Effects of magma-generation and migration on the expansion and contraction history of the Moon.

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15 **Abstract**

16 Geological and geodetic observations of the Moon from spacecraft revealed
17 that it expanded by a few km for the first several hundred million years and
18 then contracted later. The period when the planet expanded most coincides
19 with that when the mare volcanism of the Moon was active. Given the high
20 initial temperature of the deep mantle inferred from the giant impact and
21 mantle overturn hypotheses of the Moon, the observed early expansion is
22 difficult to account for by thermal expansion only. To understand the
23 observed radial change of the Moon, we numerically calculated the thermal
24 evolution of a one-dimensional spherically symmetric mantle caused by
25 transport of heat, mass, and incompatible heat-producing elements (HPEs) by migration
26 of magma that is generated by internal heating. The mantle is assumed to be enriched in
27 HPEs at its base in the initial condition. The calculated mantle expands for the
28 first several hundred million years by melting of the deep mantle and
29 upward migration of the generated magma to the uppermost mantle; the top
30 of the partially molten region rises up to the depth level of around 300 km,

shallow enough to generate mare basalts of the Moon. The migrating
magma, however, extracts HPEs from the deep interior, and the planet then
contracts gradually by cooling and solidification of the partially molten
mantle. We obtained a thermal history that is consistent with the observed
history of radial change of the Moon when the initial mid-mantle
temperature $T_M \approx 1600 \text{ K}$ and the initial ratio of the concentration of HPEs in the
crust to that of the mantle $F_{crst} \leq 12$. This initial state of the mantle inferred
from its thermal history constrains the earliest evolution of the Moon
dominated by the magma ocean and mantle overturn.

Keywords

Moon, Magma-migration, Magma-generation, Expansion/Contraction history.

Main Text

1. Introduction

The thermal history of the Moon has been a long-standing issue in studies of terrestrial planets (*e.g.*, *Toksöz et al.*, 1972; *Solomon and Chaiken*, 1976; *Cassen et al.*, 1979; *Kirk and Stevenson* 1989; *Shearer et al.*, 2006; *de Vries*, 2012; *Evans et al.*, 2014). Geological and geodetic observations from spacecraft have revealed that the Moon expanded globally in the early stage of its history (*Andrews-Hanna et al.*, 2013; *Sawada et al.*, 2016) and then contracted globally in the later stage (*Watters et al.*, 2010; *Matsuyama et al.*, 2021). The period when its radius reached the maximum coincides with that when the mare volcanism was active: the volcanism was weak before 4 Gyr ago, became active between 3.3 and 3.8 Gyr ago with the peak at ~ 3.6 Gyr ago, and then mildly continued until 1 to 2 Gyr ago (*e.g.*, *Hiesinger et al.*, 2003; *Whitten and Head*, 2015). To understand these features of the history of the Moon, we developed a spherically symmetric model of the lunar mantle evolution where magma-generation and migration as well as transport of heat, mass, and incompatible heat-producing elements (HPEs) by migrating magma are considered.

In most of earlier one-dimensional numerical models of the thermal history, the planetary expansion/contraction of the Moon is assumed to occur thermally, and the early expansion is reproduced when the initial temperature in the deep mantle is 1100 K or less (*e.g.*, *Solomon and Chaiken*, 1976): the Moon monotonously contracts throughout its history when the mantle is initially hotter because of secular cooling of the mantle. In a model where the effect of volume change from compositional differentiation is also considered, the early expansion is reproduced even when the initial temperature in the deep mantle is as high as 1200 K (*Kirk and Stevenson*, 1989). However, the initial temperature of 1200 K or less in the deep mantle is still considerably lower than that predicted from the giant impact and mantle overturn hypotheses of the Moon (*e.g.*, *Stevenson*, 1987; *Hess and Parmentier*, 1995; *Alley and Parmentier*, 1998; *Pritchard and Stevenson*, 2000; *Canup*, 2004; *Boukaré et al.*, 2018).

The early expansion of the Moon is hard to account for by three-dimensional models of mantle evolution that have been developed in the literature to understand the mare volcanism, too. Some models succeeded in reproducing the peak of mare volcanism at around 3.6 Gyr ago (*e.g.*, *Zhong et al.*, 2000; *Stegman et al.*, 2003; *Zhang et al.*, 2013a,

b). Some other models in the literature succeeded in reproducing volcanism that continues for billions of years as is observed for the lunar mare volcanism (*Konrad and Spohn, 1997; Spohn et al., 2001*). Asymmetric models where the uppermost mantle in the nearside is more enriched in HPEs than that of the farside (*Laneuville et al., 2013, 2018*) account for the long-lasting mare volcanism in the Procellarum KREEP Terrane (*Wieczorek & Phillips, 2000*). By considering the blanket effect of the crust, *Zieth et al. (2009)* suggest that the volcanism continues for an even longer period, up to 3.5 billion years. The early expansion calculated in these models are, however, too small to account for the observed globally expansion of ~0.5 to 4.9 km until 3.8 Gyr ago (*Andrews-Hanna et al., 2013; Laneuville et al., 2013; Zhang et al., 2013a; Sawada et al., 2016*), or the early expansion continues too long, 1 billion years or longer (*Zhang et al., 2013b*).

