Modeling siderophile elements during core formation and accretion, and the role of the deep mantle and volatiles

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ABSTRACT

The last decade has seen general agreement that moderately siderophile elements (MSE) in Earth’s primitive upper mantle (PUM) can be explained by metal-silicate equilibrium at mid-mantle depths in an early Earth magma ocean environment. Despite the agreement, there are some differences in the detailed modeling that has been carried out. This paper will examine siderophile element metal/silicate partitioning with respect to three different topics: (1) an examination of aspects of the modeling that one might suspect leads to differences in outcomes or in comparison between models, but actually are in agreement with experimental data and between models; (2) a discussion of the role of the deep mantle in modeling efforts; and (3) the role and/or fate of volatiles in magma ocean scenarios with an emphasis on where data are lacking.

Keywords: Core, mantle, magma ocean, siderophile, volatile, accretion

INTRODUCTION

Detailed models for the origin and accretion of the Earth grew out of early ideas developed by Eucken (1944) for heterogeneous accretion, in which the material accreting to form the Earth changed with time producing the layers of the Earth. These models were developed in more detail by Turekian and Clark (1969), Clark (1961), and Anders (1977). An alternative to heterogeneous accretion—homogeneous accretion—in which the Earth accreted from a homogeneous mixture of metallic and silicate grains and later differentiated into the core and mantle, was proposed originally by Urey (1951), Safronov (1959), Elsasser (1963), and Birch (1965) over a similar timeframe. The former models had problems explaining the light elements in Earth’s core, and the upper mantle compositions (with both refractory and siderophile elements), whereas the latter models could not explain the elevated siderophile content of the mantle, oxidized iron, and the idea that any accreting H₂O and CO₂ would be reduced to H and C in the presence of metal (core) thus eliminating sources for Earth’s hydrosphere and atmosphere (Ringwood 1979). In particular the elevated siderophile element contents in Earth’s mantle were problematic but data used to evaluate their abundances was experimental data collected at low pressures.

The development of high-pressure techniques in the 1980s and 1990s led to an abundance of studies of siderophile elements, all of which revealed that siderophile element contents of Earth’s mantle could possibly be explained by metal-silicate equilibrium at elevated P-T conditions compared to the earlier studies at 1 bar and low temperatures (e.g., Li and Agee 1996; Thibault and Walter 1995). As a result, Earth accretion models are now a combination of aspects of heterogeneous accretion and homogeneous accretion alike, with core-mantle equilibrium able to explain siderophile element contents (e.g., Righter 2011a; Wade et al. 2012), and especially if the composition of the materials changes during accretion (Rubic et al. 2011). The last decade has seen general agreement that moderately siderophile elements in Earth’s PUM can be explained by metal-silicate equilibrium at mid-mantle depths (30 to 70 GPa) in a magma ocean environment (e.g., Siebert et al. 2012; Bouhifd and Jephcoat 2011). There is some disagreement over the exact P-T conditions, and whether f O₂ was variable during accretion (e.g., Rubie et al. 2011; Righter and Ghiorso 2012; Siebert et al. 2013).

Three topics bearing on the Earth accretion models will be discussed in this paper. First, aspects of siderophile element modeling have been questioned by some, including: (1) the role of pressure in causing coordination changes in metallic and silicate melts at 5 and 20 GPa; (2) the role of absolute vs. relative oxygen fugacity in the calculations; and (3) the choice of methods for quantifying effects of alloying elements on siderophile element activities in metallic liquid. It will be shown that none of these structural effects have any bearing on the predictive expressions, and that all the observed changes in partition coefficients are fully predicted by the multiple linear regression expressions. It will also be shown that regressions using relative f O₂ (ΔIW) and absolute f O₂ predict the same behavior, albeit in two different ways. Similarly, we compare two modeling approaches for activities in metallic liquids and show that there is overall agreement in the nature and magnitude of the metallic compositional effects.

Second, modeling has not generally included deep mantle reservoirs. This has led to some models that fit Nb, V, and Cr via core formation. Yet the lower mantle may be most important reservoir. Additional studies have revealed that a deep basal magma ocean may be relevant and could harbor elements. The general role of deep mantle reservoirs in differentiation models will be discussed.

Finally, several volatile elements, volatile siderophile and highly siderophile elements have been studied only at a limited set of conditions relevant to a deep magma ocean scenario, and

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