Effect of H_2 diffusion on the H_2O systematics and redox state of glasses

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H_2 diffusion and reaction

The high diffusivity of H_2 in silicate melts and glasses relative to the more abundant dissolved species (e.g., hydroxyl, molecular H_2O) suggests that, despite its low solubility, diffusion of H_2 could be a significant mode of H transport during igneous processes, especially under low fO_2 conditions such as those experienced by lunar magmas [1]. However, the diffusion of H_2 in silicate melts and glasses is complicated by the reaction $Fe_2O_3 + H_2 \Leftrightarrow 2FeO + H_2O$, which result in changes in Fe^{3+}/Fe^{2+} (and therefore fO_2) and influences the bulk diffusion of H [2,3].

Computational model

We performed calculations using a coupled diffusion-reaction model to simulate H_2 ingassing or degassing in rhyolitic melts/glasses and the corresponding effect on H_2O_t (H dissolved as OH and molecular H_2O) and fO_2. Results for H_2 ingassing show the formation of a H_2O_t peak produced via the reaction given above, accompanied by a decrease in Fe^{3+}/Fe^{2+}. The H_2O generated by reaction diffuses much more slowly than H_2, and the overall effect is a retardation of the bulk diffusion of H into the sample. This coupled redox front/H_2O_t peak is seen in the experiments of Gaillard et al. [2,3]. Conversely, during degassing, rapid H_2 loss leads to an accompanying decrease in H_2O_t and increase in Fe^{3+}/Fe^{2+} as H_2O reacts with FeO to compensate for the loss of H_2. Critical predictions of this behaviour is that joint degassing of H_2O and H_2 will lead to much faster loss of water than degassing of H_2O alone and will act to oxidise the glass/melt.

Application to lunar melt spherules

Our modeling, although currently limited to rhyolitic rather than basaltic compositions, predicts that at lunar conditions, including the effect of H_2 degassing from melt spherules can lead to melt oxidation and a higher apparent H_2O degassing rate. This could have implications for studies considering H_2O degassing [4], and the occurance of redox profiles [5] in lunar glass spherules.

[1] Zhang (2011) *LPSC* **42**, 1957. [2] Gaillard *et al*. (2003a) *Am Min*. **88**, 308-315. [3] Gaillard *et al*. (2003b) *GCA* **67**, 2427-2441. [4] Saal *et al*. (2008) *Nature* **454**, 192-195. [5] McCanta *et al*. (2019) *Am Min*. **104**, 453-458.