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Effects of core formation on the Hf–W isotopic composition of the Earth and dating of the Moon-forming impact

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ABSTRACT

Earth's core formation set the initial compositions of the core and mantle. Various aspects of core formation, such as the degree of metal–silicate equilibration, oxygen fugacity, and depth of equilibration, have significant consequences for the resulting compositions, yet are poorly constrained. The Hf–W isotopic system can provide unique constraints on these aspects relative to other geochemical or geophysical methods. Here we model the Hf–W isotopic evolution of the Earth, improving over previous studies by combining a large number of *N*-body simulations of planetary accretion with a core formation model that includes self-consistent evolution of oxygen fugacity and a partition coefficient of tungsten that evolves with changing pressure, temperature, composition, and oxygen fugacity. The effective average fraction of equilibrating metal is constrained to be $k > 0.2$ for a range of equilibrating silicate masses (for canonical accretion scenarios), and is likely <0.55 if the Moon formed later than 65 Ma. These values of k typically correspond to an effective equilibration depth of $\sim$0.5–0.7$\times$ the evolving core–mantle boundary pressure as the planet grows. The average mass of equilibrating silicate was likely at least 3$\times$ the impactor's silicate mass. Equilibration temperature, initial fO_2, initial differentiation time, semimajor axis, and planetary mass (above $\sim$0.9 $M_\oplus$) have no systematic effect on the ^{182}W anomaly, or on $f^{Hf/W}$ (except for fO_2), when applying the constraint that the model must reproduce Earth's mantle W abundance. There are strong tradeoffs between the effects of k, equilibrating silicate mass, depth of equilibration, and timing of core formation, so the terrestrial Hf–W isotopic system should be interpreted with caution when used as a chronometer of Earth's core formation. Because of these strong tradeoffs, the Earth's tungsten anomaly can be reproduced for Moon-forming impact timescales spanning at least 10–175 Ma. Early Moon formation ages require a higher degree of metal–silicate equilibration to produce Earth's ^{182}W anomaly.

1. Introduction

The segregation of Earth's metallic core from its silicate mantle was one of the most significant geochemical events in our planet's history. Understanding how and when this process occurred informs our knowledge of the accretion and earliest state of our planet, its modern-day core composition, the timing of Moon formation, and many other phenomena. The Hf–W system is one of the most widely used geochemical tools for dating Earth's core formation (e.g., Jacobsen, 2005; Kleine et al., 2002; Touboul et al., 2007; Yin et al., 2002). It can also be used to explore the nature of the core formation process by comparing measurements with numerical models (e.g., Halliday et al., 1996; Harper and Jacobsen, 1996; Kleine et al., 2004a; Nimmo and Agnor, 2006; Rudge et al., 2010).

^{182}Hf decays into ^{182}W with a half-life of 8.9 Ma (e.g., Kleine et al., 2009), the same order of magnitude as terrestrial planet accretion timescales. During core formation, moderately siderophile W is mostly sequestered into a planet's core. Halfnium is lithophile, so if ^{182}Hf is alive during core formation, it will remain in the mantle and decay into ^{182}W, creating an excess of mantle ^{182}W relative to other W isotopes. The Hf–W system is therefore sensitive to core formation timing (e.g., Halliday et al., 1996; Harper and Jacobsen, 1996; Jacobsen, 2005). Previous studies have shown that the Hf–W system is also sensitive to the siderophility of W (Halliday and Lee, 1999; Yu and Jacobsen, 2011) and the mechanism of core formation, such as the extent of metal equilibration (e.g., Dahl and Stevenson, 2010; Kleine et al., 2004a; Nimmo and Agnor, 2006;

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Nimmo et al., 2010; Rudge et al., 2010) and the extent of silicate equilibration (e.g., Deguen et al., 2014; Harper and Jacobsen, 1996; Morishima et al., 2013). Both Nimmo et al. (2010) and Rudge et al. (2010) found that Earth's ^{182}W anomaly is best reproduced when $\sim$40% of the incoming metal equilibrates with the mantle, for example. A greater extent of metal–silicate equilibration reduces the tungsten anomaly significantly, requiring faster growth to reproduce Earth's ^{182}W anomaly (e.g., Rudge et al., 2010).

