

TESTING MODELS OF THE MOON'S ORIGIN, IV: CONDENSATION OF P AND S INTO SILICATE MELT AND METAL PRECIPITATION FROM IT. M. I. Petaev^{1,2} and S. B. Jacobsen¹, ¹Department of Earth & Planetary Sciences, Harvard University, 20 Oxford St., Cambridge MA 02138, USA; ²Harvard-Smithsonian CfA, 60 Garden St., Cambridge MA 02138, USA.

Introduction: Our previous modeling of BSE (Bulk Silicate Earth) vapor condensation in the proto-lunar disk [1-6] formed by a high energy, high angular momentum Giant Impact [7] showed that both chemical and isotopic characteristics of the Moon-Earth system, including observed depletions of the Moon in minor (e.g., Na, K) and trace (e.g., Cu, Zn) elements relative to the Earth, can be reproduced reasonably well. Condensation of two important elements, P and S, while both being included in the code, have not been discussed so far due to the limited thermodynamic data and the lack of reasonable solution models for these elements in a very high-temperature silicate melt. Here we attempt to model condensation of P and S into silicate melt and to evaluate partitioning of them, along with some siderophile elements, between liquid metal and proto-lunar silicate melt once the latter precipitates the former upon cooling.

Rationale for S and P solution models: Because of the adverse effects of S and P on metal quality, extraction of these elements from liquid metals into molten silicate slags has been extensively studied for a wide range of silicate melt compositions [e.g., 8-12]. The partitioning of P and S between liquid metal and silicate melts is typically described in terms of phosphate and sulfide capacities which describe concentrations of PO_4^{3-} and S^{2-} ions in silicate melts equilibrated with liquid metal as a function of temperature, f_{O_2} , f_{S_2} (in the case of sulfide capacity), and melt compositions at a pressure of 1 bar. It was found that the solubility of P_2O_5 in multicomponent silicate melts shows very large negative deviations from ideality. There are also petrologic models based on experimental and natural data describing partitioning of S (in terms of sulfide capacity) between silicate melts of mafic-ultramafic compositions and equilibrated sulfide melts [e.g., 13-17]. While neither metallurgical nor petrologic models of S and P solubility in silicate melts can be used directly for modelling condensation of P and S in the proto-lunar disk, they do provide important information on possible S and P end members of a complex P- and S-bearing silicate melt. Under reducing conditions of the proto-lunar disk, such end members are Ca and Mg orthophosphates and Mn, Fe, Ca, and Mg monosulfides.

Condensation model: The thermodynamic data-

base of the 34-element version of the GRAINS code [6] has been updated to include new data on P compounds [18-20], among which the liquid $\text{Ca}_3(\text{PO}_4)_2$ and $\text{Mg}_3(\text{PO}_4)_2$ species were treated as end members of an ideal silicate melt.

Because of the highly refractory nature of CaS (melts at 2723 K at 1 bar) and availability of high-temperature thermodynamic data [21], CaS was chosen as a S-bearing end member of ideal silicate melt. Since possible dissolution of other monosulfides in silicate melt and probable negative deviations from ideality of Ca and Mg orthophosphates were neglected, the calculated concentrations of S and P in silicate melts are likely to represent only lower limits.

The solution model of liquid metal was also modified to treat all end-members as ideal components. Such a treatment eliminated unrealistically high P concentrations in liquid metal, predicted by the earlier versions of the code.

In order to better quantify condensation of siderophile elements, the thermodynamic data for many gaseous species were updated and extended to include more oxides, sulfides, and chlorides of such elements as Ni, Co, Cu, W, Ga, and Ge.

Results and Discussion: The new results of modeling of the BSE vapor condensation (Fig. 1) are consistent with our previous findings [6,7], with the exception that the predicted concentrations of Ga and Ge in the silicate melt (\cong proto-Moon) no longer match the estimated BSM (Bulk Silicate Moon) composition. This is most likely a result of inadequate description of Ga and Ge condensation into silicate melt as trivalent (Ga_2O_3) and tetravalent (GeO_2) oxides. Both Ga and Ge would readily condense into liquid metal but the latter precipitates from the silicate melt at lower temperatures (by 400-500°C) than the predicted Moon accretion temperatures (Fig. 1) when the silicate melt is expected to be isolated from the ambient gas.

