Reconciling fast and slow cooling during planetary formation as recorded in the main group pallasites

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Both the main text of the manuscript an the supplementary information are included in this document.

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Abstract

Pallasite meteorites contain evidence for vastly different cooling timescales: rapid cooling at high temperatures (K/years) and slow cooling at lower temperatures (K/Myrs). Pallasite olivine also shows a variety of textures ranging from well-rounded to angular and fragmental, and some samples record chemical zoning. Previous pallasite formation models have required fortuitous changes to the parent body in order to explain these contrasting timescales and textures, including late addition of a megaregolith layer, impact excavation, or parent body break-up and recombination. We investigate the timescales recorded in Main Group Pallasite meteorites with a coupled multiscale modelling approach, using a 1D model of the parent body and a 3D model of the metal-olivine mixing region, to see if these large-scale changes to the parent body are necessary. We find that the contrasting timescales, textural heterogeneity, and preservation of chemical zoning can all occur within one simple ellipsoidal segment of an intrusion complex, with ~ 12 % of our randomly generated models returning favourable pallasite formation conditions (2200 model runs), with small intrusion volumes ($< 5\times10^6$ m^3) and colder background mantle temperatures (< 1200 K) favourable. Large rounded olivine can be explained by earlier intrusion of metal into a hotter mantle, suggesting possible repeated bombardment of the parent body. The formation of pallasitic zones within planetesimals may have been a common occurence in the early Solar System, as our model shows that favourable pallasite conditions can be accommodated in a wide range of intrusion morphologies, across a wide range of planetesimal mantle temperatures, without the need for large-scale changes to the parent body. We suggest that pallasites represent a late stage of repeated injection of metal into a progressively cooler planetesimal mantle.

1 Introduction

Main Group Pallasite meteorites (referred to from here on as "pallasites"), consisting of a mixture of silicate crystals and FeNi alloy, are believed to represent a key time in the early evolution of the solar system as metal differentiated from silicate and planetary cores began to form. However, models differ about the exact details of the process represented by the pallasite meteorites. In particular, pallasites contain evidence for cooling at contrasting timescales: the metal portion records cooling at rates of $\sim 10^{-6}$–10^{-5} Kelvin per year below $\sim$ 900 K (Ni diffusion studies; Yang et al., 1997, 2010; Goldstein et al., 2014), while orders of magnitude more rapid cooling ($\sim 10^{0}$–10^{2} Kelvin per year) has been suggested to explain chemical gradients and heterogeneity in olivine acquired at higher temperatures (Miyamoto, 1997; Tomiyama and Huss, 2006), and the halted textural equilibration post-metal-injection (Walte and Golabek, 2022). The difference between these rates cannot be explained by a simple conductive cooling model of a planetesimal that initially cools rapidly and then slows (Yang et al., 2010).

The macro-scale texture of pallasite olivine across and within samples ranges from well-rounded to fragmental and highly angular (Grossman and Nomenclature Committee of the Meteoritical Society, 2022). The degree of rounding of olivine grains scales with residence time in hot FeNi (Saiki et al., 2003; Walte et al., 2020), and so the range in degree of olivine angularity across pallasite samples adds further constraints on the cooling rate of the intruded metal in contact with said olivine. The heterogeneity of olivine textures may indicate different formation environments for rounded versus angular olivine crystals, with different temperatures, cooling rates and residence times in molten FeNi metal (McKibbin et al., 2019).

Previous models have suggested injection of metal into a planetesimal mantle via a metallic bolide (Tarduno et al., 2012) or ferrovolcanism from the planet's molten core (Johnson et al., 2020) in order to explain the delivery of molten metal into the parent body mantle. Metal intrusion formation models typically include a qualitative description of large-scale changes to the parent body following metal intrusion to explain the contrasting timescales recorded in pallasite samples, including impact-related excavation to enable rapid cooling of olivine, the late addition of a thick megaregolith blanket to slow cooling at lower temperatures after the olivine cooling rates were recorded, or the break-up and/or re-combination of the parent body (Bryson et al., 2015; Walte et al., 2020; Yang et al., 2010). Walte et al. (2020) suggest the presence of a small fraction (2–15 vol. %) of 'primary' metal trapped in the parent body mantle before the intrusion of 'secondary' metal from a bolide, either as residual metal from incomplete parent-body differentiation, or delivered by an earlier impact and subsequently texturally equilibrated (Walte and Golabek, 2022), to facilitate rounding and grain-growth of the largest fraction of rounded olivines over millions of years, and to aid later migration of metal melt through the mantle.

The observed cooling-rate constraints and textural details have previously been studied in isolation or included in descriptive formation hypotheses, and have not been integrated into a single quantitative model to address whether large-scale changes to the parent body or different formation environments are required to produce the diversity of time scales and textures seen across Main Group Pallasites.

We model the rapid thermal evolution of a metal-olivine intrusion within a slowly cooling mantle in order to test whether we can reproduce the recorded cooling rates and observed olivine textures in pallasite samples without ad-hoc changes to the parent body. We assume a separation of timescales such that there is a one-way interaction between slow cooling of the planetesimal and the fast evolution of the intrusion: the planetesimal mantle temperature sets the initial and boundary conditions of the metallic intrusion, but this small metallic intrusion does not influence the slow, large-scale cooling of the planetesimal mantle. We also investigate the effect of the inclusion of a small fraction of metal in the planetesimal mantle, both on the cooling of the parent body, and on the cooling of later intrusions into the mantle, in order to address the possibility of a multi-collisional formation with earlier stranded metal in the mantle. We discuss the existence of other meteorite groups under the umbrella textural term “pallasite” that formed in different parent bodies, in distinct regions of the Solar System, and what this implies for the planetary building process.

2 Numerical model of a metal intrusion

Our conceptual approach of coupling the large-scale, long-term cooling of the pallasite parent body, to the small-scale, rapid cooling of the intrusion region, can be summarised in five steps (labelled with corresponding numbers in Figure 1):

Step 1. We model the 1D temperature evolution of a simple three-layered parent body, using the method and planetesimal geometry of the best-fitting result of Murphy Quinlan et al. (2021a): a thick-mantled 250 km radius planetesimal with a core radius of 125 km, and an 8 km-thick megaregolith layer that does not vary in thickness with time. We repeat this body geometry, with the addition of 15 vol. % metal in the mantle. We also use an example result from Nichols et al. (2021): a thin-mantled 300 km radius body with a 250 km radius core, and an 8 km-thick blanket of megaregolith that does not vary in thickness with time.

Step 2. We use the output of step 1 (a time series of temperatures and cooling rates along radius) to calculate a residence depth for the Imilac meteorite in each parent body, based on the metallographic cooling rates recorded by Ni diffusion between kamacite and taenite (Yang et al., 2010; Bryson et al., 2015).

We infer that this cooling rate is recorded after metal injection, once the metal has cooled to the background mantle temperature of the parent body, and that it captures the large-scale cooling of the planetesimal mantle. We focus on this one meteorite as an example, but our results are general and can be applied across the suite of pallasite meteorites.

Step 3. We extract temperature profiles along the planetesimal's radius, centered at the residence depth calculated in step two, at times earlier than the metal cooling rates were recorded. We interpolate these temperature profiles so that they can be used at a smaller metre-scale grid size.

Step 4. We consider a cube of mantle material with a vertical temperature gradient set by the background mantle 1D temperature profile from step three.

Step 5. We place an ellipsoid with the material properties of mixed metal and olivine in the centre of this cartesian box, with an elevated temperature relative to the background mantle (above the liquidus of FeNi metal), and allow it to cool and crystallise while determining the region's 3D temperature field.

Steps 4 and 5 are developed and discussed in more detail below; information regarding the earlier steps can be found in Murphy Quinlan et al. (2021a). We use the Imilac meteorite due to paleomagnetic measurements that add an additional constraint regarding core crystallisation timing (Bryson et al., 2015), but our model set-up and assumptions can also be applied to other Main Group Pallasite samples. An inherent assumption of our model is that there is a separation of timescales, implying that there is only one-way interaction between the slowly cooling parent body mantle, and the rapidly cooling intrusion: while the mantle temperature sets the boundary condition and initial temperature field of the intrusion model, the intrusion does not effect the large scale cooling of the mantle. We assume instantaneous emplacement of the molten metal and do not model deformation associated with intrusion. The results of this intrusion model are then compared to the evidence from pallasite samples for preservation of chemical heterogeneity and rounding of olivines to see whether the conditions are favourable for reproducing the known pallasite samples in the meteorite record.

2.1 Modelling the intrusion region

Our intrusion model consists of an ellipsoidal region of interconnected solid olivine bridgework (Boesenberg et al., 2012), the pore space (created by impact-related inter- and intra-granular fracturing) of which has been infiltrated and saturated by initially molten FeNi metal. This intrusion region is centered in a box of mantle material (Figure 1; steps 4 and 5) that is below the FeNi solidus. We assume convection of the metal in this region is inhibited by the low porosity and permeability of the solid olivine bridgework, the crystallisation of the metal, and the low gravitational acceleration.

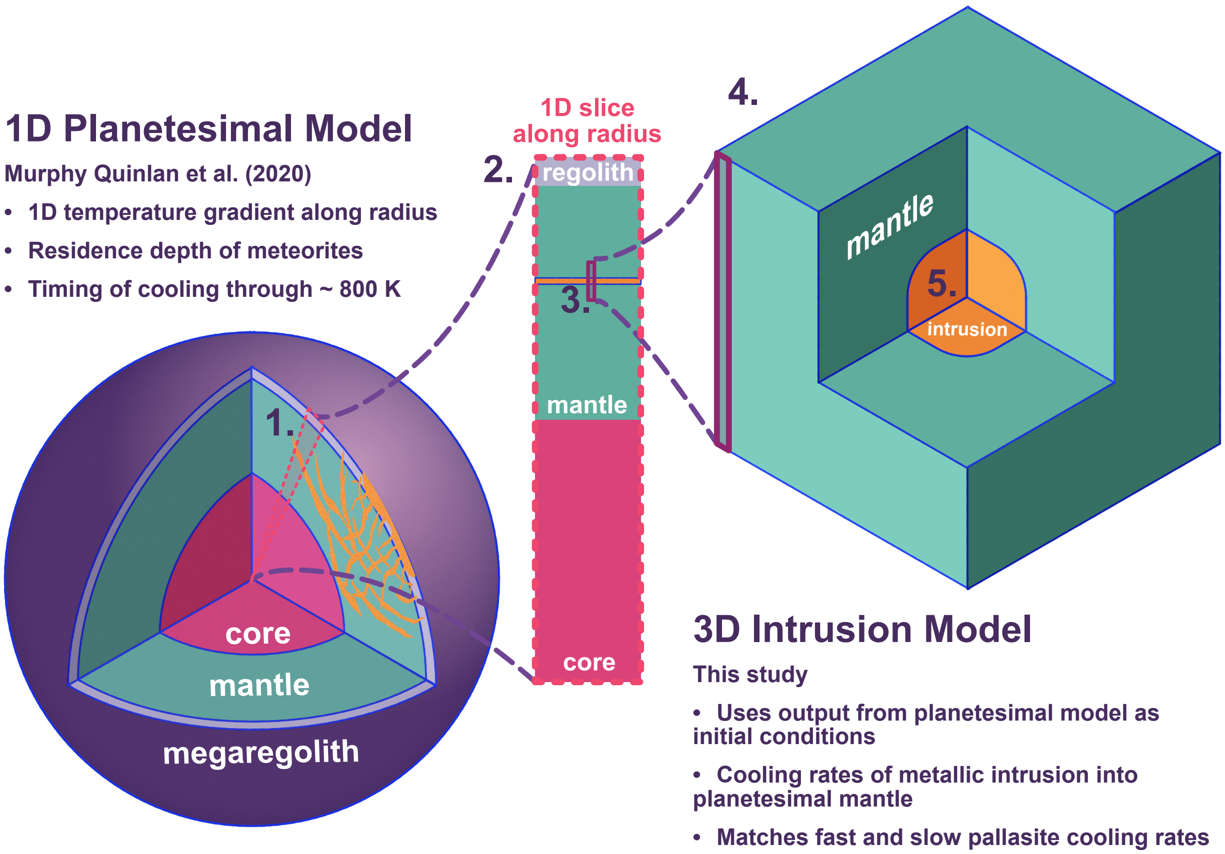

Figure 1: Cartoon sketch of model set up; not to scale. 1D temperature, cooling rate, and pallasite residence depth estimation output from the planetesimal model of Murphy Quinlan et al. (2021a) are used as input for a 3D intrusion model; the numbers refer to the modelling method steps laid out in section 2.

We consider a cartesian box of mantle material with constant temperature in the horizontal directions x and y, and the vertical coordinate z aligned with the 1D mantle temperature output from the planetesimal model (Figure 1; part three). Assuming a purely conductive system in which convective heat transport and internal heat generation are neglected, the temperature T (K) in this volume satisfies the three-dimensional heat conduction equation (Carslaw and Jaeger, 1959):

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) \tag{1}$$

where: ρ is the density of the material ($\mathrm{kg\,m^{-3}}$); c_p is the specific heat capacity ($\mathrm{J\,kg^{-1}\,K^{-1}}$); t is time (s); x, y, and z are the spatial coordinates (m); and k is thermal conductivity ($\mathrm{W\,m^{-1}\,K^{-1}}$). We choose temperature-independent k, allowing the Crank-Nicolson scheme to be applied to the problem without the complications associated with non-linearity (Carslaw and Jaeger, 1959; Özısık, 1993).

We define a uniaxial ellipsoid of volume $V = \frac{4}{3}\pi a^2 b$, where a and b are radii, which represents the intrusion region with a pallasitic mix of silicate and metal. The dimensions of the box ($X = Y = Z$), within which this ellipsoid is centered, is set by the diffusion lengthscale for the mantle material: we wish to run the model for ten years, and do not want the temperature near the model boundaries to change during that time. This allows us to apply a zero-flux condition to the boundaries of the problem.

Directly modelling the mixed-phase region of olivine crystals and metal melt would be computationally expensive and require detailed knowledge of the geometry of the phase mixture, which we do not know. Instead, we take a macroscopic approach to track the cooling and crystallisation of the metal in this area, and consider the intrusion region as a single material, using volume-averaged effective thermal properties. We adopt the method of Mottaghy and Rath (2006) to model permafrost: we assume a simple saturated two component system, where olivine forms a solid interconnected bridgework of crystals, with the pore space filled with metal.

The fraction of solid and liquid metal is controlled by a temperature-dependent function which should be one when the metal is entirely solid ($T < T_S$, the FeNi solidus temperature), and zero when the metal is fluid ($T > T_L$, the FeNi liquidus temperature). In order to account for the latent heat associated with melting or crystallisation, we apply the simple fixed-domain apparent heat capacity method (Figure S1) which correlates the heat capacity of the phase-changing material with the slope of the enthalpy-temperature curve (Zeneli et al., 2021, further details in supplementary materials).

The material properties outside the intrusion region have constant values that match that of olivine, or a mixture of olivine and 15 vol. % metal; however, phase change processes are not considered for the metal in this region. Sudden jumps and step functions in the spatially-varying diffusivity can introduce instabilities especially if these material properties boundaries intersect with the model boundary, so we surround our intrusion region with mantle material and ensure spatially-constant material properties at the model boundaries.

We apply the semi-implicit Crank-Nicolson scheme (Crank and Nicolson, 1947) with zero-flux boundary conditions to the heat equation in 1D. Forward difference is used for the time derivative of T, but the spatial derivative is evaluated at the time step $t + \Delta t/2$ instead of at t, taking the arithmetic mean between the time step t and $t + \Delta t$. We also discretise κ with respect to distance using finite differences (Langtangen and Linge, 2017).

In order to extend this scheme to three dimensions, we apply the Fractional Step Method (Cen et al., 2016; Yanenko, 1971), which evaluates the heat equation in one-third time step increments along each of the spatial dimensions.

We bench-marked our numerical model against an analytical solution from Carslaw and Jaeger (1959), and found that the maximum relative defect between the numerical and analytical models dropped to below 1 % within 150 seconds (Figure S2). We also investigated the effect of spatial resolution on our results to ensure we chose a sufficiently small spatial step size (Figure S3). Extended methods and full derivations can be found in the supplementary information.

3 Quantitative constraints on the cooling of pallasite meteorites

The results of the model at different times are analysed and compared to the meteorite record. We address two key criteria: the potential for rounding of olivine grains, and the preservation of primary igneous zoning. Each intrusion model output is scored based on whether it was consistent with observations from the meteorite record with respect to these criteria; models with a score of two reproduce both results.

3.1 Textural heterogeneity

According to the Meteoritical Bulletin Database (Grossman and Nomenclature Committee of the Meteoritical Society, 2022) and the textural descriptions compiled by McKibbin et al. (2019), pallasite meteorite samples described as having predominantly "rounded" olivine grains constitute 36 % by mass of the Pallasite Main Group (PMG) meteorite record, while samples with predominantly "angular" olivine constitute 32 % by mass of the PMG meteorite record (Figure S4). The remaining pallasites show a mix of olivine morphologies, with both angular and rounded grains present within single samples.

