# Shear-induced material transfer across the core-mantle boundary aided by the post-perovskite phase transition

Nick Petford[1], Dave Yuen[2], Tracy Rushmer[3], John Brodholt[4], and Stephen Stackhouse[4]

[1]*Center for Earth and Environmental Science Research, Kingston University, Surrey, KT1 2EE, UK*
[2]*Minnesota Supercomputer Institute, University of Minnesota, Minneapolis, MN55455, USA*
[3]*Department of Geology, University of Vermont, Burlington, Vermont, 04505, USA*
[4]*Department of Earth Sciences, University College London, WC1E 6BT, UK*

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We present a novel mechanical model for the extraction of outer core material upwards across the CMB into the mantle side region of D$''$ and subsequent interaction with the post-perovskite (ppv) phase transition. A strong requirement of the model is that the D$''$ region behaves as a poro-viscoelastic granular material with dilatant properties. Using new *ab-initio* estimates of the ppv shear modulus, we show how shear-enhanced dilation promoted by downwelling mantle sets up an instability that drives local fluid flow. If loading rates locally exceed c. $10^{-12}$ s$^{-1}$, calculated core metal upwelling rates are $>10^{-4}$ m/s, far in excess of previous estimates based on static percolation or capillary flow. Associated mass flux rates are sufficient to deliver 0.5% outer core mass to D$''$ in $< 10^6$ yr, provided the minimum required loading rate is maintained. Core metal transported upwards into D$''$ may cause local rapid changes in electrical and thermal conductivity and rheology that if preserved, may account for some of the observed small wavelength heterogeneities (e.g. PKP scattering) there.
**Key words:** Post-perovskite, dilatancy, D$''$, core metal transport, strain rate, deformation.

## 1. Introduction

The extent and mechanisms by which material from the earth's liquid outer core interacts with overlying lower mantle is currently unresolved and controversial. Recent $^{187}$Os/$^{188}$Os isotopic models (Brandon *et al.*, 2003) and Fe/Mn ratios (Humayun *et al.*, 2004) suggest that the Hawaiian plume may have sampled c. 0.5% core material, inherited from a thermal or Fe-enriched chemical boundary layer at the core-mantle interface. This picture appears consistent with the recent discovery of a post-perovskite (ppv) silicate in the D$''$ layer whose phase transition is more sensitive to composition (Fe content) than pressure (Murakami *et al.*, 2004; Mao *et al.*, 2004) but inconsistent with W-Hf isotope data, also from Hawaii and apparently contradicting the hypothesis that evidence of core-mantle interaction is preserved in surface rocks (Schersten *et al.*, 2004). Clearly, the absence of a detectable core component in erupted magmas is not in itself evidence against core-mantle interaction, the most obvious expression of which is heat transfer (e.g. Gibbons and Gubbins, 2000; Olson, 2003). However, D$''$ is also a mechanical boundary layer capable of deforming (e.g. Garnero, 2000). The strain-field measured by seismic methods has revealed a detectable anisotropy due to the alignment of crystals or lateral changes in material (elastic) properties (Karato, 1998), while numerical simulations show that large strain deformation can accumulate at high stresses along the core mantle boundary (CMB) in the region of downwelling slab material (McNamara *et al.*, 2002). In addition, seismic data further suggest the presence of a silicate melt fraction at D$''$ in the range c. 6–30% (Garnero, 2000). The latter can be explained by in-situ partial melting of perovskite (Lay *et al.*, 2004). However, density arguments make emplacing outer core material into D$''$ via buoyancy fluxing problematic, and quantification of the material transfer process(es) responsible remain speculative (Stevenson, 2003).

