Japan Geoscience Union Meeting 2010
(May 23-28 2010 at Makuhari, Chiba, Japan)

SIT041-P07 会場:コンベンションホール 時間: 5月24日17:15-18:45

熱力学計算を用いたマントル溶融のモデリング

Numerical modeling of mantle melting by thermodynamic calculation

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Partial melting is an important process for both material fractionation and cooling of the Earth. Thermodynamic modeling is a powerful approach to describe the phase relation, mass balance and energy balance during melting. In this study, thermodynamic properties of silicate liquid and rock forming minerals are developed to construct thermodynamic model of mantle melting.
Algorism to minimize total Gibbs free energy of multi-component melt-present systems including solid solution has been developed in Ueki and Iwamori (2009, AGU). The algorism calculates gradient of total Gibbs free energy of the system with respect to any tiny perturbations on molar contents of liquid and solid end-members under the constraint of a constant bulk composition. Minimum of the Gibbs free energy of the system, in other words, equilibrium phase proportion and compositions are found where the total Gibbs free energy of the system increases with respect to any tiny perturbation on molar contents of liquid and solid end-members in the system.
The energy minimization algorism has been applied to a natural system involving olivine, clinopyroxene (cpx), orthopyroxene (opx), spinel and silicate liquid at 1 GPa. Compositional space of SiO2-Al2O3-FeO-Fe3O4-MgO-CaO has been investigated to describe mantle melting. Thermodynamic parameters of silicate liquid are calibrated with compositions of silicate liquid and minerals in previously reported high-pressure melting experiments and thermodynamic properties of rock forming minerals.
The thermodynamic model predicted relationship between bulk composition, temperature and melting degree during partial melting of mantle peridotite, remarkably well in Ueki and Iwamori (2009). However, calculated composition of silicate liquid did not reproduce experimental result well. For example, calculated FeO* content is significant lower than experimental derived value at the identical condition. Besides the insufficient reproducibility of melt composition, composition of residual pyroxenes during melting is not well reproduced, in terms of FeO*/MgO exchange between olivine and pyroxene. Furthermore, cpx related parameters of silicate liquid show higher residual during calibration than the other end-members. The residual indicates clear compositional dependent non-ideality of cpx. Natural pyroxene exhibit strong compositional dependent non-ideality, as manifested in immiscibility gap (solvus). However, thermodynamic model developed in Ueki and Iwamori (2009) employed the simplest model; ideal solution model for mixing term of cpx and opx. In this study, three-site ideal mixing is newly introduced to solid solution model of opx and cpx. Pyroxene related parameters of silicate liquid is newly calibrated.
With the three site ideal mixing model, value and compositional dependence of calibration-residual of cpx is smaller than that of ideal solution model, indicating the three site ideal solution model approximates mixing model of cpx at pressure, temperature and compositional range in this study. Calculation of melting of peridotite are carried out with ideal or new employed three-site solid solution model of pyroxenes. Computed phase relation and compositions are strongly dependent on

solid solution model of opx and opx-related parameters of silicate liquid. Detailed investigation of solid solution model and thermodynamic parameters of opx have to be carried out for further improvement of the melting model to calculate both phase proportion and composition at any temperature, pressure and bulk composition.
With the new solid solution model of pyroxene and newly calibrated parameters of silicate liquid, more realistic composition of silicate liquid is derived than our previous model, both in fertile peridotite and depleted peridotite. Phase relations during melting of mantle peridotite, including relationship between melting degree and temperature, are also reproduced with the new solid solution model.

キーワード:溶融,熱力学,数値計算,マントル,メルト
Keywords: melting, thermodynamics, numerical calculation, mantle, melt