Small olivine grains of diameter 300 μm could be rounded within approximately ten years in Fe-Ni-S at temperatures at or above $\sim$ 1573 K, or within approximately three months at $\sim$ 1623 K (Walte et al., 2020; Saiki et al., 2003). Larger olivines could also be rounded on geologically short timescales at higher temperatures, or with protracted cooling, or in the presence of sulfide-rich metal melt. However, Walte et al. (2020) and Walte and Golabek (2022) suggest large rounded olivines predate the pallasite-forming metal-olivine mixing event and so do not need to be explained in the intrusion process; they are rounded by a small fraction of metal (2–15 vol. %) retained in the mantle from incomplete differentiation and core formation, or stranded after partial re-equilibration from an earlier metallic impact. We address this by increasing the diffusivity of the parent body mantle for a selection of runs to approximate 15 vol. % metal trapped in the mantle, and track the cooling history at the depth of pallasite residence to see if large-scale rounding can be achieved prior to secondary metal intrusion.

To produce a pallasite sample with a dominantly rounded olivine texture (including the largest size fraction of olivine, which requires long timescales to round, > Myr), the starting olivine must already be rounded, and then any small fragments of olivine fractured during the intrusion of metal must be sufficiently heated for long enough to round post-intrusion. To produce pallasite samples with a dominantly angular texture, the original pre-intrusion olivine must either be euhedral or "angular", or if rounded, must be extensively fractured during metal intrusion. Then, the intrusion region must cool quickly enough to not modify their angularity.

To produce a mixed-type pallasite with both rounded and angular olivine grains, the original olivine texture could be rounded, with then some fracturing on metal intrusion and subsequent rapid cooling for preservation of this angularity; or, the original texture could be angular or euhedral with rounding of smaller grains due to prolonged contact with hot metal post-intrusion. Mixed-type pallasites can also be produced by pieces of angular or rounded olivine being broken off the bridgework and entrained in the metal melt, and carried to regions with olivine of a different morphology, followed by rapid cooling which preserved the textural heterogeneity.

While we accept that the meteorite record almost certainly does not accurately and representatively sample the pallasite formation region of the pallasite parent body, it provides some suggestion of the proportion of the intrusion region that should produce rounded or angular olivines. We define a volumetric fraction of the total PMG record expected to have a rounded, angular or mixed olivine texture, by assigning a dominant texture to each sample in the database, then dividing the recorded sample mass by the average pallasite density (Grossman and Nomenclature Committee of the Meteoritical Society, 2022; Britt and Consolmagno, 2003, see supplementary information). We take the dominantly rounded fraction of the pallasite meteorite record as the minimum required volume proportion of the intrusion within which rounding occurs, and take the angular fraction of the record as the minimum required volume within which angularity is preserved. This provides upper and lower bounds on what volume of the intrusion should produce rounded olivine grains; the uncertainty between these upper and lower bounds allows for production and preservation of mixed-type pallasites.

Based on experimental results from Walte et al. (2020), to round small olivine grains we require a point within the intrusion region to be at or above 1623 K at three months after the start of the model run, or at or above 1573 K at ten years after the start of the model run. For a model to produce the textures observed in the pallasite meteorite record, at least 36 % by volume of the intrusion region must experience a temperature evolution conducive to rounding the smallest olivine grains, and at least 32 % by volume must cool quickly enough to preserve angular and fragmental olivine. We investigate the sensitivity of the model to these requirements by both varying the temperature cut-offs by $\pm10\%$ and by varying the timing of the measurement, and find that the earliest requirement ($T \geq 1623$ K at three months) is the most sensitive both to changing the time or temperature of this requirement (see Figure S5). As the temperature constraints are derived from experimental results extrapolated multiple orders of magnitude beyond the original experimental design (i.e. from hours and seconds to months and years), and the texture estimates are based on the gross statistical properties of the incomplete meteorite record, incorporating an estimate of error would imply an unrealistic level of precision.

3.2 Chemical heterogeneity

Pallasite olivines display heterogeneous core and rim compositions (Hsu, 2003), with potential oscillatory zoning in Cr, Al and V recorded in the Imilac meteorite (Chernonozhkin et al., 2021). Preservation of original igneous compositions is varied, with solid-state diffusive modification of different elements on different scales recorded across samples (Hsu, 2003). In general, Ca zoning (either diffusion profiles or original heterogeneity) is pervasive in pallasite olivine and has not been completely homogenised (Hsu, 2003).

In an olivine grain of diameter 300–500 μm, Ca will be completely homogenised within four years at $\sim$ 1573 K and within 8 years at $\sim$ 1373 K (Hsu, 2003; Jurewicz and Watson, 1988). This means that to preserve the Ca heterogeneity in pallasite olivine, including in the smallest size fraction, the majority of pallasite samples had to cool rapidly enough to prevent this erasure.

Based on diffusion studies of Hsu (2003) and Jurewicz and Watson (1988), to preserve zoning we require that a point within the intrusion region cools below 1573 K within four years, and below 1373 K within eight years. In order to reproduce the "ubiquitous" preservation of Ca zoning observed in the pallasite meteorite record Hsu (2003), we require that $>$ 95 % by volume of the intrusion region cools rapidly enough to preserve Ca zoning. We also set a more lenient requirement of $>$ 50 % by volume to allow for variations in degree of diffusional modification, to test if this changes the overall trend of results. We use this lower cut-off value of

> 50 % for our example case (Fig. 2) to better illustrate our point-by-point filtering approach, but use the stricter > 95 % cut-off when looking at the overall suite of models, and unless otherwise specified refer to this as the zoning requirement. As with the rounding criteria, we allowed the temperature requirements to vary by ±10%, and investigated the sensitivity of the model to the times these filters were applied (Figure S5).

3.3 Filtering model output

We analyse each model run's 3D temperature array at three months, four years, eight years, and ten years and find the volume of the intrusion region that meets each of the following logical criteria:

$$\begin{aligned} R &:= (T_{\text{3mnths}} \geq 1623\,\text{K}) \;\vee\; (T_{\text{10yrs}} \geq 1573\,\text{K}), \\ Z &:= (T_{\text{4yrs}} \quad \leq 1573\,\text{K}) \;\wedge\; (T_{\text{8yrs}} \;\leq 1373\,\text{K}), \end{aligned} \tag{2}$$

where R represents potential rounding, and Z denotes potential zoning. Based on the meteorite record (Grossman and Nomenclature Committee of the Meteoritical Society, 2022; see supplementary information) we assign a score to the model output:

- If between 36–67 vol.% of the intrusion will round olivine crystals, and > 50 vol.% or > 95 vol.% (depending on the suite of models) will preserve Ca heterogeneity, the output receives a score of two.
- If the intrusion region meets only one of these criteria, the output receives a score of one.
- If neither constraint is met, the output receives a null score.

We use this simple scoring criteria instead of alternative measures of goodness-of-fit as we are primarily interested in whether any models can match these criteria, as opposed to investigating in detail what region of parameter space best reproduces certain results. This can be addressed in future work, as the Euclidean norm or a similar measurement can be easily incorporated into our framework. We also test the sensitivity of the overall score to changing the rounding and zoning criteria. We find that for a spatial step $\Delta x < 4$ m, the result is not impacted by the spatial resolution of the model (Figure S3).

4 Cooling of a metal intrusion

Using the best-fitting model of Murphy Quinlan et al. (2021a), we initially modelled the temperature evolution of the mantle of a 250 km radius planetesimal and calculated the residence depth of the Imilac pallasite meteorite based on Ni-diffusion cooling rates estimated from its metal portion (Figure 2a; Murphy Quinlan et al., 2021a; Yang et al., 2010; Bryson et al., 2015). The vertical temperature gradient through the mantle at an earlier time (selected at random, Figure 2b) was then used as the initial condition for the metal intrusion model (Figure 2c and d). The parameters used for this model are given in table 1.

Each node within the intrusion region was filtered as described in section 3.3, and the volume percentage of the intrusion meeting the rounding requirements and zoning requirements were calculated independently (Figure 3). Approximately 67 % of the intrusion region cools quickly enough to preserve calcium zoning in olivine (Figure 3 a), passing the requirement of > 50 % by volume of the intrusion region meeting the zoning criterion. The rounding requirement is also met by just under 67 % of nodes in the intrusion region, passing the requirement of between 36–67 % by volume of the region meeting this criterion. The model receives a score of two, indicating that it meets both requirements.

This result demonstrates that an ellipsoidal intrusion of molten metal into a porous olivine planetesimal mantle can reproduce the necessary thermal evolution pathways both to facilitate the rounding of small olivine grains, and to allow the preservation of Ca zoning. Within the intrusion region, mean cooling rates of $\sim$ 10–150 K/Myr are reached, agreeing with the elevated cooling rates suggested by Miyamoto (1997) to explain olivine diffusion profiles (Figure 3 c). This model also agrees with recorded metal cooling rates due to the initial and boundary conditions; once the intrusion cools to the background mantle temperature (15 – 50 years by conductive cooling, depending on size of the intrusion), it will continue to cool at the same rate as the planetesimal mantle, and will cool through the required temperature window at the rate predicted by metal cooling rates (Bryson et al., 2015; Yang et al., 2010; Murphy Quinlan et al., 2021a).

Parameter	Symbol	Unit	Range/Value	Example model run	References/Notes
Initial conditions					
Intrusion radii	r_x, r_y, r_z	m	10–150	72, 72, 92	
Mean radius	$\bar{r}$	m	11–147	79	
Unique/non-unique axes	b/a		0.07–15.0	1.28	
Metal fraction (intrusion)	ϕ_m	vol. fraction	0.05–0.55	0.32	Met. Bull. Database
Trapped metal (in mantle)		vol. fraction	0–0.2	0	Walte et al. (2020)
Background mantle temp. (top)	T_t	K	250–1600	847	Murphy Quinlan et al. (2021a)
Background mantle temp. (bottom)	T_b	K	265–1665	851	Murphy Quinlan et al. (2021a)
Initial intrusion temp.	T_i	K	1600–1900	1660	Assumed above liquidus due to impact heating
Material properties					
Metal					
Density	ρ_m	kg m^{-3}	7020–7500	7260	Scheinberg et al. (2016)
Conductivity	k_m	W m^{-1} K^{-1}	30–40	35	Scheinberg et al. (2016); Touloukian et al. (1971)
Heat capacity	c_m	J kg^{-1} K^{-1}	820–850	835	Desai (1986)
Diffusivity	κ_m	m^2 s^{-1}	$k_m/(\rho_m c_m)$		
Latent heat of crystallisation	L	J kg^{-1}	1.33E05 – 2.7E+05	2.56E+05	Scheinberg et al 2016
Liquidus temperature	T_L	K	1570–1810	1600	Ehlers (1972)
Solidus temperature	T_S	K	1260–1790	1260	Ehlers (1972)
Olivine					
Density	ρ_{ol}	kg m^{-3}	3320–3360	3341	Su et al. (2018)
Conductivity	k_{ol}	W m^{-1} K^{-1}	2.5–3.4	3	Murphy Quinlan et al. (2021a); Bryson et al. (2015)
Heat capacity	c_{ol}	J kg^{-1} K^{-1}	810–830	819	Su et al. (2018)
Diffusivity	κ_{ol}	m^2 s^{-1}	$k_{ol}/(\rho_{ol} c_{ol})$		
Numerical details					
Time step	Δt	s	2.63E06	2.63E06	Approx. 1 month
Spatial step	Δx, Δy, Δz	m	2	2	Calculated from L, N
Box size	L_x, L_y, L_z	m	200–800	400	
Number of nodes	N_x, N_y, N_z		101– 401	201	L and N balanced to give $\Delta x, y, z = 2$ m
Total iterations			10– 241	121	
Boundary conditions	$\mathbf{b}^n$, $\mathbf{b}^{n+1}$		Neumann, Dirichlet	Zero flux (Neumann)	
Outputs					
Actual intrusion volume	V	m^3	4.90E03–1.38E07	1.998E06	
Percentage zoning preserved	Z %	%	0 – 100	67.2	
Percentage rounded	R %	%	0 – 100	66.7	

Table 1: Ranges of parameter values for 2200 model runs, including example model run illustrated in Figures 2 and 3. Ranges given do not include parameter variation for sensitivity testing and benchmarking (see supplementary material for further information).

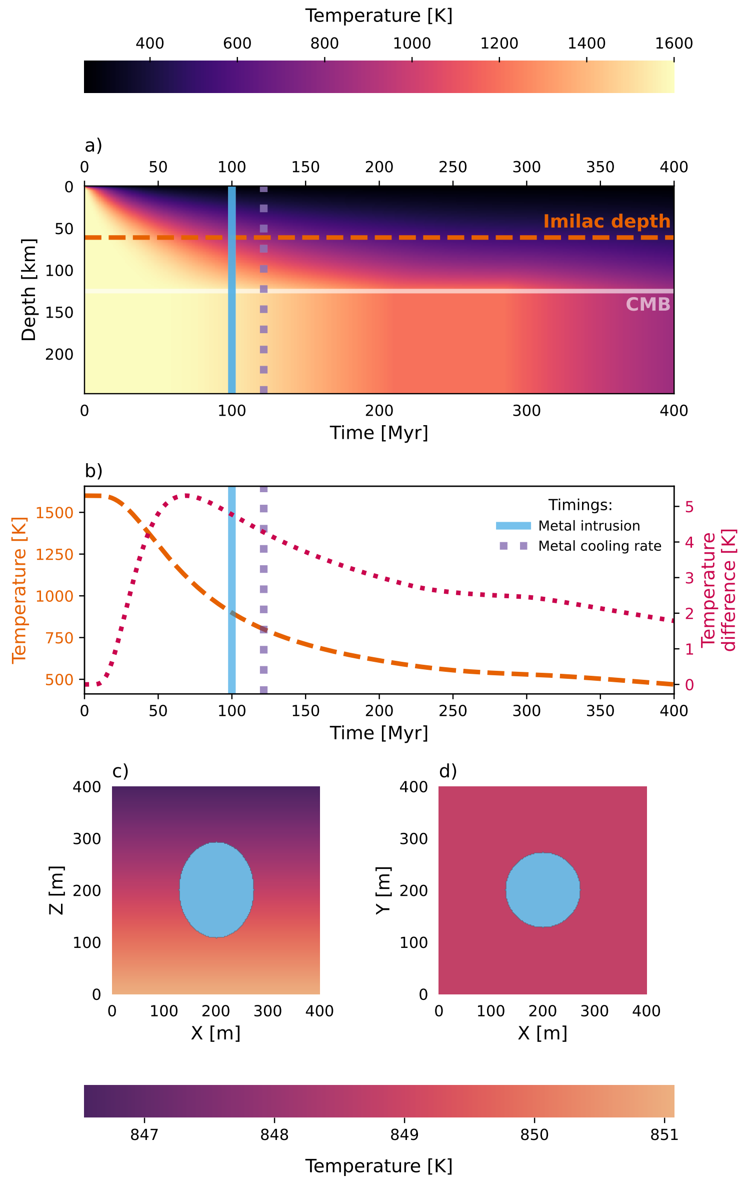

Figure 2: Initial conditions for model run. (a) The 1D temperature evolution for a 250 km radius planetesimal with a 125 km radius core and an 8 km thick porous megaregolith layer (Murphy Quinlan et al., 2021a,b). The core-mantle boundary (CMB) and residence depth of the Imilac pallasite meteorite (61 km, from metal cooling rates; Murphy Quinlan et al., 2021a) are labelled. (b) Temperature profile at this 61 km depth, and temperature difference across a 400 m slice of mantle centred at this depth. These outputs provide the initial and boundary conditions for the intrusion model. The blue vertical line shows the time of intrusion of metal into the mantle (chosen), while the purple dashed line shows the time metallographic cooling was recorded in the pallasite sample (measured). (c & d) Initial conditions for the intrusion model: two 2D slices through the 3D ellipsoid geometry (prolate ellipsoid). Z lies along the planetesimal radius, and shows the vertical temperature gradient, while X and Y have constant temperature. The blue ellipsoid represents the intrusion region, with a temperature of 1790 K.

