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Key Points:

- We estimate the effect of the Moon-forming giant impact on the siderophile trace element composition of the bulk silicate Earth
- Our models rule out Moon-forming giant impactors larger than 0.15 Earth's masses
- On the basis of siderophile trace elements, the presence of melt at the base of the mantle, after Moon formation, is possible

Supporting Information:

- Supporting Information
- Data Set S1

Correspondence to:

H. Piet,
helene.piet@asu.edu

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Geochemical Constraints on the Size of the Moon-Forming Giant Impact

Hélène Piet^{1,2,3} , James Badro^{1,2} , and Philippe Gillet² 

¹Institut de Physique du Globe de Paris, Sorbonne Paris Cité, Paris, France, ²Earth and Planetary Science Laboratory, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, ³Now at School of Earth and Space Exploration, Arizona State University, Tempe, AZ, USA

Abstract Recent models involving the Moon-forming giant impact hypothesis have managed to reproduce the striking isotopic similarity between the two bodies, albeit using two extreme models: one involves a high-energy small impactor that makes the Moon out of Earth's proto-mantle; the other supposes a gigantic collision between two half-Earths creating the Earth-Moon system from both bodies. Here we modeled the geochemical influence of the giant impact on Earth's mantle and found that impactors larger than 15% of Earth mass result in mantles always violating the present-day concentrations of four refractory moderately siderophile trace elements (Ni, Co, Cr, and V). In the aftermath of the impact, our models cannot further discriminate between a fully and a partially molten bulk silicate Earth. Then, the preservation of primordial geochemical reservoirs predating the Moon remains the sole argument against a fully molten mantle after the Moon-forming impact.

1. Introduction

The giant impact hypothesis has gained ground since its inception in the early 70s (Hartmann & Davis, 1975; Ringwood, 1970) and is now widely considered to be the leading theory explaining the formation of the Moon (Canup, 2004, 2012; Cuk & Stewart, 2012). It has been proven successful in addressing a number of outstanding characteristics of the Earth-Moon system: its angular momentum, the relative masses of both bodies, volatile-element depletion in the Moon, the small lunar core, etc. Moreover, recent planetary dynamical models of solar system formation have shown that large impacts are common events (Morbidelli et al., 2012; O'Brien et al., 2006; Raymond et al., 2006; Schenk et al., 2012), especially in the final stages of terrestrial accretion, giving more impetus to the theory.

However, the Moon-forming giant impact (MFGI) model has struggled with one of the most striking features of the Earth-Moon system: the quasi-identical isotopic (oxygen (Wiechert et al., 2001; Young et al., 2016), chromium (Bonnand et al., 2016; Trinquier et al., 2008), titanium (Leya et al., 2008; Zhang et al., 2012), and composition of lunar and terrestrial rocks. Most traditional smoothed particle hydrodynamic simulations of planetary impacts advocate that the Moon is mostly formed from material originating from the impactor and ejected into an accretion disk around the Earth (Canup, 2004; Canup & Asphaug, 2001); this is problematic since it suggests that the giant impactor and the proto-Earth (i.e., the Earth prior to the giant impact) formed from nebular reservoirs with identical isotopic compositions, which is unlikely (Kaib & Cowan, 2015; Mastrobuono-Battisti & Perets, 2017; Pahlevan & Stevenson, 2007). This conundrum has driven recent investigations toward two extreme models of Moon formation: either a huge collision between two half-Earths (Canup, 2012) that (by symmetry) contributes equal and identical amounts of material from both initial bodies to the final Earth and Moon or the very energetic collision of a small impactor (Cuk & Stewart, 2012) that forms the Moon exclusively from material in the proto-Earth, and then thoroughly mixes (Nakajima & Stevenson, 2015) with the Earth's mantle, elegantly diluting any isotopic distinction between the impactor and proto-Earth. While both end-member models achieve the designated goal of forming an Earth and a Moon with similar isotopic compositions, the extreme range of impactor size (2% to 50% of Earth's mass) precludes any inference of the geochemical and petrological evolutions of the Earth-Moon system after the impact. Our aim here is to provide an independent constraint on the mass of the giant impactor, using only reliable terrestrial geochemical observables.

