THE PARAMETERIZATION OF SOLID METAL-LIQUID METAL PARTITIONING OF SIDEROPHILE ELEMENTS.
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Motivation:

The composition of a metallic liquid can significantly affect the partitioning behavior of elements. For example, some experimental solid metal-liquid metal partition coefficients have been shown to increase by three orders of magnitude with increasing S-content of the metallic liquid [e.g. 1]. Along with S, the presence of other light elements, such as P and C, has also been demonstrated to affect trace element partitioning behavior [e.g. 2].

Understanding the effects of metallic composition on partitioning behavior is important for modeling the crystallization of magmatic iron meteorites and the chemical effects of planetary differentiation. It is thus useful to have a mathematical expression that parameterizes the partition coefficient as a function of the composition of the metal. Here we present a revised parameterization method, which builds on the theory of the current parameterization of Jones and Malvin [3] and which better handles partitioning in multi-light-element systems.

Previous parameterization:

Jones and Malvin [3] demonstrated that the partitioning between solid and liquid metal is dominantly influenced by the metallic liquid composition, not the temperature or properties of the solid metal. In the parameterization of Jones and Malvin [3], the metallic liquid is modeled as being composed of domains, the calculation of which depends on the speciation of the light element in the metallic liquid. The Jones and Malvin [3] method has had success at parameterizing element partitioning in the Fe-Ni-S, Fe-Ni-P, Fe-Ni-S-P, and Fe-Ni-C systems [3, 4].

The large majority of experimental solid metal-liquid metal partitioning data is from the Fe-Ni-S system. In this system, by the Jones and Malvin [3] method, the solid metal-liquid metal partition coefficient (D) is expressed as:

$$1/D = [(1-2\alpha_S X_S)\hat{}(-\beta_S)]/D_o \qquad \text{[eq.1]}$$

where X_S is the mole fraction of S in the metallic liquid, D_o is D in the endmember, light-element-free Fe-Ni system, α_S is a constant of 1.09 that is specific to partitioning in S-bearing systems, and β_S is a constant specific to the element being parameterized. The factor of 2 comes from assuming FeS as the speciation of S in the metallic liquid. Parameterization of partitioning in the Fe-Ni-P system is functionally similar to eq.1 for the Fe-Ni-S system:

$$1/D = [(1-4\alpha_P X_P)\hat{}(-\beta_P)]/D_o \qquad \text{[eq.2]}$$

with X_P as the mole fraction of P in the metallic liquid, α_P as a constant of 1.36 that is specific to partitioning in P-bearing systems, and β_P as a constant determined by the element being parameterized. The factor of 4 arises from using Fe_3P as the speciation of P in the metallic liquid.

By the Jones and Malvin [3] method, D_o in eq.1 and eq.2 should be the same, but β_S and β_P are different, denoting different effects from S and P in the metallic liquid. In the more complicated Fe-Ni-S-P system, the effects from both S and P need to be taken into account, leading to the following expression:

$$1/D = [(1-2\alpha_S X_S-4\alpha_P X_P)\hat{}(-\beta_{SP})]/D_o \qquad \text{[eq.3]}$$

with

$$\beta_{SP} = [2X_S/(2X_S+4X_P)]\beta_S + [4X_P/(2X_S+4X_P)]\beta_P$$

Partitioning in the multi-light-element system of Fe-Ni-S-P is thus expressed as a weighted average of the effects in the endmember Fe-Ni-S and Fe-Ni-P systems. The expression would be correspondingly more complicated for the Fe-Ni-S-P-C system.

Revised Method:

Our revised method is based upon the same theory as presented in Jones and Malvin [3]. The composition of the metallic liquid is taken to be the dominant influence on the solid metal-liquid metal partitioning behavior, and the metallic liquid is envisioned to be composed of domains. For siderophile, metal-loving, elements, the element is attracted to the light-element-free "Fe domains" in the metallic liquid. The partition coefficient is thus a function of the concentration of these available "Fe domains:"

$$1/D = [(\text{Fe domains})\hat{}\beta]/D_o \qquad \text{[eq.4]}$$

The general form of eq.4 is similar to the Jones and Malvin [3] method shown in eq.1-3. The revision to the parameterization method comes in the calculation of the Fe domains. In the Fe-Ni-S system, the Fe domains are calculated as:

$$\text{Fe domains} = (1-2X_S)/(1-X_S) \qquad \text{[eq.5]}$$

This calculation is based on using FeS as the speciation of S in the metallic liquid. In the calculation, every S is paired with an Fe, and the metallic liquid can be envisioned as being composed of Fe and FeS domains.

Figure 1 shows the experimental partitioning data for Ge and Ir in the Fe-Ni-S system plotted against the Fe domains, as calculated by eq.5, and a fit to the data using our revised parameterization method. Our revised parameterization is able to match the partitioning data as well as the original Jones and Malvin [3] method. This success shows that using eq.4 to calculate the Fe domains removes the need for the constant of α_S in the parameterization.