Motivated by the challenge of providing a physical mechanism of material transfer across the CMB, we have undertaken a set of zeroth order calculations that derive estimates of the pressure changes and subsequent fluid flow rates relevant to a deformable poro-viscoelastic matrix as a function of applied shearing stress. In this purely mechanical model, we argue that episodic, high deformation rates at the CMB, and the presence of core liquid metal in D$''$ may be intimately coupled, with mass and heat transfer across the interface driven by downwelling of more dense material from higher levels in the mantle. The macroscopic part of the problem has been modelled successfully in recent large scale numerical simulations of whole mantle flow (Kellogg *et al.*, 1999; McNamara *et al.*, 2002), and the deformation effects arising from this are summarised elegantly by Karato (1998). Our approach combines a microscale, shear-dilatancy sensitive material deformation model for the solid component of D$''$ idealised to a set of constant moduli to simplify the analytical solutions (Koenders and Petford, 2000), coupled to the macroscale dynamics. A comparable microscale formalism for two-phase flow with Maxwellian viscoelastic rheology in the upper mantle has been devel-

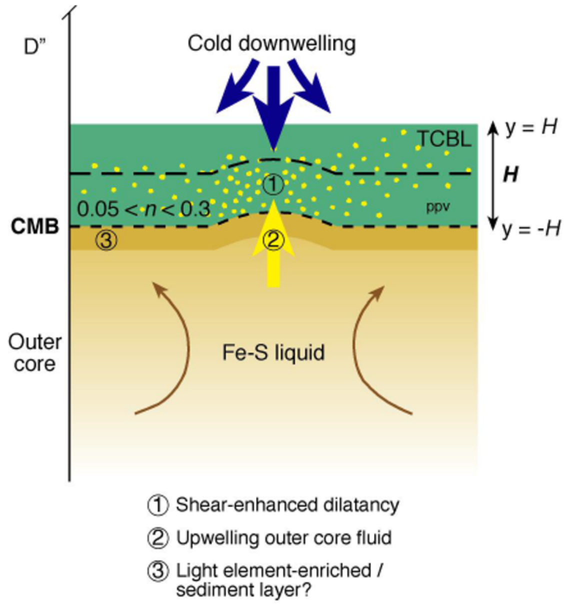


Fig. 1. Diagram showing the simplified geometry of a thermal and chemical boundary layer (TCBL) of thickness $H$ undergoing loading by downwelling dense material (blue arrows), inspired by Kellogg *et al.* (1999), and Karato (1998). Three zones are identified: (1) region of shear-enhanced (poroviscoelastic) dilatancy, (2) upwelling outer core fluid shown as yellow arrow, and (3) Compositionally buoyant upper layer of uncertain thickness and extent that may contain sediments (Buffett *et al.*, 2000; Alfe *et al.*, 2002). The thermal effect of upwelling core material on the positioning of the pv-ppv phase bounary is approximated by the upper dashed line.

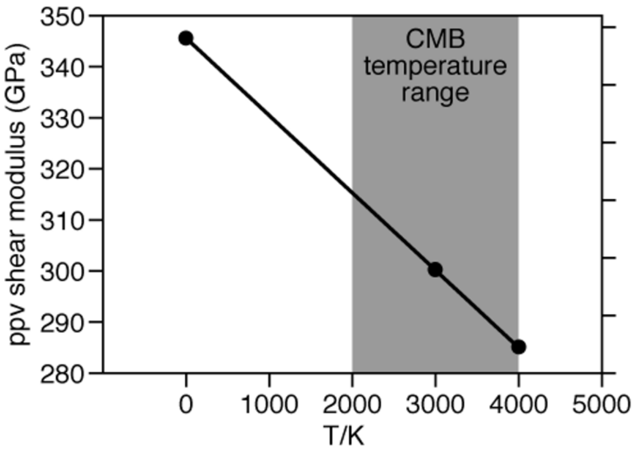


Fig. 2. Plot showing post-perovskite shear modulus ($G$) as a function of temperature corresponding to a pressure of 136 GPa, calculated using a molecular dynamics *ab-initio* approach (Stackhouse *et al.*, 2005). The estimated temperature interval in the region of the CMB is shown (shaded) for reference.

oped recently (Vasilyev *et al.*, 1998), and we expect the Deborah number ($De$), which measures the importance of elasticity in this phenomenon, to be of order 1 or greater in the D$''$ layer. For reasons outlined below, knowledge of the shear modulus ($G$) of the new post perovskite phase is most helpful in this respect.

