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THREE-DIMENSIONAL DENSITY MODEL OF THE MANTLE BENEATH THE UKRAINIAN SHIELD

Purpose. Mantle density models are key tools for understanding the fundamental geological and physical processes occurring within the Earth and are essential to our scientific and applied understanding of the planet.

Methodology. The tasks were solved by a complex research method, including analysis and generalization of literary and patent sources, analytical, experimental studies, using computer and mathematical modelling methods.

Findings. One-dimensional models simplify the mantle density distribution by assuming that it is uniform only in the vertical direction. This limitation does not allow for horizontal variations in mantle density, which may be important on a regional scale. 3D models are more complex and require more data and computational resources, so their use may be limited. In this study, we present a quasi-three-dimensional model of mantle density beneath the Ukrainian Shield. This 3D model is obtained using a basic set of one-dimensional seismic tomographic velocity models calculated for 21 mantle domains in the depth range from 50 to 2,600 km. The process of converting the P-wave velocity model into a density model includes the following stages: 1) determining seismic boundaries in the mantle based on P-wave velocity curves for each mantle domain; 2) creating a synthetic mantle model beneath the Ukrainian Shield for the P,S-wave velocity curves; 3) solving the Adams-Williamson equation for each domain, considering polynomial corrections to extract heterogeneities during its solution; 4) analysing existing models by comparing the calculated gravitational potential at the central point of the Ukrainian Shield as the standard reference for selecting one of 5 reference models. Here, we focus on the final stages of constructing the mantle density model by: 1) balancing the mass of the upper and lower mantle for each domain when determining density using the Adams-Williamson equation and introducing polynomial corrections; 2) calculating densities for each of the 21 mantle domains and their 3D integration.

Originality. The obtained mantle-density model of the Ukrainian Shield aligns well with the division of the mantle into three main layers: lithosphere, upper mantle, and lower mantle. Each of the mantle's structural layers has its representation pattern in density heterogeneities. Anomalies of decreased density in the lithosphere of the Ukrainian Shield correlate with thermal anomalies, whereas anomalies of increased density correspond to tectonic zones dividing its megablocks.

Practical value. Regions of increased density gradient are associated with mantle thrust faults, which in some cases can be boundaries between different petrological formations and serve as channels for magma ascent into the Earth's crust at certain stages of geological development of the Ukrainian shield and, in turn, be sources of minerals.

Keywords: *Ukrainian Shield, mantle, Adams-Williamson equation, density, 3-D model*

Introduction. Since the end of the last century, research has enhanced the detailed knowledge of the Earth's internal structure. Modern models are based on seismic tomographic data, which have been used to construct global seismic tomographic maps reflecting seismic heterogeneity of the Earth's interior at different depths in the mantle [1]. However, the question on whether using a single one-dimensional reference model of the Earth is suitable for reconstruction of the mantle structure under continents, oceans, platforms, folded areas and other large geotectonic structures has not yet been resolved. Thus, research questions remain open: which model should be chosen for the reconstruction of different regions? How should the reconstructions that use several one-dimensional reference models be coordinated? Geophysicists also have to solve the issues related to the sphericity of the Earth when (*i*) choosing its mediated structure and determining the level of detail of the model [2], (*ii*) accounting for velocity anisotropy [3], (*iii*) using common and consistent P- and S-wave data [4] and (*iv*) recalculating seismology data into the Earth density model [5]. These questions concerning mantle density are being studied actively.

In particular, there is active investigation to discern the structure of the mantle beneath the Ukrainian Shield. Previous studies present the preliminary stages necessary for the conversion of quasi-three-dimensional P-velocities into mantle density. Data from seismic tomographic kinematic methods was used to recalculate data on P-wave velocities in the mantle beneath the Ukrainian Shield [6]. P-wave velocities data served to determine seismic boundaries in the mantle using the first derivative of the P-velocity depth curve, $v_p(z)$ [7]. Each of these curves represents a distinct mantle domain located beneath the Ukrainian Shield. Further studies constructed a synthetic S-velocity model that is collinear with the original P-velocity model and remains within the error range of the kinematic seismic tomography method. Density heterogeneity obtained from the Adams-Williamson equation solution has been resolved by developing a method of polynomial corrections [8]. These corrections were calculated for reference models [9]: PREM, PEMA, PEMC, AK135 and IASP91. The reference model AK135, which was constructed from the gravitational field of a point potential at the shield's center [10], can be considered the reference for the Ukrainian Shield.