In these previous models, only the thermal expansion/contraction has been considered, and the planetary expansion by melting has been neglected. The occurrence of dykes and volcanism in the early Moon (*e.g., Hiesinger et al., 2003; Andrews-Hanna et al., 2013; Needham and Kring, 2017*), however, suggests that the effects of volume

change from melting are important. Magma-migration and transport of heat, mass, and HPEs by migrating magma should also be considered (*e.g.*, *Shearer et al.*, 2006). In this study, we develop a one-dimensional spherically symmetric model of magma-generation and migration in the mantle of the Moon and evaluate their effects on the radial change of the planet and volcanism, taking account of enrichment of the deep mantle in HPEs due to the mantle overturn (*e.g.*, *Hess and Parmentier*, 1995; *Alley and Parmentier*, 1998). We neglect the effect of mantle convection on the thermal history of the Moon in our study because the lunar mantle is around the threshold for the onset of thermal convection, and hence the mantle convection is probably weak at most (*Shearer et al.*, 2006; *Yanagisawa et al.*, 2016). Indeed, the thermal history of the lunar mantle calculated in the thermal convection model of *Laneuville et al.* (2013, 2018) is not so much different from that calculated from a model where mantle convection is not considered (*Wieczorek & Phillips*, 2000).

2. Model Description

We numerically simulate the thermal and structural evolution of the internally heated

one-dimensional spherically symmetric mantle of the Moon caused by thermal conduction, magma generation and migration, and transport of heat, mass, and incompatible HPEs by migrating magma. The outer radius of the spherical shell r_p is 1700 km while the inner radius r_c is 374 km (*e.g.*, Williams *et al.*, 2001; Weber *et al.*, 2011; Yan *et al.*, 2015), and the crust of 43 km ($r_{crst} = 1657$ km; Wieczorek *et al.*, 2013) in thickness enriched in HPEs is placed along the surface boundary. The mantle materials are modeled as a mixture of olivine-rich materials A and the ilmenite bearing cumulates (IBC; *e.g.*, Ringwood and Kesson, 1976) B ; their composition is denoted as $A_\xi B_{1-\xi}$. The binary system is assumed to constitute a eutectic system with the eutectic composition of $A_{0.1}B_{0.9}$, which corresponds to the basaltic composition enriched in IBC component; the composition of the magma calculated below is almost always eutectic. Magma is generated when the temperature exceeds the solidus temperature. Generated magma migrates upward as a permeable flow driven by the buoyancy of the magma through coexisting matrix (*e.g.*, McKenzie, 1984; Kameyama *et al.*, 1996; Ogawa, 2018). The temperature is fixed at $T_{sur} = 270$ K on the surface boundary, while the core is modeled as a heat bath of

124 uniform temperature. The thermal diffusivity of the crust is about half that of the mantle
 125 and the crust serves as a blanketing layer (*Ziethe et al.*, 2009). Initially, the deep mantle
 126 is more enriched in HPEs and IBC-rich component than the mid-mantle as earlier
 127 models of mantle differentiation by the magma ocean and the subsequent mantle
 128 overturn suggest (*e.g.*, *Ringwood and Kesson*, 1976; *Hess and Parmentier*, 1995).

129

130 **2.1 The basic equations**

131 The continuity equation is

$$132 \quad \nabla \cdot \mathbf{U} = -\nabla \cdot [\phi(\mathbf{u} - \mathbf{U})]. \quad (1)$$

133 Here, $\mathbf{U}$ is the velocity of the matrix, $\mathbf{u}$ that of magma, and ϕ the melt-content; $\mathbf{U}$
 134 and $\mathbf{u}$ have only radial component because of the assumed spherical symmetry. The
 135 relative velocity $\mathbf{u} - \mathbf{U}$ is proportional to the density difference between magma and the
 136 coexisting matrix $\Delta\rho$ as

$$137 \quad \mathbf{u} - \mathbf{U} = -\frac{k_\phi}{\mu\phi} \mathbf{g} \Delta\rho, \quad (2)$$

138 where k_ϕ is the permeability that depends on ϕ as $k_{\phi 0}(\phi/\phi_0)^3$; the ϕ -dependence
 139 is truncated at its value at $\phi = 0.4$. Here, $k_{\phi 0}$ is the reference permeability, the values

140 of which are given in *McKenzie* (1984) and *Miller et al.* (2014); ϕ_0 is the reference
 141 melt content; μ the viscosity of magma; $\mathbf{g}$ the gravitational acceleration; the
 142 parameter values are given in Table 1. The density difference between solid-phase and
 143 melt-phase $\Delta\rho$ depends on the chemical composition of the phases as well as the depth
 144 as

$$145 \quad \Delta\rho = \rho_0 \left\{ \beta(\xi_l - \xi_s) + \frac{\Delta V_l}{V_0} [1 + \beta(1 - \xi_l)] \right\}. \quad (3)$$

146 Here, ξ_s and ξ_l are the content of the end-member A in the solid-phase and the melt-
 147 phase, respectively; ρ_0 the reference density. $\Delta V_l/V_0$ expresses the amount of density
 148 reduction by melting that depends on the depth as

$$149 \quad \Delta V_l/V_0 = D_0 + D_1/[1 + (r_p - r)/\zeta]^2, \quad (4)$$

150 where the values of D_0 , D_1 , ζ are chosen so that the solidus temperature calculated
 151 from Equation (4) by the Clausius-Clapeyron slope becomes close to the solidus
 152 temperature of mantle materials (*Katz et al.*, 2003); r is the radial coordinate. We set
 153 $\beta = 0.135$ based on the density of olivine-rich end member A ($\rho_A = 3300 \text{ kg m}^{-3}$;
 154 *Elkins-Tanton et al.*, 2011), that of the IBC end member B ($\rho_B = 3744 \text{ kg m}^{-3}$; *Snyder*
 155 *et al.*, 1992; *Shearer et al.*, 2006), and that of the IBC-rich eutectic composition of

156 $A_{0.1}B_{0.9}$ ($\rho_e = 3700 \text{ kg m}^{-3}$; *Elkins-Tanton et al.*, 2011; *Yu et al.*, 2019).

157 The solidus temperature T_{melt} depends on the lithostatic pressure $P = \rho_0 g(r_p - r)$

158 as

159
$$T_{melt} = T_0(G + 1), \quad (5)$$

160 where

161
$$G = \frac{1}{\rho_0 \Delta h} \int_0^P \frac{\Delta V_l}{V_0} dP; \quad (6)$$

162 T_0 is the solidus temperature at the surface (*Katz et al.*, 2003); Δh the latent heat of

163 melting.