Previous numerical simulations of D$''$ suggest that dense material, concentrated in regions of downwelling, can also be entrained in upwellings. The result is to impose a topography on D$''$ that is steep and of large amplitude, and whose structure is most likely coupled to the overlying mantle (Loper and Lay, 1995; Olson, 2003). As discussed in more detail below, calculated core fluid upwelling velocities scale with the rate of deformation, and because the problem is phrased in terms of shear strain rates are independent of key intensive fluid (Fe metal alloy) properties.

## 2. Analysis

Our analysis is based on a material deformation model of the linear-elastic, isotropic relations first proposed by Biot (1941), but modified to include the effects of dilatancy under deviatoric (pure shearing) motion. Details of the model, including full analytical solutions to the governing differential equations, are given in Koenders and Petford (2000) and Petford and Koenders (2003) and not repeated in detail here. A key feature of this analysis is the coupling of pure shearing stress to volumetric strain, so that the modified Biot equation captures many important parameters relevant to deforming porous layers including the average melt displacement, melt (fluid) pressure, permeability and the set of general moduli of the solid framework. Although the latter are a source of error due to uncertainties in mantle rheology at appropriate pressures and temperatures (Mitrovica and Forte, 2004), molecular dynamics simulations of the newly discovered post-perovskite phase (Oganov and Ono, 2004; Tsuchiya *et al.*, 2004; Stackhouse *et al.*, 2005) enable estimates of some key material properties of a ppv-dominated lower mantle, specifically the bulk and shear moduli as a function of temperature, to be made with some degree of confidence. The dilatancy instability which drives fluid flow by reducing the local intergranular pressure, requires a porosity field as an initial condition. This is provided by a background silicate melt fraction of up to 30%, located in discrete regions of high heat flow close to the CMB, and responsible for observed heterogeneity in seismic velocity there (Garnero, 2000; Lay *et al.*, 2004). The porous matrix is assumed to be granular in nature so that external deformation results in a dilatant effect that can be captured mathematically. Biot's equation for the consolidation of compressible fluid flow in a porous material with position-dependent permeability takes the form

$$\frac{\partial}{\partial y}\left(k(y)\frac{\partial p}{\partial y}\right) = n\beta\frac{\partial p}{\partial t} + \frac{\partial \dot{v}}{\partial y} \qquad (1)$$

where $n$ is the porosity and $\beta$ is the fluid compressibility. The permeability is assumed constant, and depends on the granular (ppv) length scale $d$, outer core fluid viscosity ($\eta$) and the melt fraction. The total stress is $\sigma_{ij} = \sigma'_{ij} - p\delta_{ij}$, where $p$ is the excess pore pressure and $\sigma'_{ij}$ is the skeletal stress (Terzaghi, 1943). The vertical coordinate is $y$, the two horizontal coordinates are $x$ and $z$. The stress equilibrium requires that $\partial\sigma_{ij}/\partial x_{ij} = 0$, which for a problem that does not depend on $x$ and $z$ results in $\sigma'_{xy} = c(t)$ and $\sigma'_{yy} - p = d(t)$, where $c(t)$ and $d(t)$ are time dependent constants.

Under appropriate boundary conditions, Biot's equation (above) above can be solved analytically to yield explicit expressions for the excess pore fluid pressure and the local flow rate (see Petford and Koenders, 2003, appendix A for full details). A number of simplifications are introduced.