Recognizing that it is currently unfeasible to simultaneously address all issues associated with Earth's density models, this investigation examines the following matters: 1) converting 21 P- and S-velocity curves of mantle domains of the Ukrainian Shield into density using the Adams-Williamson equation and polynomial adjustments for heterogeneity on intervals identified by seismic boundaries within the depth range of 50–2,600 km (the aggregate of resultant density curves comprises a quasi-three-dimensional model); 2) appropriately linking the obtained model with the masses of the upper and lower mantle.

The aim of this study is to construct a density model beneath the Ukrainian Shield. To this end, we propose a new set of methods (approaches) for a (step-by-step) construction of a three-dimensional (quasi-dimensional) model of mantle density beneath the Ukrainian Shield. The proposed model has been obtained as a result of the solution of several problems, imposed both by the initial data and, to a large extent, by the limitations of the theoretical and practical aspects of the construction of density models. We first explain the methodology to derive these models, which equally apply to both one-dimensional density calculation problems and to their multidimensional variants. Next, we present the obtained 3D density model from depths ranging from 50 to 2,600 km. We then discuss the accurateness of our model with respect to other existing models. We finally conclude that the density anomalies beneath the Ukrainian Shield correlate with deep mantle inhomogeneities.

Methods. ***Theory.*** The presence of two types of waves with different front propagation velocities, compression – longitudinal – and shear – transverse – in a homogeneous isotropic medium was proved by Poisson. This is a consequence of the fact that there are no rotating particles in the compression-tension waves, and shear waves are not accompanied by a change in volume. The dependence of seismic velocities on density underlies the analytical Poisson solution for the wave equation in two-dimensional Euclidean space. According to the theory of elasticity, at *small deformations,* particle motions represent *elastic* waves. In a homogeneous boundless medium, the equation of elastic wave propagation is described as follows. Let us denote by X, Y, Z the components of external mass forces acting on a volume element, δV. The forces, according to Dalembert's principle, are proportional to the accelerations, i.e., to the second derivatives of the displacement components in time. The volume element is in equilibrium, which for any stress fields in the case of isotropic medium is written in the form

$$(\lambda+\mu)\frac{\partial\Theta^2}{\partial x}+\mu\nabla^2 u+\rho X=\rho\frac{\partial u}{\partial t^2}; \quad (1)$$

$$(\lambda+\mu)\frac{\partial\Theta^2}{\partial z}+\mu\nabla^2 w+\rho Z=\rho\frac{\partial w}{\partial t^2},$$

where $\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ is the Laplace operator, $\Theta = \frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}$ is dilatation, $u = u(x, t), v = v(y, t), w = w(z, t)$ are displacement fields caused by bulk forces at time $t = 0$, in general under different conditions, and λ, μ are elastic moduli or Lame coefficients.

In the absence of external forces, i.e., when only inertial forces arising during steady-state oscillatory motions act, $X = Y = Z = 0$. In this case, two fundamental equations can be obtained by formal transformations

$$\nabla^2\vec{u}=\frac{1}{v_p^2}\frac{\partial^2\vec{u}}{\partial t^2}; \quad (2)$$

$$\nabla^2\vec{u}=\frac{1}{v_s^2}\frac{\partial^2\vec{u}}{\partial t^2}. \quad (3)$$

Equation (2) describes the propagation of longitudinal (compression) waves and (3) describes transverse (shear) waves. The P- and S-velocities, v_p and v_s, respectively, are expressed in terms of elastic parameters and density as

$$v_p=\sqrt{\frac{(\lambda+2\mu)}{\rho}}; \quad v_s=\sqrt{\frac{\mu}{\rho}}. \quad (4)$$

One of the Lamé coefficients is the shear modulus, $\mu = (\Delta F/A)/(\Delta L/L)$, i.e., the ratio of a transverse deformation – specific shear force in cross section A – to longitudinal deformation (shear ΔL by length L). The other coefficient is related to the bulk modulus, $K = \Delta P/(\Delta V/V)$, i.e., the ratio of the change in hydrostatic pressure ΔP to the compression of a given volume V as

$$\lambda = K - (2/3)\mu. \quad (5)$$

The P- and S-wave velocities are expressed as a function of the bulk and shear moduli as

$$v_p^2=\frac{1}{\rho}\left(K+\frac{4}{3}\mu\right); \quad v_s^2=\frac{\mu}{\rho}. \quad (6)$$

