

Thermodynamic Calculation of polybaric Melting of Mantle Peridotite

UEKI, Kenta^{1*}, IWAMORI, Hikaru²

¹Volcanic Fluid Research Center, Tokyo Institute of Technology, ²Department of Earth and Planetary Sciences, Tokyo Institute of Technology

Partial melting is an essential process for both material differentiation and heat transportation of the Earth. Numerical forward calculation is useful approach to predict melting in the dynamic system such as the magma ocean that may have developed from surface to lower mantle depth, and the present day subduction zone where fluid addition, mantle convection and melting are tightly coupled. Thermodynamic calculation by system energy minimization is a general approach to describe dynamic melting of such multi component and multi phase system, because that can provide an internally consistent relation of phase relation and mass and energy balance during melting.

We have developed a straightforward algorithm for calculating phase equilibria of multicomponent system by energy minimization of the system, together with thermodynamic configuration to describe a molar Gibbs free energy of silicate melt. The thermodynamic model constructed with the algorithm and melt thermodynamic configuration successfully reproduced melting phase relation of mantle peridotite at 1 GPa. We have expanded a calibration database of the thermodynamic model up to 3 GPa to conduct a polybaric melting calculation, which is dominant in natural tectonic settings (e.g., mid-ocean ridges and hotspots).

Construction of equation of state of silicate melt is an essential factor to evaluate multi pressure melting. We employ two different configurations for volumetric parameters of silicate melt to investigate better approach to predict melting relation at high pressure. In the first configuration, molar volume of silicate melt end-component is represented by the difference from the volume of corresponding solid end-component (dV), and the dV is calibrated with the results of previously reported melting experiments. We also employed a set of 1 bar experimental volumetric parameters (Lange and Carmichael, 1990) for the equation of state of silicate melt, which is commonly used to calculate melt volumetric property. In this case, standard state molar volume of melt end-component is calibrated with the calibration data set. In both configurations, dC_p , which is the difference in molar specific heat between the corresponding melt and solid end-components, are also calibrated and ideal solution are assumed for silicate melt. The tested system consists of $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-FeO-Fe}_3\text{O}_4\text{-MgO-CaO}$ and includes olivine, clinopyroxene, orthopyroxene, and spinel with silicate melt. Thermodynamic parameters and enthalpy, entropy and temperature of fusion at 1 bar for solid end-components are taken from previous studies.

Our thermodynamic calculation with calibration of dV successfully reproduced experimentally determined multi pressure melting reaction of mantle spinel lherzolite at 1-3 GPa (Hirose and Kushiro, 1993), including systematics between pressure-temperature-composition of the system and melt composition and melting degree. On the other hand, calculation result with parameter of derive larger misfit with experimental result. Our model with calibration of dV makes better prediction than pMELTS (thermodynamic model to calculate phase relation of melt present system), in terms of temperature-phase proportion including melt fraction. pMELTS did not calibrate melt volumetric parameters and utilized volumetric parameters. It is deduced that our configuration, in which thermodynamic parameters for melt is calibrated based on the difference from the corresponding solid end-component at melting P-T conditions, is useful approach, rather than extrapolation from standard state properties of simple systems as have been often employed in the previous studies.

Keywords: Thermodynamics, melting, mantle, phase equilibria