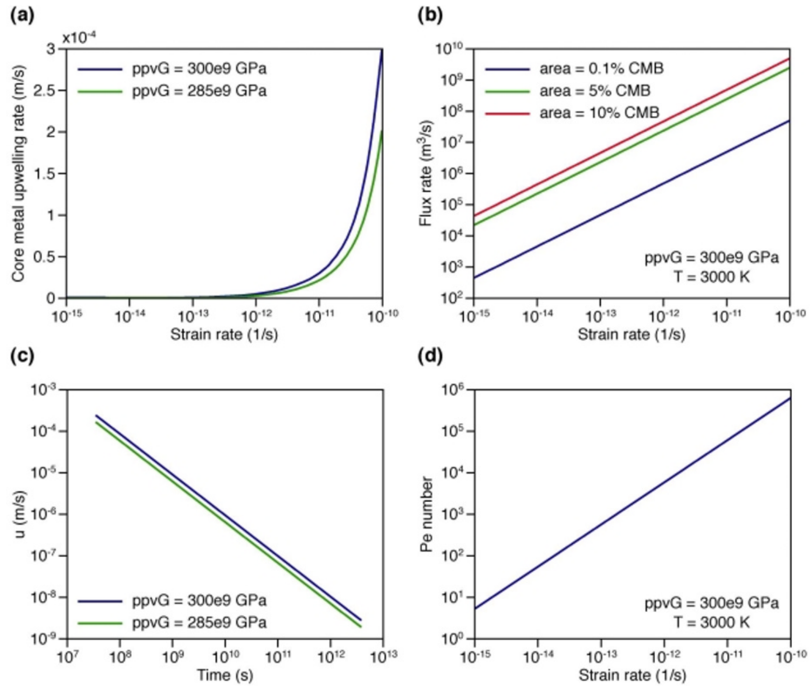


Fig. 3. (a) Calculated core liquid metal flow rates (m/s) as a function of strain rate assuming a ppv shear modulus of 300 and 285 GPa (3000 < T < 4000 K, cf. Fig. 1). The strain rate interval relevant to the problem lies in the region $10^{-15} < \dot{e} < 10^{-10}$ s. Note that flow of outer core material into D″ will only be active while loading is constant. Relaxation to strain rates $< 10^{-12}$ s$^{-1}$ will slow the rate of flow considerably, or even prevent it altogether. (b) Volumetric flux rate (m$^3$/s) into D″ as a function of loading rate for three cross sectional areas of the core mantle boundary corresponding to 0.1, 5 and 10% of the total surface area. (c). Transport (residence) time of core fluid in a 10 km deep mantle layer overlying the CMB for two values of the ppv shear modulus $G$. (d). Thermal Peclet number ($Pe = uH/\kappa$) where $u$ is the average fluid flow velocity and $\kappa$ is the thermal diffusivity of liquid Fe at 1673 K ($5.7 \times 10^{-6}$ m$^2$s). $Pe >> 1$ where $\dot{e} \gtrsim 10^{-13} s^{-1}$.

As the thickness of D″ is variable, for simplicity we define a zone within D″ of height $H$, where the behaviour of the top and bottom zones are represented by suitable boundary conditions (Fig. 1). These are an impermeable top layer ($\partial p/\partial y = 0$) and a permeable (fluid) base, corresponding to the core-mantle interface where no excess pore pressure is expected.

Fluid flow accompanying the dilatancy effect in unconsolidated, densely packed granular material is independent of fluid density (see Reynolds, 1885; Rowe, 1962). Our hypothesis rests on the assumption that dilatancy can operate in a broadly similar way in the deep earth in regions of elevated background porosity (melt fraction). In this respect it is relatively controversial. The attraction however is that Reynolds dilatancy provides a plausible mechanism, grounded in standard physics, capable of modifying locally the stable density gradient that defines the CMB region. A shear-enhanced melt migration model also overcomes problems relating to percolation of Fe-liquid metal through a silicate matrix constrained by high dihedral angles (Rushmer *et al.*, 2000; Bruhn *et al.*, 2000; Terasaki *et al.*, 2005). Experimental evidence for the shear-enhanced mobility of liquid metal (although not at the required PT conditions), comes from rock deformation studies on natural Fe-bearing H-chondrites loaded at laboratory strain rates (c. $10^{-5}s^{-1}$) where a dilation effect is observed, causing partially molten liquid metal to flow into sites of low pressure (Rushmer *et al.*, 2005). Clearly any model of fluid transfer between the outer core and D″ based on buoyancy forces alone (e.g. McKenzie, 1984), *would* need significant modification (Kanda and Stevenson, 2004).

## 2.1 Time constants and flow rates

Typical values for the time constant of the process are now estimated. The maximum value of the pressure at the top of the region is obtained at $t = t^* H^2 (1 + n\beta\theta) / (\theta k)$. The stiffness $\theta$ is the dilatant modulus for the densely packed ppv granular layer, currently a poorly known quantity, and taken in the range $10^9 - 10^{10}$ Pa. The lengthscale $H$ under investigation is of the order 10 km, chosen to correspond with the lower end of wavelength scattering (e.g. the range in smallest scale heterogeneities) observed seismically at the CMB (Garnero, 2000). Taking a mean ppv grain size of 1 mm in the vicinity of the CMB gives a characteristic timescale of the problem of some $10^2 - 10^4$ yrs. Note that the time constant of the problem is independent of the shear rate $\dot{c}_0$.

