Thermodynamic models of mantle melting to very high pressures: Objectives, motivations and sources of data

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A quantitative understanding of the chemistry and physics of major-element differentiation of silicate planetary bodies requires thermodynamic data and solution models that facilitate calculation of liquid-solid phase equilibria to pressures on the order of 135 GPa. At present, the development and calibration of such databases and models is hampered by both a lack of direct experimental phase-equilibrium constraints and by uncertainty regarding the structures of the constituent phases – especially liquids – at elevated pressures. Few experimental data are available to infer structural characteristics of silicate melts at pressures higher than 35 GPa, yet spectroscopic studies of glasses quenched from melts made at high pressure, and density-pressure systematics of melts inferred from analysis of mineral fusion curves, mineral buoyancy experiments and shock-compression studies, suggest that variation in melt structure with pressure is systematic and has a first order effect on bulk thermodynamic properties. One of the primary goals that must be achieved in order to construct melting models of the Earth's deep interior is a quantitative understanding of the relation of melt structure – or alternately, the configurational entropy of a melt – and density; from such a relation all thermodynamic properties of the liquid can be derived. A technique that generates data that are ideally suited for unambiguous correlation of density with melt structure is molecular dynamics (MD) computer simulation. Recent advances in computer hardware/software and the routine use of parallel computing platforms has made feasible the systematic application of MD simulation for the generation of data sets relevant to the calibration of thermodynamic models of silicate liquids at elevated pressures. The successful exploitation of these simulations depends on a suitable and robust set of transferable interatomic potentials, which are utilized to calculate forces between atoms. Such potentials are available for liquids and solids in the system CaO-MgO-Al_2O_3-SiO_2; this system is an excellent analogue for investigating the chemistry of melting in the lower mantle. Several examples of the use of MD data to calibrate thermodynamic models of liquids will be presented.

Petrographic clues to overturn and eruption of open-system magma chambers: Santorini, Greece

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Over the last 3000 years, post-caldera eruptions of Santorini, Greece, resulted in the formation of the Kameni Islands, which comprise a series of compositionally similar dacitic lava flows. Each lava flow has a distinct population of partially-crystalline mafic enclaves, which were derived from the break-up of a layer of replenishing magma responsible for triggering the eruption. Five of the flows (erupted in 1570, 1939, 1940, 1941 and 1950) include enclaves with essentially identical andesitic bulk compositions. The absence of phenocrysts in the enclaves shows that they formed from the crystallisation of originally aphyric melt which intruded the uppermost chamber prior to eruption.

The crystal framework of the enclaves comprises euhedral plagioclase, with prominent hopper-like extensions due to quench growth. Angles subtended at the junctions between pairs of plagioclase grains are modified from the original angle formed by random impingement of euhedral grains. Prominent re-entrants result in curved pore corners and reduced angles, and are best developed where the initial impingement angle was low, occurring entirely in an outer, quench-related zone. We interpret these re-entrants as a consequence of diffusion-limited growth during a period of rapid crystallisation. Thus the extent of angle reduction reflects the amount of growth during quenching.

Measurement of angle populations using the Universal Stage shows that the enclave population in each flow is distinct. We suggest that this reflects differences in the timing of cooling, crystallisation and attainment of neutral buoyancy of the replenishing layer. For magma which reached the density of the host dacite while relatively hot, overturn would result in significant quenching and angle reduction compared to a layer which had to cool and crystallise more in order to trigger overturn. Since the CSD and bulk composition of the andesite in the 5 flows are indistinguishable, we suggest that small differences in pre-eruptive H_2O content of the andesite and/or the host dacite control the details of chamber overturn and eruption triggering.