Perspectives on shallow mantle melting from thermodynamic calculations

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Introduction

Understanding the relationship between mantle processes and formation of oceanic crust requires a method for modeling the composition and amount of melt produced as functions of temperature, pressure, and mantle composition. Empirical parameterizations constructed for this purpose have greatly enhanced our understanding of mantle melting, but they do not incorporate self-consistent relationships between phase equilibria and melting energetics. Here we describe a different approach, in which the melting process is calculated from thermodynamic models for minerals and silicate melts. These calculations represent the first attempt to use thermodynamic predictions to explore the connection between melting reactions and the energetic quantities (entropies, volumes, and heat capacities) that control mantle melting. This method holds particular promise for understanding aspects of mantle melting that cannot easily be inferred from empirical parameterization of phase equilibrium experiments (e.g. melt compositions at very low melt fraction, melt production during fractional fusion, and adiabatic paths for partially molten peridotite, with and without melt segregation.)

Thermodynamic calculations of peridotite partial fusion have been performed using MELTS, which calculates silicate liquid–mineral equilibria by thermodynamic potential minimization (Ghiorso and Sack, 1994; Ghiorso et al., 1994). MELTS was developed to simulate low pressure crystallization of silicate liquids, but has been adapted to model peridotite melting at pressures up to 3 GPa. We approximated fractional fusion by calculating 1% melting increments, removing the melt, and repeating the melting step with the residue. Batch fusion along adiabatic paths was simulated by locating T–P trajectories of constant entropy; fractional fusion during upwelling was approximated by holding the entropy constant for each incremental ascent/melting step.

Isobaric batch melting

Isobaric calculations of partial melting of fertile peridotite show realistic phase relations and qualitatively good agreement with liquid compositions from the 1 GPa experiments of Baker and Stolper (1994), which are not part of the MELTS database (Fig. 1). Relative to the experiments, calculated liquids have too much MgO and too little SiO_2, reflecting the overstability of orthopyroxene by about 2 kJ at 1 GPa. The high calculated MgO concentrations lead to temperatures that are systematically high (by ~ 50–$75°$) for a given melt fraction. Na contents of the calculated liquids are also too high (Fig. 1), reflecting either the necessity for small adjustments in the free energy of formation of the jadeite component or the absence of a ureyite component. Such adjustments, which can be easily incorporated to improve the details of the calculated melt compositions, will be made in the future.

An important feature of the calculated fusion path is the behaviour at < 5% melting. This is a region for which there are few experimental constraints, but that may be very important to MORB petrogenesis because total amounts of melting may be only 5–20% for most MORBs and because it is in the early stages of incremental melting that geochemical characteristics related to highly incompatible elements (e.g. U/Th systematics) are set. Our calculations indicate that during the first stages of melting of fertile peridotite, the amount of melt produced per temperature increment is small (< 0.1%/°C). Liquid composition changes rapidly in the early stages of melting
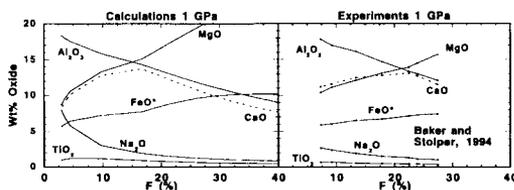

FIG. 1.

as Na_2O is diluted and these large changes in melt composition are accompanied by significant changes in temperature. This effect is exaggerated in our calculations relative to that expected in natural systems because calculated Na_2O concentrations are too high.

Predicted mineral/liquid partition coefficients of some trace elements change in response to the rapid changes in liquid composition at low melt fraction. For example, we predict that Ti is increasingly compatible in pyroxenes at low melt fraction. We speculate that similar effects will result in large increases in partition coefficients of other highly charged trace elements (e.g., Zr, Hf, U, and Th) at low melt fractions.

Fractional fusion

In simple systems with solid solutions, fractional fusion usually produces less melt per temperature increment than does batch fusion, but our calculations indicate that behavior of actual peridotites is more complex. During the initial stages of melting, isobaric fractional fusion of fertile peridotite does produce less melt per temperature increment than batch fusion (and at any given temperature, the total melt produced by fractional fusion is less than that produced by batch fusion; Fig. 2). However, once the residue from fractional fusion becomes highly depleted in Na ($\sim5\%$ total melting), significant melt is produced over small temperature intervals. In fact, we predict that above a few percent melting, fractional fusion produces slightly more melt per temperature increment ($\sim2.3°C/\%$) than batch fusion ($\sim3°C/\%$).

Adiabatic decompression

Comparison of the calculated results of adiabatic upwelling for both batch fusion and for fractional fusion reveals (as for isobaric melting) that only small amounts of melt are generated when the solidus is first intersected, but larger amounts of melt are generated after the Na_2O in the residue is largely depleted. For both batch and fractional melting, calculated adiabatic upwelling produces less than 5% melt in the first GPa of ascent, but from F = 5% to exhaustion of clinopyroxene, both processes generate melt at rates that are with the range of previous estimates for melt production by adiabatic batch fusion (10–20%/GPa). In general, after the first 3–5% of melting, 'fractional fusion adiabats' produce melt at approximately the same rate as batch fusion adiabats. Other interesting results include: (1) melt compositions calculated along adiabatic paths show less
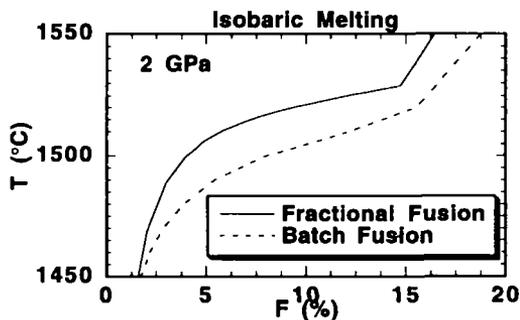

FIGURE 2.

variation with melt fraction than those calculated for isobaric melting; and (2) before clinopyroxene is exhausted, calculated fractional adiabats are only slightly ($\sim10°C$) hotter than batch adiabats with the same solidus intersection.These calculations imply that melt production during adiabatic upwelling of the mantle may be heterogeneously distributed, with smaller degrees of melting produced from a relatively thick interval at greater depth and higher degrees of melting produced from a relatively narrow, interval at shallower depth (i.e., in the sense of the residual melt column concept of Plank and Langmuir, 1992, melt fraction contours are predicted to be widely spaced over a great depth in the deeper parts of the column, but closely spaced at shallow levels). The differences in melt composition produced between these two regimes may also be affected by differences in partition coefficients at low and at high melt fraction. More specific estimates of the role of these effects on MORB petrogenesis must await refinement of the thermodynamic models.

References

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