Combining the P- and S-wave velocities from Equation (6), the seismic parameter F can be obtained as

$$\frac{K}{\rho}=v_p^2-\frac{4}{3}v_s^2=F. \quad (7)$$

From the definition of the bulk modulus, and taking into account that density changes are directly proportional to volume, $K = \Delta P/(\Delta\rho/\rho)$, and considering (7) yields

$$F=\frac{\Delta P}{\Delta\rho}. \quad (8)$$

If we assume that the change in pressure depends only on the weight of the overlying layer of thickness Δl, then,

$$\Delta P=\rho g\Delta l, \quad (9)$$

or

$$\Delta\rho F=\rho g\Delta l, \quad (10)$$

where g is the gravity force. Passing from finite increments to infinitesimal ones, we obtain the Adams-Williamson equation

$$\frac{d\rho}{dl}=-\frac{g\rho}{F}. \quad (11)$$

P- and S-wave velocities. Problem definition and its solution arise from the nature of the used initial data. Our input data are the seismic tomographic P-velocity model for the mantle beneath the Ukrainian Shield [6], which we want to reconvert into a density model. The P-velocity model was constructed taking into account the known crustal thicknesses and using the kinematic method based on the solution of the seismic problem by decomposing the slowness function into a Taylor series [11]. The obtained solution of the seismic tomography problem represents the exact lower boundary with respect to the solution obtained by the classical linearization method and contains fewer limitations on the velocity function. The method does not depend on the choice of the initial approximation (one-dimensional reference model) and is correct according to Tikhonov. The model itself represents a set of one-dimensional curves of the P-wave velocity with depth, $v_p(z)$, characterizing some volume of the petrophysical medium, the size of which depends on the sampling window of the P-phase seismic wave first arrival times in the midpoint format, i.e., the data for the hodograph. The inversion of the hodograph gives the solution $v_p(z)$ as a smooth, non-decreasing function, with the constant velocity function inside the waveguide (if any), and calculated from the velocity values at the upper and lower boundaries of the waveguide. This smooth and non-decreasing representation of the velocity function $v_p(z)$ carries information about the layers and seismic boundaries in an implicit way. Seismic boundaries were determined from the kinks in the first derivative of $v_p(z)$. The obtained results demonstrate that the mantle beneath the Ukrainian Shield in the depth interval of 50–2,600 km has a layered structure, with depth-varying layers whose morphology is correlated with large tectonic units and has significant deviations from all known seismic boundaries of Earth reference models (AK135, PREM, IASP, PEMA, PEMC). The main obstacle for using this velocity model for the calculation of the density and other physical parameters of the mantle, like temperature and viscosity, is the availability of velocities of P-waves. Since the Adams-Williamson equation (10), $F=\left(v_p^2-\frac{4}{3}v_s^2\right)$ and, thus, the seismic velocities v_p and v_s, should be known.

To recalculate the P-velocities into S-velocities, we follow the approach proposed in [4]. It has been shown that if the ratio v_p/v_s is recalculated using the arithmetic mean of five reference seismological models, the obtained synthetic S-velocity model has acceptable deviations, which are comparable to the resolution of the method used to produce it, i.e., the kinematic Taylor approximation of the seismic problem solution. The calculated velocity errors from determining the maximum depth of the refracted apparent ray are of the same order as the deviations for one-dimensional reference models ($v_s - v_{s1}$), where *vs* is the velocity value from literature and *vs*1 is the velocity value obtained by conversion and are much lower than the error of ± 0.1 km/s, which can be achieved by other seismic methods [12]. That is, the synthetic S-velocity model obtained by recalculation of the P-velocity model has the property of commensurability with the original model, which gives advantages in accuracy for further joint use of two collinear models (P, S) during transformations into petrophysical (physico-lithological) models of the mantle.

1D density model. When both P and S velocities are available, it is possible to calculate the mantle density by using the Adams-Williamson equation (10). This calculation is feasible under some imposed restrictions, namely, the Earth has a homogeneous composition, the pressure builds-up in the Earth's mantle according to the hydrostatic law, i.e., the pressure increases $\Delta\rho$ as the depth increases by Δr (r is the sphere radius), and it is equal to the weight of the substance of this layer per unit area. That is, the material compression under the action of gravity forces is prevented mainly by elastic forces, i.e., Hooke's law is valid. (10) includes the seismic parameter F, which is a function of the already known seismic velocities v_p and $v_{s.}$

Using the Adams-Williamson equation, we obtain a density model for the homogeneous Earth's mantle, which is far from reality. The densities according to the five reference mantle models (AK135, IASP91, PREM, PEMA, PEMC) obtained using the Adams-Williamson equation were considered by Shumlianska and Pigulevskiy [8]. It has been shown that the differences between the densities are significant and a solution was proposed to obtain the first approximation of the density values $\rho(v)$. Comparing a homogeneous model after Adams-Williamson equation by data from one reference model (AK135, IASP91 PREM, PEMA, PEMC, digital data on models taken from the IRIS website and the "real" heterogeneous values, the following reference model was made [8]:

1. The Adams-Williamson equation (10) provides a solution for a homogeneous model of the Earth. We calculated the density using the Adams-Williamson equation with input data (v_p, v_s, ρ_0 – initial density) from reference models (PREM, PEMA, PEMC, IASP91, AK135), and obtained corresponding $\rho_{A\text{-}W}$ values for each model.
2. The density $\rho_{A\text{-}W}$ was approximated using polynomials within seismic boundaries for each model.
3. Density data (ρ) from reference models were also approximated on the same intervals as $\rho_{A\text{-}W}$ at the specific site.
4. The polynomial correction of heterogeneity is determined by the variation between the polynomials ($\rho - \rho_{A\text{-}W}$) in each interval within the seismic boundaries.

The density distribution in a one-dimensional model within a single layer, bounded by seismic boundaries, is described by a linear function of the form $\rho(z) = \rho_0 + k(z)$, where $\rho(z)$ represents the density value at depth z, ρ_0 represents the density value at the upper point of the layer (note that the upper point of one layer simultaneously serves as the lower point for the layer above it) and k is the angular coefficient, which determines the density variation with depth.

Method for selecting an optimal reference model. The total contribution of the spherically symmetric layers of the Earth to the total gravity field in the centre of the Ukrainian Shield at the point 31.5 E and 48.5 N is 981,658.94 mGal. The gravimetric database [10] was used to calculate the total gravitational field. For the core, the value of the gravitational effect was defined as 367,131.8 mGal. The gravitational effects from the upper and lower mantle were calculated using the data obtained from the five reference models (AK135, IASP91, PREM, PEMA, PEMC), adding the values for the crust at the point of calculation according to the data on the density of the crust of the Ukrainian Shield given by Svistun, et al. [10], Kurlov, et al. [13], Azarov, et al. [14, 15], Antsiferov, et al. [16, 17]. By comparison of the total amount with the value of 981,658.94 mGal, it was found that the value of the total gravity field calculated using the AK135 model has the smallest deviation.

Calculation of the 3D density model. We propose a methodology to recalculate synthetic P and S velocity three-dimensional models into density values, and we apply the proposed methodology to the mantle beneath the Ukrainian Shield. The calculation of the synthetic P- and S-velocity three-dimensional model was carried out according of the method described [4]. The calculation into density values will be done by making polynomial corrections for heterogeneity. The AK135 reference model is chosen as the "initial" model for the mantle beneath the Ukrainian Shield.

The calculation of the density model consists of several stages, which are briefly formulated below:

1) determination of the seismic boundaries by the inflection points of the first derivative of the velocity curves $v_p(z)$ from the seismic tomographic model of the mantle beneath Ukrainian Shield [6]. This is a quasi-3D model, represented by a set of one-dimensional velocity curves obtained by solving the seismic problem by the method of kinematic approximation [11];

2) calculation of the synthetic S-velocity model using the P-velocity model, which has the property of commensurability (proportionality) with the original model, giving advantages in accuracy when the two collinear models (P, S) are used together for conversion to the density mantle models [4];

3) calculation of one-dimensional density curves by solving the Adams-Williamson equation, using P and S velocity values for each mantle domain beneath the Ukrainian Shield as input data;

4) transformation of the obtained density curves representing one-dimensional, homogeneous models of different mantle domains using polynomial corrections from reference model AK135, which is selected as optimal for modelling mantle density beneath the Ukrainian Shield [8].

The Adams-Williamson equation (10) for the first iteration step requires initial density parameters ρ_0. The initial densities at the 50 km level were provided by Kurlov, et al. [13], Azarov, et al. [14, 15], Antsiferov, et al. [16, 17].

Seismic boundaries of mantle beneath the Ukrainian Shield vary with depth and do not follow boundaries for the AK135 model. Significant depth variations of seismic boundaries are also known and recorded by other seismological methods.

The calculated density results are checked for compliance against the AK135 reference model. The mass of the upper and lower mantle is calculated from the obtained density results. The masses are compared with the corresponding masses in the AK135 model. Corrections are made as the arithmetic mean value separately for the upper and lower mantle if there is an excess or deficiency of mass in the experimental model. The formula for calculating the mass, m, is the following system of equations

$$\begin{cases} \rho(r-\Delta r) = \rho(r) - \Delta\rho = \rho(r) + G\dfrac{\rho(r)m(r)\Delta r}{Fr^2} \\ m(r-\Delta r) = m(r) - \Delta m = m(r) - 4\pi\rho(r)r^2\Delta r \end{cases}, \qquad (12)$$

where ρ is density; $\Delta\rho$ is an increment of density; m is the mass of the Earth; Δm is an increment of the mass; r is the radius of the Earth; Δr is an increment of the layer thickness*;* G is the gravitational constant.