Earth accretion and core formation are coeval processes during which accretion of planetesimals melted the silicate mantle of the Earth, thus creating a magma ocean at the surface of the proto-Earth (Murthy, 1991;

Stevenson, 1981). Earth's core progressively formed by separation and equilibration of the metal from accreting bodies in this magma ocean, scavenging siderophile elements on its way down to form the core.

This left a clear chemical imprint still observed today in mantle-derived rocks, which has, in turn, been used to infer the conditions of core formation on Earth (Badro et al., 2015; Fischer et al., 2015, 2017; Rudge et al., 2010; Siebert et al., 2012, 2013; Wade & Wood, 2016). The MFGI is the last major accretion event in Earth's history, which occurred 30 to 100 Myr after solar system formation (Connelly & Bizzarro, 2016; Jacobson et al., 2014; Touboul et al., 2009; Yin et al., 2002), after the main phase of core formation had taken place on Earth (~30 Myr; Kleine et al., 2002; Yin et al., 2002). It therefore also constitutes the last major metal-silicate differentiation event in Earth's history (Wade & Wood, 2016), and its chemical effect on both Earth's core and mantle can be modeled by core formation models (Badro et al., 2015). Here we adapted the model of Badro et al. (2015) to account for the specificities of a large final impact, by introducing partial equilibration between the impactor's core and the proto-Earth's magma ocean, and allowing for a surge in (the degree of) mantle melting after the impact.

2. Simulations

Earth accretion was modeled as a multistage process: accretion was discretized in 100 steps, with core separation, equilibration, and segregation occurring at each step in the growing (i.e., deepening) magma ocean. The evolution of core and mantle composition was calculated at each step for several siderophile (Fe, Ni, Co, Cr, and V) and lithophile (Si and O) elements using the same thermodynamic metal-silicate equilibrium model as in Badro et al. (2015) (see also the supporting information; Ma, 2001; Siebert et al., 2011; The Japan Society for the Promotion of Science, 1989; Wade & Wood, 2005). The first 99 stages of pre-MFGI proceeded with a small constant mass flux (<0.01 Earth mass). The final accretion event (100th stage) consisted of the MFGI, where the mass of the impactor was varied between 5% and 25% of Earth's total mass (Figure S1 in the supporting information). Temperature was varied along four tested different geotherms (Figure S2). We also tested different compositional paths of the mantle during accretion to reflect accretion from different families of accretionary building blocks (Figure S3). The final composition of the core and mantle was then obtained, and the moderately siderophile element (MSE) abundances in the mantle were compared to their observed present-day values (see the supporting information for details about the parameters scanned in the simulations; Andrault et al., 2011; Badro et al., 2016; Fiquet et al., 2010; Wood et al., 2008)