The flow rate at the end (the steady state) of the process in the vicinity of $y = H/2$ (Fig. 1) is now considered (the short time solution is given in Koenders and Petford, 2000). The outcome is

$$t \to \infty : k\frac{\partial p}{\partial y} = \frac{-HR\dot{c}_0}{2\theta} = \frac{-HG\dot{e}}{\theta} \tag{2}$$

with both pressure and flow rate dependent on the shear stress rate $\dot{c}_0$. Typically this value is of the order of the product of the principal modulus $G$ and the strain rate $\dot{e}$. Recent *ab-initio* molecular dynamics calculations are used to provide estimates of $G$ for the post perovskite phase (Fig. 2), whose material properties are likely to govern the rheology of the lowermost mantle. At conditions relevant to

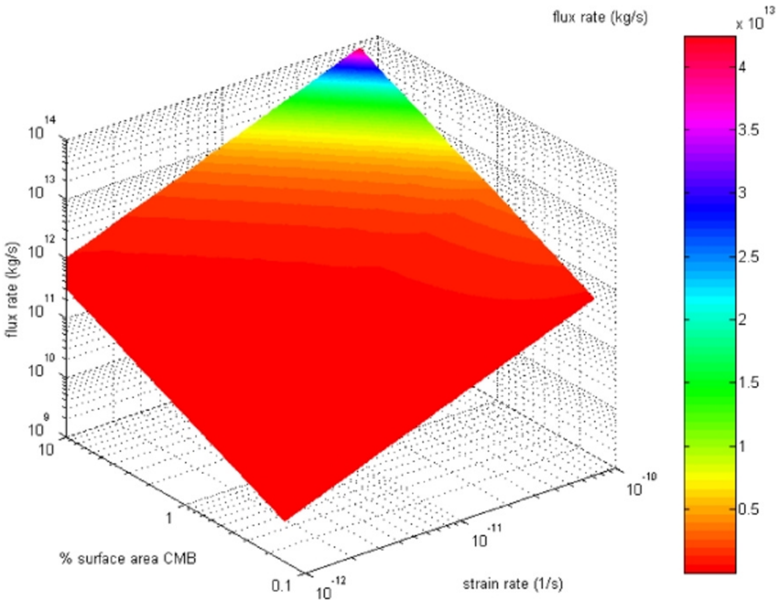


Fig. 4. Plot showing mass flux rate ($\rho = 10^4$ kg/m$^3$) as a function of loading rate interval and area of CMB deformed (defined arbitrarily as 0.1 to 10% total CMB surface area). Mass flux rates during constant loading where $Pe >> 1$ are in excess of $10^{11}$ kg/s.

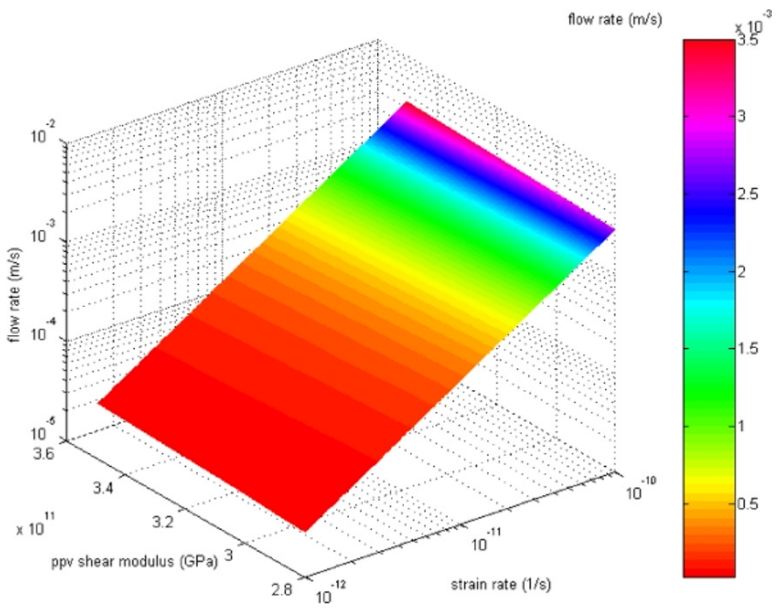


Fig. 5. Plot showing the effect of changing ppv shear modulus ($G$) on average upwelling flow velocity. The rate of flow appears relatively insensitive to the precise value of $G$.