The same calculation must be done for the reference model AK135. The differences between the masses of the upper mantle according to the AK135 and the masses from density curves constructed for each of the domains of the Ukrainian Shield are introduced as a correction. It is calculated separately for each of the experimental curves as an average over the whole section above from the upper mantle boundary. Fig. 1 shows an example of the procedure of mass corrections for a density curve which is constructed for the upper mantle domain with a midpoint coordinate of 31.5E and 48.5N. It can be seen that we are able to preserve individual features of the initial P-velocity curve while keeping the mass balance in accordance with the reference model AK135. These operations are performed for each of the mantle domains beneath the Ukrainian Shield.

Results. The obtained results are presented as a set of one-dimensional density curves for each of the mantle domains beneath the Ukrainian Shield, calculated in the depth range of 50–2,600 km, with a step of 25 km. The results of the density calculations are presented in the form of horizontal sections for depths from 50 to 1,500 km (Fig. 2).

In spite of the direct relationships between the solution of the Adams-Williamson equation and the initial density values chosen for the first iteration, we manage to eliminate such a dependence by applying subsequent transformations as described above. We obtain a three-dimensional density model that corresponds to (is collinear to) the initial P-velocity model. Fig. 2 shows a variation with depth of the mantle density beneath the Ukrainian Shield. Its comparison with the 75 km section, where densities are calculated according to the P-velocity model, shows a significant difference in the geometry of anomalies, which reflects the heterogeneity beneath different tectonic units of the Ukrainian Shield. Considering the sections 75–200 km, which depict the lithosphere structure, we note that at these depths the general geostructural plan of the Ukrainian Shield is broken by a submeridional zone in its central part (Fig. 2, 75–100 km). The density difference from 3.2 to 3.6 g/cm^3 is confined to this zone. The central part of this zone corresponds to the transregional tectonic Inhul fault zone, which correlates well on 150–200 km sections with the pattern of the lithosphere lower boundary depths, identified by thermal anomalies [18]. It also agrees with the deep mantle heterogeneities, identified by complex analysis of potential physical fields and seismic studies of the Ukrainian Shield [19].

Sections constructed at depths of 500 and 600 km correspond to the lower boundary of the upper mantle. Below 500 km, the density anomalies in the upper mantle reflect changes in the pressure and temperature (PT) conditions and, possibly, the composition of the mantle rocks. The spatial correlation of mantle density anomalies with surface structures at such depths is meaningless. Low-density anomalies completely change their shape below 800 km, being localized beneath of the centre of the Ukrainian Shield and expanding along the boundaries of the Dnieper–Donets Basin. Down to 1,500 km, the density anomalies generally retain this pattern. Below 1,500 km, an equant anomaly of high density begins to form under the south part of the Holovaniv suture zone. At these depths, the submeridional zone becomes less contrasting, which may be related to the PT conditions, which level the density features. Moving into the lower mantle, starting from the depths of 800 km and below, this zone is practically not visible (Fig. 2, 800–1,500 km). Interpretation of deep anomalies in the upper and lower mantle for such a small area as the Ukrainian Shield is practically meaningless since it would be necessary to extend the area of research for geodynamic modelling, including calculations of rock composition, viscosity, and temperature.

Discussion. The proposed methodology for recalculating (transforming) the initial P-velocity model into a 3D density model has been applied for the first time to the Ukrainian Shield. We now discuss its suitability by comparing it with the methods used by other researchers. There are two general approaches to solve the problem of finding the density of the Earth's mantle. One of them assumes the creation of one-dimensional reference models with radial distribution of density, with an a priori assumption regarding the mantle composition. Density is presented in general terms as

$$C = a + b\rho; \qquad (13)$$

$$C = (v_p^2 - 4/3v_s^2)^{1/2}, \qquad (14)$$

where C is acoustic wave velocity, and a and b are coefficients, which depend on the atomic weight of the substance. For bulk wave velocities, the experimental relations with density are