In most of these previous models, the partitioning behavior of W was treated as a constant and constrained to match the present-day mantle tungsten concentration, whereas experimental data show that it depends strongly on pressure (P), temperature (T), oxygen fugacity (fO_2), and composition (Cottrell et al., 2009; Ohtani et al., 1997; Righter and Drake, 1999; Righter et al., 1997; Shofner, 2011; Shofner et al., 2014; Siebert et al., 2011; Wade et al., 2012; and references therein), which changed within the Earth's interior as it grew. More sophisticated models of core formation now exist in which elements partition between metal and silicate in multiple stages as the Earth grows and oxygen fugacity evolves self-consistently (e.g., Fischer et al., 2017; Rubie et al., 2011), but these models have focused on elemental chemistry and have not included isotopic calculations.

The goal of this study is to combine Hf–W modeling with a core formation model (Fischer et al., 2017) to better understand the process of core formation. Relative to previous Hf–W models, we introduce several novel concepts. Here the partitioning behavior of W varies with P, T, fO_2, and composition. A large number of accretion simulations are used for growth histories (Fischer and Ciesla, 2014), to illustrate how stochastic variability in accretion history affects the Hf–W system. Because we incorporate a full core formation model, the composition of Earth's mantle provides additional constraints that the model must reproduce. This type of model can be used to improve interpretations of Hf–W measurements and to better understand the timing and mechanism of core formation.

2. Numerical methods

Modeling Hf–W isotopic evolution requires an understanding of impact history, modeling of core formation, and an isotopic model. Information about impact history was taken from a suite of 100 N-body simulations (Fischer and Ciesla, 2014), which provide plausible accretion histories of the planets (e.g., timing of impacts, masses/provenance of impactors). Fifty of the simulations are consistent with the Nice model (Circular Jupiter and Saturn, CJS), and fifty have Jupiter and Saturn on their modern-day orbits (Eccentric Jupiter and Saturn, EJS). CJS and EJS represent two of many possible models of Solar System formation, considered here as examples of growth histories for the Earth; other styles of accretion may have different implications (Section 6). The simulations began with $\sim$80 Moon- to Mars-mass planetary embryos and $\sim$3000 smaller planetesimals. When two bodies passed within the sum of their radii, they were assumed to merge (Section 6). After 200 Ma of orbital evolution, the 100 simulations had formed 73 Earth analogues, defined here as the largest surviving planet with a semimajor axis of 0.75–1.25 AU and a mass within a factor of 1.5 of Earth's mass ($M_\oplus$). These Earth analogues have a mean mass of 1.0 $\pm$ 0.2 $M_\oplus$ and semimajor axis of 0.98 $\pm$ 0.14 AU.

In the post-processing of these simulations, they are combined with a core formation model (Fischer et al., 2017, which uses similar methodology to Rubie et al., 2011). Each body is assigned an initial composition, then the model steps through the accretion histories of all bodies, allowing them to undergo high P–T metal–silicate equilibration with each impact. Compositions of the resulting cores and mantles are calculated for a variety of major, minor, and trace elements, with the metal–silicate partitioning behaviors of these elements calculated as functions of P, T, fO_2, and composition as constrained by experimental data (e.g., Fischer et al., 2015). Pressures are determined using Earth's density variations with depth as a pseudo equation of state (Fischer et al., 2017). Oxygen fugacity is expressed in log units relative to the iron–wüstite (IW) oxygen fugacity buffer and is approximated as:

$$\Delta \mathrm{IW} \approx 2 \log\left(\frac{X_{\mathrm{FeO}}}{X_{\mathrm{Fe}}}\right) \tag{1}$$

where X_{FeO} is the FeO content of the mantle and X_{Fe} is the Fe content of the core, expressed as mole fractions. An initial oxygen fugacity is prescribed, but subsequently it is evolved self-consistently (e.g., Rubie et al., 2011) according to experimentally-determined partitioning data, to ensure that only viable fO_2 histories are produced.