164 The energy equation is

165
$$\frac{\partial(\rho_0 h)}{\partial t} + \nabla \cdot (\mathbf{U} \rho_0 h) = -\nabla \cdot [\rho_0 h_l \phi (\mathbf{u} - \mathbf{U})] - \frac{\Delta V_l}{V_0} \rho_0 \mathbf{g} \phi \mathbf{u} + \nabla \cdot [k \nabla T + \kappa_{edd} \nabla(\rho_0 h)] + \rho_0 q, \quad (7)$$

166 where the enthalpy h is written as

167
$$h = C_p T + \phi \Delta h (1 + G); \quad (8)$$

168 $h_l = h(\phi = 0)$; C_p is the specific heat; T the temperature; $k = \rho_0 C_p \kappa$ the thermal

169 conductivity; κ the thermal diffusivity; q the internal heating rate. In addition, we

170 assumed that matrix disintegrates and that a strong turbulent diffusion occurs with the

171 eddy diffusivity of $\kappa_{edd} = 50\kappa$ in largely molten regions with $\phi > 0.4$. κ_{edd}

172 is assumed to gradually increase with increasing ϕ as ϕ^3 to avoid
 173 numerical instability. Migration of magma is calculated in the energy equation as a
 174 transport of the latent heat of melting by migrating magma (the first term on the right-
 175 hand side of Equation 7). We also assumed that the thermal diffusivity in the crust κ_{crst}
 176 is lower than that in the mantle κ_{mantle} to take account of the blanketing effect of the
 177 crust and regolith layer (e.g., *Zieth et al.* 2009), that is

$$178 \quad \kappa = \begin{cases} \kappa_{crst} & \text{at } r > r_{crst} \\ \kappa_{mantle} & \text{at } r < r_{crst} \end{cases} \quad (9)$$

179 Following the method described in *Zieth et al.* (2009), we assumed that
 180 $\kappa_{crst}/\kappa_{mantle} = 0.48$.

181 The internal heating rate changes with time as

$$182 \quad q = q_{tr} Q_0 \exp(-\lambda t), \quad (10)$$

183 where Q_0 is the initial amount of HPEs, λ the decay constant (Table 2). q_{tr}
 184 changes with time as

$$185 \quad \frac{\partial q_{tr}}{\partial t} + \nabla \cdot (q_{tr} \mathbf{U}) = -\nabla \cdot [\phi q_{liq} (\mathbf{u} - \mathbf{U})] + \nabla \cdot [\kappa_{edd} \nabla q_{tr}], \quad (11)$$

186 where $q_{liq} = q_{tr}/[\phi + D(1 - \phi)]$, D is the partition coefficient of HPEs between
 187 melt-phase and solid-phase, and q_{tr} is normalized so that $\int_V q_{tr} dV = 1$ holds where

188 the integration extends over the entire spherical shell.

189 The bulk composition $\xi_b \equiv \phi \xi_l + (1 - \phi) \xi_s$ changes with time as

190
$$\frac{\partial \xi_b}{\partial t} + \nabla \cdot (\xi_b \mathbf{U}) = -\nabla \cdot [\phi \xi_l (\mathbf{u} - \mathbf{U})] + \nabla \cdot [\kappa_{edd} \nabla \xi_b]. \quad (12)$$

191 In the estimate of the radial expansion of the Moon, we consider the effects of
192 temperature change (*Solomon and Chaiken, 1976*) and expansion by melting: the radial
193 change ΔR is given by

194
$$\Delta R = \frac{1}{r_p^2} \int_{r_c}^{r_p} \left[\alpha \Delta T + \frac{\Delta V_l}{V_0} \Delta \phi \right] r^2 dr, \quad (13)$$

195 where α is the thermal expansivity, and ΔT and $\Delta \phi$ are the deviation of temperature
196 and melt-content from the values assumed in the initial condition.

197

198 **2.2 Initial distribution of temperature, HPEs, and bulk composition**

199 Figure 1 shows an example of the initial distributions of enthalpy, temperature,
200 internal heating rate, and composition. This initial condition is motivated by earlier
201 models of the mantle overturn that is expected to have occurred after solidification of
202 the magma ocean (*e.g., Snyder et al., 1992; Alley and Parmentier, 1998; Elkins-Tanton*
203 *et al., 2011; Boukaré et al., 2018*). Crystal fractionation in magma ocean is expected to

204 have formed a dense layer composed of IBC and urKREEP (materials enriched in K,
 205 rare-earth elements, and P) at the top of the mantle. The gravitationally unstable mantle
 206 is suggested to have overturned to form a layer enriched in the residual materials at the
 207 base of the mantle (hereinafter, termed the “Overturned layer”; *e.g.*, Ringwood and
 208 Kesson, 1976; Hess and Parmentier, 1995; Zhao *et al.*, 2019). The materials in the
 209 overturned layer are enriched in HPEs; the overturned materials with the composition of
 210 $A_{0.1}B_{0.9}$ are assumed to be 7.5 times more enriched in HPEs than the bulk Moon (Hess
 211 and Parmentier, 1995) in the present model. We estimated the distribution of the
 212 overturned materials in the mantle after the mantle overturn based on the distributions
 213 of internal heat source q_{init} calculated in the models of Yu *et al.* (2019) and Zhao *et al.*
 214 (2019). We first approximated the distribution of HPEs they calculated by

$$215 \quad q_{init} = q_0 + \Delta q \exp\left[-\frac{r - r_c}{L}\right], \quad (14)$$