$$v_p = a_p + b_p\rho; \quad v_s = a_s + b_s\rho. \qquad (15)$$

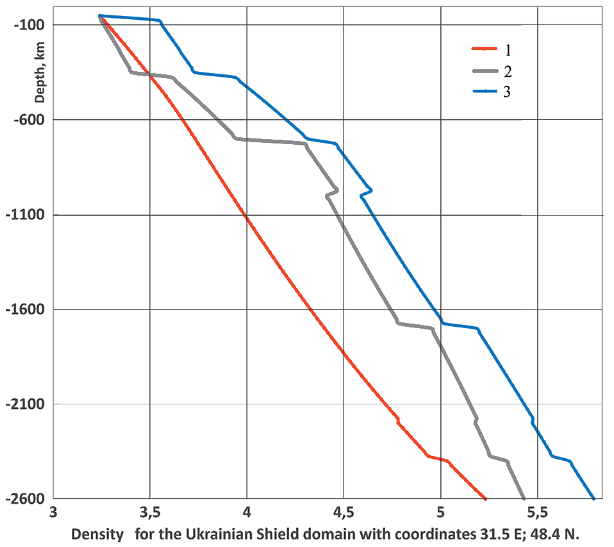

Fig. 1. Example of the application of the mass correction to the density curve constructed for the upper mantle domain with midpoint coordinates 31.5E and 48.5N:

1 – Density according to the Adams-Williamson equation; 2 – Polymial Heterogeneity Corrected Density; 3 – Polynomial Heterogeneity Corrected Density mass-balanced

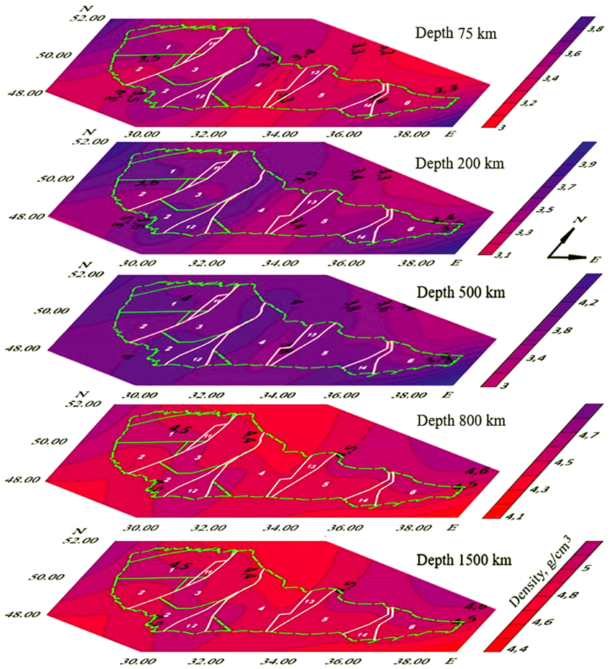

Fig. 2. Horizontal sections of the mantle density beneath the Ukrainian Shield, g/cm^3, for several depths ranging from 50 to 2,500 km. Tectonic division of the Ukrainian Shield [13]. *Domains:*

1 – Volyn; 2 – Dniester-Bouh; 3 – Ros-Tikych; 4 – Inhul; 5 – Middle Dnieper; 6 – Azov. Suture zones: 11 – Nemyriv-Kocheriv; 12 – Holovaniv; 13 – Krivyy Rih–Kremenchuh; 14 – Orikhiv-Pavlohrad

In this approach, it is necessary to know the coefficients *a* and *b*. The Birch's approach has been widely applied for resolving the problems of calculation of the density of the crustal and mantle rocks beneath the Ukrainian Shield by Gordienko, et al. [20, 21], Krasovsky, et al. [22].

In these standard Earth-density models, the solutions are based on the sequential differentiation of the gravity equation for spherical layers along their radii. The basic analytical relations for a spherical Earth with homogeneous stratification along the radius are given in [23]. This approach takes into account conditions at the boundaries of the piecewise-radial density distribution according to the Roche law and Gauss model [24]. With this approach, if the density of the Earth is set at the surface, it is possible to calculate the values of the seismic function at each of the known seismic boundaries of the Earth. The representation of the mantle structure by seismic wave velocity anomalies, supplemented by seismic boundaries, allows using the technique of layer-by-layer density finding at fixed layer boundaries. Our proposed methodology refers to this approach, where the coefficients *a* and *b* are found as polynomial corrections to the solution of the Adams-Williamson equation (10).

The other approach is based on modern seismic tomography studies of the mantle density structure and phase state that show that the influence of inelasticity in the mantle must be taken into account [25, 26] and his followers derive density, temperature, and other parameters in the mantle through nonlinear components, namely the absorption time of the seismic energy by a medium through which waves with different frequencies pass. This approach shifts the attention to the elastic properties of the crystal lattice, i.e., it is necessary to know at least the composition of rocks and the pressure. A complete solution of the mantle density problem is possible only by jointly solving it using the two approaches, linking the physical macro and micro models of the mantle.