the CMB ($P = 136$ GPa) the calculated ppv shear modulus ranges from 285 GPa ($T = 4000$ K) to 300 GPa at $T = 3000$ K (Stackhouse *et al.*, 2005). These values are used to inform the analytical calculations that follow.

## 3. Results

Specimen calculations that illustrate the consequences of dilational instability and explore the sensitivity of outer core fluid upwelling over a strain rate interval $10^{-15} < \dot{e} < 10^{-10}$ s$^{-1}$ are now given. The lower limit is characteristic of background mantle convection (Turcotte and Schubert, 2002), while the upper limit corresponds to a total strain in layer thickness $H$ of 10% in 10 years. Figure 3 summarises the results of several calculations aimed at determining order of magnitude flow and mass flux rates of upwelling outer core liquid across the CMB in response to deformation-driven dilatancy in D$''$. The flow rate calculations are shown for two values of the post-perovskite shear modulus that correspond to a temperature difference of 1000 K at constant pressure (136 GPa).

The key variable governing the rate of upwelling is the strain rate. In contrast, the effect of matrix temperature on flow rates expressed through the ppv shear modulus is small, on the order of 5%. Average flow rates into the D$''$ layer are negligible ($< 10^{-6}$ m/s) until the local strain rate exceeds $10^{-12}$ s$^{-1}$. Above this value, regarded as a minimum for significant upwards transport of liquid core metal, flow rates increase steadily to a maximum of c. $3 \times 10^{-4}$

m/s at $\dot{e} = 10^{-10} s^{-1}$ (Fig. 3(a)). Estimates of volumetric flux rates into the base of D″ are shown in Fig. 3(b) as a function of area fraction of CMB deformed. To emphasize the locality of the effect (clearly the entire CMB cannot be deformed simultaneously), three cross sectional areas corresponding to 0.1, 5 and 10% of the total CMB surface area (c. $1.5 \times 10^{14}$ m$^2$) are used. As with average flow rates, volume flux rates increase with increasing strain rate for a given area of CMB deformed, from a minimum of c. 500 $m^3/s$ ($\dot{e} = 10^{-15}$ s$^{-1}$, area fraction CMB $= 1 \times 10^{-3}$), to c. $10^9$ m$^3$/s ($\dot{e} = 10^{-10}$ s$^{-1}$, area fraction CMB $= 0.1$). It is instructive also to consider the potential transport time of infiltrating core fluid. Consider a vertical distance ($H$) upwards from the CMB to a height of 10 km, a lengthscale characteristic of the observed small scale geophysical heterogeneity in D″ (Garnero, 2000). Outer core material could in principle be transported this distance in $10^2$ to $10^3$ years provided loading remains constant at $\dot{e} = 10^{-12}$ s$^{-1}$. If higher rates of strain ($10^{-10}$ s$^{-1}$) can be achieved, transport times are of the order $10^8$ s (several years). We do emphasise however that these results are tentative and should be treated accordingly. Indeed, an important aspect of the infiltration process not considered in detail here are thermal effects, in particular the possibility that liquid core metal will freeze during upwards flow. A crude analysis of the thermal regime is shown in Fig. 3(d), where the thermal Peclet number ($Pe$) is plotted against strain rate. For plate tectonic loading rates, $Pe$ is close to 1, and does not significantly exceed unity until strain rates exceed c. $10^{-12}$ s$^{-1}$.