Since the impactor was a differentiated object, the compositions of its core and mantle were calculated similarly to the Earth's (see the supporting information for details; Kleine et al., 2004). After the impact, the simplest model assumes that its core merges with the proto-Earth's core after some degree of chemical interaction with the silicate magma ocean (Nimmo et al., 2010; Rubie et al., 2003; Rudge et al., 2010). The extent of partial equilibration between the core and mantle (Kleine et al., 2009; Rudge et al., 2010) is described by the fraction k of the impactor core that equilibrates with the whole mantle. The remaining fraction $(1 - k)$ merges directly with the Earth's protocore retaining its initial composition. The equilibration parameter k was fixed at 1 (full metal-silicate equilibration) for all core formation stages prior to the giant impact and then varied for all values between 0 and 1 (by steps of 0.1) for the final MFGI stage. During the main phase of accretion, full metal-silicate equilibration (i.e., $k = 1$) was considered for two reasons, one practical and one fundamental. Practically, it generates the most diverse family (or ecosystem) of proto-Earths owing to the full mass of core and mantle chemically interacting; if Earth was accreted with partial core-mantle equilibration during the main phase, only a fraction (k) of the core would interact and drive the compositions of both core and mantle, and hence, their final composition would be found somewhere in the "full equilibrium family," albeit at different P , T , and composition (which does not matter here since we will be testing all possibilities). At the other extreme, $k = 0$ will always generate the same proto-Earth regardless of P , T , and composition, because the core does not interact with the mantle. Hence, forcing $k = 1$ to the main stage of accretion yields the broadest range of compositions prior to the impact and allows the broadest range of giant impacts, so that any scenario that does not satisfy mantle MSE abundances with $k = 1$ will certainly not satisfy them with $k < 1$; in other words, we could be accepting certain implausible models, but we certainly are not ruling out any plausible models, so that any models that are effectively ruled out by our models can be safely discarded. Fundamentally, $k = 1$ prior to the impact is necessary to satisfy the ^{182}W isotopic composition of the Earth

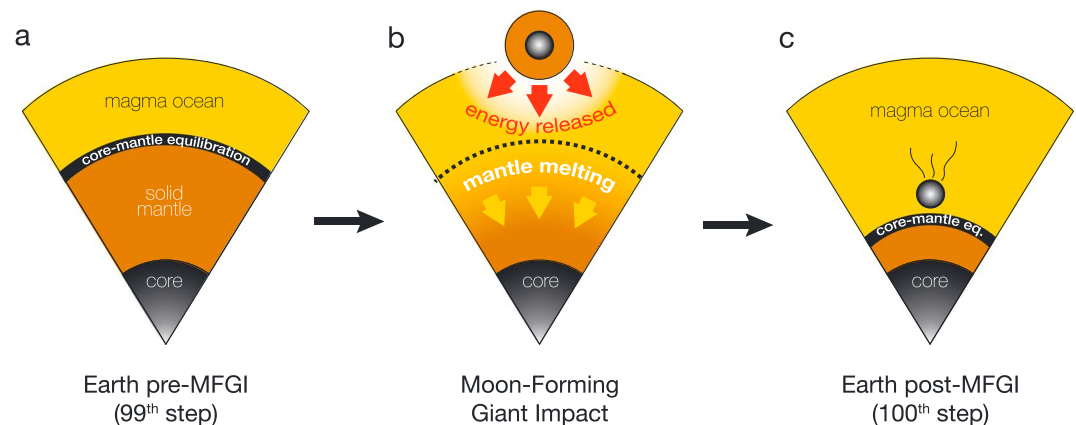


Figure 1. Mantle melting induced by the collision of the Moon-forming giant impactor with the proto-Earth. (a) Prior to the MFGI, the proto-Earth is covered by a magma ocean ensuing from repeated impacts along the course of Earth's accretion and core formation. The average conditions of metal-silicate equilibration are those prevailing at the base of the magma ocean, which iteratively deepens with time as the Earth grows by accretion. (b) At the end of accretion, the collision between the MFGI and the proto-Earth releases a lot of energy that might have contributed to melting a far more significant portion of the mantle than before the impact, (c) pushing the base of the magma ocean toward greater depths where the impactor's core would (partially) equilibrate at higher pressure and temperature. Here we consider a (azimuthally) global magma ocean that can be described by a radial model.

and Moon (Kleine et al., 2009). Introducing any partial equilibration in this phase would take the apparent age of core formation above 30 Myr (see Figure 18 in Kleine et al., 2009), which is inconsistent with current planetary formation models (Morbidelli et al., 2012; Walsh et al., 2011).

