INSTABILITY OF A REACTION ZONE AT THE CORE-MANTLE BOUNDARY (CMB)

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Abstract. The core-mantle reaction proceeds on two scales: the short-scale chemical reaction leading to local equilibrium and the large-scale dispersal of reaction products. The second process is connected with a growth of the CMB-radius and may be described with application of the diffusion equation. The departure from a stationary interface is calculated using the gravitational body force as the mechanism controlling the "tension" of the distorted spherical core body. Stability analysis with the help of angular harmonics leads to the result that undulations of CMB are stable for very long wave lengths only.

1. Introduction

The core-mantle boundary (CMB) marks the largest change in bulk composition inside the Earth, separating the liquid iron alloy of the outer core from the crystalline silicates of the mantle. The processes near CMB play a key role in the dynamics and evolution of the Earth (e.g. Young and Lay, 1987). Laboratory investigations by means of diamond-anvil cells (Jeanloz, 1990; Knittle and Jeanloz, 1991; Goarant *et al.*, 1992) have demonstrated that at the relevant thermodynamic conditions of the Earth's deep interior liquid iron reacts chemically with silicates of the lower mantle. The main point of this process is the infiltration of liquid iron into the mantle and a chemical reaction with the silicates producing metallic alloys (e.g. FeO) and nonmetallic silicates (e.g. SiO_2 stishovite). In this way a reaction zone, ≈ 10 to 10^3 m thick, is created at the interface between mantle and core (Stevenson, 1991). A quantitative estimate by Poirier and Le Mouel (1992) shows that infiltration can be about 10^2 m. The short-scale chemical reaction is followed by a large-scale dispersal of reaction products as shown in Figure 1.

The purpose of this paper is to investigate the large-scale dispersal of reaction products with the help of the diffusion equation in spherical symmetry and to perform a stability analysis on such a reaction zone using methods from the theory of interface stability (e.g. Delves, 1974).

2. Model for Large-Scale Dispersal of Reaction Products

In our simplified model the dispersal of reaction products can be thought of as the dissolution of FeO from the reaction zone into the core. In a slow process FeO has to diffuse down a concentration gradient from the mantle concentration

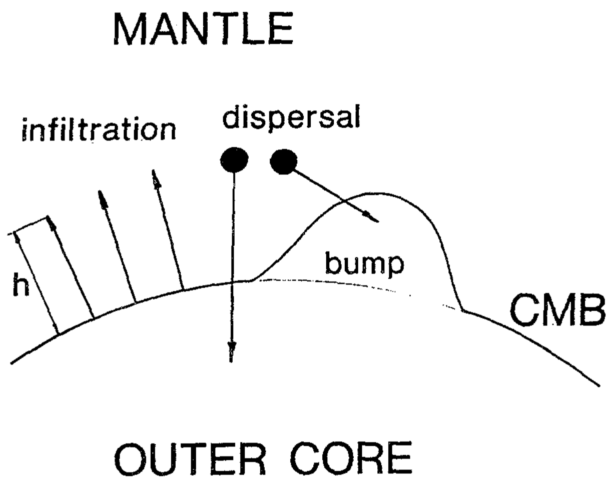

Fig. 1. Infiltration of fluid iron into the mantle and large-scale dispersal of reaction products.

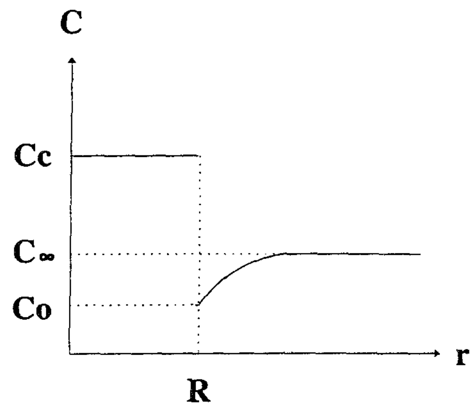

Fig. 2. Model for large-scale dispersal of reaction products.

C_∞ to the equilibrium concentration Co for dissolving in the core alloy with the concentration C_0 (see Figure 2). This dissolution is a STEFAN-problem (e.g. Carslaw and Jaeger, 1959) and results in a growing core radius $R(t)$.