216 where $q_0 = 5.77 \text{ pW kg}^{-1}$ is the internal heating rate of the olivine-rich materials
 217 beneath the IBC and urKREEP layer before mantle overturn (Yu *et al.*, 2019), L the
 218 thickness of the basal layer enriched in the overturned materials, and Δq is calculated
 219 from the assumption that the excess internal heating rate in the overturned layer Q_{OL}

220 defined by

$$221 \quad Q_{OL} = \int_{r_c}^{r_{crst}} 4\pi r^2 \Delta q \exp\left[-\frac{r-r_c}{L}\right] dr, \quad (15)$$

222 satisfies

$$223 \quad Q_{OL} = \int_{r_c}^{r_p} 4\pi r^2 q_{bulk} dr - \int_{r_{crst}}^{r_p} 4\pi r^2 q_{crst} dr - \int_{r_c}^{r_{crst}} 4\pi r^2 q_0 dr. \quad (16)$$

224 Here, $q_{bulk} = 14.70 \text{ pW kg}^{-1}$ is the average initial heating rate of the Moon at 4.4

225 Ga (*McDonough and Sun, 1995; Taylor and Wieczorek, 2014; Lodders, 2003*; see Table

226 2), while q_{crst} that of the crust which is treated as a free parameter (See Figure 1a).

227 Then, we calculated the initial distribution of chemical composition ξ_b in the mantle

228 from q_{init} as

$$229 \quad \xi_b = 1 - \frac{\Delta q \exp[-(r-r_c)/L]}{7.5q_{bulk}}, \quad (17)$$

230 and $\xi_b = 1$ in the crust. On the other hand, the initial distribution of enthalpy h is

$$231 \quad h = \min(h_{sur}, h_{mantle}), \quad (18)$$

232 where,

$$233 \quad h_{surf} = C_p T_{sur} + f_{sur} \left(1 - \frac{r}{r_p}\right), \quad (19)$$

$$234 \quad h_{mantle} = \begin{cases} C_p T_M & \text{if } r > r_{OL} \\ C_p T_M + (T_c - T_M) \left(\frac{r_{RL} - r}{r_{RL} - r_c}\right)^2 & \text{if } r < r_{OL} \end{cases}. \quad (20)$$

235 Here the initial temperature in the bulk of the mantle T_M is a free parameter, f_{sur}

236 and r_{OL} are constants arbitrarily chosen to be $6 \times 10^4 \text{ J kg}^{-1}$ and 550 km (*Hess and*
 237 *Parmentier*, 1995), respectively, and $T_c = 1900\text{K}$ is the initial temperature of the core
 238 (*e.g.*, *Ziethé et al.*, 2009; *Zhang et al.*, 2013a, b); we assumed that the core is hotter than
 239 the mantle 4.4 Gyr ago (*e.g.*, *Alley and Parmentier*, 1998; *Boukaré et al.*, 2018). We
 240 illustrate the assumed enthalpy distribution in terms of the equivalent temperature
 241 $T_{eq} = h/C_p$ in Figure 1c.

242

243 **2.3 Free parameters**

244 There are four free parameters in our model: the initial temperature in the mid-mantle
 245 T_M , the reference permeability $k_{\phi 0}$ (see Equation 2), the ratio of the concentration of
 246 the HPEs in the crust to the mantle F_{crst} , and thickness of the overturned layer L ;
 247 instead of $k_{\phi 0}$, we will use its normalized form $M = \frac{k_{\phi 0} \rho_0 g r_0}{\mu \kappa}$ hereinafter (Table 3).
 248 We varied the normalized permeability M in the range estimated from the parameter
 249 values of Table 1, F_{crst} is estimated from a value adapted in earlier models (*Konrad*
 250 *and Spohn*, 1997; *Spohn et al.*, 2001), and L from earlier mantle overturn models
 251 (Figure 6 of *Li et al.*, 2019; Figures 6, 7 of *Yu et al.*, 2019; Figure 3 of *Zhao et al.*,

2019).

3. Results

3.1 Thermal and structural evolution of the mantle

3.1.1 Reference model

We present the radial change of the planet calculated in the reference case in Figure 2a. The assumed parameter values are $T_M = 1550K$, $M = 28$, $F_{crst} = 8$, and $L = 1/5.5$. The radius of the planet changes with time by two reasons, thermal expansion and melting (see also Equation 13), as indicated by the green and light blue lines in the figure, respectively. Thermal expansion consistently causes radial contraction of the planet over the calculated 4.4 Gyr history. On the other hand, the history of radial change by melting consists of three stages: in Stage I, the planet rapidly expands until around 0.6 Gyr; in Stage II, the planet slowly expands until around 1.3 Gyr; in Stage III, the planet gradually contracts. In total, the planet expands by 1.14 km because of mantle melting in Stage I but shrinks in Stage III because of thermal contraction and solidification of the mantle. The planet shrinks by 1.08 km for the last 800 million years

268 of the calculated history (Figure 2a).

269 A closer look at Figures 2c and 2e shows more clearly how mantle melting
270 contributes to the calculated radial expansion/contraction history of the planet. A large
271 amount of magma is generated in the deep mantle due to the strong internal heating by
272 the HPEs-enriched overturned layer nearby the core-mantle boundary assumed in the
273 initial condition. The upward extension of the partially molten region in the deep mantle
274 caused by internal heating and upward migration of the generated magma (Figures 2c,
275 2e) causes the conspicuous radial expansion of Stage I (Figure 2a). The maximum melt-
276 content of the region is around 0.4 and occurs at the top of the region. The migrating
277 magma concentrates HPEs and the end-member *B* enriched materials to the top of the
278 region (Figures 2d and 2f). When the magma enriched in HPEs ascends to the
279 uppermost mantle (radius $r = 1300$ to 1400 km), however, the effect of conductive
280 cooling from the cold surface boundary heat overcomes the internal heating by the
281 HPEs in the magma, and the magma solidifies (1.0 Gyr in Figure 2b); the radial
282 expansion of the planet almost stops accordingly (Stage II in Figure 2a). According to
283 decay and depletion of the HPEs, the partially molten region then gradually shrinks

(Stage III in Figure 2a).