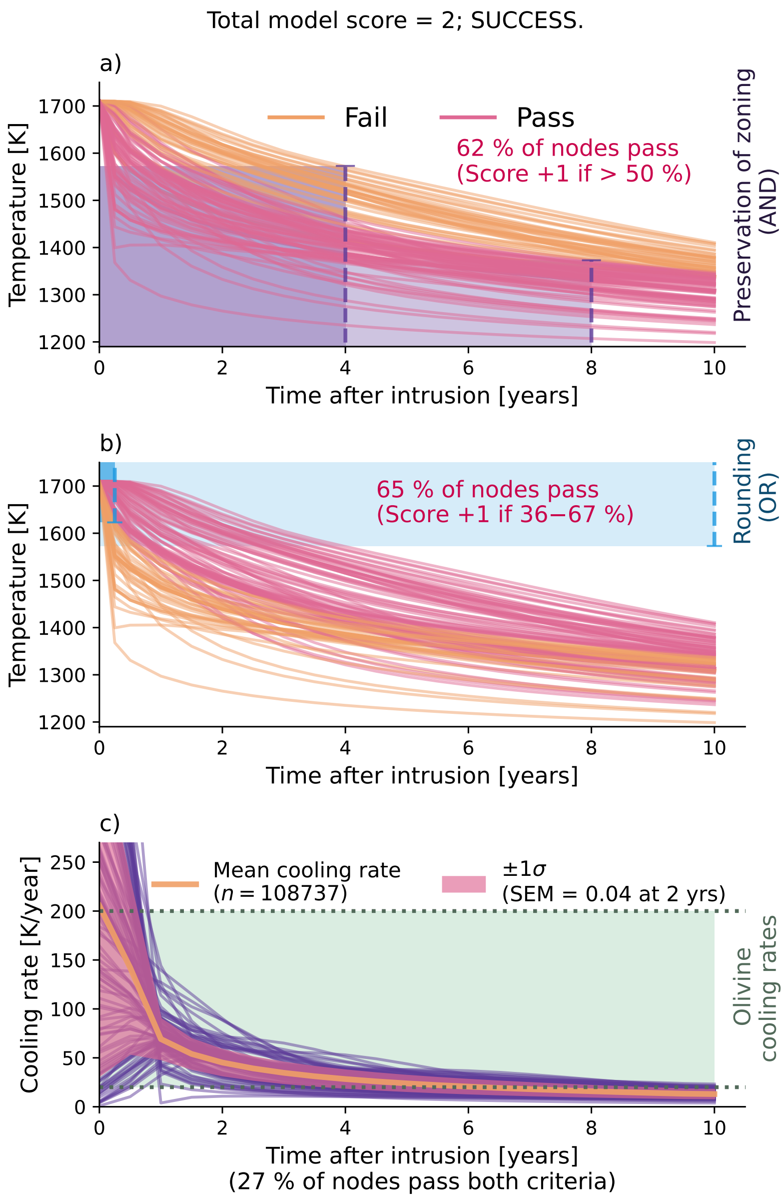

Figure 3: Results and output for a single model run with initial conditions in Figure 2. Each line is a temperature or cooling rate time-series for a volume element within the intrusion described in Figure 2 (e.g. within the blue ellipsoid). Each model is initially assigned a score of zero. Panel (a) shows a sample of nodes (200) within the intrusion filtered according to whether olivine zoning would be preserved at that location. If the model "passes" the zoning preservation criteria (> 50 % of points will preserve zoning, as is true in this example with 67.2 % passing), one is added to the model's score. Panel (b) shows the same nodes filtered according to whether olivine grains will be rounded at that location. If the model "passes" the olivine rounding criteria (36–67 % of points will round olivine, as is true in this example with 66.7 % of nodes passing), one is added to the model's score. A score of two is deemed "successful". The full array of nodes within the intrusion area is used to calculate these percentages (108,737 in this example). Panel (c) shows the cooling rates for the same selection of nodes. The mean cooling rate and standard deviation were calculated with all nodes in the intrusion ellipsoid (108,737). The green shaded region highlights the range of cooling rates suggested by Miyamoto (1997) to explain pallasite olivine zoning.

5 Exploring the parameter space

In order to explore how commonly pallasite formation models can yield conditions that preserve the disparate cooling rates, the model procedure was repeated for different intrusion times in the 250 km radius planetesimal (300 models), and for a 300 km radius planetesimal with a 250 km radius core, and an 8 km megaregolith layer (300 models, reproducing a case from Nichols et al., 2021) with randomised intrusion geometry. Randomised initial mantle temperatures were also chosen to approximate different parent body geometries and a range of different intrusion depths (600 models). The summarised results of these 1200 model runs are shown in Figure 4, and ranges within which parameters were varied in table 1. We also ran a suite of 1000 models with varying material properties including density, heat capacity, and crystallisation temperature in addition to randomly selected mantle temperatures and intrusion geometry, which allowed us to approximate the effect of adding a small percentage of trapped metal to the mantle or changing the composition of the intruding metal, as well as testing the model's sensitivity to these parameters.

Neither initial intrusion temperature (Figure 4, third column) nor metal fraction (by volume, Figure 4, fourth column) strongly control whether the intrusion region will match both constraints. Intrusion volume is a strongly controlling parameter (Figure 4, first column), with the majority of models with a volume greater than 5×10^6 m^3 meeting neither constraint. While background mantle temperature displays a weak negative relationship with the overall model score, it is strongly negatively correlated with zoning preservation, and moderately positively correlated with rounding potential (Figure S6). Cooler mantle background temperatures (Figure 4, second column) result in higher mean cooling rates and favour meeting both constraints (Figure 4n). These trends hold true not only for model results that use mantle temperature inputs from the planetesimal model, but also for the randomised input parameters that cover a larger parameter space, when material properties are varied randomly, and in the more specific sensitivity tests (Table S1, Figures S7, S8, S9).

Varying the trapped metal content in the mantle or the mantle diffusivity does not systematically change the mean intrusion temperature after ten years, the zoning preserved or the rounding expected (Figure S10), with no significant correlation found between either olivine or metal material properties and model results (Figure S11).

Based on the mean temperature of the intrusion through time, we calculated the mean cooling rate and average temperature of the intrusion between three months and ten years; this allows for an approximate overview of the cooling rate over the model run time, excluding the extremely rapid cooling on initiation of the model. Figure 5 highlights the temperatures and cooling rates relevant to rapid pallasite olivine cooling suggested by Miyamoto (1997); sufficiently high cooling rates are reached in the first few years of cooling.

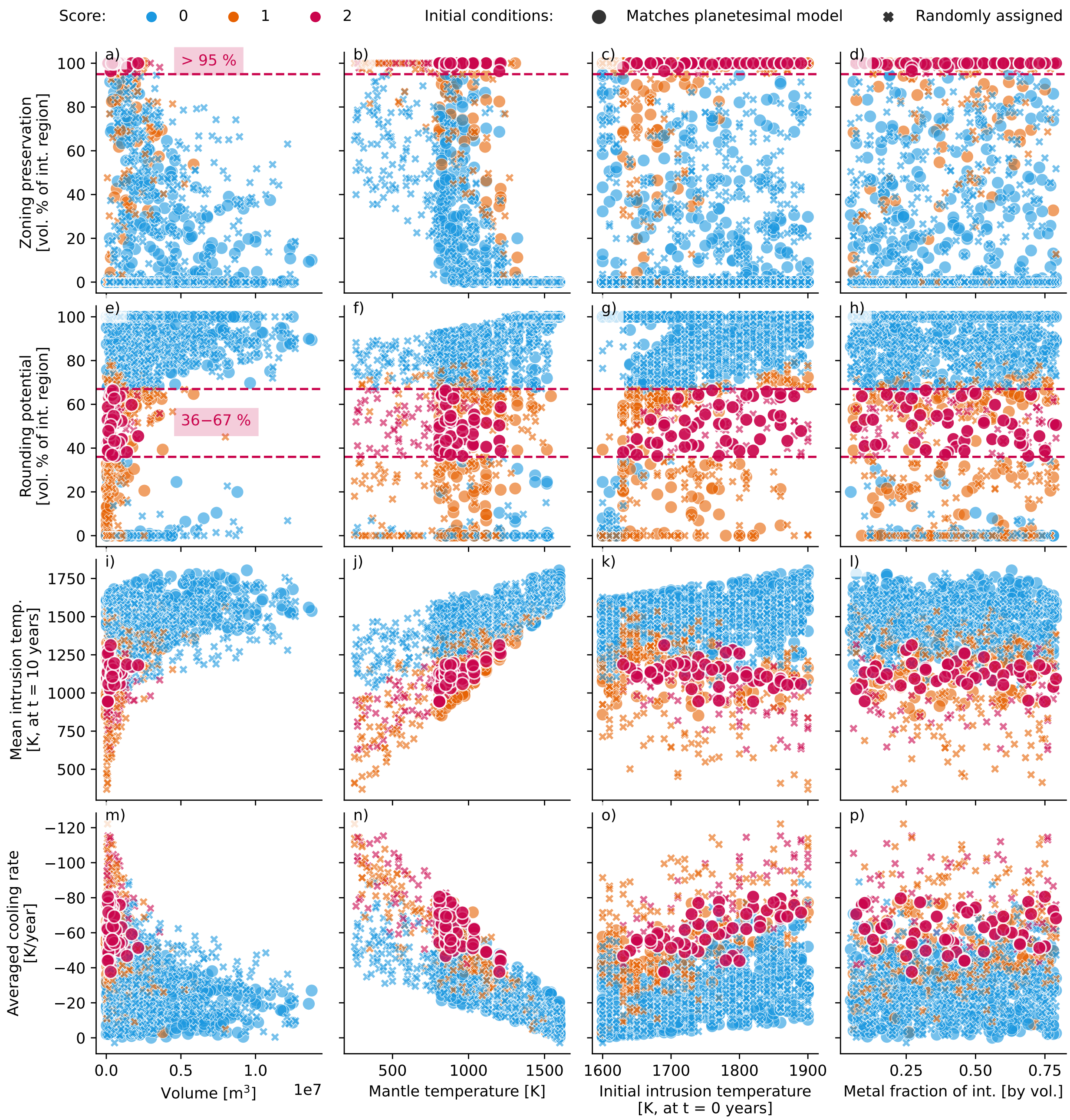

Figure 4: Summary of results for 1000 model runs. Colour denotes score: 0 means neither constraint was matched, 1 means one constraint was matched, and 2 means both constraints were matched. Marker shape describes the initial temperature conditions: either output from a planetesimal model, or randomly assigned. Parameters were not varied in isolation. Large pink circles match both constraints and used input from a planetesimal model.

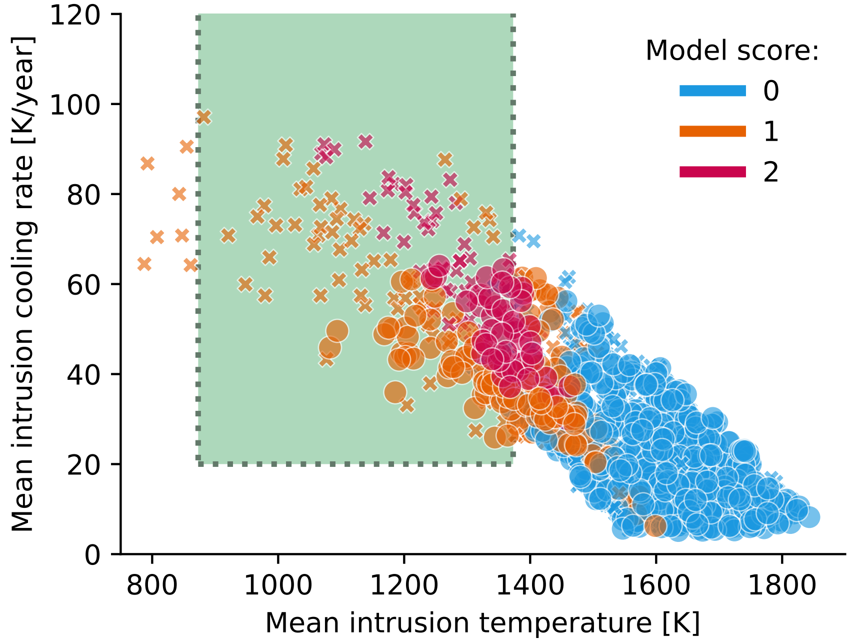

Figure 5: Mean intrusion temperatures and cooling rates over the model run time (from 3 months to 10 years) for the intrusion region for 1200 model runs. The shaded region highlights the cooling rates and temperatures suggested by Miyamoto (1997), estimated from olivine diffusion profiles (Hsu, 2003). Model results that fall within this region reproduce the required rapid cooling in the relevant temperature window. Colour denotes score: 0 means neither constraint was matched, 1 means one constraint was matched, and 2 means both constraints were matched. Marker shape describes the initial temperature conditions: either output from a planetesimal model, or randomly assigned.

This suggests that both short-term, rapid cooling of olivine in molten metal, followed by much slower cooling of the FeNi metal, are explained by the intrusion of hot metal into a warm mantle.

6 Discussion

A simple model of a metallic intrusion into the mantle of a planetesimal reproduces the gross statistical properties of olivine texture and diffusive modification observed in pallasite meteorites, and replicates the contrasting slow metal and rapid olivine cooling rates estimated from various elemental diffusion profiles. This model reproduces these results without the need for impact-exhumation or parent body break-up to explain rapid olivine cooling rates, or the addition of a late thick megaregolith layer to explain slow cooling, as have been invoked by previous models (Yang et al., 2010; Bryson et al., 2015; Walte et al., 2020; Walte and Golabek, 2022).

Walte and Golabek (2022) list the observational constraints from pallasite samples that formation models much match, comprising: remnant magnetisation, a warm mantle prior to pallasite formation, rapid cooling at high temperatures (>1200 K), slow cooling at lower temperatures (1000–700 K), varied residence depths (from metal cooling rates), and low Ir concentrations implying differentiation of the injected molten metal. Their qualitative model of a non-destructive two-body collision agrees with all the available constraints; however, it requires impact rebound or a similar effect to produce rapid cooling after impact and development of a megaregolith layer to support later slow cooling (Walte et al., 2020). We show quantitatively that an intrusion of molten metal into a planetesimal mantle can meet the above constraints without the need for an impact rebound or development of a late thick megaregolith layer to slow cooling. While our results do not preclude large-scale changes to the parent body, it removes the need for them; this means that future work can seek lines of evidence for these planetary-scale processes instead of them being assumed a requirement for pallasite formation.

We show that the required criteria for pallasite formation can be met for a wide range of intrusion morphologies (Figure 6d), at a wide range of mantle temperatures (as a proxy for both timing of intrusion and residence depth). For models using planetesimal mantle temperature as initial conditions, criteria were met more often later in the planetesimal's history (shortly before the slow metal cooling rates were recorded), when the mantle was cooler and faster intrusion cooling rates could be achieved (Figure 6a, b); the zoning preservation requirements cannot be met unless the temperature of the mantle is below 1373 K, as the intrusion needs to cool below this temperature within 8 years. Small intrusion regions with mean radii between 20 and 140 m produce the rapid cooling required to preserve olivine chemical heterogeneity (Figure 6c). Similarly, high aspect ratio morphologies (more pipe- or sheet-like) with a minimum radius < 50 m more

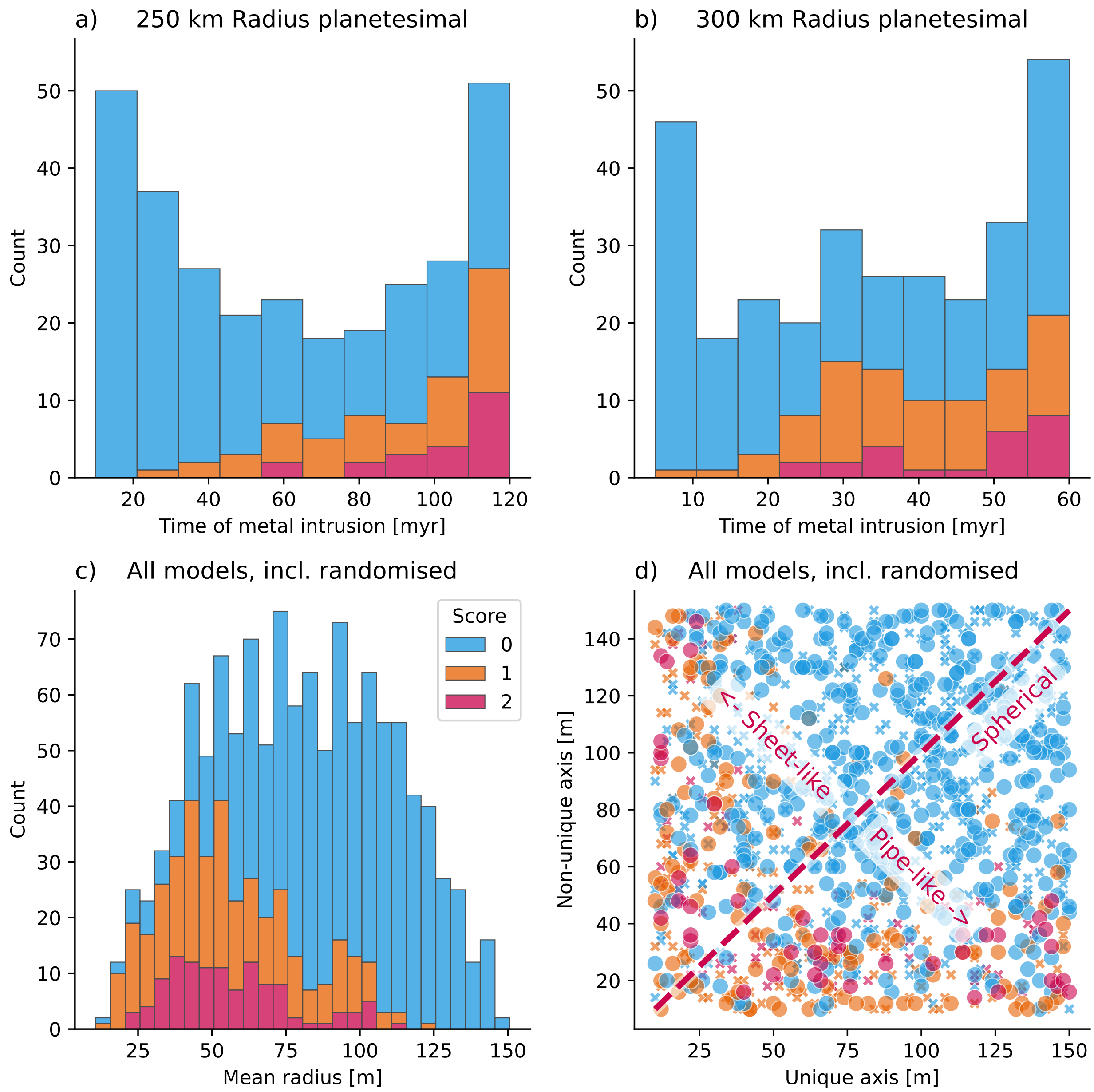

Figure 6: Dependence of score on timing of intrusion, volume of intrusion region, and geometry of intrusion region. a & b) Histograms of score for timing of metal intrusion (in millions of years after initiation of model/crystallisation of magma ocean) for both planetesimal models. Maximum time on both histograms is the time the metal cooling rate was recorded. c) Histograms of score for mean radius of intrusion region for all models with constant material properties (1200 model runs). d) Dependence of score on intrusion region volume and aspect ratio for all models with constant material properties (1200 model runs).

frequently meet the constraints as opposed to intrusion segments that are more spherical in shape with both maximum and minimum radii above ~ 50 m. (Figure 6d), with a weak non-monotonic correlation measured (Figure S6). This suggests that pallasite-material formation is constrained to intrusions with a sufficiently small minor axis (of ~ 50 m).

