A Thermodynamic Model for High-Ti Silicate Melts

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Thermodynamic phase equilibrium modeling serves as a powerful tool for investigating petrogenesis of diverse igneous rock types. Recent advancements in thermodynamic models demonstrate robust capabilities in reproducing subsolidus phase abundances/compositions in both experimental and natural samples, while accurately predicting solidus positions and melt-residue relationships for various peridotitic compositions[1]. However, when compared to extensive experimental datasets, these models exhibit some discrepancies: they overestimate MgO while underestimating FeO and Al_2O_3 in high-MgO melts (>10 wt.%), and they struggle to accurately predict TiO_2 contents in high-Ti melts. These shortcomings hinder their capacity in modeling the origin and evolution of high-titanium basalts and lunar basalts.

To address these limitations, we have developed an optimized thermodynamic model, building on the framework established by Tomlinson and Holland (2021). This refined model was calibrated using over 600 experimental results from anhydrous systems. It operates within the chemical system K_2O-Na_2O-CaO-FeO-MgO-Al_2O_3-SiO_2-TiO_2-Fe_2O_3-Cr_2O_3 and covers a pressure-temperature range of 0.01–60 kbar and 600°C up to the peridotite liquidus. Key advancements include: (1) Enhanced predictive capability for phase relations and melting processes, accurately reproducing phase assemblages across various peridotite compositions under both subsolidus and suprasolidus conditions; (2) Improved concordance between modeled and experimental melt compositions, notably in predicting melt TiO_2 concentrations up to 18 wt%.

The optimized model also effectively replicates experimental simulations of the fractional crystallization of the lunar magma ocean (e.g., [2][3]). This advancement enables investigations into fractional mantle melting and basalt generation, as well as explorations of lunar magma ocean evolution and lunar basalt genesis. A significant breakthrough of this model is its ability to overcome previous limitations in modeling titanium-enriched magmatic systems, thereby establishing a novel thermodynamic framework for lunar petrological studies.

Reference:

[1] Tomlinson & Holland (2021), Journal of Petrology, 62(1): egab012.

[2] Schmidt & Kraettli (2022), Journal of Geophysical Research: Planets, 127(5): e2022JE007187.

[3] Charlier, Grove, Namur & Holtz, (2018), Geochimica et Cosmochimica Acta, 234: 50-69.