Verification by an independent method of the obtained data at this stage is possible only at the qualitative level. We have already mentioned the similarity of anomalies obtained from different geophysical fields at different depths [19] and density anomalies. A similar picture was obtained for the depths of the lithosphere lower boundary [18].

The quantitative verification of the model will be possible when the three-dimensional density model of the mantle for the Earth as a whole will be calculated. In such case, not only will it be possible to calculate the moment of inertia and compare it with the observed data, but also to determine the orbital height of any artificial satellite and compare it with its actual orbit by calculating the gravitational potential. The proposed model can be used as a reference for modelling the mantle convection and long-term dynamics of the lithosphere. If the convection is considered as a slow deformation of a highly viscous liquid, then the Navier-Stokes equation can be used with some general assumptions and simplifications. For instance, as long as the compressibility has not a significant effect, the deviations from a reference density profile do not exceed several per cent. The equations can be simplified by the introduction of common approximations that assume a temporally constant, but depth-dependent reference profile for the density (the inelastic liquid approximation), or a complete lack of the compressibility and usage of a constant reference density (the Boussinesq approximation). However, such simplification results in significant errors when the models of the layered environment or the ones having significant temperature gradients are considered.

The most accurate approximations of the Navier-Stokes equations for geodynamics were proposed by Gassmoler, et al. [27] and implemented in the open-source modelling software ASPECT [28]. These authors proposed using a density which takes into account the effects of the varying temperature and composition, but neglected changes in dynamic pressure, which could cause volume changes in the order of 0.1 % or smaller.

The proposed mantle density model beneath the Ukrainian Shield is suitable for such geodynamic modelling. The model has all the necessary properties: density variations in the order of about 0.1 %, and density variations that are caused by the changes in the rock composition or temperature [27]. The density change in the proposed model is revealed by a step in isolines. In turn, the isoline pitch directly depends on the resolution of the seismic tomography method, i.e., on the Fresnel zone's size. It has been shown that for the upper mantle, the resolution of the method is 30 km, and for the lower mantle it is 50 km [7].

The heterogeneous structure of the mantle beneath the Ukrainian shield, shown as seismic tomography velocity anomalies [6], has also been confirmed by geochemical studies. For instance, Tsymbal [29], who studied geochemical anomalies in the upper mantle beneath the Ukrainian Shield, showed that the upper mantle under the Ukrainian Shield is heterogeneous both horizontally and vertically in terms of the degree of differentiation, depletion, and metasomatic reworking. The upper mantle beneath the Volyn and Dniester-Bouh domains is differentiated, and the rocks are weakly depleted; beneath the Ros-Tikych domain, the mantle is weakly metasomatized; beneath the Inhul Domain, mantles are moderately differentiated, depleted and variably metasomatized, whereas mantle beneath the Middle Dnieper Domain is depleted and beneath the Azov Domain it is weakly depleted and largely metasomatized. It is worth noting that the areas of mantle depletion defined by [29] roughly correspond to the areas beneath the Ukrainian Shield that host positive density anomalies. In contrast to the seismic tomography data, which reflects the current state of the mantle, the geochemical data refers to certain moments in the past when the corresponding mantle-derived rock complexes were formed. This observation may indicate the long-lasting nature of the mantle (lithospheric) density anomalies. They correspond to certain domains of the continental crust that have experienced different geological histories and were formed at different moments in the past [30, 33]. Some of the density anomalies may correspond to the eclogite-bearing buried ancient subduction zones [31].

A complex heat flow pattern was obtained for the territory of Ukraine by Gordienko, et al. [32]. The coincidence of anomalies of the low density of mantle rocks with anomalies of the increased heat flow is apparent from consideration of horizontal sections of the mantle density (Fig. 2) and the heat flow. These anomalies can be traced to a depth of 200 km, which corresponds to the lower boundary of the lithosphere [18, 34]. So, we can conclude that there is a significant influence of temperature on rock density, at least in the lithosphere layer.