One last parameter considered here is the mean pressure of metal/silicate equilibration after the giant impact. The tremendous energies involved in the giant impact should melt very large fractions of the mantle (Nakajima & Stevenson, 2015; Tonks & Melosh, 1993), deepening the magma ocean and shifting the thermodynamics conditions of core/mantle equilibration (see Figure 1); however, the extent of this shock-induced melting is difficult to evaluate. We therefore implemented this additional parameter in our simulations by testing three different mean pressures of equilibration after the impact: 106 GPa, 120 GPa, and 135 GPa (Figure S4). Core formation models without a giant impact provide a bound on the depth of the magma ocean providing a mean pressure range of 42–75 GPa for core-mantle equilibration (Badro et al., 2015). A final giant impact interacting (albeit partially) with the magma ocean at very high pressures due to shock-induced melting thus leaves a chance for shallower magma oceans to exist in the main phase of Earth accretion prior to the impact.

Each set of values for the input parameters yields a multistage core-formation simulation, where the abundance of four MSE can be tracked as shown in Figures 2 and 3. The final composition of the mantle in the simulation was compared to the present-day abundance of Ni, Co, Cr, and V in the Earth's mantle, which constitute the most reliable set (Fischer et al., 2015; Li & Agee, 1996; Siebert et al., 2012, 2013; Wood et al., 2008) of MSE abundances in the bulk silicate Earth (Lyubetskaya & Korenaga, 2007; McDonough & Sun, 1995). Only simulations producing terrestrial mantles (i.e., matching simultaneously all four abundances, within uncertainties; see Table S1 in the supporting information) were considered successful "models," and the others (i.e., where one or more MSE abundance is violated) were discarded. Figures 2 and 3 showcase two such examples of a successful and an unsuccessful scenario, respectively.

In order to constrain the broadest distribution of sizes for the giant impactor, we ran an extensive set of ~2 million simulations such as the ones shown in Figures 2 and 3: instead of arbitrarily fixing core-formation conditions, we simulated every combination of parameters that were systematically varied over their entire plausible range (see Badro et al., 2015): (1) giant impactor mass, (2) depth and (3) temperature of the magma ocean before and after impact, (4) FeO content (also referred to as "redox" of " f_{O_2} " in other publications) of the magma ocean, and (5) degree of equilibration of the giant impactor in the magma ocean. This scan covers all of parameter-space and hence allows defining an all-encompassing solution space; any outlying