In our implementation, the volume of the intrusion region required to satisfy the rounding criteria is set by the volume (sample mass/average pallasite density) proportion of the meteorite record described as having angular, rounded, fragmental or mixed textures as the dominant sample texture (Figure S4). This neglects the variation in density and metal/olivine proportion in samples, varying sulfur content of metal pockets, and suffers from bias due to a number of outlying massive samples in the record. We bootstrapped (with replacement) the Meteoritical Bulletin Database (Grossman and Nomenclature Committee of the Meteoritical Society, 2022) and found the sample size too small to assign robust statistics. We also recognise that the pallasite meteorite record may not proportionally sample the formation region. However, we apply the available constraints to our model to show that we can match the meteorite samples available. Despite these limitations, our model shows that parameters such as the metal fraction of the pallasite region and the proportion of metal trapped in the planetesimal mantle do not systematically change whether pallasite-like material can be produced. Our results also highlight the importance of the timing of metal intrusion into the parent body mantle, and the temperature at which the intruded mantle is residing. Changing the proportion or volume percentage of rounding required by a small percentage does not change the conclusions of our study within the parameter range explored: that rounded olivine and preserved chemical zoning can be recovered from the same pallasite intrusion volume.

Hsu (2003) describes calcium zoning in pallasite olivine as ubiquitous, which in combination with detailed diffusion of Ca in olivine studies, makes it a sensible choice for first steps in calculating erasure or preservation potential in a metallic intrusion. We set the zoning preservation requirement to $> 95\%$, implying that essentially all pallasites must preserve some degree of Ca heterogeneity. However, we also considered a lower requirement of > 50 % to also allow regions of erasure and more intensive diffusional modification (see Figure S15). Across all model runs, this lower zoning requirement increased the number of model runs that meet both constraints from 263 (12.0 % of 2200 model runs) to 343 (15.6 % of 2200; see table S2). The same dependence on mantle temperature and intrusion volume is seen and rapid olivine cooling rates are still met between four and eight years after intrusion (Figure S9) .

As mentioned previously, the time and temperature pairings used to estimate grain rounding and zoning preservation are associated with unquantifiable errors. In order to assess the sensitivity of the model to the temperature requirements, we varied the temperature of each filter by ± 10 % of the original temperature (Table S2, Figures S12, S13). While the absolute number of successful models changed, the overall relationship between model score and parameters such as initial temperature, background mantle temperature or intrusion volume remained essentially the same (Figure S14). We also assessed the change through time in intrusion volume that satisfies each temperature requirement, for the example model run illustrated in Figure 3. We found that the rounding requirement of $T_{3\mathrm{mnths}} \geq 1623\,\mathrm{K}$ was most strongly dependent on timing of the measurement, as the intrusion is still rapidly cooling at this time. The intrusion region satisfying this requirement will change by approximately ± 10 vol. % per month at this stage in the intrusion process (Figure S5), whereas by four, eight and ten years when the other temperature requirements must be matched, the change in the intrusion region that matches each constraint is ~ 1 vol. % or less per month. At three months, changing the temperature requirement by ± 10 % may result in a model no longer passing the rounding criterion (Figure S5); however, this does not change the overall relationship between the input parameters and the results (Figure S14).

The inclusion of a small fraction of metal within the planetesimal mantle may explain the presence of large (radius ~ 5 mm), well rounded olivine crystals: Saiki et al. (2003) estimated that olivine grains with a radius of 5 mm would be fully rounded in the presence of FeNi after 7 Myr at or above 1673 K, 29 Myr at or above 1573 K, or 241 Myr at or above 1473 K. While we primarily focus on models of the pallasite parent body with a purely olivine mantle, we also modelled a parent body with 15 vol. % metal trapped in the mantle as in Walte et al. (2020). We assumed that the sole effect of adding this small fraction of metal is to increase the mantle diffusivity, which in turn accelerates planetary-scale cooling by a small degree (Figure 7). We find that hotter mantles (post magma ocean solidification, with higher olivine solidus temperatures) better facilitate this large-scale, long term rounding of olivine grains (Figure 7). We also varied the metal content in the mantle region surrounding the intrusion in our intrusion-scale model between 0–20 vol %, but found no systematic effect on the score of models (Figure S10).

While hotter initial mantle temperatures are required for this earlier period of olivine rounding, the final stage of metal intrusion that is recorded in pallasites was most likely injected into a cooler mantle that was approaching ~ 800 K (Figure 6 a, b, Figure 7). We find that intrusions of all sizes into mantles of ~ 1200 K and hotter cannot cool below 1373 K quickly enough to preserve Ca zoning (Figures 4, 7). In order to reproduce the cooling rates through 873 K suggested by Miyamoto (1997), the background mantle must be below this temperature at the time of intrusion (Figure 7). This restricts the timing of the pallasite-forming metal intrusion to between ~ 10–30 Myr before cooling through the metallographic cooling rates at approximately 800 K.

Our simple model could also be developed by incorporating more complex grain-growth and rounding mechanisms, such as that of Solferino and Golabek (2018), which focuses on olivine grain growth in contact with solid Fe-Ni-S at different depths within a planetesimal mantle. While we take a macroscopic approach

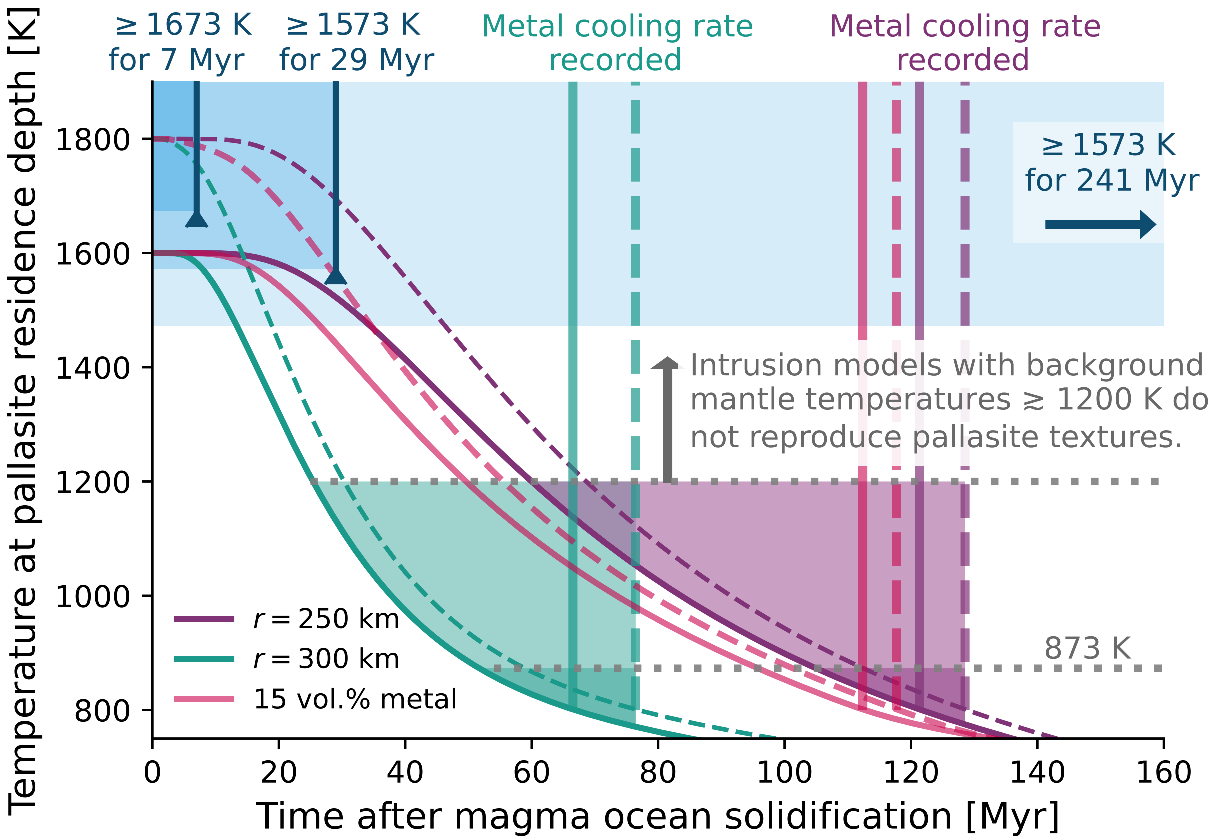

Figure 7: Temperature time series at depth of Imilac pallasite residence, based on FeNi cooling rates (Yang et al., 2010), for a 250 km radius planetesimal with a 125 km radius core (Murphy Quinlan et al., 2021a), a 300 km radius planetesimal with a 200 km radius core (Nichols et al., 2021), and a a 250 km radius planetesimal with a 125 km radius core, and 15 % by volume metal trapped in the mantle. Blue boxes represent temperature criteria suggested by Saiki et al. (2003) to explain rounding of large (5 mm radius) olivine crystals; the model cooling time series must pass through one of the blue lines. The two horizontal grey dashed lines indicate maximum background mantle temperature at time of final metal intrusion to meet different criteria: in order to preserve Ca zoning, background mantle temperature must be below 1200 K, which in order to cool through temperature window at the cooling rates suggested by Miyamoto (1997), the background mantle temperature must be below 873 K.

to modelling the olivine-metal mixing region, a micro-scale investigation of the crystallisation of metal in contact with olivine and the potential volume change, localised reactions textures and microstructures would provide further constraints on the pressure, temperature and time of mixing between these phases.

An interesting area of research outside the scope of the current study is the details of metal intrusion into the parent body mantle and the dominant mode of transport of the metal through the mantle. While previous models have suggested that the metal may have an internal source (eg., the molten core of the planetesimal, suggested by a ferrovolcanism origin; Johnson et al., 2020), recent isotopic studies show a statistically significant disequilibrium between the metal and silicate phases in pallasites, strengthening the argument for an external source delivered via impact (Windmill et al., 2022). Studies of core formation via percolative flow (Solferino et al., 2020; Berg et al., 2018) and intrusion propagation and emplacement (Walker et al., 2021; Stephens et al., 2021) alongside microstructural evidence from pallasite samples can be utilised to better understand this. Our model can aid in this research, as it provides a range of mantle temperatures over which pallasite-like textures can be produced.

Instead of attempting to recover specific details of the pallasite parent body, we have taken a statistical approach and instead look at the range of parameters over which pallasite formation is possible. Our results show that the development of conditions favourable to pallasite formation are common across the parameters we tested, but are constrained by the mantle temperature, which can be considered a proxy for the timing of metal intrusion. The two-stage formation hypothesis of Walte and Golabek (2022) suggests that an earlier impact injected metal into the pallasite parent body mantle, but did not produce "pallasite-like textures" as observed in meteorite samples, because the mantle was too hot at the time. Instead, the region of intrusion achieved textural equilibrium, only retaining a small fraction of metal which aided olivine grain growth and rounding. A later impact is proposed to then deliver more molten metal into the cooler mantle, producing the textures observed in samples. Our model reproduces the timescales suggested by both these different stages of formation. These metal-injection events may be a recurrent stage in planetesimal development, representing a halted core-growth event where cooler mantle temperatures do not facilitate migration of metal all the way to the centre of the planetesimal before solidification.

Framed in this way, perhaps the unusual feature of pallasite meteorites is that they were excavated in such a way that preserved them and allowed them to be delivered to Earth, as opposed to their formation being a unique event. This is supported by the evidence for planetesimal growth in two distinct reservoirs in our Solar System (Morbidelli et al., 2022), both of which are sampled by pallasitic material: while we specifically discuss and model the parent body of the Main Group Pallasite meteorites, the umbrella group of pallasites including the Eagle Station Pallasites, the Pyroxene Pallasites, and anomalous ungrouped samples, must sample multiple parent bodies sourced from both the carbonaceous and non-carbonaceous reservoirs

(Jacquet, 2022). These similar lithologies, samples from different regions of the early Solar System, from isolated planetesimals, suggests that this process was repeated on multiple bodies. Jacquet (2022) suggests a renaming of the pallasite class to "dunite-iron" meteorites to highlight the textural similarities instead of inferring a genetic link.

It is possible that multiple metal impacts delivered metal to the mantle of the pallasite parent body over the course of its life span: some of which may have supported core growth during the magma ocean stage of differentiation; others which stalled in the hot, newly-solidified mantle and eventually reached textural equilibrium, producing regions of well-rounded, large olivine grains; and later still an intrusion into a cooler mantle that facilitated rounding of some smaller olivine grains fractured during intrusion, preservation of chemical heterogeneity in areas previously untouched by prior intrusions, and rapid heating, cooling, and subsequent diffusional modification of olivine rim compositions. Following this intrusion, the body continued to cool, the core crystallised and paleomagnetism was recorded in some samples (Bryson et al., 2015; Nichols et al., 2021; Murphy Quinlan et al., 2021a), and the body became geologically frozen in place until its destruction $\sim$ 100 Myr ago (Herzog et al., 2015).

7 Conclusions

Different formation environments are not required to explain varied levels of rounding of olivine grains in pallasite meteorites: large, well-rounded grains may predate metal intrusion and be linked to contact with primordial metal pockets (Walte et al., 2020) or an earlier injection of metal into a hotter planetesimal mantle (Walte and Golabek, 2022), while angular grains existed within dunite aggregates away from these melt pockets before metal intrusion. Fragmental grains may have been fractured during metal intrusion. All grains in the intrusion region then were rounded according to their location in the intrusion - grains near the periphery would have cooled rapidly and preserve their initial state (whether well-rounded, fragmental, or angular), while olivine grains nearer the centre of the intrusion region would cool more slowly, allowing a greater degree of rounding that would be size-dependent on a macro-scale.

Large-scale disruption of, or accretion to, the pallasite parent body are not required to reproduce the contrasting cooling timescales suggested by olivine and metal diffusion. Instead, the rapid injection of hot metal into a slowly cooling, warm planetesimal mantle creates a temperature perturbation leading to rapid initial cooling in the local area, matching that required to preserve olivine compositional heterogeneity, followed by equilibration with the mantle and a return to the slow planetesimal-scale cooling rates recorded in the Ni diffusion profiles in the Widmanstätten texture. While Walte and Golabek (2022) suggest that the pallasite-forming metal intrusion event was aided by still-molten trapped metal pockets, residing in a parent-body mantle above the metal solidus, the later impact and large scale injection of metal could have re-melted these preexisting FeNi pockets locally, enabling impact into a marginally cooler mantle.