The theory of this parameterization method is based on the availability of Fe domains. In that sense, S affects the partitioning behavior in a passive way, by reducing the concentration of available Fe domains. It then follows that the identity of the light element is not really important. What is important is understanding how the light element affects the Fe domains that are available. To calculate the effect of a light element on the concentration of available Fe domains, it is necessary to know the speciation of the light element in the metallic liquid. For P and C, the use of Fe_2P and Fe_2C respectively as the species in the metallic liquid produced the best fits to the limited data. The Fe domains in the Fe-Ni-S-P-C system can thus be calculated as:

$$\text{Fe domains} = (1\text{-}2X_S\text{-}3X_P\text{-}3X_C)/(1\text{-}X_S\text{-}2X_P\text{-}2X_C) \quad \text{[eq.6]}$$

The calculated Fe domains are then used in eq.4 to parameterize the partition coefficient. In contrast to the Jones and Malvin [3] method, there is only one β for each element, and β is independent of the identity of the light element. Having only one β simplifies the dealing of element partitioning in multi-light-element systems. Along with partitioning data for the Fe-Ni-S system, Fig. 1 also plots data for Ge and Ir in the Fe-Ni-P, Fe-Ni-S-P (Ge only), and Fe-Ni-C systems. Our revised parameterization method is able to fit all of the experimental data as a function of the Fe domains.

It is important to note that this parameterization method is for elements that exhibit siderophile behavior when partitioning in solid metal-liquid metal systems. In this parameterization, the siderophile behavior is expressed as a function of the concentration of Fe domains. For elements that exhibit chalcophile, S-loving, behavior, the availability of the S-bearing domains, not the Fe domains, will have the dominant effect on the partitioning behavior [5]. Similarly, for elements that are attracted to P or C, those light element-bearing domains will influence the partitioning behavior.

In conclusion, for the solid metal-liquid metal partitioning of siderophile elements, the partition coefficient can be expressed as a function of the concentration of Fe domains in the metallic liquid. The identity of the light element, such as S, P or C, affects the concentration of Fe domains but the observed partitioning behavior is the same function of the Fe domains, regardless of the light element. This simplifies the parameterization of partitioning in multi-light-element systems relative to the Jones and Malvin [3] method.

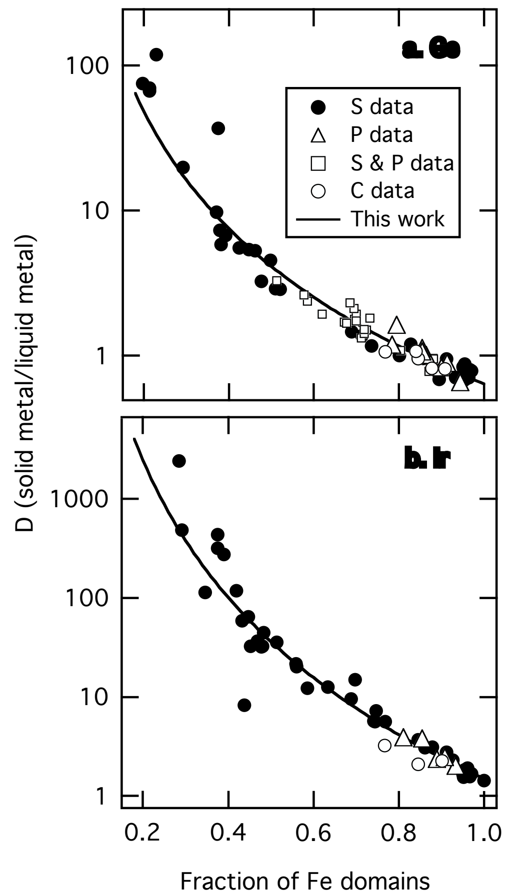

Fig.1. The solid metal-liquid metal partition coefficients for **(a)** Ge and **(b)** Ir are plotted as a function of the concentration of Fe domains in the metallic liquid. Our revised parameterization method is able to match experiments conducted in the Fe-Ni-S, Fe-Ni-P, Fe-Ni-S-P, and Fe-Ni-C systems. References for the experimental data are given in [2,3,6].

References: [1] Jones J. H. and Drake M. J. (1983) *GCA* **47**, 1199-1209. [2] Willis J. and Goldstein J. I. (1982) *LPSC XIII, JGR* **87**, A435-A445. [3] Jones J. H. and Malvin D. J. (1990) *Met. Trans*. **21B**, 697-706. [4] Lauer H. V. Jr. and Jones J. H. (1999) *LPSC* **XXX**, #1617. [5] Chabot N. L. and Jones J. H. (2002) *MAPS* **37**, A30. [6] Chabot N. L. et al. (2003) *MAPS*, in press. **Acknowledgements:** This work is supported by NASA RTOP 344-31-20-18 to J. H. J. and NASA grant NAG5-11122 to R. P. Harvey.