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Chemical boundary of the cratonic lithoshere from the geophisycal and petrological data

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1. Introduction

The lithosphere–asthenosphere boundary (LAB) represents the base of the Earth's lithosphere, the rigid and relatively cool outer shell characterised by a conductive thermal regime, isolated from the convecting asthenosphere. The lithosphere is underlain by a weak layer (the asthenosphere), which is characterised by pervasive plastic deformation (solid-state creep) on time scales of tens of thousands of years. The lithosphere is composed of discrete plates and the lithosphere–asthenosphere boundary (LAB) separates each plate from the underlying convecting mantle. The continental crust and underlying subcontinental lithospheric mantle (SCLM) are highly heterogeneous. The ranges in thickness of the lithosphere are from a few tens of kilometers beneath rift zones, to >250 km beneath some Archean cratons. Chemically, the LAB should divide a lithospheric mantle that is variably depleted in basaltic components from a more fertile asthenosphere. In xenolith suites from cratonic areas, the bottom of the depleted lithosphere is marked by a rapid downward increase in elements such as Fe, Ca, Al, Ti, Zr and Y, and a rapid decrease in the median Mg# of olivine. The petrologic (PLAB), based on xenolith and xenocryst data, thermal boundary (TLAB), based on termobarometry data and thermal physics models; the rheological LAB, based on numerical modelling of mantle creep and stress regime; the seismological LAB, based mainly on studies of surface waves and S-receiver functions; and the electrical LAB, based on magnetotelluric surveys are discussed.

In the present paper, using physicochemical modeling methods, we adjust thermal boundary layer and petrologic lithosphere-asthenosphere boundary layer of the lithosphere Archean Kaapvaal and Siberian craton. Petrologycal LAB is calculated under the assumption of local isostatic equilibrium with the compensation depth at the base of the numerical domain. According to the principle of isostasy, all regions of the Earth with identical elevation must have the same buoyancy when referenced to a common compensation level. In order to estimate absolute elevation one needs to perform a density ρ(H) for the craton and reference column. With the help of physicochemical modeling methods, bulk composition models can be converted into equilibrium phase assemblages and the related seismic and density characteristics (the forward problem), while the velocity structures can be converted into composition and/or temperature distribution models (the inverse problem) [*Kronrod and Kuskov,* 2007; 2010]. Based on the method developed in [*Kuskov et al.,* 2006], we reconstructed the temperature of the lithosphere at depths of 70–300 km from the composition of xenoliths from kimberlite pipes of the craton and absolute values of *P* and *S* wave velocities. The forward and inverse problems are solved by the minimization of the Gibbs free energy and equations of state of mantle material incorporating phase transformations, anharmonicity (thermal expansion and compressibility), and attenuation effects (anelasticity of mantle material at high temperatures), which should be taken into account due to nonlinear variations in thermodynamic and seismic properties with rising temperature and pressure. Equilibrium compositions of phase assemblages, elastic wave velocities, and density were calculated with the use of the THERMOSEISM software complex [*Kuskov et al.,* 2006, *Kuskov and Kronrod,* 2007].

The thermal structure of continental lithosphere (the thickness of the thermal lithosphere, temperature, heat flows, and heat generation in the crust and lithosphere) is reconstructed from geothermal, seismic, and petrologic data. The first step is the determination of the temperature profile from absolute wave velocities (T_S). The T_S profile is then adjusted to a thermophysical model of conductive transfer. A feature inherent in the solution of the thermophysical inverse problem obtained in this paper is the use of constraints derived from the temperature reconstruction by seismic data inversion. As a result, the analytical dependence of the temperature on depth, the intensity of radiogenic heat sources in the crust, and heat flow components in the crust and lithosphere are determined. Profiles of the density, temperature, wave velocity in the craton lithosphere and the petrologic PLAB and thermal boundary are constructed. The results are compared with data of seismology, petrology, thermal models, and thermobarometry.