Within one small ellipsoidal segment of intrusion, a diversity of textural and diffusive modification of olivine can be achieved. This does not preclude different formation environments for pallasite meteorites with differing olivine textures or diffusion profiles, rather it removes this as a requirement. Our simple model shows that further understanding of the small-scale processes related to the mixing of olivine and metal in the pallasite region is required to understand the planetesimal-scale processes. The model also highlights the importance of the temperature of the mantle on the evolution of the pallasite region, and how this is linked to relative timing of the injection of metal following the crystallisation of the magma ocean, and shows how different regions of one small intrusion can experience very different temperature-time paths.

We produced a simple, first-step model to address the contrasting timescales preserved in pallasite meteorites and suggest that the simplest explanation (injection of metal into the mantle of a planetesimal) without ad hoc changes to the parent body, can explain the heterogeneity seen across pallasite meteorites. We suggest that pallasite meteorites represent a late, preserved metallic intrusion into a planetesimal mantle and speculate that this parent body potentially experienced earlier metal-injections: previous intrusions would have delivered material to the core, leaving a small fraction trapped within the mantle.

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Supplementary materials for: Reconciling fast and slow cooling during planetary formation as recorded in the main group pallasites

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1 Extended methods

Our intrusion model consists of an ellipsoid region of interconnected solid olivine bridgework (Boesenberg et al., 2012), the pore space (created by inter- and intra-granular fractures) of which has been infiltrated and saturated by initially molten metal. This intrusion region is surrounded by a portion of the planetesimal mantle. We assume convection of the metal in this region is inhibited by the low porosity and permeability of the solid olivine bridgework, the rapid crystallisation of the metal, and the low gravitational acceleration.

We consider a cartesian box of mantle material with constant temperature in the horizontal directions x and y, and the vertical coordinate z aligned with the 1D mantle temperature output from the planetesimal model. Assuming a purely conductive system in which convective heat transport and internal heat generation are neglected, the temperature T (K) in this volume satisfies the three-dimensional heat conduction equation (Carslaw and Jaeger, 1959):

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) \tag{1}$$

where: ρ is the density of the material ($\mathrm{kg\,m^{-3}}$); c_p is the specific heat capacity ($\mathrm{J\,kg^{-1}\,K^{-1}}$); t is time (s); x, y, and z are the spatial coordinates (m); and k is thermal conductivity ($\mathrm{W\,m^{-1}\,K^{-1}}$). We choose temperature-independent k, allowing the Crank-Nicolson scheme to be applied to the problem without the complications associated with non-linearity (Carslaw and Jaeger, 1959; Özısık, 1993).

We define a uniaxial ellipsoid centered in the box, of volume $V = \frac{4}{3}\pi a^2 b$, where a and b are radii, which represents the intrusion region with a pallasitic mix of silicate and metal. The dimensions of the box ($X = Y = Z$) enclosing this ellipsoid is set by the diffusion lengthscale for the mantle material: we wish to run the model for ten years, and do not want the temperature near the model boundaries to change during that time. This allows us to apply a zero-flux condition to the boundaries of the problem.

Directly modelling the mixed-phase region of olivine crystals and metal melt would be computationally expensive and require detailed knowledge of the geometry of the phase mixture. Instead, we take a macroscopic approach to track the cooling and crystallisation of the metal in this area, and consider the intrusion region as a homogeneous, isotropic material, using volume-averaged effective thermal properties. We adopt the method of Mottaghy and Rath (2006) to model permafrost: we assume a simple saturated two component system, where olivine forms a solid interconnected bridgework of crystals, with the pore space filled with metal.

The volume fraction of metal-saturated pore space is denoted by ϕ_m, while the olivine fraction is labelled ϕ_{ol}, with $\phi_{ol} + \phi_m = 1$. We can then replace ρc_p in equation 1 with the arithmetic mean of ρc_p for metal and olivine ($\rho_m c_m$ and $\rho_{ol} c_{ol}$), and k with the square-root mean for both phases (k_m and k_{ol}) as this is more physically realistic for a randomly distributed mixture (Mottaghy and Rath, 2006; Roy et al., 1981):

$$\rho c_p = \phi_m \rho_m \, c_m + \phi_{ol} \rho_{ol} \, c_{ol} \, , \quad k = \left(\phi_m \sqrt{k_m} + \phi_{ol} \sqrt{k_{ol}} \right)^2 . \tag{2}$$

The metal-filled porosity can be further divided into the solid ($\phi_{m(s)}$) and liquid ($\phi_{m(l)}$) fractions:

$$\phi_m = \phi_{m(s)} + \phi_{m(l)}. \tag{3}$$

The fraction of solid and liquid metal is controlled by a temperature-dependent function which should be one when the metal is entirely solid ($T < T_S$, the solidus temperature), and zero when the metal is fluid ($T > T_L$, the liquidus temperature). We use the differentiable equation suggested by Mottaghy and Rath (2006):

$$\Theta = \begin{cases} \exp\left[- \left(\frac{T - T_\mathrm{L}}{w} \right)^2 \right] & \text{if} \quad T < T_\mathrm{L}, \\ 1 & \text{if} \quad T > T_\mathrm{L}, \end{cases} \tag{4}$$

where w is just $\frac{\Delta T}{2} = \frac{T_L - T_S}{2}$. This is differentiable:

$$\frac{d\Theta}{dT} = \begin{cases} -\frac{2(T - T_\mathrm{L})}{w^2} \exp\left[- \left(\frac{T - T_\mathrm{L}}{w} \right)^2 \right] & \text{if} \quad T \leq T_\mathrm{L}, \\ 0 & \text{if} \quad T > T_\mathrm{L}. \end{cases} \tag{5}$$

We apply this to the crystallisation of meteoritic Fe-Ni-S metal (Fig. S1), with $T_L = 1600$ K and

$T_S = 1260$ K (Wasson and Choi, 2003, Ehlers, 1972).

To account for the latent heat associated with melting or crystallisation, we apply the simple fixed-domain apparent heat capacity method which correlates the heat capacity of the phase-changing material with the slope of the enthalpy-temperature curve (Zeneli et al., 2021). We add a term to the heat capacity of the component that experiences the phase change—in this case, the metal—to define a new apparent volumetric heat capacity ($\rho c_{m,app}$; Sarbu and Sebarchievici, 2017):

$$\phi_m \rho c_{m,app} = \phi_{m(l)}\, \rho_{m(l)}\, c_{m(l)} + \phi_{m(s)}\, \rho_{m(s)}\, c_{m(s)} + \rho_{m(l)}\; L\, \frac{\partial \phi_{m(l)}}{\partial T}, \tag{6}$$

where L is the specific latent heat of fusion (J kg^{-1}). This can then be substituted in to equation 2 to find the overall apparent heat capacity of the mixed region; similarly, the conductivity can be modified to accommodate the solid and liquid metal phase. Diffusivity (κ, m^2 s^{-1}) can be defined for all the phases in the mixed region, including the phase change effects:

$$\kappa = \frac{k}{\rho c_p} = \frac{\left(\phi_{m(l)} \sqrt{k_{m(l)}} + \phi_{m(s)} \sqrt{k_{m(s)}} + \phi_{ol} \sqrt{k_{ol}}\,\right)^2}{\phi_{m(l)}\rho_{m(l)}c_{m(l)} + \phi_{m(s)}\rho_{m(s)}c_{m(s)} + \rho_{m(l)}L\, \frac{\partial \phi_{m(l)}}{\partial T} + \phi_{ol}\rho_{ol}\; c_{ol}}. \tag{7}$$

While diffusivity inside the ellipsoidal intrusion region is defined by equation 7, the material properties outside the intrusion have either constant values that match that of olivine, or use the same equations but with a smaller fraction of metal (to approximate metal trapped in the mantle). Sudden jumps and step functions in the spatially-varying diffusivity can introduce instabilities especially if these material properties boundaries intersect with the model boundary. We ensure this does not happening by centering our intrusion ellipsoid within mantle material with spatially-constant material properties, so that the model boundary never crosses the mantle-intrusion boundary.

1.1 Numerical approach

To illustrate our approach, we first consider the heat equation in 1D and write it in terms of spatially varying diffusivity:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial T}{\partial x}\right) + \text{I.B.C.}, \tag{8}$$

where I.B.C. stands for initial and boundary conditions. We apply the semi-implicit Crank-Nicolson scheme (Crank and Nicolson, 1947) with zero-flux boundary conditions. Forward difference is used for the time derivative of T, and the spatial derivative is evaluated at the time step $n + 1/2$ instead of at n, taking the arithmetic mean between the time step n and $n + 1$. We also discretise κ with respect to distance, i, using finite differences (Langtangen and Linge, 2017).

After expansion and simplification, the resulting system of linear equations can be represented in matrix form: $A\mathbf{T}^{n+1} + \mathbf{b}^{n+1} = B\mathbf{T}^{n} + \mathbf{b}^{n}$, where A and B are $N \times N$ matrices, $\mathbf{T}^{n+1}$ and $\mathbf{T}^{n}$ are column vectors of temperature at times $n+1$ and n, and $\mathbf{b}^{n}$ and $\mathbf{b}^{n+1}$ are boundary condition column vectors. For zero-flux boundary conditions, these column vectors are zero. We define a new parameter in place of the Fourier number, with variable diffusivity: $\mathbf{r}_i = \kappa_i \Delta t / \Delta x^2$, where Δt is the time step and Δx is the spatial step. We can then define the upper, lower and diagonal coefficients of A and B:

$$
\begin{aligned}
R_i^U &= r_i + r_{i+1}, \\
R_i^L &= r_i + r_{i-1}, \\
R_i^D &= 2r_i + r_{i+1} + r_{i-1}.
\end{aligned} \tag{9}
$$

The matrix equation can then be written:

$$
\begin{aligned}
&\begin{pmatrix}
4+R_0^D & -2R_0^U & & & \\
-R_1^L & 4+R_1^D & -r_1 & 0 & \\
& & \ddots & & \\
& 0 & -R_{N-1}^L & 4+R_{N-1}^D & -R_{N-1}^U \\
& & & -2R_N^L & 4+R_N^D
\end{pmatrix}
\begin{pmatrix}
T_0^{n+1} \\ T_1^{n+1} \\ \vdots \\ T_{N-1}^{n+1} \\ T_N^{n+1}
\end{pmatrix} \\
= &\begin{pmatrix}
4-R_0^D & 2R_0^U & & & \\
R_1^L & 4-R_1^D & R_1^U & 0 & \\
& & \ddots & & \\
& 0 & R_{N-1}^L & 4-R_{N-1}^D & R_{N-1}^U \\
& & & 2R_N^L & 4-R_N^D
\end{pmatrix}
\begin{pmatrix}
T_0^{n} \\ T_1^{n} \\ \vdots \\ T_{N-1}^{n} \\ T_N^{n}
\end{pmatrix}.
\end{aligned} \tag{10}
$$

This requires that $\mathbf{r}$ is a column vector with two ghost points at r_{-1} and r_{N+1}. In order to find the temperature distribution at the next time step, we multiply across by the inverse of A: $\mathbf{T}_i^{n+1} = \left(A^{-1}B\right)\mathbf{T}_i^{n}$. The full derivation of these matrix equations can be found in the supplementary information.

In order to extend this scheme to three dimensions, we apply the Fractional Step Method (Cen et al., 2016; Yanenko, 1971), which evaluates the heat equation in one-third time step increments along each of the spatial dimensions i, j and k:

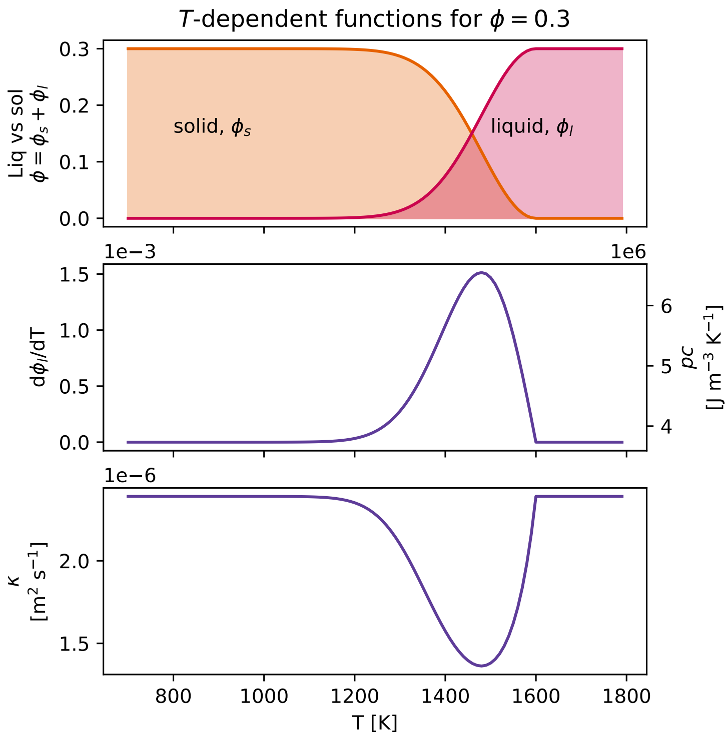

Figure S1: Temperature dependent functions for a mixed region of 30 % phase-change material (PCM - in this case, metal - ϕ), and 70 % non-PCM, in this case olivine $(1-\phi)$. The functions for κ and ρc are for this mixture. To simplify the problem, we have set the material properties for liquid and solid metal as equal; however, the code allows these to be varied independently.

$$
\begin{aligned}
A\mathbf{T}_{j,k}^{n+\frac{1}{3}} &= B\mathbf{T}_{j,k}^{n}, \\
A\mathbf{T}_{i,k}^{n+\frac{2}{3}} &= B\mathbf{T}_{i,k}^{n+\frac{1}{3}}, \\
A\mathbf{T}_{i,j}^{n+1} &= B\mathbf{T}_{i,j}^{n+\frac{2}{3}},
\end{aligned}
\tag{11}
$$

where the superscript $\left(n+\frac{1}{3}\right)$ refers to the fractional time step $t^{n+\frac{1}{3}} = t^n + \frac{1}{3}\Delta t$ and so on. The temperature distribution at the next time step is found by evaluating these three one-dimensional equations in turn instead of one three-dimensional equation (Sahijpal, 2021).

We bench-marked our numerical model against an analytical solution from Carslaw and Jaeger (1959), and found that the maximum relative defect between the numerical and analytical models dropped to below 1 % within 150 seconds (Figure S2).

2 Additional figures relating to benchmarking and sensitivity analyses

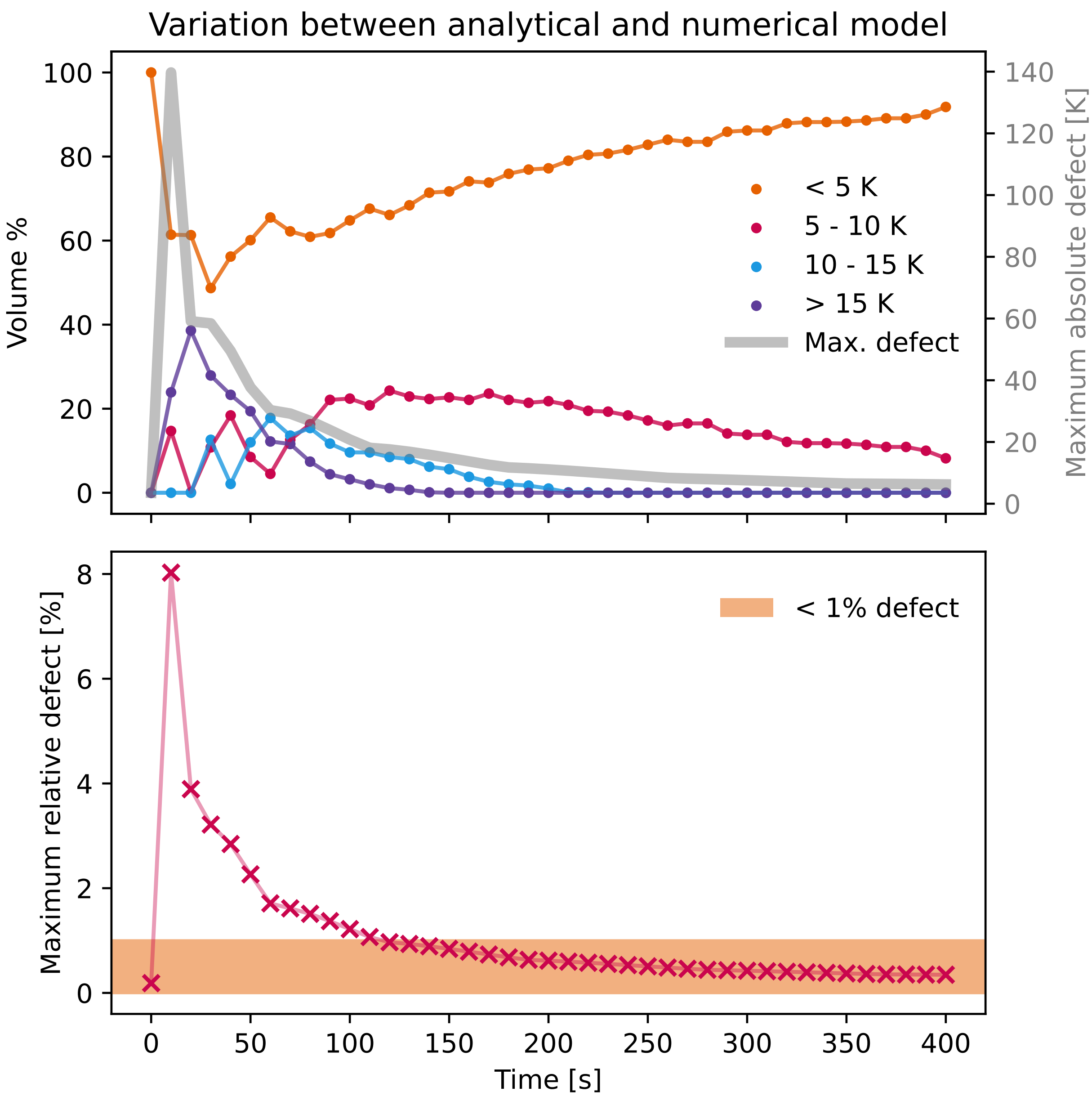

Figure S2: The numerical model was set up to closely approximate a cube with fixed-temperature boundary conditions and spatially constant diffusivity, and the results were compared to the output of an analytical solution for the same geometry (Carslaw and Jaeger, 1959). Within 150 seconds, the maximum relative defect drops below 1 %, with the majority of the numerically modelled region within 5 K of the analytical solution (comparing pixel to equivalent pixel).