An interesting feature of melt-distribution shown in Figures 2c, 2e is that two regions with elevated melt-content develop in the mantle after around 1.5 Gyr, one at the radius r around 600 km and the other at r around 1300 km. The shallower region arises because the magma migrates upward concentrating the HPEs there. On the other hand, the deeper region arises because upward migrating magma has extracted the compositionally dense end-member B from the region by 1.5 Gyr (see the depth range of 500 to 1200 km in Figure 2f). Because of the depletion in the end-member B , the density of matrix becomes almost equal to that of magma that is more enriched in the end-member B . Owing to the almost neutral buoyancy of magma in the deep mantle, the partially molten region persists there until today (Figures. 2c, 3e).

3.1.2 Radial expansion/contraction by magma

To more clearly show how the radial expansion in Stage I and contraction in Stage III of the reference case occur, we calculated three more models: Model 1 where only the effects of thermal diffusion, internal heating, and melt-generation are considered; Model

300 2 where magma migration (the second term on the left hand side and the first term on
301 the right hand side in Equation 7) is added to Model 1; Model 3 where HPE-transport
302 by migrating magma (Equation 11) is added to Model 2. (In Models 2 and 3, $\beta = 0$ is
303 assumed in Equation 3.) The difference between the reference model and Model 3 is
304 whether or not the transport of the end-member B by migrating magma (Equation 12) is
305 taken into account. The values of free parameters assumed in these models are the same
306 as those assumed in the reference model shown in Figure 2.

307 In Model 1, the planet first shrinks until around 0.4 Gyr and then expands owing to
308 melting of the deep mantle by internal heating (Figure 3). A totally molten region
309 develops at the base of the mantle after 0.4 Gyr and becomes thicker with time because
310 the effect of conductive cooling from the cold surface boundary is negligible at such a
311 great depth; the totally molten region occupies the deeper part of the mantle with radius
312 r less than around 1000 km at 4.4 Gyr.

313 The large-scale melting shown in Model 1 does not occur in Model 2 (Figure 4)
314 where magma-migration is considered. Migrating magma extracts heat from the deep
315 mantle and transport it to uppermost mantle. The carried heat is further transported to

316 the cold surface boundary by conduction. The melt-content in the deep mantle is less
317 than 0.1, and there is no total melting as observed in Model 1. Consequently, the planet
318 radially expands only during the period of ~0.3 to ~0.7 Gyr.

319 When HPE-transport by migrating magma is also considered (Model 3 in Figure 5),
320 the partially molten region persists in the mantle only until around 2 Gyr and the entire
321 mantle becomes solid after that. Most of the HPEs in the region migrates upward to its
322 top within the first 0.5 Gyr (Figure 5c). The magma solidifies quickly in the top of the
323 partially molten region due to the strong conductive cooling from the surface boundary,
324 and the partially molten region shrinks (Figure 5b). Note that the early radial expansion
325 by melting observed in Model 3 is 0.15 km smaller than that observed in the reference
326 model shown in Figure 2a. The smaller expansion in Model 3 is a consequence of a
327 faster upward migration of magma calculated in Model 3 compared with that calculated
328 in the reference model. Magma velocity is proportional to the density difference
329 between magma and the coexisting matrix (Equation 3). The compositional density
330 difference (the first term on the right hand side of Equation 3) is, however, neglected
331 and melt is always substantially less dense than matrix, leading to the faster upward

migration of magma in Model 3. The changes of the chemical composition by magma migration also have important influences on the history of the lunar radial expansion/contraction history.

3.2 Radial expansion/contraction at various parameters

We explored how the radial expansion in Stage I and contraction in Stage III depend on the four free parameters, T_M , F_{crist} , L , and M by carrying out an extensive parameter search as shown in Figure 6.

The initial mid-mantle temperature T_M influences the timing and magnitude of radial expansion (Figure 6a). Higher T_M (1700 to 1750 K) leads to an earlier expansion (0.2 to 0.3 Gyr) with a smaller amplitude of less than 0.4 km as well as a longer period of Stage III. This tendency arises because a higher T_M implies a higher melt-content in the initial mantle, which causes the earlier expansion of the partially molten region, and the radial contraction due to solidification of the melt works more strongly. F_{crist} and L strongly affect the presence or absence of the expansion. Lower F_{crist} and L imply more HPEs in the deep mantle, leading to more expansion in Stage I (Figures 6b, 6c). The

permeability M strongly affects the magnitude of expansion/contraction when $M \leq 4$ as shown in Figure 6d because a higher permeability induces quicker drainage of magma from the mantle. (Note that the case at $M = 0$ in Figure 6d is Model 1 in Figure 3.) At $M \geq 4$, however, this effect of increasing M becomes saturated and the history of planetary expansion/contraction becomes almost independent of M .

4. Discussions

The spherically symmetric mantle calculated in our model radially shrinks for the first ~300 million years because the magma generated in the shallow mantle by the assumed high initial temperature solidifies. Then, the mantle radially expands by up to 1.4 km ($M = 12$ in Figure 6d) as magma is generated in the deep mantle and migrates upward to the uppermost mantle that is cooled by conduction from the surface boundary until 0.6 Gyr of the calculated history. The migrating magma extracts HPEs from the deep mantle. After 1 to 2 Gyr since the start of the calculated history, the mantle radially contracts (~1 km for the last 800 million years) owing to its solidification and cooling that result from the HPE-depletion at depth (Figure 7).

