Examining the Geochemical Behavior of Sulfur in Highly Reduced Planetary Bodies: Insights from X-Ray Absorption Near Edge Structure (XANES) Spectroscopy at the S K-edge

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The oxidation state(s) and speciation of S imparts a major geochemical control on the chemical affinity and behavior of S in magmatic systems. Under reducing conditions (< IW +3), oxygen (O^{2-}) is replaced by sulfide (S^{2-}) on the anion sub-lattice of the silicate melt, and complexes with cations [M], where: $0.5\ S_2 + [M]O^{\text{(silicate melt)}} = 0.5\ O_2 + [M]S^{\text{(silicate melt)}}$. The limiting solubility of sulfide in a silicate liquid is defined by the S content at sulfide saturation (SCSS), where: $[M]S^{\text{(silicate liquid)}} \Leftrightarrow [M]S^{\text{(sulfide liquid)}}$. The SCSS is sensitive to temperature, degree of melt polymerization (i.e., SiO_2 content), oxygen fugacity (fO_2), FeO content, and to a minor degree pressure. In highly reduced systems similar to those seen on Mercury and the aubrite meteorite parent bodies (APB) (IW-3 to IW-8), the SCSS is highly sensitive to FeO concentrations of the melt. SCSS estimates for mercurian lavas and APB remain enigmatic, in part due to their low-FeO (< 2 wt% FeO), high-S (> 1 wt% S) and exceedingly low fO_2 characteristics. Additionally, initial experimental results under highly reduced conditions show a preference for Mg to be incorporated into the sulfide phase over Ca. However, there is a much stronger correlation between Ca and S on the surface of Mercury compared with Mg and S. Micro-XANES spectroscopy is a synchrotron based technique used to probe the electronic and chemical structure of materials and compounds and is a well-established method that enables *in situ*, high-resolution, and non-destructive analyses. Here we examine S speciation at low fO_2 using a sulfur-rich diopside melt composition and silicon-rich metal at 1 GPa and 1600°C. All sulfur was added to the experiments as S^0 or FeS to examine the effect of Fe on S speciation. Results from this experimental study, compared with previous literature data, will help to elucidate the preference of Ca and Mg in sulfides and provide insights into the oxidation state, speciation, and bonding environment of S in the experimental charges.