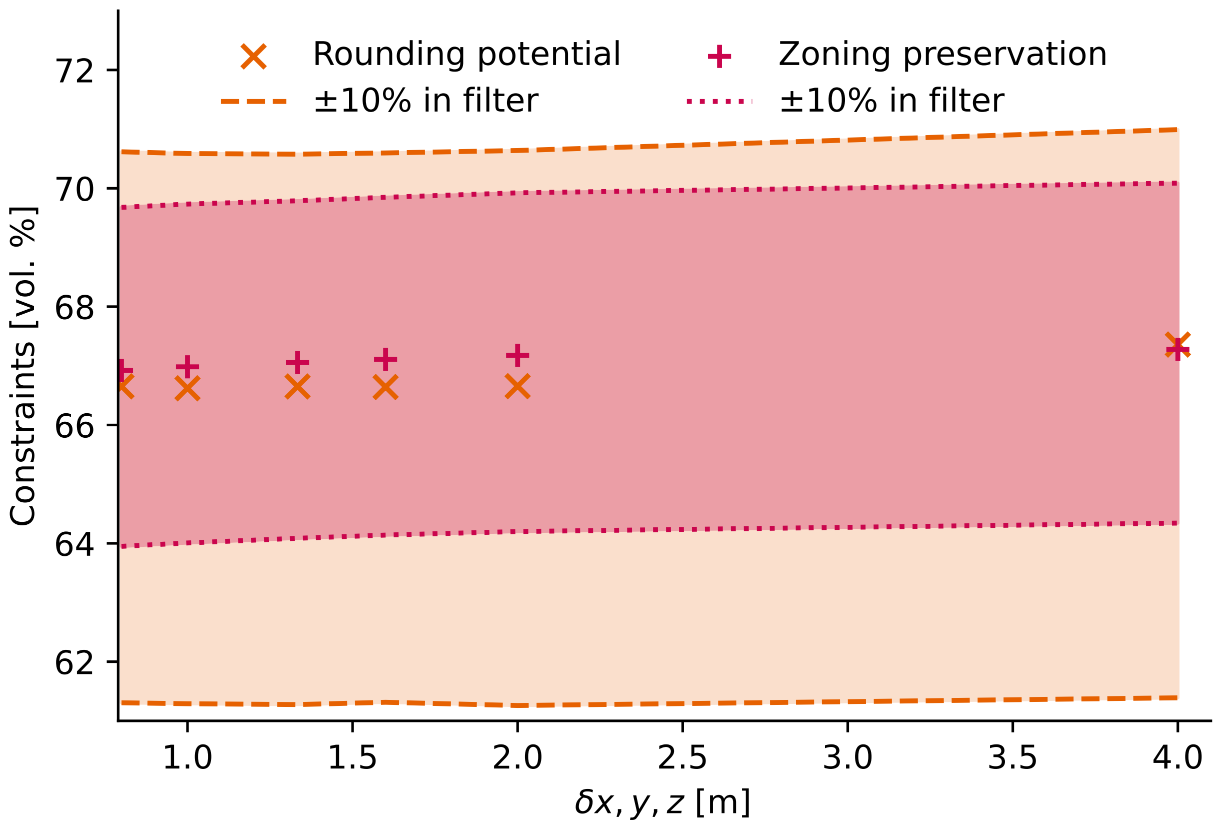

Figure S3: Exploration of effect of model resolution and rounding potential/zoning preservation. Spatial step size of < 4 m results in a change in either result by < 1 %. These are compared to the effect of increasing or decreasing the temperature cutoffs for the rounding and zoning criteria.

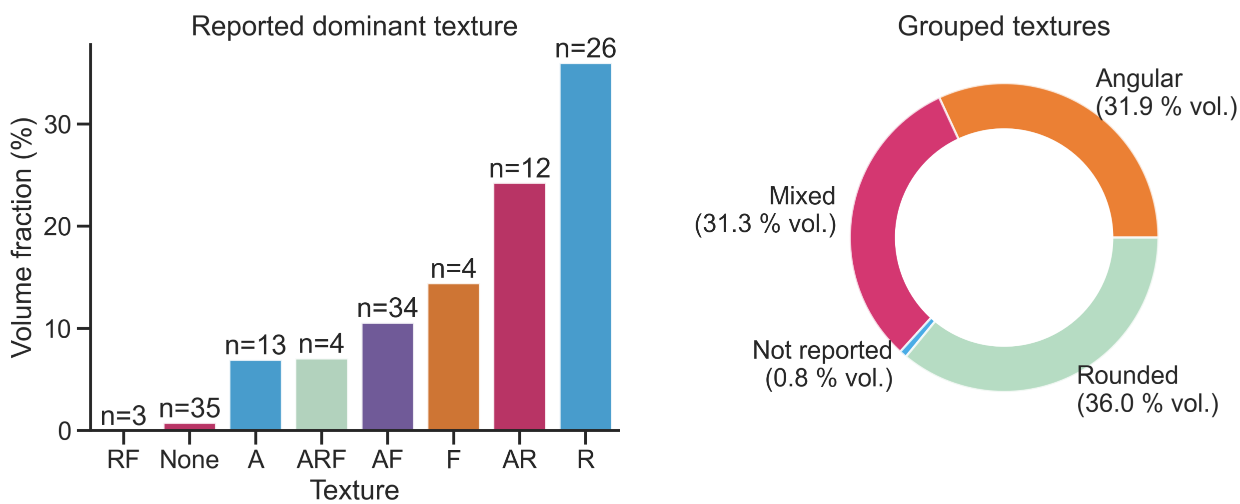

Figure S4: Pallasite olivine macro-textures based on qualitative descriptions from the Meteoritical Bulletin and collated results from McKibbin et al. (2019), shown as volume fraction of the total pallasite record. RF: rounded fragmented; None: no texture mentioned in description; A: angular; ARF: mixed texture; AF: angular fragmental; F: fragmental; AR: mixed texture; R: rounded. The pie chart shows these grouped as used in the model constraints, with groups A and AF combined into "Angular", and groups RF, ARF and AR combined into "Mixed". "Rounded" contains only the group R. For the model to "pass" the rounding constraint, the volume that can potentially support rounding needs to fall between "Rounded" (36 vol. %) and "Rounded" + "Mixed" (67 vol. %).

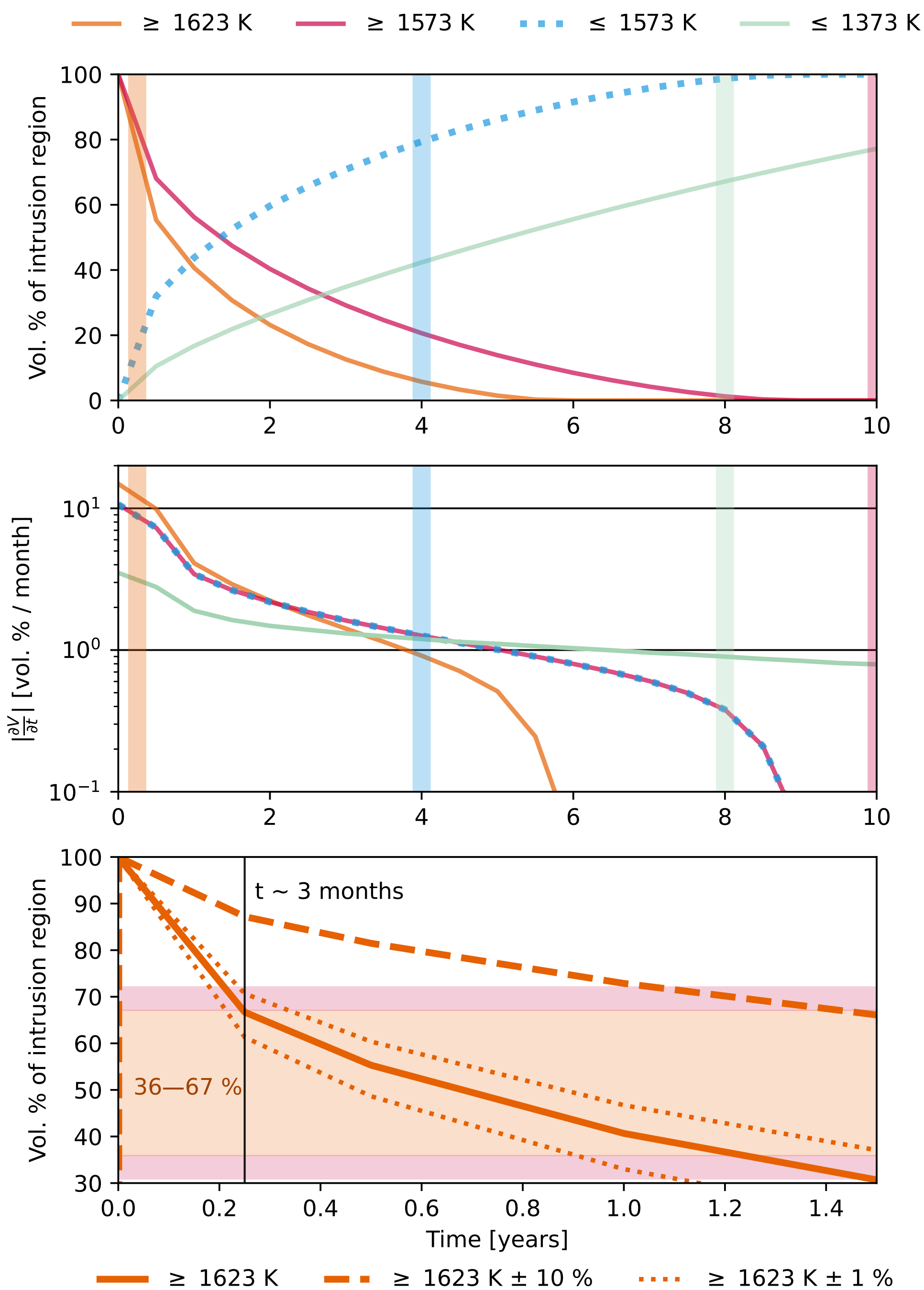

Figure S5: Exploration of the effect of time of measurement for each of the rounding and zoning criteria. The top panel shows the volume % of the region of the intrusion that matches each requirement through time, and the corresponding time that this measurement is taken (matching colour vertical line). The second panel shows the rate of change of intrusion volume that matches each criterion, per month (where the timestep is $\sim$ 1 month). The botom panel is a zoomed view of the first criteria ($T_{3\text{mnths}} \geq 1623$ K), which is the most sensitive to timing. This plot also shows the volume % of the region that matches the criteria if the temperature requirement is varied by ± 10 % or ± 1 %. The rounding requirement volume is shown in shaded orange, with an additional ± 5 % shown in pink.

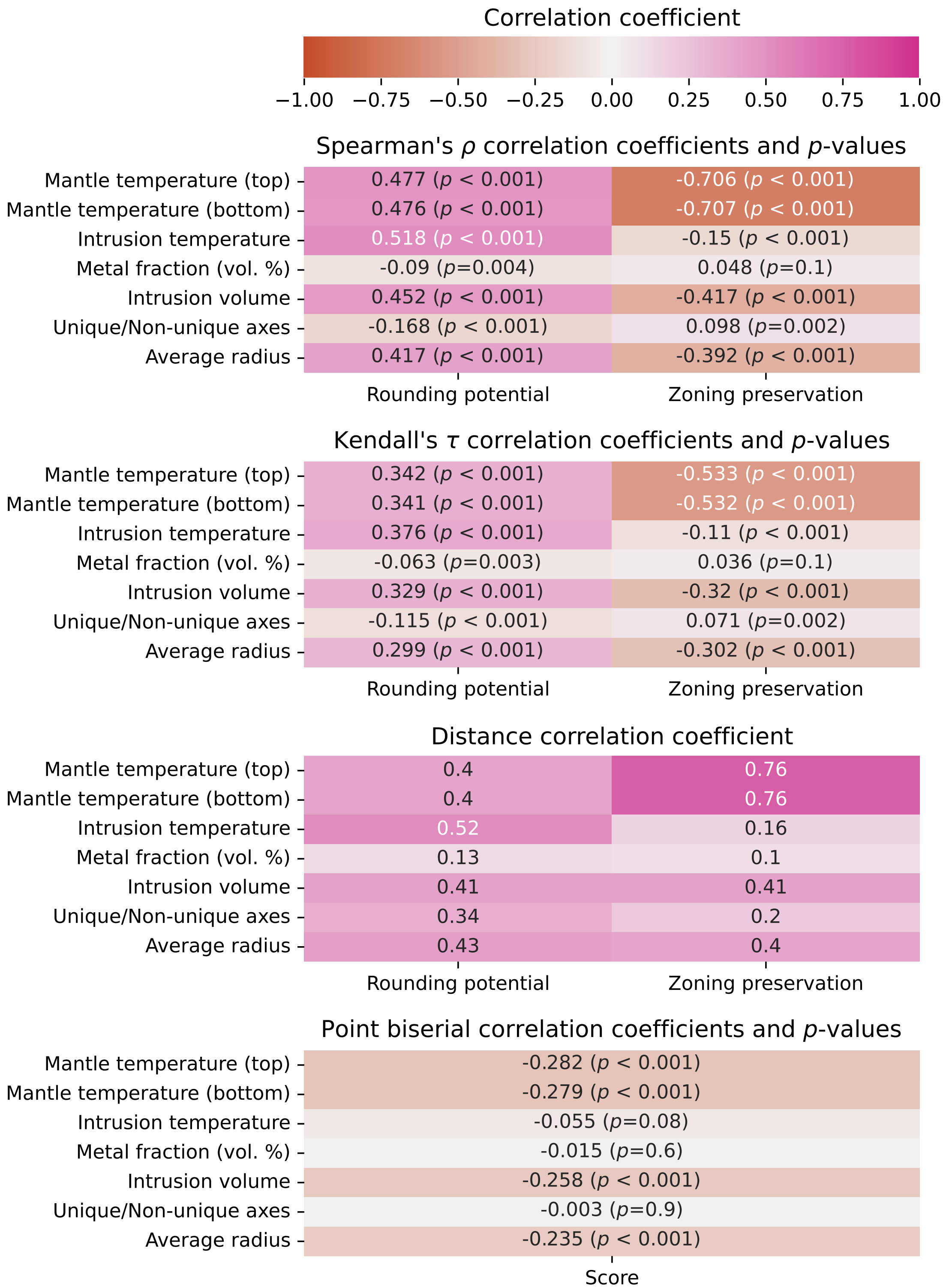

Figure S6: Monotonic and non-monotonic estimations of correlation with p value where relevant, for a suite of initial conditions and resulting volume % that match the rounding and zoning preservation criteria, as well as the overall score (where score was reduced to a binary pass/fail, with scores of 0 and 1 grouped into the fail category).

