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A note on the sensitivity of mantle convection models to composition-dependent phase relations

Craig R. Bina

Department of Geological Sciences, Northwestern University, Evanston, Illinois

Mian Liu

Department of Geological Sciences, University of Missouri, Columbia, Missouri

Abstract. Numerical simulations of mantle convection are highly sensitive to the dependence of phase relations upon pressure, temperature, and composition. Phase transitions in the (relatively silica-poor) olivine components of the mantle tend, with increasing iron content, to inhibit convective mass transfer between the upper and lower mantle. Those occurring in the (relatively silica-rich) non-olivine components fail to inhibit (and indeed promote) such mass transfer. Behavior in the real mantle must entail an interplay between such competing effects, with the finite width of multivariant phase fields acting to mitigate impediments to flow. Attempts to directly correlate computed flow or temperature fields with models derived from physical observables should be approached with caution, given the sensitivity of the former to compositional heterogeneity and uncertainties in phase relations.

Introduction

The occurrence of mineralogical phase transitions in the Earth's mantle [*Ringwood*, 1970] has long been inferred to impose significant constraints upon the convective dynamics of the interior. Early work [*Richter*, 1973; *Schubert et al.*, 1975; *Christensen and Yuen*, 1984, 1985] demonstrated that the sign and magnitude of the Clapeyron (pressure-temperature) slopes of phase transitions are important in determining the extent to which the upper and lower mantle may mix or remain stably stratified. More recent studies [*Nakakuki et al.*, 1994; *Solheim and Peltier*, 1993, 1994; *Tackley et al.*, 1993, 1994; *Honda et al.*, 1993; *Weinstein*, 1992, 1993; *Peltier and Solheim*, 1992; *Zhao et al.*, 1992; *Liu et al.*, 1991; *Machetel and Weber*, 1991] have suggested that, because of its negative Clapeyron slope, the disproportionation of γ-spinel into magnesiowüstite and silicate perovskite (the $\gamma \rightarrow pv + mw$ transition) at 660 km depth has the potential to inhibit mantle circulation and to induce time-dependent instabilities so that even a stably stratified mantle may occasionally mix through catastrophic overturn events. We may briefly summarize such work by noting that the local body forces induced by thermal distortion of phase boundaries with negative Clapeyron slopes tend to inhibit mantle circulation across such phase transitions and that strong time-dependent instabilities may be induced near phase boundaries.

In such studies, the phase transitions are approximated by univariant phase boundaries with fixed Clapeyron slopes in simple compositions (e.g., the $\alpha \rightarrow \beta$ transition in pure Mg_2SiO_4). Thus, the 660 km seismic discontinuity is represented by the univariant $\gamma \rightarrow pv+mw$ transition in Mg_2SiO_4, whose fixed negative Clapeyron slope inhibits transport between the upper and lower mantle. Similarly, the 410 km seismic discontinuity is represented by the univariant $\alpha \rightarrow \beta$ transition in Mg_2SiO_4, whose fixed positive Clapeyron slope does not inhibit transport.

The magnitudes of such Clapeyron slopes, however, are not necessarily constant; they may be functions of pressure and temperature [cf. *Bina and Helffrich*, 1994]. Moreover, the actual identity of the relevant phase transition, and thus the magnitude and sign of the corresponding Clapeyron slope, may change with pressure and temperature. This was explored recently by *Liu* [1994], who noted that the $\gamma \rightarrow pv + mw$ transition in endmember Mg_2SiO_4 olivine is replaced by the $\beta \rightarrow pv + mw$ transition at high temperatures (Figure 1a). While the former possesses a negative Clapeyron slope, so that descent of cool downwellings whose geotherms pass below the triple point is inhibited, the latter possesses a zero or weakly positive Clapeyron slope (due to its greater volume decrease and more negative entropy change), so that ascent of warm upwellings whose geotherms pass above the triple point is not inhibited. The striking asymmetry which results, in which the phase boundary resists the descent of subducting slabs but not the ascent of rising plumes, can be seen in Figure 2a. Higher Rayleigh numbers serve to amplify mixing.