We use the time independent form of the diffusion equation (which corresponds to the Laplace-equation) for the concentration C_m in the reaction zone near CMB:

$$\frac{D_m}{r^2}\left[\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta}\sin\Theta\frac{\partial}{\partial\Theta}+\frac{1}{\sin^2\Theta}\frac{\partial^2}{\partial\Phi^2}\right]C_m=0, \tag{1}$$

where D_m is the diffusion coefficient of FeO in silicates near to their melting temperature. The solution of Equation (1) is

$$C_c = \text{const.} \qquad \text{for } r < R, \tag{2}$$

$$C_m(r) = C_\infty + (C_0 - C_\infty)\frac{R}{r} \qquad \text{for } r \geq R. \tag{3}$$

At the core radius $R(t)$ the conservation condition for dissolving material has to be fulfilled:

$$D_m \left[\frac{\partial C_m}{\partial r}\right]_{r=R} = (C_c - C_o)\frac{\mathrm{d}R}{\mathrm{d}t}. \tag{4}$$

Equations (2)–(4) should also fulfil the condition of mass conservation at CMB: The flux of FeO down the concentration gradient into the core must be also accompanied by a corresponding flux of Fe for keeping C_c = Const. in the core. There are at least two ways out of this problem:

First, according to Knittle and Jeanloz (1991), the reaction at CMB may be presented as

$$Mg_{0.9}Fe_{0.1}SiO_3 + 0.15Fe = MgSiO_3 + 0.20FeO + 0.05FeSi + 0.05SiO_2.$$

From this equation we can see that indeed iron from the lower mantle perovskite goes effectively (as FeSi) into the core so that (at least approximately) the mass conservation can be fulfilled at the condition of constant solute concentration C_c in the core and growing core radius R. The other argument consists in the fact the reaction between core and mantle concerns only a thin shell of about 10^3 m thickness which is only a small part compared to the volume of the whole (outer) core.

In the following we will investigate two models for the concentration gradient on the left-hand side of Equation (4).

Model A: As shown in Figure 2, we assume that FeO is transported to the CMB only by diffusion. In this case the concentration gradient follows from Equation (3):

$$\left[\frac{\partial C_m}{\partial r}\right]_{r=R} = \frac{(C_\infty - C_0)}{R}. \tag{5a}$$

Model B: We assume that diffusion of FeO is the only transport mode within a diffusional boundary layer near CMB while outside this layer there is a general downward flow of material with a prescribed uniform speed U_0 and a removal in plumes (Stacey, 1992). According to Loper (1992) this uniform speed U_0 is about 7×10^{-12} m/sec. So the thickness D of the diffusional boundary layer can be found from $D = D_m/U_0 \approx 10^2$ m if $D_m \approx 10^{-9}$ m^2/sec (Vitjazev and Majeva, 1980). In this case we approximate the concentration gradient as

$$\left[\frac{\partial C_m}{\partial r}\right]_{r=R} = \frac{(C_\infty - C_0)}{D}. \tag{5b}$$

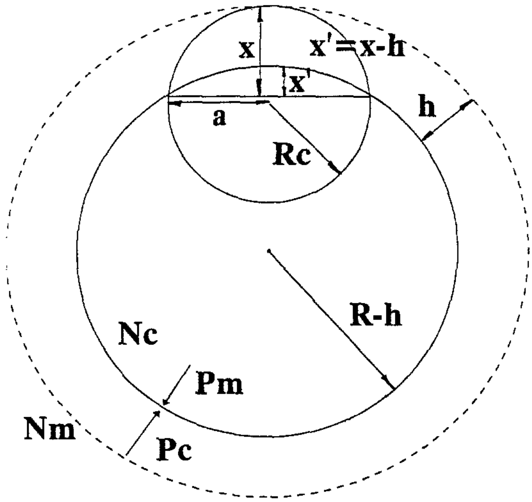

Fig. 3. Sketch of a bump at the interface, where h = infiltration depth equal to the height of a bump; N_m, N_c = number of FeO particles in mantle and core, respectively; P_m, P_c = pressure in mantle and core, respectively; R = core radius; R_c = radius of curvature of protrusion; x, x' and a = geometrical quantities used in Appendix A.

