crystallization, most of the mantle had solidified, and the final melt dregs began to crystallize above the mantle. With that crystallization came the enrichment of dense ilmenite, radiogenic elements, and other incompatible elements (K, REEs and P; collectively known as KREEP). That ilmenite has been modeled to sink into the mantle, as far down as the core-mantle boundary in some cases, dragging incompatible elements down with it. Therefore, it is the titanium-induced mantle overturn that helps gives Apollo basalt samples their diverse compositional character, as none are believed to reflect partial melting of a primitive mantle composition. By honing in on the titanium signatures (as well as ages and textures) of lunar basalts, we can begin to model the lunar mantle's compositional structure in more detail. ***In short, surface composition helps approximates internal composition.***



NEXT STEPS

Our understanding of terrestrial planet formation is more intimately linked to our understanding of the Moon's formation than to any other body in the inner solar system except Earth. The genesis shared by the Earth and Moon continues to be a focus in planetary science, most recently in the context of space resources. New versions of the Giant Impact Hypothesis (e.g. Lock et al. 2018; a new idea on lunar formation and reconciling compositional similarities, angular momentum, rotational inclination, etc.) drive reconsiderations of early lunar geochemistry. It is becoming increasingly apparent that the Moon's composition is the same as that of Earth but with reduced amounts of volatile elements.

An outstanding issue in lunar evolution concerns the original water content in the early lunar mantle. The amount of water, combined with varying proposed ranges of bulk silicate Moon compositions and the Moon's thermal state, together determine what the primary composition and structure of the lunar mantle and crust should ideally be.

The problem is that most published models are based on assumptions of an anhydrous lunar mantle; current research increasingly suggests otherwise. Given our new understanding of juvenile water in the lunar mantle (including potential late-stage addition through cometary ices), investigating the cooling of the lunar mantle requires new models.

We continue our work with experimental petrology, scheduled for the Spring of 2021:

1) High P-T piston-cylinder runs will simulate early lunar mantle thermal states and compositions; from these runs, probable crystallization schemes will be established considering a hydrous young lunar mantle.

Thermodynamic phase modeling will continue through a joint venture between Colorado School of Mines and the University of Oxford:

2) Thermodynamics modeling will be compared with the above experimental results to better constrain probable lunar bulk silicate compositions and mantle density profiles.

Finally, we continue with machine learning, moving to supervised methods:

3) Machine learning algorithms (SML) will be chosen based on the results from 1) and 2) as well as on previously published findings.

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ABSTRACT

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