Conclusion. A 3D mantle density model beneath the Ukrainian Shield is presented in this paper. The density model is obtained by recalculating the P-velocity seismic tomographic model of the mantle. The velocity model is represented by a set of twenty-one one-dimensional velocity curves, each obtained by inverting a hodograph (a travel-time curve) representing a single mantle domain beneath the shield. Each P-velocity curve has individual features, retaining a layered structure in general. The set of density curves that are recalculated from these P-velocity curves constitutes a 3D density model (quasi-3D). Three layers are identified in the mantle: the lithosphere, upper and lower mantle, each of them significantly differing in terms of the density distribution. The analysis of the 3D model of the mantle density beneath the Ukrainian Shield shows the correlation of the density anomalies with deep mantle inhomogeneities identified from the results of a comprehensive analysis of potential physical fields and deep seismic studies. The tectonic and geological structure of the Ukrainian Shield are reflected in the density anomalies in the lithosphere. The domains of the Ukrainian Shield have lower lithosphere densities than the suture zones separating them. The denser lithospheric mantle beneath the sutures likely indicates the presence of eclogitic rocks. Besides, the density model shows the link between the anomalies of low density and the anomalies of increased heat flow, reflecting the significant effect of temperature on rock density, at least in the lithosphere. Finally, areas of mantle depletion roughly correspond to the areas beneath the Ukrainian Shield that host positive density anomalies. In contrast to the seismic tomography data which reflects the current state of the mantle, the geochemical data refers to certain moments in the past when the corresponding mantle-derived rock complexes were formed. This observation may indicate the long-lasting nature of the mantle (lithospheric) density anomalies. The link between the tectonic structure of the crust and lithospheric density anomalies can be traced to depths of 200 km and then they vanish at the depth of 500 km, showing the influence of the lithosphere as a colder layer on the rock properties of the upper mantle. The obtained three-dimensional model of mantle density beneath the Ukrainian Shield allows establishing a correlation between the deep layers: the lithosphere, upper mantle, and lower mantle. The transition from the velocity model of wave propagation to the distribution of density opens possibilities for further determination of other physical parameters, such as temperature and viscosity. This, in turn, unveils the potential for geodynamic modelling.

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Тривимірна модель густини мантії під Українським щитом

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Мета. Розробка моделі густини мантії для розуміння фундаментальних геологічних і фізичних процесів, що відбуваються всередині Землі, і є важливим для нашого наукового та практичного розуміння будови планети.

Методика. Поставлені завдання вирішувалися комплексним методом дослідження, що включає аналіз й узагальнення літературних і патентних джерел, проведення аналітичних, експериментальних досліджень із використанням методів комп'ютерного та математичного моделювання.

Результати. Одновимірні моделі спрощують розподіл густини мантії, передбачаючи, що він є однорідним лише у вертикальному напрямку. Це обмеження не дозволяє враховувати горизонтальні варіації густини мантії, що можуть бути важливими на регіональному рівні. Тривимірні моделі більш складні та вимагають більше даних й обчислювальних ресурсів, тому їхнє використання може бути обмеженим. У цьому дослідженні ми презентуємо квазітривимірну модель густини мантії під Українським щитом. Ця 3D-модель отримана за допомогою базового набору одновимірних сейсмічних томографічних швидкісних моделей, розрахованих для 21 мантійного домену в діапазоні глибин від 50 до 2600 км. Процес перетворення моделі швидкості P-хвиль у модель густини включає такі етапи: 1) визначення сейсмічних границь у мантії на основі кривих швидкостей P-хвиль для кожного мантійного домену; 2) створення синтетичної моделі мантії під Українським щитом для кривих швидкостей P,S-хвиль; 3) вирішення рівняння Адамса-Уільямсона для кожного домену, ураховуючи поліноміальні поправки для врахування неоднорідності; 4) аналіз існуючих моделей шляхом порівняння розрахованого гравітаційного потенціалу та поля, що спостерігається в центральній точці Українського щита в якості еталону для вибору однієї з 5 референтних моделей (ПРЕМ). У нашому дослідженні ми акцентували увагу на останніх етапах конструювання моделі густини мантії: 1) збалансування маси верхньої й нижньої мантії для кожного домену при визначенні густини за допомогою рівняння Адамса-Уільямсона та уведення поліноміальних поправок; 2) розрахунок густин для кожного з 21 мантійних доменів і їх 3D-інтеграція.

Наукова новизна. Отримана модель густини мантії Українського щита добре відповідає поділу мантії на три основні шари: літосферу, верхню мантію й нижню мантію. Кожен структурний шар мантії має свій патерн представлення в неоднорідностях густини. Аномалії зменшеної густини в літосфері Українського щита корелюють із тепловими аномаліями, тоді як аномалії збільшеної густини відповідають шовним зонам, що їх розділяють.

Практична значимість. Регіони зі збільшеним градієнтом густини пов'язані з мантійними аномаліями, які в деяких випадках можуть бути межею між різними петрологічними формаціями, та служити каналами для підняття магми до земної кори на певних етапах геологічного розвитку Українського щита, та привносити геохімічні елементи для утворення корисних копалин.

Ключові слова: *Український щит, мантія, рівняння Адамса-Уільямсона, густина, 3-вимірна модель*

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