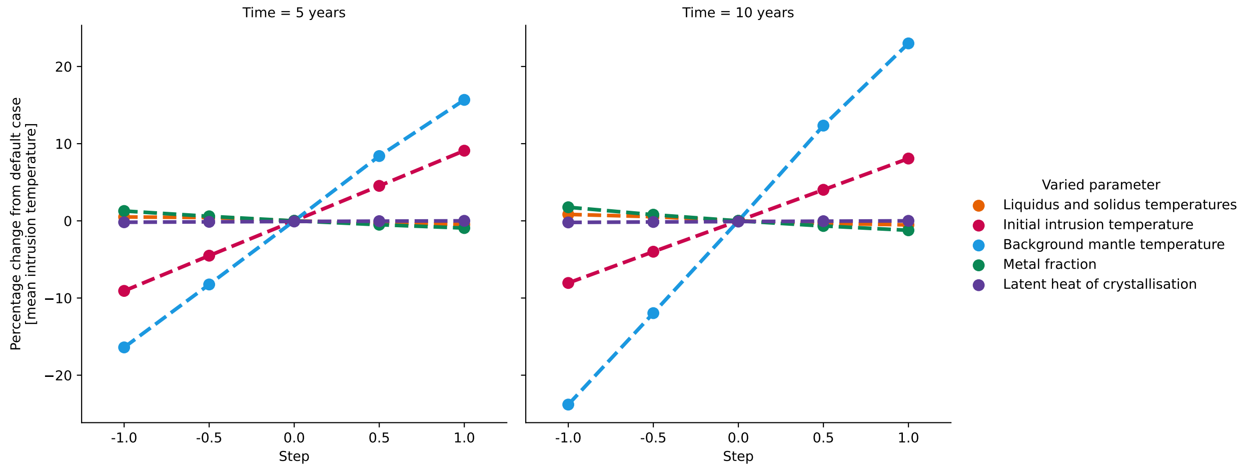

Figure S7: Sensitivity testing; varying parameters individually across a maximum, minimum and mean value. Details given in Table S1.

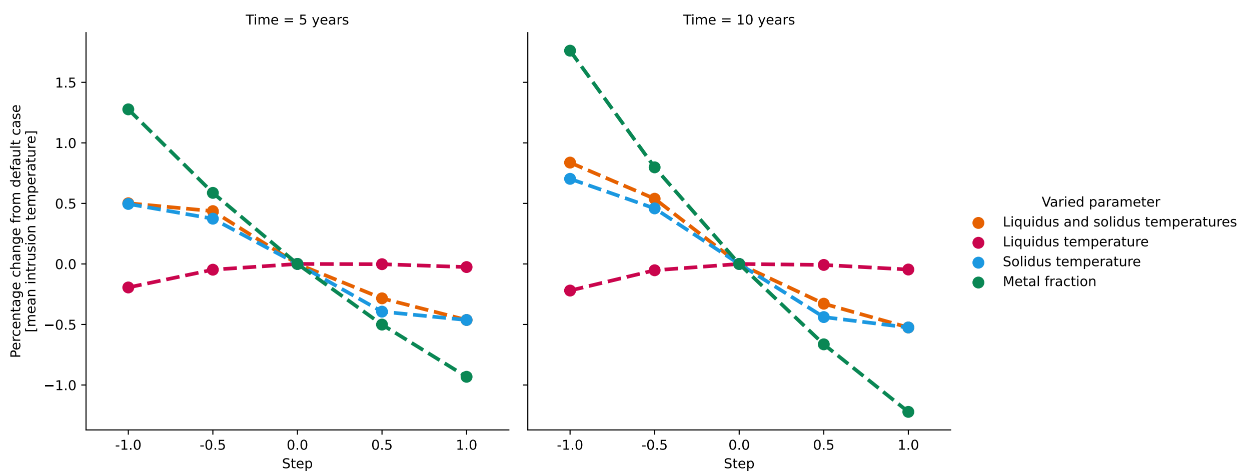

Figure S8: Sensitivity testing; varying parameters individually across a maximum, minimum and mean value, zoom in on less sensitive paramters. Details given in Table S1.

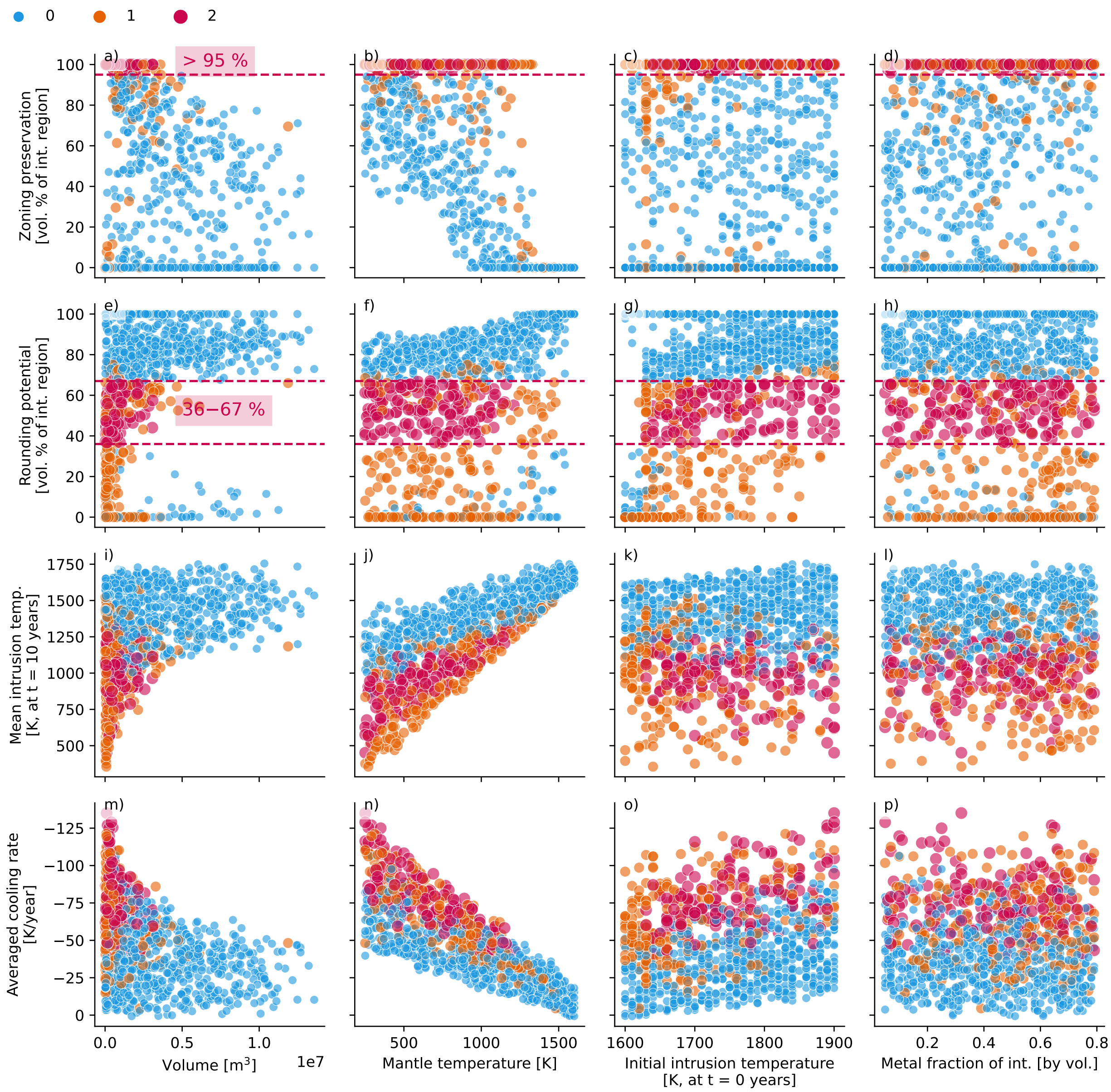

Figure S9: Summary of results for 1000 model runs where material properties were allowed to vary randomly in addition to geometry-related parameters. Colour denotes score: 0 means neither constraint was matched, 1 means one constraint was matched, and 2 means both constraints were matched. Marker shape describes the initial temperature conditions: either output from a planetesimal model, or randomly assigned. Parameters were not varied in isolation. Large pink circles match both constraints and used input from a planetesimal model.

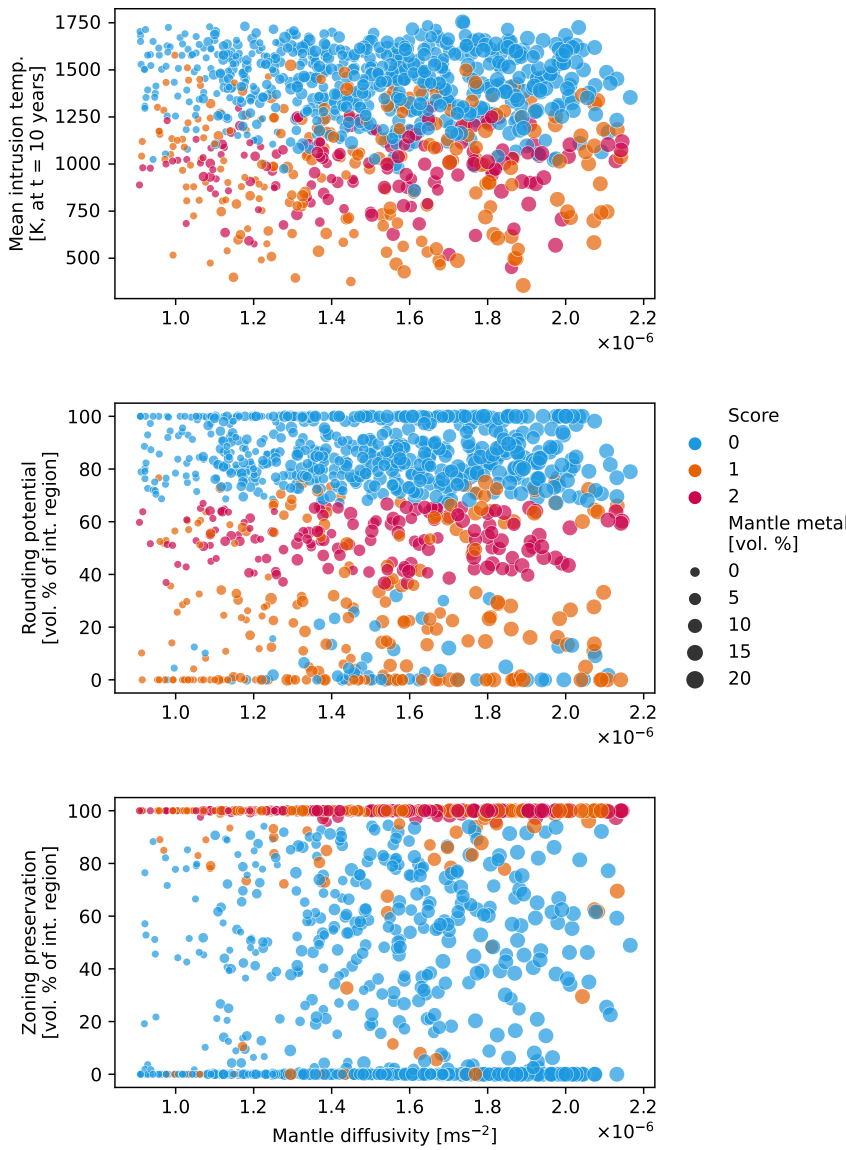

Figure S10: Summary of results for 1000 model runs where material properties were allowed to vary randomly in addition to geometry-related parameters, highlighting the effect of varying the proportion of trapped metal in the mantle and mantle diffusivity. Colour denotes score: 0 means neither constraint was matched, 1 means one constraint was matched, and 2 means both constraints were matched. Marker shape describes the initial temperature conditions: either output from a planetesimal model, or randomly assigned. Parameters were not varied in isolation. Large pink circles match both constraints and used input from a planetesimal model. No significant correlation was found between fraction of metal trapped in the mantle and model score.

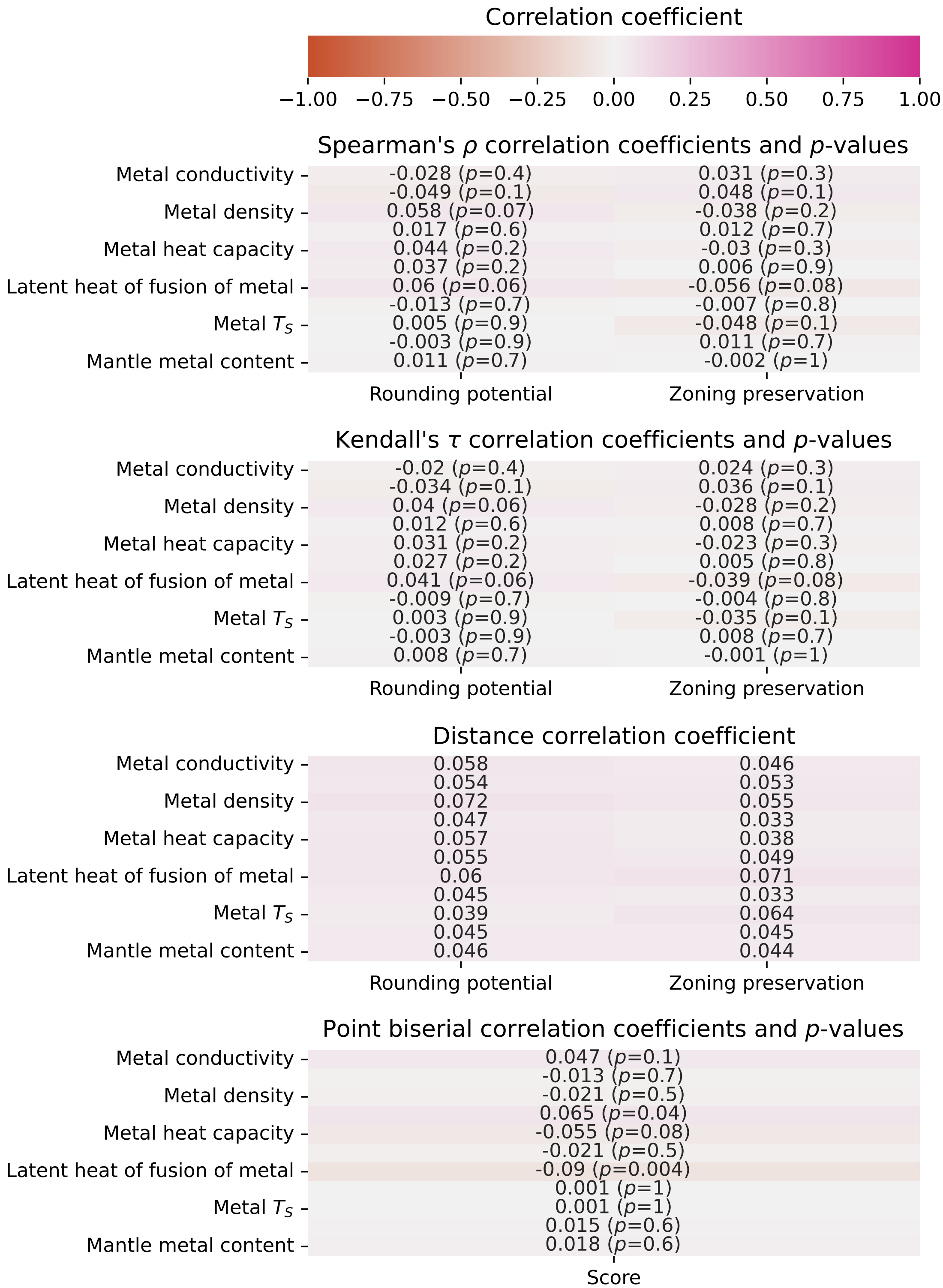

Figure S11: Monotonic and non-monotonic estimations of correlation with p value where relevant, for a suite of initial conditions (specifically relatin to material properties) and resulting volume % that match the rounding and zoning preservation criteria, as well as the overall score (where score was reduced to a binary pass/fail, with scores of 0 and 1 grouped into the fail category).