Here we expand upon the work of *Liu* [1994], noting that phase relations depend not only upon pressure and temperature but also upon composition. The identity of the relevant phase transitions, and thus the nature of any corresponding Clapeyron slopes, are functions of chemical composition. Because the mantle is a complex multicomponent chemical system, and because it should be characterized by varying degrees of compositional heterogeneity [e.g., *Metcalfe et al.*, 1995], we explore the sensitivity of mantle convection simulations to such composition-dependent variations. Compositional heterogeneity may also induce chemical buoyancy effects [*Liu and Chase*, 1991], such as the reversal whereby oceanic crustal compositions become intrinsically less dense than pyrolite mantle compositions over the 670-710 km depth

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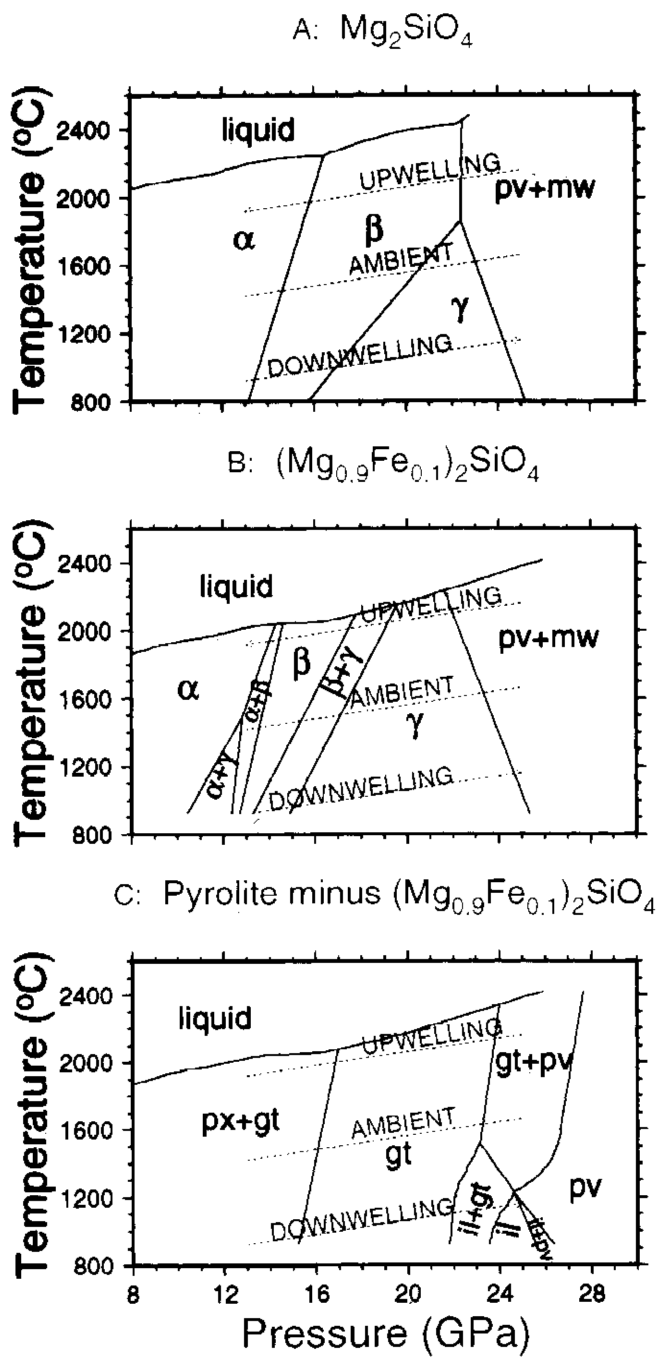

Figure 1. Schematic phase diagrams for Mg_2SiO_4 olivine (A), $(Mg_{0.9}Fe_{0.1})_2SiO_4$ olivine (B), and pyroxene-garnet components (C), after *Gasparik* [1990] and *Ita and Stixrude* [1992]. Phases are olivine (α), modified spinel (β), spinel (γ), perovskite (pv), magnesiowüstite (mw), pyroxene (px), garnet (gt), and ilmenite (il). Broken lines depict highly schematic geotherms for ambient mantle, cold downwellings, and hot upwellings.

interval [*Irifune and Ringwood*, 1987], but we restrict the focus of this study to the effects upon convection models of changes in phase relations.