364

365 **4.1 Comparison with earlier models**

366 The most important feature of our model is that the mantle radially expands by up to
367 1.4 km for the first hundreds of millions of years despite that the initial temperature in
368 the mid-mantle T_M is as high as ~ 1600 K because of the expansion caused by melting.
369 In earlier one-dimensional models where expansion/contraction of the planet occurs
370 only thermally, the initial temperature in the deep mantle must be less than 600 K to
371 1200 K at most to account for the early expansion of the Moon (*Solomon and Chaiken*,
372 1976; *Kirk and Stevenson*, 1989; *Andrews-Hanna*, 2013; *Sawada et al.*, 2016).
373 Otherwise, the earlier researchers found that the calculated mantle monotonously
374 shrinks or expands at the beginning of its history only slightly at most. The same
375 conclusion has been reached in three-dimensional models where heat-transport by
376 mantle convection is considered, too. Although the global expansion of the early Moon
377 is as large as 2 km in some earlier models (*Zhang et al.* 2013a,b), the consumption of
378 latent heat by melting is neglected and the effect of thermal expansion is overestimated
379 in these models. Besides, the early expansion of the model (see H50E100MR2500 of

380 *Zhang et al.* 2013b, for example) continues for so long as 1 Gyr as is the case for our
381 model that start with the initial mantle temperature T_M of 1400 K (Figure 6a); the
382 period of early expansion is substantially longer than that for the Moon. In a model
383 where HPEs are assumed to be enriched in the uppermost mantle of the nearside
384 (*Laneuville et al.*, 2013), the farside mantle shrinks by about 5 km although up to 7 km
385 expansion is observed on the nearside, and this model does not account for the globally
386 expansion. In our model where planetary expansion by melting is considered, we found
387 not only the planetary contraction in the later stage but also the planetary expansion by
388 up to 1.4 km for the first several hundred million years of the calculated history of the
389 mantle (Figures 2, 6), suggesting that melting of the mantle has played a crucial role in
390 the observed expansion/contraction history of the Moon (*Watters et al.*, 2010; *Andrews-*
391 *Hanna et al.*, 2013; *Sawada et al.*, 2016; *Matsuyama et al.*, 2021).

392 Our models also show that a careful modeling of magma generation and migration is
393 crucial to realistically reproduce the melting history of the lunar mantle. In earlier one-
394 dimensional models where the initial temperature is more than 1000 K lower than the
395 solidus temperature in the deep mantle (*Wood*, 1972; *Solomon and Teksöz*, 1973;

396 *Toksöz and Solomon, 1973*), a partially molten region is first induced by the high initial
397 temperature in the uppermost mantle and then shifts toward the deep mantle as it is
398 internally heated by HPEs; the mantle becomes totally molten at its base today in some
399 models (see Figure 6 of *Solomon and Toksöz (1973)*, for example). This melting history
400 is similar to that of Model 1 where the mantle thermally evolves only by thermal
401 diffusion and internal heating (Figure 3). The melting history, however, substantially
402 depends on magma-migration, transport of HPEs and materials by migrating magma.
403 When heat transport by migrating magma is added to Model 1, a partially molten region
404 extends upward to the uppermost mantle (Model 2; Figure 4). When HPE-transport by
405 migrating magma is further considered, the deep mantle becomes depleted in HPEs
406 within around 0.5 Gyr since the beginning of the calculation, and the partially molten
407 deep mantle becomes solidify within 2 Gyr (Model 3; Figure 5). In the reference model
408 where changes in the chemical composition by magma segregation is added to Model 3,
409 depletion of matrix in the end-member *B* allows a partially molten region to persist for 4
410 billion years in the deep mantle (Figure 2). To account for the melting history of the
411 lunar mantle that exerts control over the history of planetary expansion/contraction and

412 mare volcanism, a careful modeling of magma generation and migration as well as
413 transport of heat, HPEs, and materials by magma is indispensable.

414 To further extend the model presented here, it is important to include the effects of
415 mantle convection on the melting history of the lunar mantle. In three-dimensional
416 spherical models of lunar mantle convection (*e.g.*, *Konrad and Spohn*, 1997; *Spohn et*
417 *al.*, 2001; *Ziethe et al.*, 2009; *Laneuville et al.*, 2013), magma is generated only in the
418 shallow mantle at the beginning of the calculated history. The partially molten region
419 then gradually shrinks owing to cooling from the surface boundary; the deep mantle
420 does not melt throughout the calculated history because of convective heat extraction.
421 Some three-dimensional models suggests that evolution of compositional structure of
422 the mantle caused by mantle convection also plays an important role in the thermal and
423 volcanic history of the Moon (*Hess and Parmentier*, 1995; *Stegman et al.*, 2003; *Zhang*
424 *et al.*, 2013a, b). (Note, however, that many of earlier models of the lunar mantle are
425 calculated at a condition much more favorable for thermal convection than that of the
426 real lunar mantle as suggested in Figure 8 of *Yanagisawa et al.* (2016). The mantle
427 evolution in a model where mantle convection is calculated at a more realistic condition

(Laneuville *et al.*, 2013) is indeed not so different from a corresponding earlier model where mantle convection is neglected (Wieczorek and Phillips, 2000).)

Keeping the caveat about the effects of mantle convection on mantle evolution in mind, we apply our one-dimensional model of mantle evolution caused by magma-generation and migration to the Moon in the next section.

