"WATER" IN LUNAR BASALTS: THE ROLE OF MOLECULAR HYDROGEN (H₂), ESPECIALLY IN THE DIFFUSION OF THE H COMPONENT
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Introduction: Water solubility and diffusion in terrestrial rocks have been investigated extensively. The data show that dissolved water is present in two species: H₂O molecules (H₂Oₘ) and hydroxyl (OH) groups [1,2]. Other possible forms, such as molecular hydrogen (H₂), have not been observed. Experimental data indicate that the diffusion of the hydrox component (H₂Oₘ and OH) in silicate melts is due to diffusion of H₂Oₘ, whereas OH groups are essentially immobile compared to H₂Oₘ [3-8]. Furthermore, oxygen diffusion under hydrous conditions is also carried by the diffusion of H₂Oₘ [9-11].

Recently, significant concentration of the H component in lunar rocks [12,13] has been demonstrated through SIMS measurements (but also see [14]). The exact species of the H component have not been determined. In discussion of the pre-loss "water" content, water diffusion data and model [4] have been applied [12]. However, because lunar rocks equilibrated under much more reducing conditions, it is possible that there is dissolved H₂ in lunar basaltic melt. Furthermore, because H₂ diffusivity is very high, diffusion of dissolved H₂ could contribute significantly to the diffusion of the H component even when H₂ concentration is relatively low. This report evaluates possible role of molecular H₂ in lunar basalts following the work of [11].

In this report, the hydrous component (or "water") means both H₂Oₘ and OH. The H component means all hydrogen species (including molecular H₂ and the hydrous component).

H₂/H₂O Ratio in the gas Phase as a Function of $f_{O_2}$: First, the H₂/H₂O ratio in the gas phase as a function of oxygen fugacity is calculated. This is a relatively easy and reliable evaluation from thermodynamic data. Using the following reaction:

$H₂(gas) + (1/2)O₂(gas) = H₂O(gas)$

the equilibrium constant $K = f_{H₂O} / f_{H₂ · f_{O₂}^{1/2}}$ can be calculated from $exp[-ΔG_i^0/(RT)]$, and then $[H₂]/[H₂O]$ can be calculated from $1/(K · f_{O₂}^{1/2})$. The results are shown in Fig. 1. The oxygen fugacity of NNO±2 (black curves in Fig. 1) is the range for terrestrial basalts [15], and IW to IW-2 (red curves in Fig. 1) is the range for lunar basalts [16]. It can be seen that under lunar redox conditions, H₂/H₂O ratio is $> 1$, and H₂ content is greater than H₂O in the gas phase.

Dissolved H₂/H₂O Ratio in the Melt: Molecular H₂ solubility data in silicate melts are limited. To the author's knowledge, solubility of H₂ is only known for silica melt [17-18] (in other melts, H₂ might be oxidized and hence it is more difficult to pin down H₂ solubility). However, H₂Oₘ solubility in silica melt is not available. Hence, I use H₂Oₘ solubility in a high-silica rhyolitic melt [19] and H₂ solubility in silica melt to estimate H₂/H₂O ratio in silicate melts. The estimation is not expected to be accurate, but may be viewed as an order of magnitude approximation.
Fig. 2 shows estimated ratio of dissolved molecular H$_2$ over dissolved H$_2$O$_m$ in silicate melt. Dissolved H$_2$/H$_2$O ratio is smaller than the ratio in the gas (fluid) phase. In highly reducing melt (such as IW-2), dissolved H$_2$ concentration exceeds dissolved H$_2$O$_m$ concentration.

**Relative Contributions of H$_2$ and H$_2$O$_m$ to the Diffusion of the H Component:** Molecular H$_2$ diffusion data in silicate melts are limited. To the author's knowledge, only in silica melt, are reliable H$_2$ and D$_2$ diffusion data available [18, 20-23]. But no reliable H$_2$O$_m$ diffusion data in silica melt are known. Again, H$_2$O$_m$ diffusion data in high-silica rhyolitic melt [6] are used together with H$_2$ diffusion data in silica melt. Hence, the estimation is only an order of magnitude approximation. Molecular H$_2$ diffusivity is very high, about 10 times molecular H$_2$O$_m$ diffusivity at 1673 K, and about 10,000 times at 665 K.

The contribution by H$_2$ diffusion to that by H$_2$O$_m$ diffusion on the diffusion of total H component can be compared using the ratio of $D_{H_2}[H_2]$ to $D_{H_2O_m}[H_2O_m]$ [11]. If this ratio is $> 1$, then molecular H$_2$ diffusion is the major diffusing species in total H-component diffusion. If the ratio is $< 1$, then H$_2$O$_m$ is the major diffusing species in total H-component diffusion.

**Discussion:** The discussion below is tentative because H$_2$ and H$_2$O$_m$ solubility and diffusivity have not been determined in the same melt. On the basis of Figs 2-3, a significant fraction of the H component dissolved in lunar melts may be molecular H$_2$, rather than H$_2$O$_m$ or OH. Because elemental hydrogen is likely present (and possibly dominates) in lunar melts, H in lunar rocks should be referred to as the H-component (including elemental H$_2$, and the hydrous species of H$_2$O$_m$ and OH), rather than “water”.

The diffusion of molecular H$_2$ is very rapid. At 380 K (the average daytime temperature on Moon), $D_{H_2}$ in silica is still significant, $6\times10^{-14}$ m$^2$/s, with a diffusion distance of 1.4 mm in one year, meaning that any molecular H$_2$ in lunar glasses would be lost (ignoring implantation of solar wind H).

At high temperatures as lunar magma is cooling down, H$_2$ rather than H$_2$O$_m$ is likely the dominant diffusing species in the melt. That is, modeling H-component diffusion assuming “water” diffusivity underestimates the diffusion rate. Accurate modeling of lunar degassing of the H-component requires quantification of the role of elemental H$_2$ in the diffusion of the component.

**References:**