The corresponding mass flux can also be estimated, assuming a constant value for the liquid metal density. Results are summarised in Fig. 4, which shows the changing mass flux as a function of loading rate and CMB area deformed. For example, provided flow is continuous (itself a major assumption), a mass flux rate of $10^{11}$ kg/s, corresponding to a strain rate of order $10^{-12}$ s$^{-1}$ and $Pe >> 1$ would in principle deliver 0.5% outer core material by mass into the lowermost mantle, a requirement based on geochemical arguments (Brandon *et al.*, 2003), in $<< 10^6$ yrs. Clearly the flux rate is sensitive to the cross sectional area and strain rate, (although relatively insensitive to exact value of the ppv shear modulus, Fig. 5), and could vary by several orders of magnitude around this value. Cessation of loading might prolong the process indefinitely. The point is made however, that the viscoelastic dilatancy instability, while sustained, offers a means of transporting substantial amounts of material across the CMB on geologically very short timescales.

## 4. Discussion

While acknowledging that further experimental and computational mineral physics work is needed to constrain and test the validity of the proposed dilatancy mechanism, a strong feature of the model as it stands is that a dynamic coupling between the liquid outer core and overlying lowermost mantle is a necessary (albeit transient) condition. Here, the lower mantle responds on the microscale (characteristic lengthscale mm to m), to macroscopic convective motions (characteristic lengthscale >> km). This contrasts with previous models for material transfer across the CMB such as electrochemical transfer of Fe and Ni (Ringwood, 1959) and upwards percolation of Fe metal alloy due to capillary effects (Poirier, 1993), which are passive processes. These effects are small, with lengthscales on the order of metres, compared with the potential mass flux due to the shearing mechanism described here, even if the required dilational instability is short lived.

Although possibly a rare event restricted in space and time, a number of important geodymanical implications flow from our model of material transfer. Firstly, it provides a mechanism for upwards transport of outer core material into D″ capable of imparting a distinctive HSE chemical signature into the lowermost mantle, that couples known large scale mantle flow processes with recent geochemical observations for core-mantle interactions (e.g. Humayun *et al.*, 2004). Secondly, given the strong dependence of the post-perovskite phase transition on composition, periodic excursions of infiltrating Fe-rich fluid from the uppermost outer core into the lowermost mantle, possibly enriched in incompatible elements (Alfe *et al.*, 2002), may have profoundly affected the positioning of this transition over time. For example, Fe can stabilise the ppv structure at pressures of c. 10 to 20 GPa lower than the pure $MgSiO_3$ end member for a given CMB temperature (Mao *et al.*, 2004), with the estimated drop in inversion temperature along an isotherm of c. −1 GPa per 1 mol% Fe. Charged coupled substitutions analogous to those described for Mg-perovskite (Walter *et al.*, 2004) may also help to modify the chemical potential of D″ close to the CMB. Large amounts of Fe may be responsible for ultra low velocity zones (Mao *et al.*, 2004), although other mechanisms related to topography such as sedimentation in CMB basins should not be ruled out (Buffett *et al.*, 2000; Olson, 2003). In this case, the analogy between sedimentary ULVZs and the granular deformation model proposed here is striking and worthy of further investigation. Indeed, the dilatant effect may be more pronounced in outer core sediments, should they exist, than in the overlying silicate mantle.

Even if upwelling core metal does not install a surface measurable, radiogenic isotopic potential in D″, it is likely to produce a rheological effect that could influence the elastic properties of ppv and produce changes in electrical and thermal conductivity (Manga and Jeanloz, 1996). In particular, trapping by surface tension effects of pockets of isolated, immiscible core melt as the loading event wanes, provides a both a mechanism and resulting geometry to account for the intense small-scale heterogeneity (large PKP precursors) at the CMB in addition to any seismic heterogeneity and anisotropy due to ferromagnesian ppv silicate (e.g. Tsuchiya *et al.*, 2004). Finally, we emphasise that the ppv phase transition itself will aid the extraction mechanism due to stress changes related to negative volumetric changes in downwelling regions and positive (expansive) changes during upwelling. Critically, no similar phase transitions occur in the lithosphere or upper mantle.

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N. Petford (e-mail: n.petford@kingston.ac.uk), D. Yuen, T. Rushmer, J. Brodholt, and S. Stackhouse