3. Distortions of a Stationary Interface

Up to now we have assumed that the interface has spherical symmetry and is connected with the stationary equilibrium concentration C_0. In the Earth's deep interior there may be some processes that cause distortions of the interface resulting in deviation from spherical symmetry. One example is the entrainment of material by overlying mantle convection (Sleep, 1988). For a calculation of a correction term ΔC to the stationary equilibrium concentration C_0 we start from Figures 1 and 3. We divide the total Helmholtz free energy F into the parts of core F_c, mantle F_m and interface:

$$F = F_c + F_m + \gamma A_c. \tag{6}$$

The quantity γ describes the change of free energy with change of surface area A_c. In the theory of crystal growth γ is the surface tension that acts against distortions of the interface. Concerning our problem we can calculate this quantity γ for the case of gravitational body force acting against distortion of the CMB. This can be done in a simple calculation of the change in gravitational energy ΔF when a "bump" with excess density $\Delta\rho$, volume change ΔV and change of surface area ΔA, extends into the mantle with depth h under the action of gravity g (see Figure 3 and Appendix A).

$$\Delta F = \alpha \cdot \Delta\rho \cdot g \cdot h \cdot \Delta V, \tag{7}$$

where α is a factor taking into account that the mean elevation of the material in a bump is smaller than h. According to our estimation α is in the order of 1/2.

$$\Delta V = \frac{\pi h^2[4R_c(3R - 2h) - h(4R - 3h)]}{3 \cdot 4(R - R_c)}, \tag{8a}$$

$$\Delta A = 2\pi \left[\frac{h}{2}\left(\frac{2R - h}{R - R_c}\right)(R_c - R + h) + (R - h)h\right]. \tag{8b}$$

Where R is the core radius and R_c is the radius of curvature of the protrusion.

$$\gamma = \frac{\Delta F}{\Delta A}. \tag{9}$$

For the definition of a new, nonstationary interface that has distortions as shown in Figure 3 we introduce a new equilibrium concentration C_e:

$$C_e = C_0 + \Delta C. \tag{10a}$$

According to a generalized Van't Hoff relation (Delves, 1974) the relative change in concentration $\Delta C/C_o$, which corresponds to the relative change in molar fraction of the solvent, is proportional to the volume V_{mol} of core material per mole of solute in the core:

$$\frac{\Delta C}{C_o} = \frac{\Delta N_{FeO}}{N_{FeO}} = \frac{\gamma K}{R_G T_{CMB}} V_{mol} = \Gamma \cdot K. \tag{10b}$$

Table I lists the parameters and working values for variables used in Equations (7)–(10b). With the help of these values we can find:

$$\gamma \approx 4 \cdot 10^{13} \frac{J}{m^2}, \tag{11}$$

$$\Delta C/C_o \approx 0.01, \tag{12}$$

$$\Gamma \approx 20\,\text{km}. \tag{13}$$

4. Growth Rate of the CMB-Interface

Starting from the conservation condition Equation (4) we can introduce the correction term ΔC given in Equations (10a) and (10b). After a simple transformation we arrive at the following formulae for the growth rate of the CMB radius.

Model A:

$$\frac{dR}{dt} = \frac{D_m}{R}[C_\infty - C_0 - (2C_0\Gamma/R)][C_c - C_0 - (2C_0\Gamma/R)]^{-1}, \tag{14a}$$

TABLE I

Nomenclature and working values for some used parameters and variables

Symbol	Definition	Working value
$\Delta\rho$	density difference	5×10^3 kg/m^3
g	gravity	10 m/s^2
h	infiltration depth	10^3 m
R	core radius	3×10^6 m
R_c	radius of curvature of protrusion	10^5 m
V_{vol}	volume of the core per mole of solute (equal to molar mass of FeO divided by $\Delta\rho$)	1.4×10^{-5} m^3/mol
R_G	gas constant	83 J/K/mol
T_{CMB}	temperature at CMB	4×10^3 K
K	curvature $\approx 2/R$	0.7×10^{-6} m^{-1}

Model B:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \frac{D_m}{D}[C_\infty - C_0 - (2C_0\Gamma/R)][C_c - C_0 - (2C_0\Gamma/R)]^{-1}. \tag{14b}$$

Using $C_c = 0.30$, $C_\infty = 0.15$, $C_0 = 0.05$ and parameters already given in previous chapters we calculate the growth rate of CMB for the present CMB radius of about 3×10^6 m. We find that this growth rate is in the order of about meters per billion years (model A) and about 100 km per billion years (model B), respectively. The value of the growth rate of model B is a maximum value not taking into account the removal of material by other processes.

