ASSESSMENT OF CHEMICAL COMPOSITION OF THE CONTINENTAL UPPER MANTLE OF THE EARTH

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Thermodynamic approach and method of calculation. For computation of the seismic velocity profiles in the Earth's mantle (direct problem), we need a chemical model and a model for the temperature distribution. Since composition of the entire mantle is uncertain, it will take a great variety of input compositions. Another approach involves the computation of the geophysically admissible bulk composition and density distribution models in the mantle layers (inverse problem). Thermodynamic modeling of the phase relations and physical properties of the multicomponent mineral system at high pressures and temperatures was used to develop a method for solving the inverse problem of determining the bulk composition, density and temperature distribution in the continental upper mantle of the Earth from the totality of geophysical evidence [1]. The goal of the inversion procedure is to find a self-consistent petrological-geophysical model that minimises the discrepancies between the calculated parameters and "reference model". The determination of bulk composition from the seismic data generally can have many solutions. To choose the best one from a range of solutions, we should impose some extra conditions, for example, a close agreement of the temperature and bulk composition derived from the solution of the inverse problem with the parameters for a "reference model". For this purpose, we have used the following conditions.

The temperature distribution in the mantle has been modelled by the continental geotherm [2]. Seismic velocity profiles as a function of depth have been taken from the recent seismic model IASP 91 [3]. Chemical composition of the continental upper mantle at depths of 50-400 km has been modelled by the average composition of the spinel and garnet peridotites [4-6]. The chemical and phase compositions of the mantle were modelled within the system CaO-FeO-MgO-Al_2O_3-SiO_2 (CFMAS) including the pure phases and solid solutions: olivine, spinel, garnet (almandine, grossular, pyrope); orthopyroxene and clinopyroxene (5-component solutions). The observed and calculated values of the thermophysical properties were correlated with the THERMOSEISM software [3]. The package contains thermodynamic databases and subroutines for calculating mineral equilibria at high pressures and temperatures by the method of the minimisation of the total Gibbs free energy. It can be used to calculate the equilibrium mineral composition of a multicomponent system, compute the physical properties of a mineral assemblage (including the densities and seismic velocities), and obtain the petrological and geophysical constraints on the bulk chemical composition of a planetary body. Typical errors in calculating +the mantle density are better than 1%.

The solution of the inverse problem is based on the minimisation of the function [7]:

$$\vartheta = \sum_{i=1}^{N} \sum_{F} \alpha_F (F_i^0 - F_i)^2 ,$$

(F=V_p, V_s, T, C_m), (m=FeO, MgO, Al_2O_3, CaO), where F_i^o are the parameters of the "reference model", N is the number of points along the depth. C(FeO, MgO, Al_2O_3, CaO) are the oxide concentrations; the concentration of SiO_2 is determined from normalisation. With proper selection of the weight coefficients α_F, the influence of the F function on the solution can be adjusted, and the solution can be made to meet extra conditions. In making inverse problem, we require a non-negative density gradient in the mantle ($d\rho/dH$>0) and assume using the arguments on $C_{Al_2O_3}/C_{CaO}$ ratios and ratio's increments $\delta C_{Al_2O_3}/\delta C_{CaO}$ in the mantle [4] that δC_{Al2O3} = B$C\delta_{MgO}$, C_{CaO} = KC_{Al2O3} (B < 0). We have obtained that B=-0.325, K=0.97 (H=70-80 км); B=-0.325, K=0.7+0.0018(H(км)-120) (H=90-210 km); B=-0.5, K=0.8 (H=220-400 км).

*Results and Discussion***.** Chemical composition of the continental upper mantle, seismic velocities, temperature and density distribution based on minimising deviations of the calculated values of seismic velocities, concentrations, and temperature from corresponding seismic, petrological, and thermal data are shown in table 1. The calculated temperatures and velocity profiles are within the reasonable limits of all uncertainties involved in geophysical observations [2, 3]. The results of calculation show the radial compositional variations in the upper mantle.

The average bulk composition model of the upper mantle is presented in Table. 2. According to the calculated chemical composition, the continental upper mantle may consist of: spinel peridotites at depths of < 70-80 km, low-temperature peridotites at depths of 80-210 km, and high-temperature peridotites at depths of > 210-230 km. Our analysis of the composition of the upper mantle leads to the conclusion that the upper mantle of the Earth may consist of two regions with a chemical boundary at depths of 210-230 km. Such a model gives the best fit to the mantle seismic properties. It should be emphasised that the derived composition is model-independent in geochemical context but the degree of its reliability is almost completely defined by the accuracy of seismic and thermal data.

Table 1

The calculated chemical composition (wt.%) and physical properties of the continental upper mantle

H_{km}	T^oC	C_{MgO}	C_{FeO}	C_{Al2O3}	C_{CaO}	C_{SiO2}	V_p^o	V_p	V_s^o	V_s	ρ	Mg#
71	841	41.5	8.20	1.95	1.90	46.45	8.04	8.05	4.48	4.56	3.295	.900
120	1120	43.5	8.10	1.20	.84	46.36	8.05	8.12	4.50	4.54	3.295	.905
171	1329	43.3	7.90	1.27	1.02	46.51	8.19	8.20	4.51	4.53	3.317	.907
210	1400	43.2	7.90	1.29	1.12	46.49	8.30	8.30	4.52	4.55	3.346	.907
271	1434	42.7	8.35	2.20	2.13	44.62	8.52	8.52	4.63	4.62	3.42 0	.901
371	1491	40.0	8.37	3.50	2.80	45.33	8.89	8.80	4.80	4.72	3.530	.895
400	1508	38.0	8.40	4.50	3.60	45.50	9.03	8.89	4.87	4.76	3.560	.890

V_p^o and V_s^o are from [3].

Table 2

Bulk composition models (wt.%) of the continental upper mantle

Oxides	H≤70 км	70<H≤210 км	H > 230 км
SiO_2	≅46	≅46 (<$(C_{SiO2})_{70}$	44.5-45.5
Al_2O_3	≅2	1.2-1.3	≥ 2.0
FeO	≅8	≅8 (<$(C_{FeO})_{70}$	8.3-8.5
MgO	≅41	>43	38.0-42.7
CaO	≅1.9	0.8-1.2	≥ 2.0

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