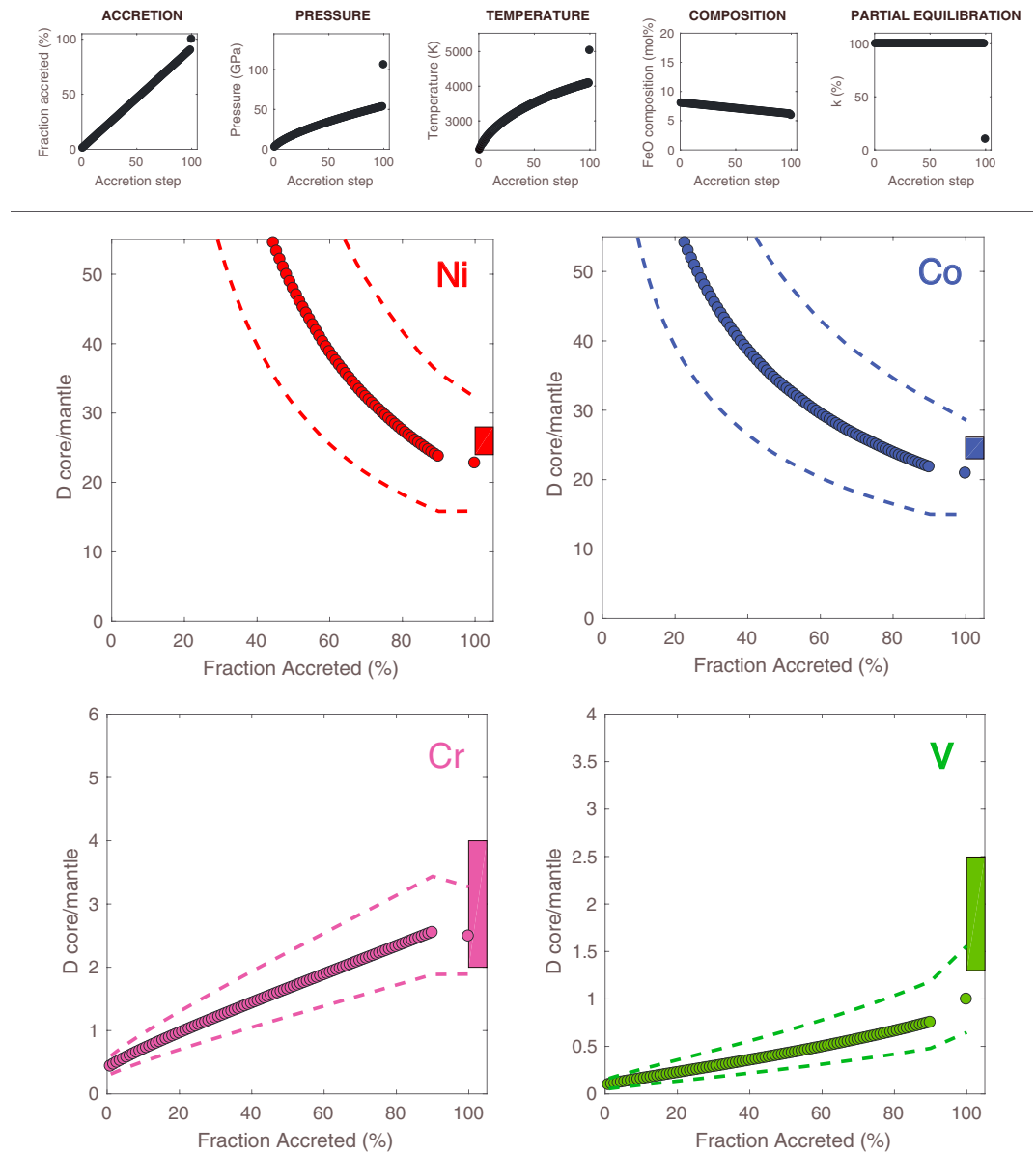


Figure 2. Successful scenario of core formation. (top) Input parameters of the model and (bottom) the output results. In this case, input parameters (from left to right) correspond to an accretion model with a MFGI size of $0.10 M_E$ at the last step of accretion, a final pressure before and after the MFGI of 57 GPa and 106 GPa, respectively, temperatures taken along a hot liquidus (Figure S2), FeO mantle content linearly decreasing during accretion (path 8, Figure S3), and 10% (i.e., $k = 0.1$) of the MFGI's core equilibrating with the mantle. The lower panel shows the output evolution of calculated core/mantle distribution coefficients D for Ni, Co, Cr, and V (see supporting information for details on the calculations) as a function of accreted mass during accretion, along with the observed value (colored shaded box) for the present-day Earth representing the constraints that need to be matched. For each element, the colored circles correspond to calculated D values at each step; the dashed contours correspond to the uncertainty on calculated values. The calculated final D values match the observables (Table S1) within uncertainties for all four elements. This scenario is thus considered a successful scenario of core formation. It is noteworthy that the specific sets of conditions would not work without the MFGI, because the V concentration in the mantle would be too high (D too low in the lower right panel). In this sense, the MFGI extends the range of parameters under which Earth's core may have formed, by providing two additional ingredients: partial metal-silicate equilibration and a surge in mantle melt fraction due to postimpact melting.