4.2 Comparison with observed features of the Moon

The evolution of partially molten region observed in the reference model that account for the radial expansion/contraction history of the Moon (see Figure 2) mesh with the history of mare volcanism of the Moon. After the initial deepening to the depth level of around 400 km until ~0.4 Gyr, the top of a partially molten region in our model becomes shallower and reaches the depth level of around 300 km at around 0.8 to 1.3 Gyr owing to magma-migration, and then again becomes deeper with time (Figures 2c, e). The deepening of the top of partially molten region until around 0.4 Gyr is consistent with the period when mare volcanism on the Moon was not so active (*e.g.*, Hiesinger *et al.*, 2003; Whitten and Head, 2015), while its shallow depth level at around 0.8 to 1.3

444 Gyr accounts for the peak of mare volcanism, which occurred at ~ 3.6 Gyr ago (*e.g.*,
445 *Hiesinger et al.*, 2000, 2003). The shrinking partially molten region observed after ~1.3
446 Gyr in our model may correspond to the deepening of the source region of mare
447 volcanism inferred from the variation of the Ti concentration in mare basalts (*e.g.*, *Hess*
448 *et al.*, 1978; *Pieters et al.*, 1980; *Taylor*, 1982; *Morota et al.*, 2011). (Although a
449 thermal diffusion model where magma-generation is not considered also show the
450 deepening of partially molten region (*Wieczorek & Phillips*, 2000), this earlier model
451 does not account for the weak volcanism of the Moon before about 4 Gyr ago.)

452 Temperature profile calculated at 4.4 Gyr in our model (Figure 2b), which is basically
453 a diffusion profile in the shallow mantle, is qualitatively consistent with the temperature
454 profile of today's Moon obtained from analysis of lunar seismic data and electrical
455 conductivity (*e.g.*, *Karato*, 2013; *Khan et al.*, 2006, 2014). The presence of a partially
456 molten zone at 4.4 Gyr in our model is also consistent with that in today's mantle of the
457 Moon inferred from its seismic observations (*e.g.*, *Latham et al.*, 1973; *Nakamura et al.*,
458 1973; *Weber et al.*, 2011). However, the molten region in our model occurs in the mid-
459 mantle and is ~500 km in thickness with the degree of melting of up to 4% (Figures

2c,e), while geophysical evidence suggests that the partially molten region occurs at the base of the mantle with its thickness around 150 km and its degree of melting 5 to 30% (Weber *et al.*, 2011). The difference in the depth, melt-content, and the thickness of partially molten region calls for further improvements of the models. In particular, it is important to consider the effects of heat transport by mantle convection.

4.3 Implication for evolution on the Moon

The initial condition assumed in our preferred models that account for the observed features of the Moon imposes a constraint on the magma ocean and mantle overturn that are expected to have occurred in the earliest stage of its evolution. Among the models presented in Section 3.2, those calculated at the initial temperature in the mid-mantle $T_M \approx 1600$ K, the initial crustal fraction of HPEs $F_{crst} \leq 12$, and the extent of the enriched layer at the base of the mantle $L \leq 1/2$ (Table 4) are consistent with the observed expansion/contraction history of the Moon (Watters *et al.*, 2010; Andrews-Hanna *et al.*, 2013; Sawada *et al.*, 2016; Matsuyama *et al.*, 2021). The early planetary expansion does not occur, and the planet monotonously contracts with time at higher

476 T_M as 1700 to 1750 K, whereas the early expansion continues for a period too long to
477 be consistent with the observed history at lower T_M as 1400 to 1450 K.

478 The preferred value of T_M is substantially lower than that immediately after the giant
479 impact (*e.g.*, *Stevenson, 1987; Pritchard and Stevenson, 2000; Canup, 2004; Lock et al.,*
480 *2018*). The lower T_M obtained in our model suggests that the mantle temperature just
481 after the planetary formation was lower than that calculated from giant impact
482 hypotheses, or that the mantle temperature was reduced by several thousands of Kelvins
483 in the course of solidification of the magma ocean and the mantle overturn (*e.g.*, *Hess*
484 *and Parmentier, 1995; Alley and Parmentier, 1998; Shearer et al., 2006; Boukaré et al.,*
485 *2018*). The value of T_M calculated in our models is, however, still substantially lower
486 than the temperature that most of the mantle overturn models predict (*Li et al., 2019; Yu*
487 *et al., 2019; Maurice et al., 2020*). The lower temperature T_M imposes a constraint on
488 the thermal history of the earliest Moon.

489 The range of F_{crst} in the preferred models implies that the average content of Th is
490 around 51.3 ppb or higher in today's mantle of the Moon. This content is higher than
491 that of the current lunar mantle inferred from the Th mass-balance model (40 ppb;

Jolliff et al., 2000) and the composition of H-chondrite (25 ppb; *Warren and Wasson*, 1979). The rather high content of Th, and hence HPEs, suggests that mantle overturn brought a large amount of urKREEP materials to the base of the mantle, or the primitive mantle was more enriched in HPEs than inferred in these studies. This result also places important constraints on the initial conditions of the Moon.

5. Conclusions

We developed a one-dimensional spherically symmetric numerical model of the thermal history of the lunar mantle, taking magma generation and migration into account. We found that transport of heat, incompatible heat-producing elements (HPEs), and materials by migrating magma play a crucial role in the thermal history. The planet radially expands by up to 1.4 km during the first around 600 million years in the calculated history as magma is generated in the deep mantle and migrates upward to the uppermost mantle. The migrating magma extracts HPEs from the deep mantle, and the planet then radially contracts due to solidification and cooling of the mantle. The radial expansion/contraction history in our model is consistent with the observed history of the

508 Moon, and the melting history of the mantle in our model accounts for the mare
509 volcanism of the Moon. We obtained this favorable model when we started the
510 calculation from the initial condition that the initial mid-mantle temperature $T_M \approx$
511 1600 K , the initial ratio of the concentration of the HPEs in the crust to the mantle
512 $F_{crst} \leq 12$, and the initial thickness of the overturned layer at the base of the mantle
513 $L \leq 1/2$. This range of the initial condition assumed imposes a constraint on the magma
514 ocean and mantle overturn that are inferred to have occurred in the Moon. In future
515 works, it is important to extend our model by taking account of heat and mass transport
516 by mantle convection.