2. Input data and method of solution

The equilibrium composition of phase assemblages, seismic velocities, and density (a forward problem) are calculated with the help of the THERMOSEISM software package [*Kuskov et al.,* 2006, *Kuskov and Kronrod,* 2007], whose database contains internally consistent values of such thermodynamic parameters as enthalpy, entropy, heat capacity, the Gruneisen parameter, thermal expansion, bulk and shear moduli of minerals, and mixing parameters of solid solutions. The model system NaTiCFMAS includes the following phases: plagioclase, Fe–Mg olivine, ilmenite, and spinel; pyrope–almandine–grossular garnet; and orthopyroxene and clinopyroxene (five- and six-component solutions). The chemical composition of the phases and their percentages are determined by the minimization of the Gibbs free energy. The equation of state of the minerals is calculated in the quasiharmonic Mie–Gruneisen–Debye approximation [*Kuskov et al.,* 2006]. Hence, we determine the density and the isotropic velocities of the phase assemblage, which depend on the chemical and phase composition of rocks; the bulk modulus and the density are estimated from the equation of state, whereas a linear dependence is adopted for the shear modulus; and the elastic moduli are determined by the Voigt–Reuss–Hill averaging. The database contains self-consistent data on such thermodynamic parameters as the enthalpy, entropy, heat capacity, Gruneisen parameter, thermal expansion, and bulk and shear moduli of minerals and on mixing parameters of solid solutions. The model multisystem (NaTiCFMAS) includes the following phases: plagioclase, Fe–Mg olivine, ilmenite, and spinel; pyrope–almandine–grossular garnet; and ortho- and clinopyroxene (five- and six-component solutions).

The method of reconstructing the temperature from seismic information is described in detail in [*Kronrod and Kuskov,* 2007; *Kronrod and Kuskov,* 2010]. The procedure for converting seismic profiles into thermal profiles in the NaTiCFMAS multisystem with phases of a variable composition is based on the equations of state of mantle material taking into account phase transformations, anharmonicity, and anelastic effects. The temperature profiles (T_S) consistent with thermodynamic properties of minerals and the phase composition of the mineral assemblage at a given depth are determined by inverting absolute velocities with a fixed bulk rock composition. The inversion is based on the minimization of standard deviations of calculated seismic velocities adjusted to the state diagram (and corrected for anharmonicity and anelasticity) from their observed values. The minimization is performed by the Newton method. As a result of the inversion, we find a temperature–depth profile and an equilibrium phase composition of the mineral assemblage (percentages of phases and their chemical compositions) under given *P–T* conditions. The depth dependence of pressure is taken from the global PREM model.

The seismic profile was inverted on the basis of low and high temperature xenoliths from kimberlite pipes of the craton. Thus, regardless of the composition of deep xenoliths of the Kaapvaal and Siberian craton, the temperature reconstruction from the seismic velocity profiles in the regional models [*Simon et al.,* 2002] and [*Pavlenkova and Pavlenkova,* 2006], leads to a temperature inversion at depths of 70-300 km. On the basis of the methods of determining the temperature in the lithosphere from seismic data (*TS*) and the 1-D model of heat conduction (*T*cond), we formulate the following inverse problem. Using the surface heat flow and the *TS* temperature profile, we have to determine the TLAB, heat generation in the upper crust, middle crust, heat flows in the crust and lithosphere. This problem is solved by minimizing a functional *f* characterizing the misfits between the temperature profile *TS* derived from seismic data and the temperature profile *T*cond calculated from model of heat conduction [*Kronrod and Kuskov*, 2007].

We are used reference column at a mid-oceanic ridge (MOR) [*Afonso et al.,* 2008], where average elevations, petrogenetic processes, and lithospheric structures are known in greater detail than in any other tectonic setting, and are obtained absolute elevation are similar to those of [*Afonso et al.,* 2008].

3. Results

Here, we present the results of estimating the lithosphere–asthenosphere boundary and thermal boundary layer. The chemical composition of the petrological models are listed in the table 1, 2 in recalculation to the NaTiCFMAS system [*Afonso et al.,* 2008, *Gregoirea et al.,* 2005, *Griffin et al.,* 2003, *McDonough et al.,* 1990, *McDonough and Sun,* 1995]. The K1, K2 petrological models for the Kaapvaal craton, K1, K2, C for Siberian craton and P model for regions Early and Middle Proterozoic are used. Temperature of the regions Early and Middle Proterozoic we are finded from the temperature at the depths 50, 100, 150 km and surface heat flow according to [*Artemieva,* 2006]. Temperature profiles, values of crustal radiogenic heat sources, and heat flow components in the crust and mantle are determined. Table 2 show our reconstructions of the petrological models, petrologic lithosphere–asthenosphere boundary (PLAB) and thermal boundary (TLAB) in comparison with thermobarometric data.