The calculated P and S depletions are pressure-dependent and approach the available estimates [22-24] at pressures below 15 bars, which are on the lower end of the Moon's accretion pressure range (15-25 bars) estimated by the physical models of the proto-lunar disk [7]. We consider this as a fairly good match, given the uncertainties associated with modeling condensation of P and S into

silicate melt.

Perhaps more interesting is the fate of these elements during the initial stages of the Moon's core formation when the still completely molten Moon cools by ~400 - 500°C after the accretion resulting in precipitation of ~ 1 wt% Fe,Ni-rich metallic liquid from the silicate melt. The chemical composition of metallic liquid evolves with the Ni/Fe, Si/Fe, and P/Fe ratios decreasing as the system cools. Only small fractions (<0.1) of Ni, Co, and Cu will remain in the silicate melt. Most of the P (Fig. 2 top panel) and all S (Fig. 2 bottom panel) would remain in the silicate melt.

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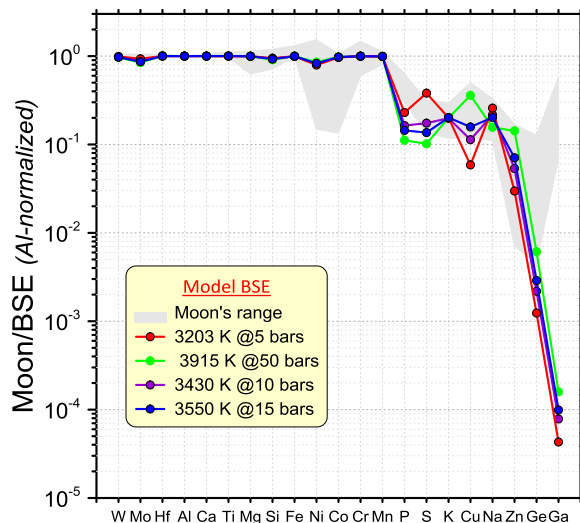


Fig. 1. BSE and Al-normalized model compositions of the Moon calculated at different P-T conditions (see legend). At each pressure, the temperature of the best fit was chosen based on the K depletion factor of 0.2.

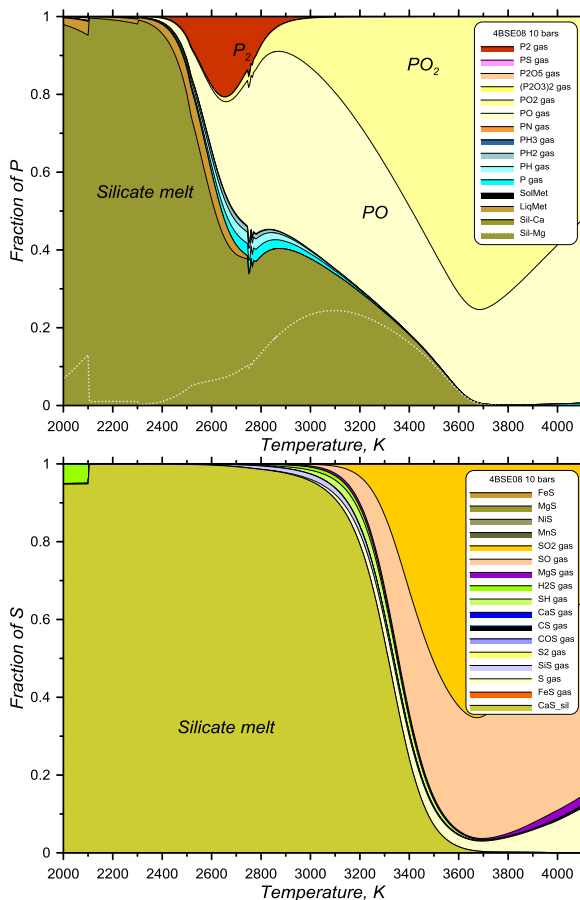


Fig. 2. Partitioning of P (top panel) and S (bottom panel) in the system of BSE composition at 10 bars.