Geophysical Research Abstracts
Vol. 13, EGU2011-52, 2011
EGU General Assembly 2011

Thermodynamic modeling of phase equilibria in magmatic systems: Progress and future directions (2010 Robert Wilhelm Bunsen Medal Lecture)

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Research over the past thirty years has established that thermodynamic modeling is extremely useful for illuminating the production, transport, chemical differentiation, and eruptive potential of magmas. The key to successful modeling of this kind is the formulation of an internally consistent thermodynamic database that includes properties of liquid and solid endmember components, and - most importantly - a cohesive set of models that describe the thermodynamics of mixing of both liquid (± fluid) and mineral solid solutions. Despite numerous successes in the application of thermodynamic modeling to liquid-solid phase equilibria under crustal and upper mantle pressure-temperature conditions, there are critical and relevant areas of application where the models fail to generate useful results. Importantly, these applications include phase equilibria in hornblende- and biotite-bearing magmas and the melting relations of silicate mantle-like bulk compositions at pressures above 3 GPa. Research is underway to address many of these modeling deficiencies. Approaches include (1) the development of new solution models for igneous pyroxenes and garnets, including majoritic garnet components, (2) the reformulation of thermodynamic models for liquid solution properties in order to implement non-deal associative solutions and a more robust equation of state that allows extrapolation of liquid density and free energy to high-pressures, (3) the creation of an experimental program to generate data necessary for the calibration of solution theory for igneous hornblendes and mica, and (4) the use of molecular dynamics simulations to facilitate the creation of a data base of liquid thermochemical properties at high-pressures that will serve as a basis for the calibration of phase equilibria models under Earth-like lower mantle conditions. All of these approaches give hope that in the future it will be possible to compute melting and melt-rock reaction over a much broader range of pressures, temperatures and bulk compositions than is currently possible, and that consequently a more extensive series of petrologic and geochemical questions will be addressable via the application of thermodynamic modeling of magmatic phase equilibria.