Computational Petrology and Pyroxene Thermodynamics

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We have developed a thermodynamically based algorithm to describe phase equilibria between coexisting clinopyroxene and orthopyroxene as a function of composition, temperature and pressure. The chemical composition of phases has been unambiguously expressed through their number of cations per formula unit (‘*constituents*’, symbol ‘*N*’), which are subject to constraints by both stoichiometry and charge balance.

For each phase, the molar free energy (G^{ϕ}) is given by the sum of contributions from: 1) the Gibbs free energy of all possible stoichiometric, charge-balanced end-members, 2) ideal entropy mixing on sites, and 3) excess mixing terms. The principle underlying the formulation of the term due to the Gibbs free energy of the end-members has been elucidated. As an example, the expression of this term for a general (Na-Ca-Mg-Fe^{2+}-Al-Cr-Fe^{3+}-Si-Ti) pyroxene system (32 end-members) has been derived.

At any given temperature and pressure a closed multi-phase system is at its equilibrium condition when the chemical composition of the phases present in the system and the number of moles of each are such that the Gibbs free energy of the system reaches its minimum value.

From a mathematical point of view, the determination of equilibrium phase assemblages can, in short, be defined as a constrained minimization problem. To solve the Gibbs free energy minimization problem two different approaches (‘*inverse*’ and ‘*forward*’) have been undertaken. For the ‘inverse’ problem, a *chi-square* measure method of data-fitting is used while in the ‘forward’ the minimization is carried out with a ‘Feasible Iterate Sequential Quadratic Programming’ method (FFSQP). The system’s Gibbs free energy is minimized under mass balance, stoichiometry, charge balance and positivity constraints.

Initial application of the programs is to assemblages of coexisting pyroxenes (orthopyroxene, and low Ca- and high Ca clinopyroxene) in CaO-MgO-FeO-SiO_2 (i.e. CMFS), CaO-MgO-Al_2O_3-SiO_2 (i.e. CMAS) and CMFAS systems. Phase relations within such systems and their subsystems are calculated over a wide range of temperatures and pressures and compare favourably with experimental constraints.

Umlekan-Ogodzha Early Cretaceous magmatic belt (Amurian Region): duration of magmatism

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The Umlekan-Ogodzha magmatic belt stretches to the East from the upper reaches of the Amur river for over 500 km in WE direction along the margin of the Amurian block. Basing on $^{40}Ar/^{39}Ar$ datings we established several stages of magmatic activity in the history of the belt.

I stage (140-127 Ma) is characterized by granitoid associations. They have the same geochemical features as granites of both I- and S- types (Rb=40-140 ppm, Ba=560-780 ppm, Th=7.5-19.8 ppm, La=15.5-31.0 ppm, Yb=0.9-1.4 ppm, Y=9.4-13.2 ppm, Nb=5.1-8.4 ppm) and correspond to granitoids of subduction settings. High ratios of $^{87}Sr/^{86}Sr(o)$= 0.70626-0.70803 and low values of Nd(t)= -3.5..-4.7 are indicative of that the source of these rocks might have been a mixture of crust matter and depleted mantle of DMM type.

II stage (125-124 Ma) is presented by high aluminiferous volcanics of andesite-dacite association. They are characterized by enrichment in Ba=650-830 ppm, Rb=61-119 ppm, Th=6.3-15.6 ppm, Sr=460-660 ppm, La=23.4-33.8 ppm. At the background of them the negative anomalies of Nb=1.0-4.0 ppm, Ta=0.2-0.5 ppm, Y=9.7-12.3 ppm, Yb=0.9-1.6 ppm are distinguished. A comparative analysis indicate the similarity of the latter to volcanics of active continental margins. At the same time, relatively high LILE concentrations, moderately high ratios of $^{87}Sr/^{86}Sr(o)$=0.70626-0.70803 and low values of Nd(t)=-3.5..-4.7 are the evidence of a considerable impact of crust contamination.

III stage (118-115Ma) is presented by bimodal trachybasalt-rhyolite association with dike complex consisting of granosyenite, granite-porphyry. The rocks are characteristic of dual geochemical features. On the one hand they have rather high REE and HFSE contents being indicative of intraplate origin. On the other hand there is a relative depletion of Nb, Ta, Y, Ti, P, HREE which is indicative of the impact of subduction processes. Thus, the most probable geodynamic setting is the rupture of a subducted slab. Moderate ratios of $^{87}Sr/^{86}Sr(o)$=0.70566-0.70629 at negative values of Nd(t)= -1.4..-4.6 are indicative of that that melting substratum experienced a significant impact of such a source as the enriched mantle of EM-I type.

IV stage (100-94 Ma) is expressed in the formation of trachybasalts and trachyandesites. According to their geochemical features they are similar to volcanics of III stage.

We suggest that the Umlekan-Ogodzha belt started to form along the margin of the Amurian block in the beginning of the Early Cretaceous and had been developing as an active continental margin during 140-124 Ma. During the period between 120-95 Ma there occurred a sharp change in the character of magmatism. We connect this with the ending of subduction process and rupture of the slab.