Method and Results

To obtain our results, we have used the finite difference method to solve a numerical model formulated within the extended Boussinesq approximation in a two-dimensional Cartesian box, employing a sheet of anomalous mass at the phase boundary to approximate the local body force induced by phase boundary distortion. The thickness of the sheet is determined by the Clapeyron slope and the lateral temperature contrast. To isolate phase transition effects, we have assumed an isoviscous mantle. The Rayleigh number is 1×10^6, and adiabatic and viscous heating effects are included. Our grid is 100 by 100, giving a spatial resolution of 15 km vertical and 45 km horizontal. (For further details of the method, see *Liu* [1994].)

To investigate compositional effects, we examine the above case of pure Mg_2SiO_4, extending it to natural mantle $(Mg_{0.9}Fe_{0.1})_2SiO_4$ olivine compositions. As can be seen in Figure 1b, the entropy of mixing contributed by Fe solid solution shifts the β and γ stability fields to lower pressures. Thus, the point at which the relevant Clapeyron slope increases (due to high-temperature stabilization of β at the expense of γ) shifts to higher temperatures (indeed, above the solidus [*Chopelas et al.*, 1994]). Hence, both upwellings and downwellings now are inhibited by the negative Clapeyron slope, as can be seen in the results of the corresponding numerical model in Figure 2b. Higher Rayleigh numbers amplify this blocking effect.

Furthermore, we may consider the behavior of more silica-rich mantle components such as $MSiO_3$ pyroxene and $M_3Al_2Si_3O_{12}$ garnet (M = Mg, Fe, Ca, etc.). Phase relations in the pyrolite components other than $(Mg_{0.9}Fe_{0.1})_2SiO_4$ olivine are depicted in Figure 1c. The relevant change in Clapeyron slope now occurs where the $il \rightarrow pv$ transition gives way to the $gt \rightarrow pv$ transition with increasing temperature. Again, the former transition possesses a negative Clapeyron slope, and the latter possesses a zero or weakly positive slope (due to the greater volume decrease and more negative entropy change). The point at which the the relevant Clapeyron slope increases, however, now occurs at significantly lower temperatures (since the large entropy of the garnet structure restricts the stability field of ilmenite to low temperatures). Hence, neither upwellings nor downwellings are inhibited for these components, as illustrated in the results of the corresponding numerical model in Figure 2c.

Discussion

In the above analyses, while considering the dependence of phase relations upon pressure, temperature, and composition, we have consistently treated the phase transitions as occurring nonlinearly over a finite depth interval (i.e., Gaussian depth-distributed with 2σ of 15 km). Strictly speaking, since these are multivariant transitions (Fe solid solution, for example, giving rise to a $\beta + \gamma$ divariant field in the olivine phase diagram of Figure 1b), strict thermodynamic Clapeyron slopes are undefined. Thus, we are actually employing some sort of "effective" Clapeyron slope [cf. *Bina and Helffrich*, 1994; *Helffrich and Bina*, 1994]. Furthermore, the broadening of phase transitions from univariant lines in simple systems to multivariant fields of finite width in multicomponent systems serves to diminish the blocking effects of boundaries with negative Clapeyron slopes [*Tackley*, 1994].

