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Multi pressure thermodynamic calculation of partial melting of peridotite by system energy minimization

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Throughout the Earth's history from early Earth when a dense melt could have accumulated at the bottom of the mantle to present day setting where melting at ridges, subduction zones and hotspots drives material differentiation, partial melting of the mantle is an essential process for its material and thermal evolution. Thermodynamic modeling is a general approach suitable for describing such material and thermal evolution during melting. It can provide an internally consistent model in terms of phase assemblage, mass- and energy-balance. We have been developing a general energy minimization algorithm for describing such mantle melting. The algorithm calculates gradient of total Gibbs free energy of the system with respect to any tiny mass of melting or solidification of melt and solid end-components under the constraint of closed system at constant pressure and temperature. Molar contents of solid and melt end-components are recalculated along the steepest gradient of total Gibbs free energy of the system at each calculation step. Equilibrium state of the system is found where the gradient becomes zero with respect to any tiny mass perturbation. Thermodynamic model had constructed with the algorithm, thermodynamic formulation of silicate melt and calibrated thermodynamic parameters for silicate melt successfully reproduced melting phase relations of mantle peridotite at 1GPa.

Here we present a new multi pressure thermodynamic calculation with newly calibrated thermodynamic parameters for silicate melt. Calibration data source is expanded to include higher-pressure experiment, up to 2 GPa. The thermodynamic model describes melting of spinel lherzolite at 1-2GPa. The calculation is carried out in a system $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-FeO-Fe}_3\text{O}_4\text{-MgO-CaO}$ with olivine, clinopyroxene, orthopyroxene, spinel and silicate melt. The dC_p values, which are a difference of specific heat between solid and melt end-component, and dV , which is a difference of volume between solid and melt end-component have been calibrated utilizing previously reported results of high-pressure melting experiments of mantle peridotite and thermodynamic properties of rock forming minerals. Simple ideal solution is employed for the activity model of silicate melt in this study.

Thermodynamic calculation with newly calibrated parameters successfully predicted multi pressure melting relation of mantle peridotite, including elevated solidus temperature at higher pressure. At 1.5 or 2 GPa calculation, temperatures 50-100 degrees higher than that of 1GPa are required to derive a certain degree of melting, which coincides well with experimentally predicted effect of pressure on melting degree (e.g.; Falloon et al., 1999; Hirose and Kushiro, 1993). Effects of pressure on partial melt compositions are well reproduced, though FeO/MgO partition between melt and solid are not well reproduced with the ideal solution activity model. Decrease of SiO_2 content and increase of FeO in a partial melt with increasing pressure and increase of MgO content with increasing temperature, as shown in Hirose and Kushiro (1993), are well reproduced. In addition to the effects of temperature and bulk composition, effect of pressure on melting relation is successfully introduced to our thermodynamic calculation with relatively simple thermodynamic formulation for silicate melt.

Keywords: thermodynamics, melting, mantle, magma