5. Stability Analysis of a Growing CMB with the Help of Angular Harmonics

Our starting point is the Laplace Equation (1) for the distribution of reaction products (FeO) in the reaction zone near CMB. We consider that any small disturbance of the spherical CMB-interface can be analyzed with the help of a sum of angular harmonic terms. The angular harmonics $Y_{lm}(\Theta, \phi)$ are labeled by the two integers l and m. We write the radius of the slightly perturbed sphere as

$$r(\Theta, \phi, t) = R(t) + Y_{lm}(\Theta, \phi)\delta(t), \tag{15}$$

where $R(t)$ is the spherical radius of the interface and $\delta(t)$ is the amplitude of a small perturbation corresponding to the height h from Figure 3. Using the well-known property of spherical harmonics:

$$\left[\frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta}\sin\Theta\frac{\partial}{\partial\Theta} + \frac{1}{\sin^2\Theta}\frac{\partial^2}{\phi^2}\right] Y_{lm} = -l(l+1)Y_{lm}, \tag{16}$$

we can find the following solution for the concentrations in the mantle and the core:

$$C_m = C_\infty + (C_e - C_\infty)\frac{R}{r} + \frac{Y_{lm}\delta B_m(t)}{r^{l1,}}, \tag{17}$$

$$C_c = \text{const} + Y_{lm}\delta r^l B_c(t), \tag{18}$$

B_m and B_c have to satisfy the boundary conditions. Furthermore, we have to introduce the curvature of a slightly distorted sphere

$$K = \frac{2}{R} - \left(\frac{2Y_{lm}\delta}{R^2}\right) + \left(\frac{Y_{lm}l(l+1)\delta}{R^2}\right), \tag{19}$$

which is independent of m.

The evaluation of the conservation condition Equation (4) for the slightly perturbed concentrations Equations (17) and (18) at the slightly perturbed radius Equation (15) requires the following conditions.

Model A:

$$\frac{\mathrm{d}\delta}{\mathrm{d}t} = \delta\frac{(l-1)D_m}{R^2}\cdot(C_c - C_e)^1\left[(C_\infty - C_e) - \frac{(l+1)(l+2)\Gamma C_0}{R}\right]. \tag{20a}$$

Model B:

$$\frac{\mathrm{d}\delta}{\mathrm{d}t} = \delta\frac{(l-1)D_m}{RD}\cdot(C_c - C_e)^1\left[(C_\infty - C_e) - \frac{(l+1)(l+2)\Gamma C_0}{R}\right]. \tag{20b}$$

Equations (20) are the main equations of the present paper. They describe the time derivative of a small perturbation δ. If this quantity is negative, the interface is stable. Any perturbation decays with time. On the other hand, if $\mathrm{d}\delta/\mathrm{d}t$ is positve, any small perturbation of the interface grows. In this case the original (spherical) interface is unstable. It is very interesting that the stability of the interface depends on the two terms inside the square brackets of Equation (20). The first term is the driving force for instability, coming from the concentration gradient in the mantle and the second term, resulting from the restoring effect of gravitational body force on a bumpy interface, drives stability. This stabilizing term depends on the degree l of the angular harmonics. Therefore the problem of interface stability is related to the length scale of the perturbation via l. Figure 4 shows the result of our stability estimation with $\delta \approx 10^3$ m. The interface is only unstable for long-wavelength perturbations with components $2 \leq l \leq 15$, with a maximum instability at $l = 9$.

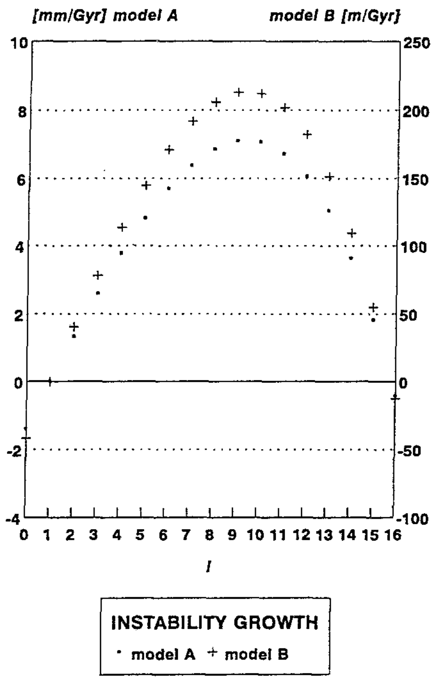

Fig. 4. Growth rate of a perturbation δ in dependence of the degree l of a spherical harmonic expansion.