Metal–silicate partitioning of W has been added to the core formation model of Fischer et al. (2017), based on the experimental results of Shofner (2011) and Shofner et al. (2014). This work combines new W metal–silicate partitioning data obtained in a laser-heated diamond anvil cell at pressures up to 50 GPa with data from many previous studies (Cottrell et al., 2009; Ohtani et al., 1997; Righter and Drake, 1999; Righter et al., 1997; Siebert et al., 2011; Wade et al., 2012; and references therein). The partition coefficient D of tungsten is expressed as a function of fO_2, P, T, silicate melt composition (SiO_2, Al_2O_3, CaO, and MgO), and metallic melt composition (C and S, which are not utilized here; see Section 6). For tungsten, $D_{\mathrm{W}} = X_{\mathrm{W}}/X_{\mathrm{WO_3}}$, while Hf is assumed to be perfectly lithophile.

Between impacts, radiogenic ^{182}W is produced in the mantle from the decay of ^{182}Hf, and with each impact, the ^{182}W abundance is modified by a core formation event. Earth's mantle W isotopic composition is tracked as a ^{182}W anomaly, defined using epsilon notation:

$$\varepsilon_{182\mathrm{W}} = \left[\frac{(X^{182\mathrm{W}}/X^{183\mathrm{W}})}{(X^{182\mathrm{W}}/X^{183\mathrm{W}})_{\mathrm{CHUR}}} - 1\right] \times 10^4 \tag{2}$$

equal to 1.9 $\pm$ 0.1 for the present-day Earth (Kleine et al., 2002, 2004b; Yin et al., 2002), where $X^{182\mathrm{W}}$ and $X^{183\mathrm{W}}$ are the ^{182}W and ^{183}W contents of the mantle, respectively, expressed as mole fractions; and *CHUR* indicates the composition of a chondritic uniform reservoir. Earth's mantle Hf/W ratio is described as:

$$f^{\mathrm{Hf/W}} = \frac{(X^{180\mathrm{Hf}}/X^{183\mathrm{W}})}{(X^{180\mathrm{Hf}}/X^{183\mathrm{W}})_{\mathrm{CHUR}}} - 1 \tag{3}$$

equal to 13.6 $\pm$ 4.3 for the present-day Earth (Kleine et al., 2009). However, there is disagreement over this value; for example, Dauphas et al. (2014) report an Earth $f^{\mathrm{Hf/W}} = 25.4 \pm 4.2$ based on a reevaluation of literature data, with the main difference from the Kleine et al. (2009) value being in the chondritic Hf/Th ratio assumed. Here we apply the constraint that Earth's mantle W abundance must be reproduced on average (Palme and O'Neill, 2007; though there is significant uncertainty in this value, see Section 6), which typically corresponds to $f^{\mathrm{Hf/W}} \approx 13.6$, depending on the core mass fraction. Other values used in the isotopic calculations, such as $^{182}\mathrm{W}/^{184}\mathrm{W}_{\mathrm{initial}}$, $^{182}\mathrm{Hf}/^{180}\mathrm{Hf}_{\mathrm{initial}}$, and $^{180}\mathrm{Hf}/^{183}\mathrm{W}_{\mathrm{CHUR}}$, are taken from Kleine et al. (2009).

Adjustable parameters within the model include the effective depth (pressure and temperature) of metal–silicate equilibration, fraction k of incoming metal that equilibrates, mass of equilibrating silicate, thermal profile, initial fO_2, and timing of first differentiation event. The depth of equilibration, expressed as a fixed fraction of the core–mantle boundary (CMB) pressure, was allowed to vary between 0 and 1. The depth for each set of model parameters