Table 1. The chemical composition of the petrological models (wait %) in recalculation to the NaTiCFMAS system

Chemical composition	**SiO_2**	**TiO_2**	**Al_2O_3**	**FeO**	**MgO**	**CaO**	**Na_2O**
Garnet peridotites [a] (**GP**) McD 1990	45.42	0.08	1.32	7.03	45.28	0.78	0.09
Primitive Mantle[b] (**PM**) McD 1995	45.2	0.2	4.51	8.13	37.6	3.6	0.36
Garnet lherzolite (Daldyn)[c] (**GL**) Grif 2003	46.15	0.05	1.21	6.55	45.25	0.71	0.08
Coarse-grained garnet peridotites (Premier) [d] (**CGP**) (GR 2005)	46.23	0.08	1.64	6.83	44.12	0.98	0.12
Coarse-grained spinel peridotites (Premier)[d] (**CSP**) (GR 2005)	45.32	0.03	1.27	6.97	45.55	0.77	0.09
High-T lherzolite (Kaapvaal)[e] (**HTL**)(Af 2008)	44.76	0.17	1.76	8.17	43.74	1.28	0.12
Protons (mean garnet SCLM+massiv xenoliths) [c] (**P**) (Grif 2003)	45.0	0.07	1.91	8.1	43.1	1.7	0.12

Note: [a] composition of [*McDonough,* 1990]; [b] composition of [*McDonough and Sun,* 1995]; [c] composition of [*Griffin et al.,* 2003]; [d] composition of [*Gregoirea et al.,* 2005]; [c] composition of [*Afonso et al.,* 2008].

Table 2. Petrological models, petrologic (PLAB) and thermal (TLAB) lithosphere–asthenosphere boundary

Region	Kaapvaal craton		Siberian craton			Early Proterozoic	Middle Proterozoic
Petrological model	K1	K2	K1	K2	C	P	P
0 – Moho[a]	34 km crust	34 km crust	40 km crust	40km crust	40km crust	37.7km crust	39.3km crust
Moxo – PLAB	GP	-----	GP	-----	GL	P	P
PLAB +10 – 400 km	PM	-----	PM	-----	-----	PM	PM
Moxo – 75 km	-----	CSP	-----	CSP	-----	-----	-----
80 km – PLAB	-----	CGP	-----	CGP	-----	-----	-----
PLAB - PLAB + 35km	-----	HTL	-----	HTL	HTL	-----	-----
PLAB + 35 – 400 km	-----	PM	-----	PM	PM	-----	-----
Petrologic lithosphere–asthenosphere boundary (computing), km	173	160	210	205	197	155	110
Lithosphere–asthenosphere boundary (termobarometry[b]), km	~ 170		~190–205			~150	-----
Thermal boundary layer (computing), km	220		300			186	165

Note: The chemical composition of the petrological models GP, GL, CSP,CGP, HTL, PM, P according to Table 1;[a] Density and thickness of the crust according to [*Afonso et al.,* 2008, *Artemieva,* 2006]; [b] Petrologic lithosphere–asthenosphere boundary according to [*O'Reilly, Griffin, 2006, Griffin et al.*, 2003]

4. Conclusions

In the present paper we adjust thermal boundary layer and petrologic lithosphere-asthenosphere boundary layer of the lithosphere Archean Kaapvaal craton and Siberian craton using physicochemical modeling methods. Petrologycal lithosphere-asthenosphere boundary is calculated under the assumption of local isostatic equilibrium with the compensation depth at the base of the numerical domain. A specific feature of the method developed for solving the inverse thermophysical problem is the incorporation of constraints obtained from the seismic data inversion for the reconstruction of temperature. The input data are seismic velocities, surface heat flows, and the petrologic models. The solution is based on the fitting of the temperature profiles derived from seismic velocities to the conductive model of heat transfer in the crust and lithosphere. The procedure of converting seismic profiles into thermal ones is based on the equations of state of mantle material taking into account phase transformations and anharmonicity and anelasticity effects. Our modeling results show good agreement with modern petrological and geothermal models.

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