517

518 **Declarations**

519 **Ethics approval and consent to participate**

520 Not applicable.

521 **Consent for publication**

522 Not applicable.

523 **List of abbreviations**

524 HPEs: heat-producing elements; IBC: ilmenite bearing cumulates.

525 **Availability of data and materials**

526 The data and the numerical code of this study are available upon reasonable
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528 **Competing interests**

529 The authors declare that they have no competing interests.

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534 **Authors' contributions**

535 KU and HH developed the numerical code. KU carried out the
536 calculations, analyzed the numerical results, prepared the manuscript.
537 MO supervised the work. KU and MO discussed the numerical results.
538 All authors read and approved the final manuscript.

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543

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547 **Endnotes**

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821

822 **Figure Legends**

823

824 **Figure 1 Initial condition.**

825 Illustration of the initial distribution of (a) internal heating rate, (b) bulk composition,
826 and (c) temperature. The assumed parameter values in the figure are: the temperature
827 of the mid-mantle $T_M = 1650K$; the ratio of the concentration of HPEs in the crust to
828 the mantle $F_{crst} = 8$; the thickness of the high-density layer after mantle overturn $L =$
829 $1/5.5$.

830

831 **Figure 2 Reference model.**

(a) a plot of radius changes against time, (b) temperature profile as a function of time, and the evolution of the distribution of (c) temperature, (d) internal heating rate, (e) melt-content, and (f) bulk composition ξ_b . The assumed parameter values are $T_M = 1550K, M = 28, F_{crst} = 8, L = 1/5.5$. In (a), the green and light blue lines indicate the contribution of thermal expansion and melting, respectively, to the total radius change (the purple line). In (c), the contour lines show the distribution of melt-content with the contour interval of 0.05 starting from 0 (indicated by the dashed line); in (e), the contour lines show the distribution of temperature.

Figure 3 Model 1.

(a) and (b) the same as Figures 2a and 2c, respectively, but for Model 1 where only the effects of thermal diffusion, internal heating and melting are considered; magma does not migrate. The assumed parameter values are $T_M = 1550K, M = 28, F_{crst} = 8, L = 1/5.5$. In (b), the contour lines show the distribution of melt with the contour interval of 0.2 starting from 0 (indicated by the dashed line).

Figure 4 Model 2.

The same as Figure 3 but for Model 2 where magma migration is added to Model 1 shown in Figure 3. In (b), the contour lines show the distribution of melt with the contour drawn at 0.01 intervals from 0.05. The dashed line indicates the molten region ($\phi = 0$).

Figure 5 Model 3.

(a), (b) the same as Figures 4a, b but for Model 3 where HPE-transport by migrating magma is added to Model 2 shown in Figure 4; transport of the end-members A and B by migrating magma is not considered. (c) The evolution of HPE-distribution for Model 3. In (b), the contour lines show the distribution of melt with the contour interval of 0.01 starting from 0 (indicated by the dashed line).

Figure 6 Radial change at various free parameters.

Plots of radial change against time calculated at various values of (a) T_M , (b) F_{crst} , (c) L , (d) M . The dotted lines show the reference model indicated by the purple line in Figure 2a.

Figure 7 Illustration of thermal and structural history of the Moon.

For each stage, see Section 3.1.1.

Table Legends

Table 1 The meanings of the symbols and their values.

Table 2 Internal heating from heat-producing elements (HPEs).

Rates of decay heat release and decay constants are after *Turcotte and Schubert* (2014).

For the current concentration ratio of the HPEs in the bulk Moon, see Section 2.2.

Table 3 The variable parameters of the numerical models.

The * parameters are dimensionless.

Table 4 The favored values of the variable parameters.

The planetary expansion calculated at these values is consistent with the observed history of radial changes of the Moon (*Andrews-Hanna et al.*, 2013; *Sawada et al.*, 2016).

Figures

Figure 1

Initial condition.

Illustration of the initial distribution of (a) internal heating rate, (b) bulk composition, and (c) temperature. The assumed parameter values in the figure are: the temperature of the mid-mantle $T_M=1650K$; the ratio of the concentration of HPEs in the crust to the mantle $F_{crist}=8$; the thickness of the high-density layer after mantle overturn $L=1/5.5$.

Figure 2

Reference model.

(a) a plot of radius changes against time, (b) temperature profile as a function of time, and the evolution of the distribution of (c) temperature, (d) internal heating rate, (e) melt-content, and (f) bulk composition ξ_b . The assumed parameter values are $T_M=1550K$, $M=28$, $F_{crist}=8$, $L=1/5.5$. In (a), the green and light blue

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(a) and (b) the same as Figures 2a and 2c, respectively, but for Model 1 where only the effects of thermal diffusion, internal heating and melting are considered; magma does not migrate. The assumed parameter values are $T_M=1550K$, $M=28$, $F_{crst}=8$, $L=1/5.5$. In (b), the contour lines show the distribution of melt with the contour interval of 0.2 starting from 0 (indicated by the dashed line).

Figure 4

Model 2.

The same as Figure 3 but for Model 2 where magma migration is added to Model 1 shown in Figure 3. In (b), the contour lines show the distribution of melt with the contour drawn at 0.01 intervals from 0.05. The dashed line indicates the molten region ($\phi=0$).

Figure 5

Model 3.

(a), (b) the same as Figures 4a, b but for Model 3 where HPE-transport by migrating magma is added to Model 2 shown in Figure 4; transport of the end-members *A* and *B* by migrating magma is not considered. (c) The evolution of HPE-distribution for Model 3. In (b), the contour lines show the distribution of melt with the contour interval of 0.01 starting from 0 (indicated by the dashed line).

Figure 6

Radial change at various free parameters.

Plots of radial change against time calculated at various values of (a) T_M (b) F_{crst} (c) L, (d) M. The dotted lines show the reference model indicated by the purple line in Figure 2a.

Figure 7

Illustration of thermal and structural history of the Moon.

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