6. Conclusions and Discussion

Chemical reactions at CMB are connected with processes of short-scale infiltration and large-scale dispersal of reaction products. The second process corresponds to an outward growing of the outer core radius. If gravitational body force acts as the tension against distortions of a growing CMB we find growth rates in the order of $\mathrm{d}R/\mathrm{d}t \approx$ m/Ga and $\mathrm{d}R/\mathrm{d}t \approx$ 100 km/Ga for our models A and B, respectively. The interface is always unstable for perturbations with $2 \leq l \leq 15$. Therefore our mechanism, if real, may be an explanation for the generation of large-scale undulations of CMB. The local distribution of undulations cannot be calculated from our model. We assume that processes in the mantle, as for example entrainment of lower mantle material by overlying convection, provide favoured regions for the development of instabilities of the reaction zone. It is interesting to note that from an analysis of the Earth's external gravitational field and from geomagnetic data Hide and Horai (1968) have already found that topography of the CMB should have such a structure that $4 \leq l \leq 8$ is realized, although the used geoid coefficients are different from those accepted now. Garland (1957) explained lower harmonics of the gravity field ($l = 3, 4, 5$) by bumps and valleys of CMB. A simple estimation (Melchior, 1986) provides small heights of about 200 m but large surface extensions in accordance with our results. Vogel (1960) already suggested an irregular shaped CMB of low-degree harmonic components on the basis of earthquake waves reflected at the CMB in good agreement with results of modern tomography (see e.g. Morelli and Dziewonski, 1987) and also with our estimations as shown above. Concerning the importance of our model for other terrestrial planets the application to Venus is evident while in the case of Mars it is not clear up to now if the transition pressure to the silicate perovskite stability field is really reached in the Martian mantle (Severova, 1991).

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Appendix A

Based on Figure 3 we first calculate the volume of a spherical cap of height x:

$$V_1 = \frac{\pi x^2}{3}(3R_c - x). \tag{A1}$$

Using geometrical relations we can express x with the help of given quantities:

$$R_c^2 - (R_c - x)^2 = a^2, \tag{A2}$$

$$(R - h)^2 - (R - h - x')^2 = a^2, \tag{A3}$$

$$x' = x - h, \tag{A4}$$

$$x = \frac{h}{2}\left(\frac{2R - h}{R - R_c}\right). \tag{A5}$$

This gives for V_1:

$$V_1 = \frac{\pi h^2}{2 \cdot 3 \cdot 4}\frac{(2R - h)^2}{(R - R_c)^3}(6RR_c - 6R_c^2 - 2Rh + h^2). \tag{A6}$$

Next we calculate the volume of a spherical cap of height x':

$$V_2 = \frac{\pi x'^2}{3}[3(R - h) - x']. \tag{A7}$$

Using similar relations as in (A2)–(A4) we find:

$$x' = \frac{h}{2}\frac{(2R_c - h)}{(R - R_c)}, \tag{A8}$$

$$V_2 = \frac{\pi h^2}{2 \cdot 3 \cdot 4}\frac{(2R_c - h)^2}{(R - R_c)^3}(6R^2 + h^2 - 6RR_c - 6Rh + 4R_c h). \tag{A9}$$

The volume change ΔV, caused by the protrusion is given by

$$\Delta V = V_1 - V_2, \tag{A10}$$

$$\Delta V = \frac{\pi h^2[4R_c(3R - 2h) - h(4R - 3h)]}{3 \cdot 4(R - R_c)}, \tag{A11}$$

which is used in the main text in Equation (8a).

In a similar way we can calculate the surface area of spherical caps of height x and x', respectively:

$$A_1 = 2\pi R_c x, \tag{A12}$$

$$A_2 = 2\pi(R - h)x'. \tag{A13}$$

With the help of Equations (A4) and (A5) we find for the change in surface area ΔA, caused by the protrusion:

$$\Delta A = A_1 - A_2, \tag{A14}$$

$$\Delta A = 2\pi\left[\frac{h}{2}\left(\frac{2R - h}{R - R_c}\right)(R_c - R + h) + (R - h)h\right], \tag{A15}$$

which is used in the main text in Equation (8b).

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