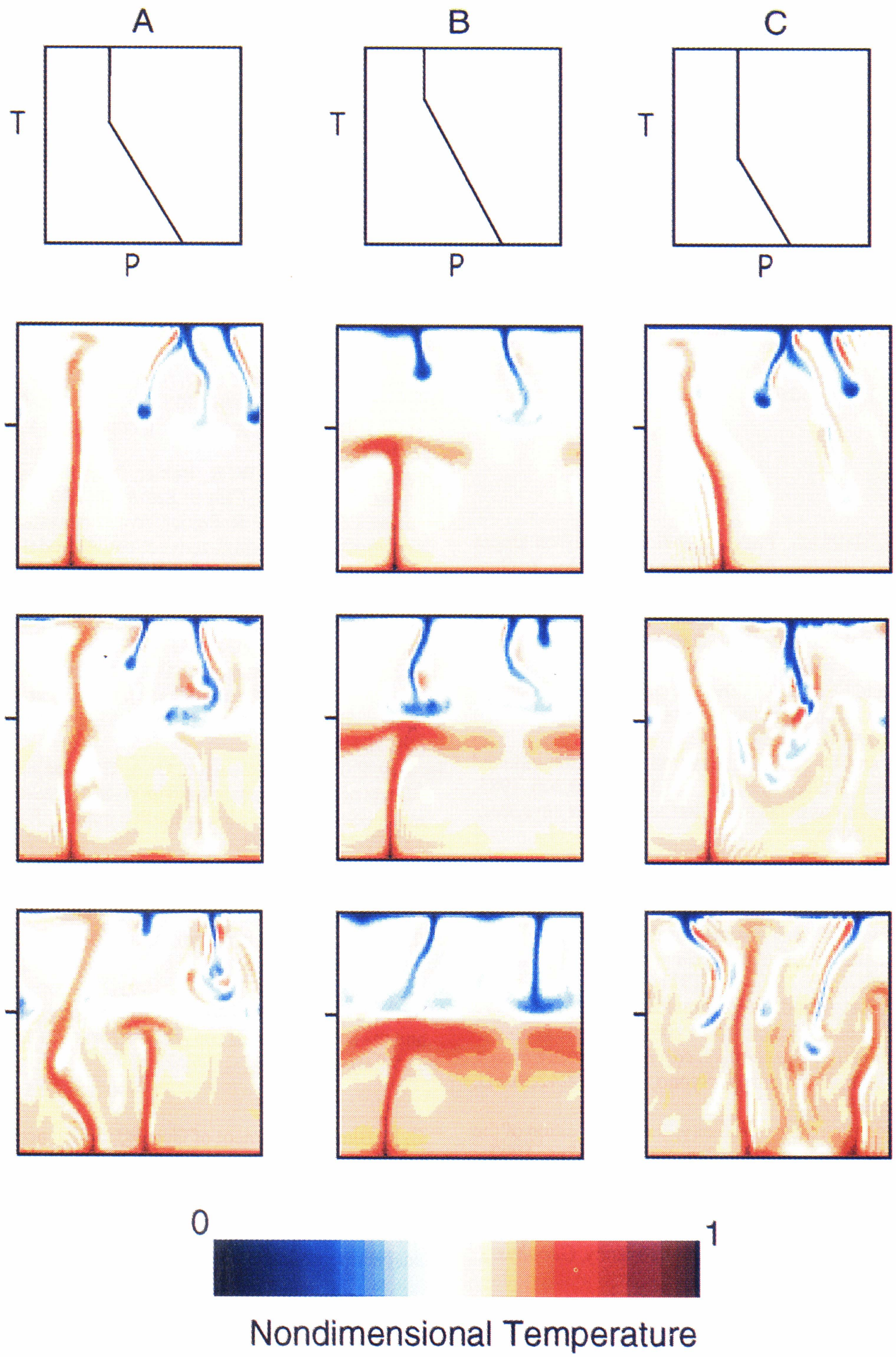

Figure 2. Numerically simulated evolution of mantle thermal field for three phase diagram topologies. Phase transitions change Clapeyron slope from -4 to 0 MPa/K above 1800°C (A), 2100°C (B), or 1350°C (C). Rayleigh number in all cases is 1×10^6. Tick marks indicate 660 km depth. Aspect ratio is three (horizontal) to one (vertical). Images in each column are sequential snapshots of thermal field. Top panels: beginning of experiment, convection has gone through one overturn. Middle panels: after two to three overturns. Bottom panels: after four to five overturns.

While phase transitions in the (SiO_2-poor) olivine components of the mantle tend, with increasing Fe content, to inhibit convective mass transfer between upper and lower mantle, those occurring in the (SiO_2-rich) non-olivine components of the mantle fail to inhibit (and indeed enhance) such mass transfer. Further compositional broadening of multivariant transitions (by solid solution effects) should act to further mitigate impediments to flow. Behavior in the real mantle must represent some complex balance between such competing effects. We conclude that the details of computed mantle convection simulations are highly sensitive to the details of phase relations as functions of pressure, temperature, and composition. Therefore, attempts to directly correlate computed flow or temperature fields with models derived from physical observables (such as three-dimensional seismic velocity structures) should be approached with caution, given the sensitivity of the former to compositional heterogeneity and uncertainties in phase relations.

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C. R. Bina, Department of Geological Sciences, Locy Hall, Northwestern University, Evanston, IL 60208-2150. (e-mail: craig@earth.nwu.edu)

M. Liu, Department of Geological Sciences, University of Missouri, Columbia, MO 65211. (e-mail: mian@earth.geosc.missouri.edu)

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