Thermodynamic modeling of mantle melting

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Partial melting of mantle peridotite is an important process for both material fractionation and cooling of the Earth, yet there remain a number of fundamental questions for the actual processes. Thermodynamic modeling is a useful approach to describe the phase relation, mass balance and energy balance of mantle melting consistently. However, there exists number of problems to handle phase relation, mass balance and energy balance of mantle melting with previously constructed thermodynamic models. In this study, newly calibrated thermodynamic parameters of silicate liquid with revised equations for apparent molar Gibbs energy and new calculation algorism are provided to make better descriptions of energy balance between silicate liquid and minerals during mantle melting.

In this study, compositional space of SiO2-Al2O3-FeO-Fe3O4-MgO-CaO with mineral assemblage of spinel lherzolite (olivine, clino-pyroxene, ortho-pyroxene and spinel) is employed to describe mantle melting. The equations of silicate liquid have been established with a revised formulation to improve the reproducibility of apparent molar Gibbs energies of pure liquid at a given temperature and pressure. In revised equation, apparent molar Gibbs free energies of silicate liquid end-components are anchored to the Gibbs free energies of solid components. Values of apparent molar Gibbs free energies of silicate liquid end-components are described as difference between Gibbs free energies of corresponding solid components. With the equation, specific heat and compressibility of silicate liquid are newly calibrated in this study. Melting temperature and enthalpy of melting is also calibrated if melting temperature of the component has not been determined. Parameters are calibrated with previously reported high pressure melting experiment of peridotite and previously reported thermodynamic properties of rock forming minerals. New energy minimization algorism is also developed to make better prediction of phase relation and energy balance for melt-present system. Stable phase assemblage and composition to minimize Gibbs free energy of the system at given temperature, pressure and whole rock composition are calculated with the algorism.

Thermodynamic calculation model is establishes with the revised equation, calibrated parameter and new algorism. Melt proportion, composition and enthalpy of fusion of anhydrous mantle peridotite at given temperature, pressure and whole rock composition are computed with the newly establishes model. The model predicts relationship between composition of the system, temperature and melting degree well.