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Calcium and Magnesium Distribution between Sulfide and Silicate Melts: Thermodynamic Modeling and Insights into Mercury's Mantle-Crust Differentiation

TAYLOR MCCOMBS[1], RICHARD GWYN[1], BRENDAN A ANZURES[2], SARAH LAMBART[3] AND ASMAA BOUJIBAR[1]

[1]Western Washington University

[2]Jacobs/NASA Johnson Space Center

[3]University of Utah

Presenting Author: mccombt@wwu.edu

Mercury stands out as the terrestrial planet with the lowest degree of oxidation among all planets of our solar system. It is characterized by a high abundance of sulfur, which is expected to replace oxygen in silicate melts. This sulfur enrichment could lead to sulfide saturation in its mantle, potentially resulting in the formation of sulfides rich in calcium and magnesium. Utilizing experimental data from the literature, we developed a thermodynamic model to explore the partitioning of calcium and magnesium between sulfide and silicate melts. This model aims to improve our comprehension of the chemical equilibria driving the process of mantle-crust differentiation on Mercury. Our models indicate that increased temperature, decreased pressure, and low concentrations of iron, oxygen, and carbon within the sulfide phase, along with low sulfur concentrations in the silicate phase, favor calcium's partitioning into the sulfide melt. Additionally, magnesium partitioning into the sulfide melt is favored with decreased pressure, decreased temperature, low concentrations of iron and calcium within the sulfide phase, and low concentrations of sulfur within the silicate phase. Our results suggest that up 9.4 wt.% and 5.6 wt.% Ca and Mg, respectively, can be present in sulfides equilibrated with sulfide-saturated silicate melts during mantle-crust differentiation. Further investigation will focus on the distribution of sulfide phases within the mantle and crust to better constrain Mercury's internal structure.