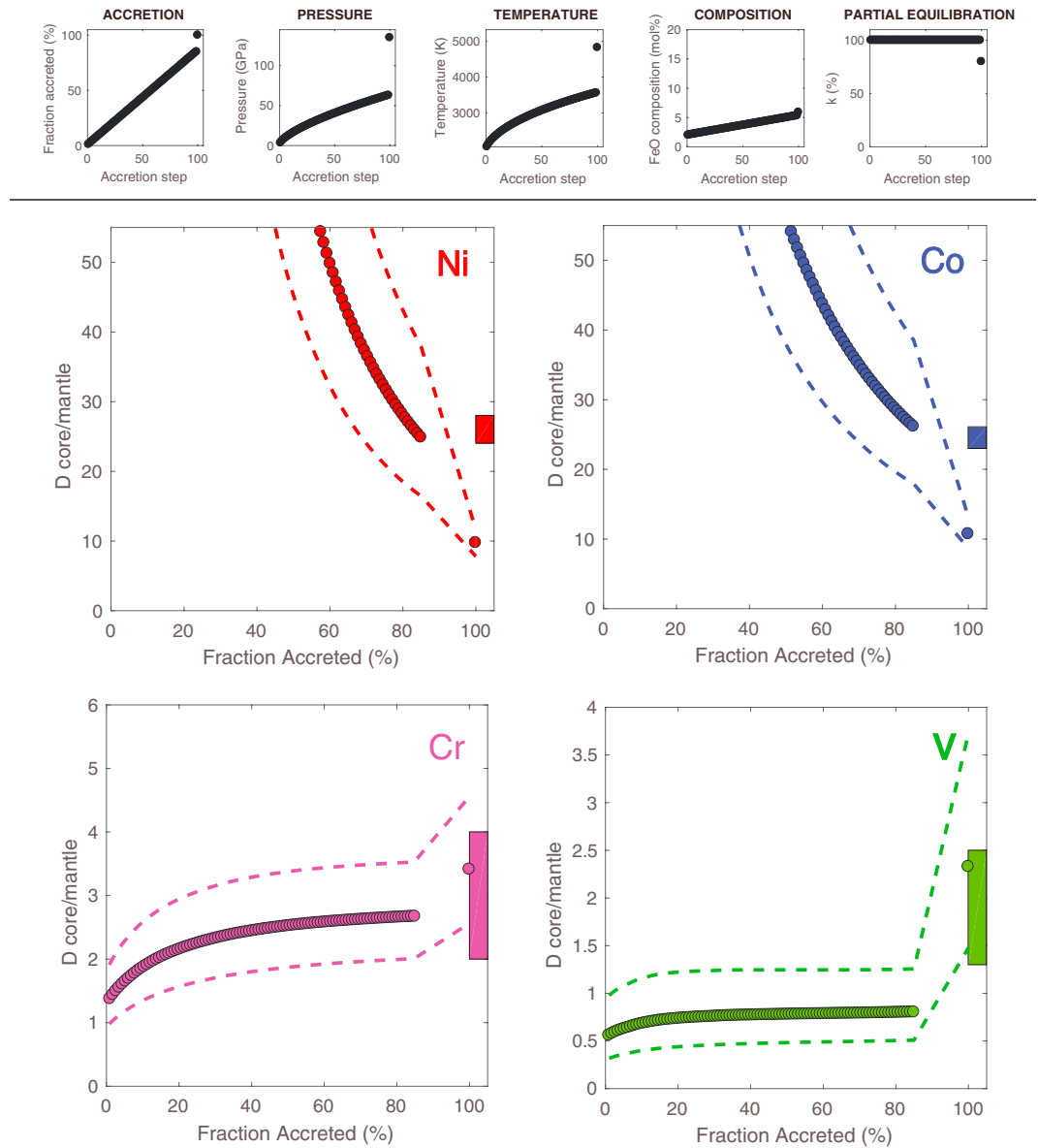


Figure 3. Unsuccessful scenario of core formation. Same as in Figure 2 above, except input parameters correspond to an accretion model with an MFGI size of $0.15 M_E$ at the last step of accretion, a mean pressure before and after the MFGI of 70 GPa and 135 GPa, respectively, corresponding temperatures taken along a cool liquidus (Figure S2), FeO mantle content linearly increasing during accretion (path 3, Figure S3), and 80% (i.e., $k = 0.8$) of the MFGI's core equilibrating with the mantle. Here the calculated final D values do not match the observables (Table S1) within uncertainties for both Ni and Co. It is clear here that the MFGI has a destabilizing effect on MSE concentration in the mantle. Clearly, the preimpact accretion model was slowly evolving toward getting all four MSE abundances in the suitable range, but the large surge in impact-induced melting increases the final pressure of equilibration, which dramatically decreases the D for Ni and Co, setting the final mantle value too low. One way to avoid such effects is to either reduce the partial equilibration parameter k or reduce the mass of the impactor: Both these will affect the mass balance in such a way as to mitigate the consequential effects of such an MFGI on final mantle composition.

conditions can assertively be ruled out as plausible for the formation of Earth's core, its mantle, and the Moon. It is noteworthy that we discarded all assumptions (that translate into other input parameters to the model) that are not substantiated by direct (e.g., the elemental or isotopic composition of the impactor) or reliable (e.g., the elemental or isotopic composition of the bulk Moon) observables.