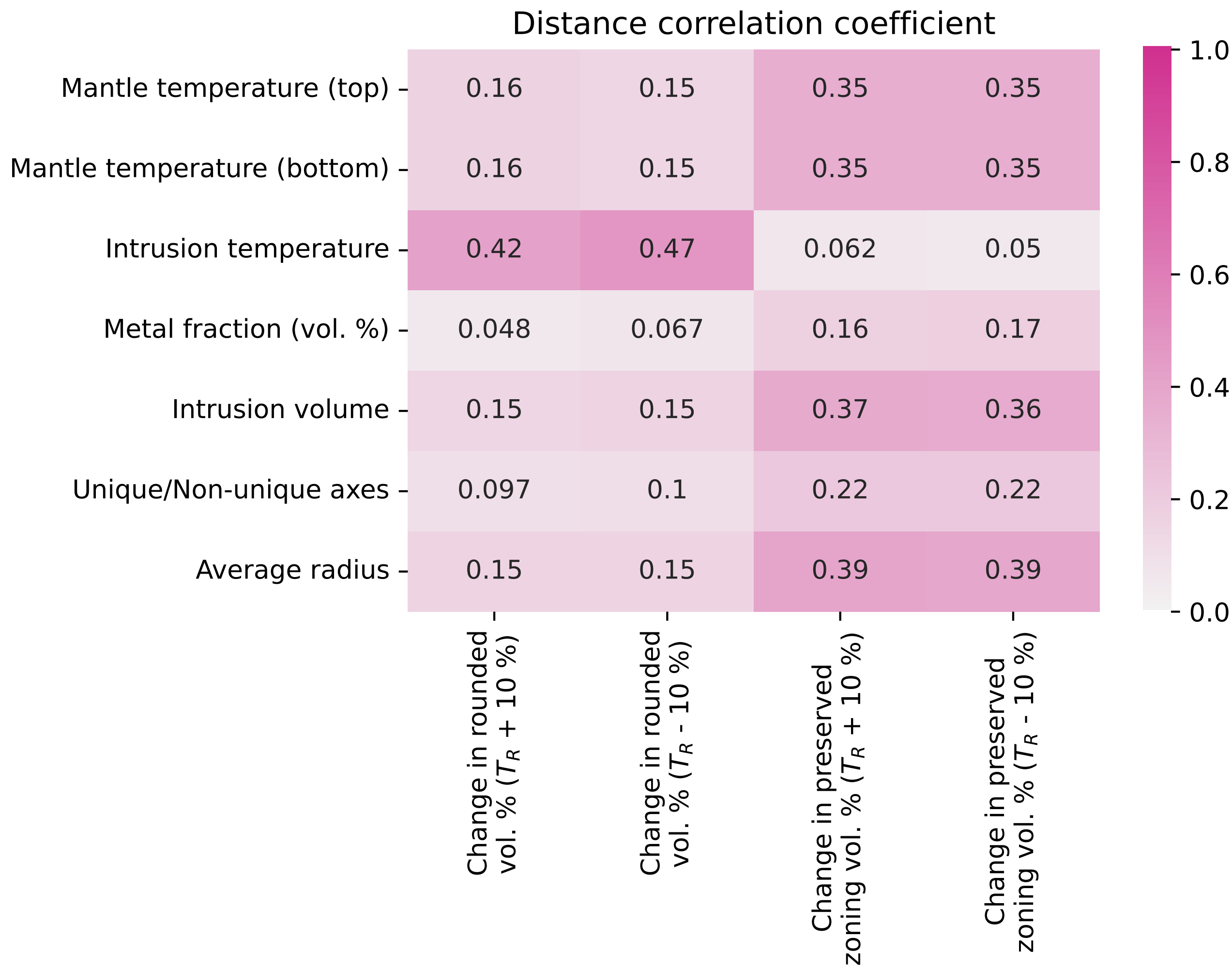

Figure S12: Non-monotonic distance correlation between change in volume % rounded and volume % zoning preserved when the temperature filters are changed by ± 10 % of the original temperature, and parameters such as mantle temperature, intrusion temperature, and intrusion geometry.

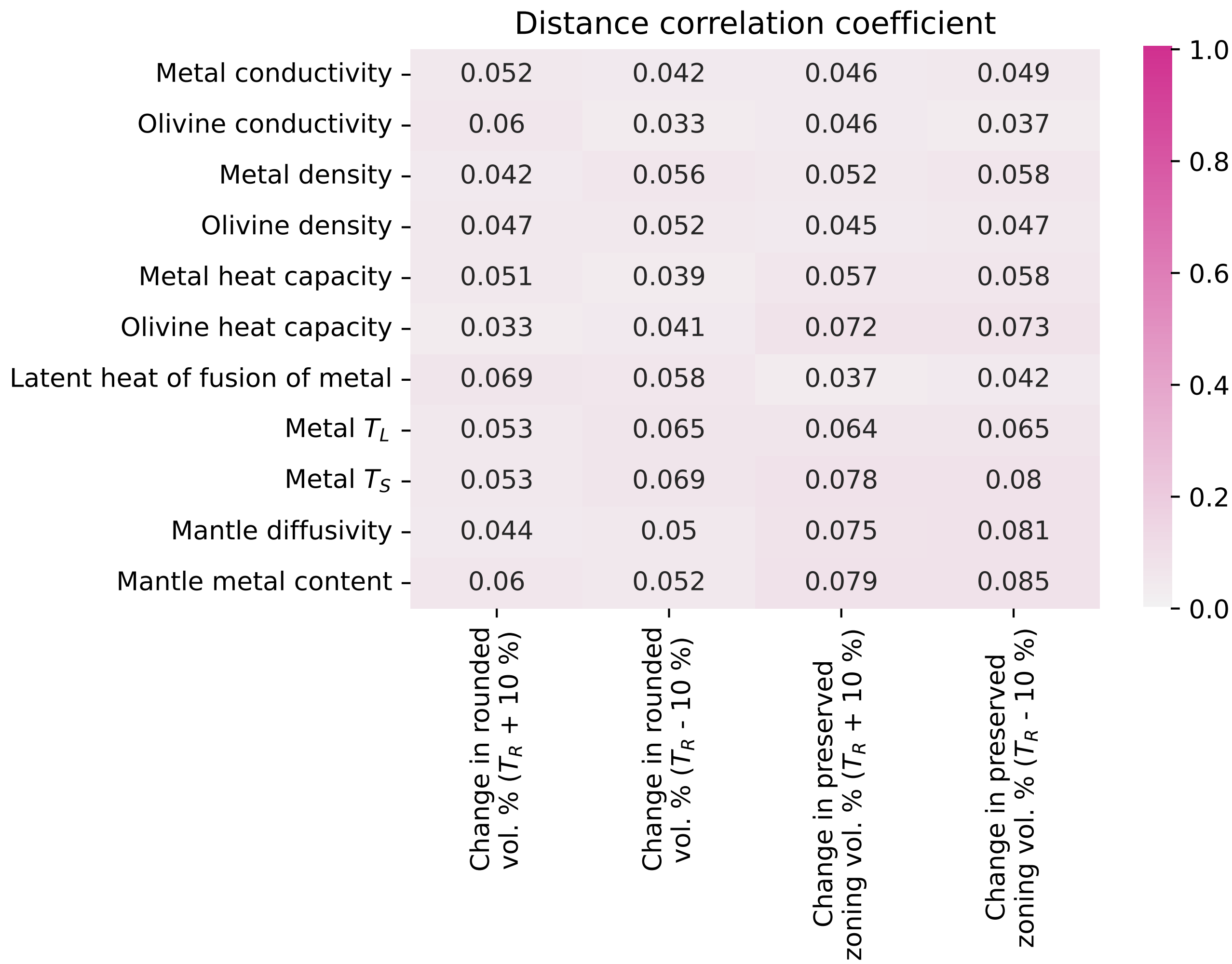

Figure S13: Non-monotonic distance correlation between change in volume % rounded and volume % zoning preserved when the temperature filters are changed by ±10 % of the original temperature, and parameters relating to the material properties of the intrusion region.

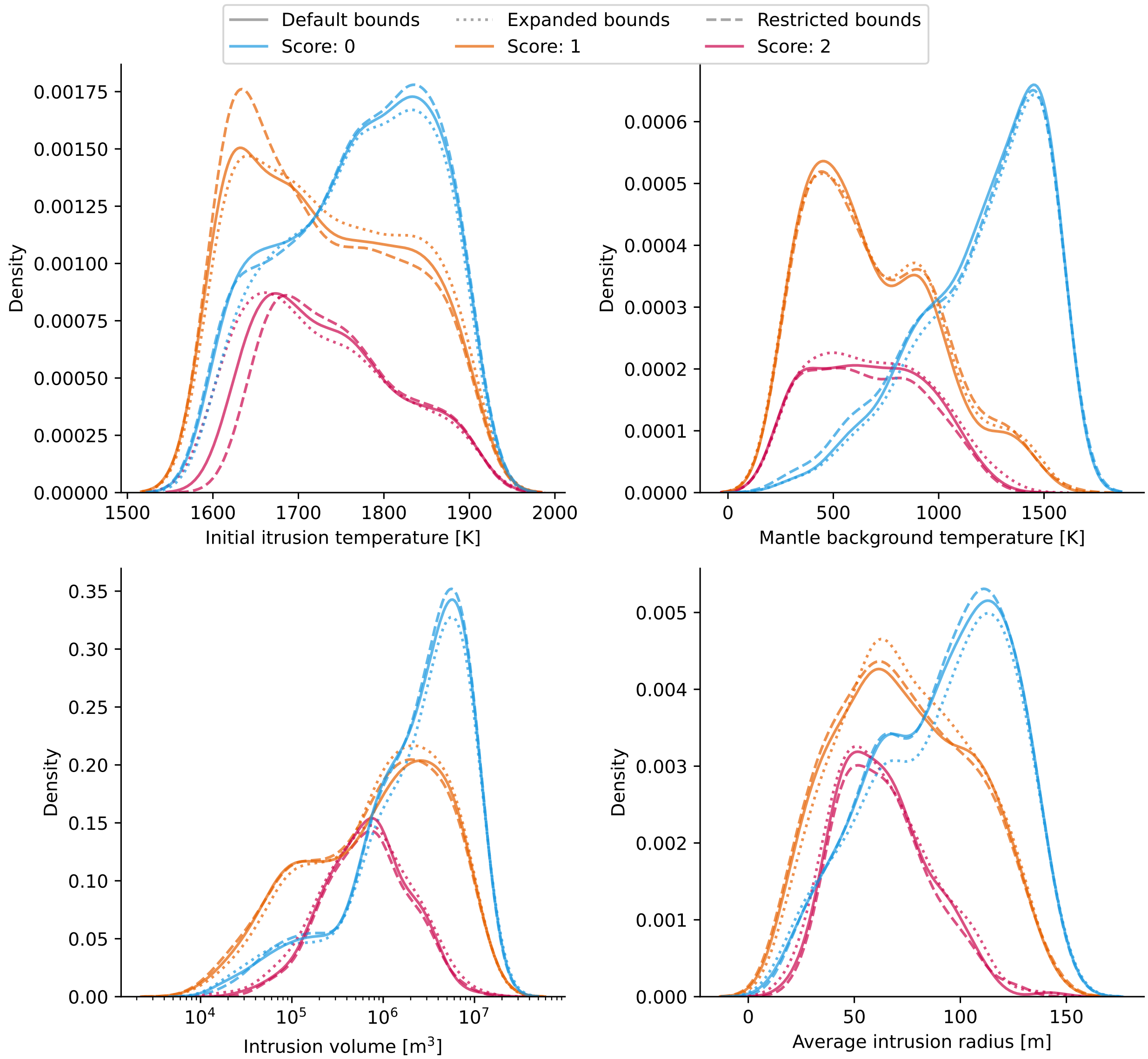

Figure S14: Kernel density estimates for model score vs. initial intrusion temperature, background mantle temperature, intrusion volume (log scale) and average intrusion radius, showing change with “restricted” and “expanded” bounds (±10 %). “Restricting” the bounds makes it more difficult for a model to pass the requirements, by increasing the rounding temperature cut-off by +10 %, and decreasing the zoning temperature cut-off by −10 %. “Expanding” the bounds is the opposite; by increasing the zoning temperature cut-off by +10 %, and decreasing the rounding temperature cut-off by −10 %, resulting in more models with a score of 2.

Table S1: Summary of model runs for sensitivity testing; results shown in Figures S7, S8. $L_{x,y,z} = 400$ m, $\Delta x, y, z = 2$ m, $r_{x,y,z} = 80$ m, material properties of metal and olivine set equal to example case in the main text. Values listed below were set to the mean value (in **bold**) unless they were being varied.

	Step:	**-1**	**-0.5**	**0**	**0.5**	**1**
Parameter varied	**Unit**	Minimum		Mean		Maximum
Liquidus Temperature	K	1570	1630.25	**1690.5**	1750.75	1811
Solidus Temperature	K	1260	1395	**1530**	1665	1800
Liquidus and Solidus Temperatures	K					
Initial intrusion temperature	K	1600	1700	**1800**	1900	2000
Background mantle temperature	K	250	637.5	**1025**	1412.5	1800
Metal fraction	Volume fraction	0.1	0.2	**0.3**	0.4	0.5
Latent heat	J/kg	133000	163750	**194500**	225250	256000

Table S2: Summary of results, with absolute numbers of models receiving each score, and percentage of the model set.

Dataset	Score = 0	Score = 1	Score = 2	Total number	% Score = 0	% Score = 1	% Score = 2
Full dataset	1438	499	263	2200	65.4	22.7	12.0
Planetesimal input	430	124	46	600	71.7	20.7	7.7
r = 250 km	226	51	22	299	75.6	17.1	7.4
r = 300 km	204	73	24	301	67.8	24.3	8.0
Full dataset, with lower req.	1100	757	343	2200	50.0	34.4	15.6
Randomly varied material prop.	626	225	149	1000	62.6	22.5	14.9
Inc. filters by +10 pc	609	246	145	1000	60.9	24.6	14.5
Dec. filters by -10 pc	628	214	158	1000	62.8	21.4	15.8
Expand filters by 10 pc	618	216	166	1000	61.8	21.6	16.6
Restrict filters by 10 pc	619	244	137	1000	61.9	24.4	13.7

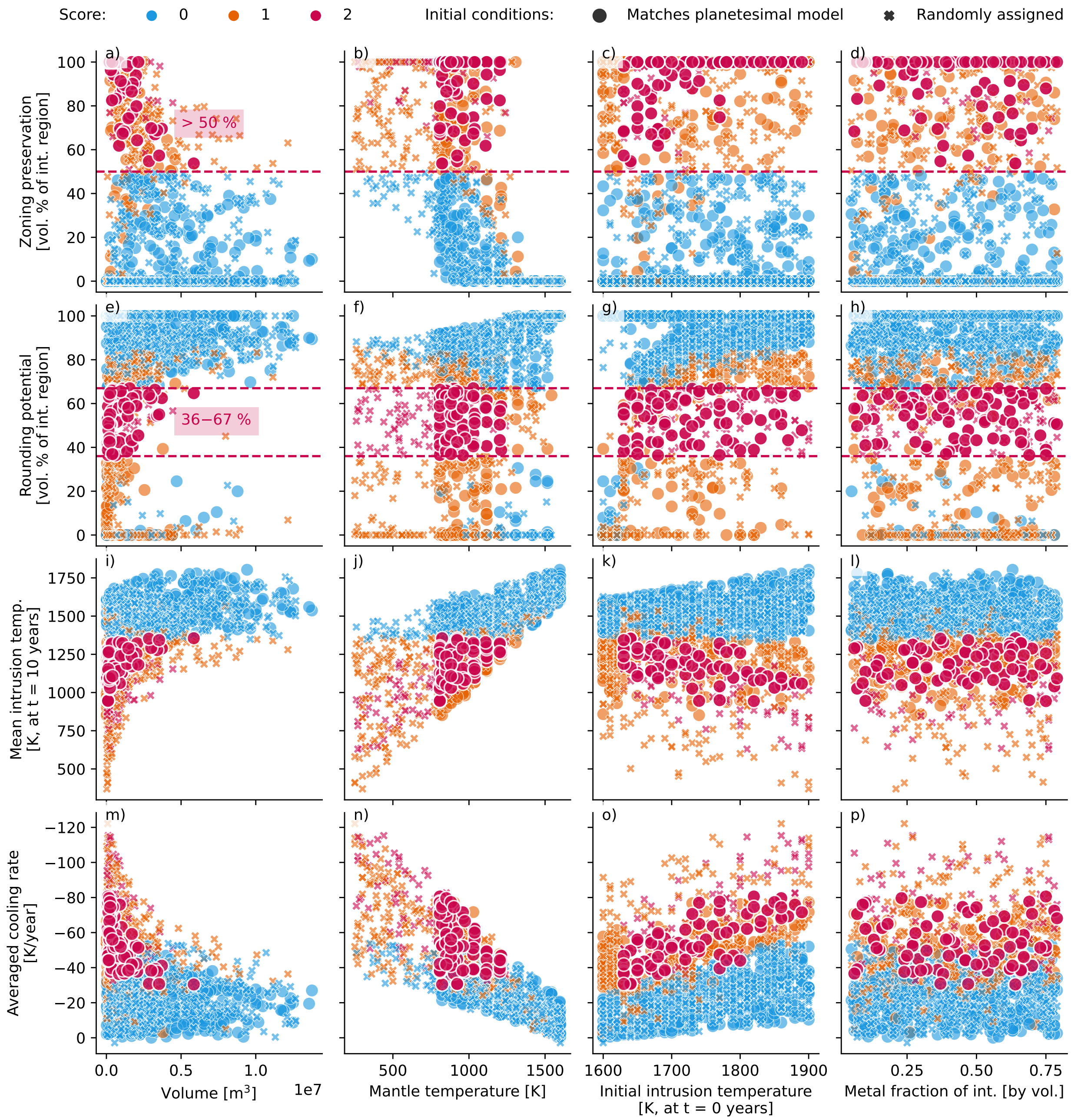

Figure S15: Summary of results for 1200 model runs with a less restrictive zoning criterion > 50 %, showing that overall trends and conclusions stay the same. Colour denotes score: 0 means neither constraint was matched, 1 means one constraint was matched, and 2 means both constraints were matched. Marker shape describes the initial temperature conditions: either output from a planetesimal model, or randomly assigned. Parameters were not varied in isolation. Large pink circles match both constraints and used input from a planetesimal model.

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