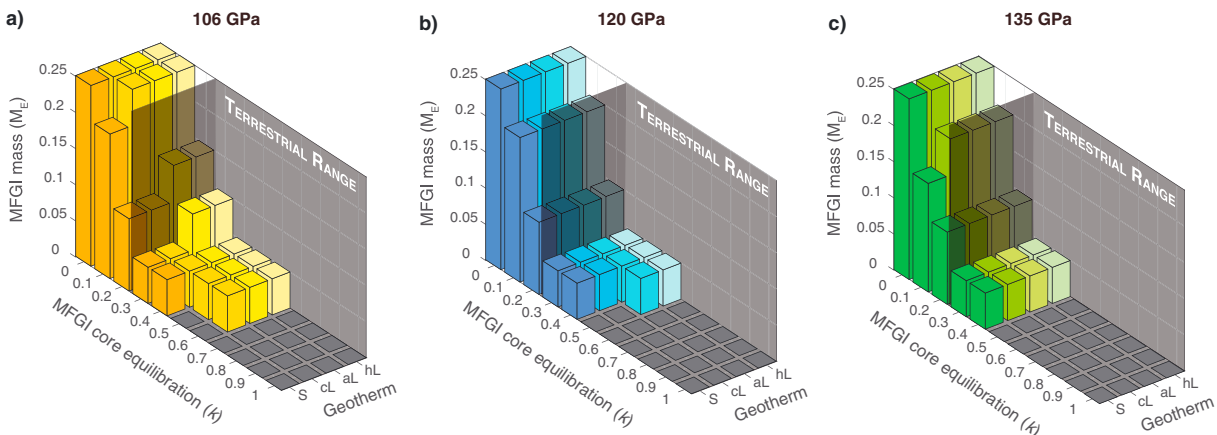


Figure 4. Giant impact models consistent with mantle geochemistry, as a function of impactor size, core partial equilibration, and geotherm. Results are displayed for each mean pressure of equilibration after the MFGI: (a) 106 GPa (yellow), (b) 120 GPa (blue), and (c) 135 GPa (green). The colored bars denote conditions where core-formation models produce a mantle consistent with observable Ni, Co, Cr, and V abundances; for each degree of partial equilibration k , giant impactor size and geotherm (S: solidus, cL: cool liquidus, aL: average liquidus, hL: hot liquidus). The grey shaded box label “terrestrial range” depicts the range of k values imposed by timing constraints and the evolution of the Hf-W chronometer (Nimmo et al., 2010) for the Earth. If there is no chemical interaction between the Earth and the giant impactor ($k = 0$), then all models find solutions. However, when considering only models with at least 30% impactor-Earth equilibration (inside the grey shaded box), a constraint established by the short-lived Hf-W chronometer, then only impactors smaller than 10–15% Earth masses can satisfy mantle geochemistry, regardless of the extent of mantle melting after the impact and other equilibration parameters explored in the models. See Figures S5–S7 for more granularity on the results.

3. Results and Discussion

The six-dimensional solution space is plotted in Figure 4, where all solutions for a given impactor size, geotherm, and degree of core-mantle equilibration are condensed. More granularities (details of composition) can be found in Figures S5–S7. The first observation in Figure 4 is that solutions can be found for all impactor sizes if no additional constraints are imposed. The constraint on the degree of partial metal-silicate equilibration is brought by calculations of the Hf-W isotopic evolution of planetary bodies during accretion using N-body simulations (Dwyer et al., 2015; Fischer et al., 2017; Nimmo et al., 2010; Rudge et al., 2010). Scenarios producing Earth-like planets with mantle tungsten anomaly within the range observed for the present-day mantle ($\varepsilon_W = 1.9 \pm 0.1$) require a minimum value of $k = 0.3$ for the Earth.

Based on this constraint, if values of k are restricted to those larger than 0.3 (grey box in Figure 4), as required to match the tungsten anomaly ε_W of the current mantle (Dwyer et al., 2015; Fischer et al., 2017; Nimmo et al., 2010; Rudge et al., 2010), then all models assuming impactors larger than 15% Earth mass systematically fail. This is due to the fact that impactor core equilibration (even if partially) at very high pressure and temperature induces a surge in Ni and Co concentrations in the magma ocean (as can be seen in the giant impact stage of the model in Figure 3). The rest is a question of mass balance: impactors larger than 15% Earth mass are so massive that no preimpact mantle composition has low-enough Ni and Co to offset that surge, and the mantle always ends up with higher Ni and Co concentrations than observed. Smaller impactors, however, can all successfully reproduce Earth’s mantle’s composition, for a range of parameters that gets larger as the impactors become smaller (as shown by larger solution spaces for small impactors in Figures 4 and S5–S7). This again is the expected behavior, with regard to the mass balance argument described above. Intermediate sized impactors (between 10 and 15% Earth mass) can marginally satisfy core formation conditions, but under the condition that the magma ocean does not get much deeper after the impact, which is problematic to reconcile with the fact that such large impacts should produce a large degree of mantle melting.

We can therefore confidently conclude that the Moon-forming giant impactor was at most a 10–15% Earth mass (roughly Mars-sized) object, plausibly smaller, and certainly not larger. This conclusion proceeds from two observations: the siderophile composition of the Earth’s mantle and the timing constraint on core formation from the Hf-W chronometer. Our results are therefore consistent with scenarios involving smaller

impactors (Canup & Asphaug, 2001; Cuk & Stewart, 2012), which would have well mixed with the Earth after the formation of the Moon (Connelly & Bizzarro, 2016; Lock & Stewart, 2016; Lock et al., 2015, 2016; Nakajima & Stevenson, 2015; Pahlevan & Stevenson, 2007; Young et al., 2016).

Since smaller impactors are more likely to preserve a large fraction of the mantle from melting (Cuk & Stewart, 2012; Stewart, et al., 2015) and remixing with the magma ocean (Figure 1), the preimpact solid residue could bear a distinct and primordial geochemical signature, predating the giant impact (i.e., older than 4.5 Ga). Such reservoirs, if they persisted to the present day, could hence constitute a putative reservoir for the source of ^{182}W (Yin et al., 2002) and ^{129}Xe (Mukhopadhyay, 2012) anomalies in the mantle. Geochemical sampling and modeling of this preimpact reservoir, if possible, could allow addressing the bulk composition and the accretionary building blocks of Earth during the main phase of accretion, predating the giant impact.

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