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**MINERALOGY**

# SYMMETRY AND STRUCTURAL COMPLEXITY OF MINERALS OF THE EARTH DEEP GEOSPHERES (PYROLITE MODEL)

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**Abstract.** Using the Dolivo-Dobrovol'sky index and information-based parameters on the basis of new experimental data, the problem of symmetry and structural complexity of the mineral matter of the deep geospheres is considered in the framework of the pyrolite model of the Earth's mantle. It is shown that, in contrast to the previously made conclusions about the increase of the symmetry of minerals with depth, the behavior of the quantitative parameters of symmetry and structural complexity is nonlinear. The symmetry increases (and the structural complexity decreases) to the boundary of the decomposition of ringwoodite into bridgmanite and "magnesiowustite" (660 km), after which there is a decrease of the Dolivo-Dobrovol'sky index to 18.40 and an increase of the atomic parameter of structural complexity to 2.786 bit/atom. This behavior is due to the uneven and opposite effect of temperature and pressure on the symmetry and complexity of the crystalline substance, which is caused by the nonlinear nature of the averaged geotherm of the Earth's crust and mantle. Information parameters of structural complexity are a more sensitive indicator of symmetry than the Dolivo-Dobrovol'sky index, which is due to the former taking into account the features of the crystal structure of specific minerals.

**Keywords:** *symmetry, structural complexity, information, mineralogy, deep Earth geospheres, mantle geotherm, temperature, pressure*

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## INTRODUCTION

Symmetry is one of the most fundamental properties of mineral matter [1]. The large amount of accumulated data on the symmetry of crystal structures of minerals allows analyzing the frequency of occurrence of various types of symmetry and space groups [2] and drawing conclusions about the evolution of symmetry and complexity of crystalline matter in the geological history of Earth [3-5]. More than forty years ago, V.V. Dolivo-Dobrovol'sky studied – based on the data available at that time – the evolution of the symmetry of Earth's shells and concluded that there is a "regular increase in the symmetry of Earth's matter with depth" [6]. As a measure of symmetry, V.V. Dolivo-Dobrovol'sky used an averaged symmetry value σ , later called the Dolivo-Dobrovolsky index (see below) [4, 5]. Relatively recently, the conclusion about the increase in the average symmetry of minerals with depth was repeated by S.K. Filatov [7] based on calculations made in a 1984 paper [6]. However, a large number of experimental studies conducted over the past 20 years using modern methods for studying matter at high temperatures and pressures (see reviews [8, 9]) have significantly expanded and deepened our understanding of the mineral composition and structure of Earth's geospheres. The purpose of this work is to analyze the depth evolution of symmetry and structural complexity of Earth's crystalline matter using the latest experimental data and theoretical methods. As will be shown below, V.V. Dolivo-Dobrovol'sky conclusion about the increase in mineral symmetry with depth needs significant clarification.

## METHODOLOGY

To study the structure of the Earth's mantle, T. Ringwood [10] proposed the so-called pyrolite (pyroxene + olivine) model, according to which the average composition of the mantle is expressed in molar percentages as follows: 44.71 $SiO_2$, 38.73

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MgO, 8.18 FeO, 3.98 $Al_2O_3$, 3.17 CaO, 0.13 $Na_2O$. Despite the fact that the pyrolite model is not the only one, in this work it is used as one of the generally accepted models of the composition and structure of the Earth's mantle. A generalized diagram of the mineral structure of the Earth's shells, compiled on the basis of geophysical data and experimental studies, is presented in Fig. 1 (works [11] and [12] were used). Based on this diagram, percentage ratios (in atomic quantities) of mineral species comprising the Earth's shell were calculated for different depths with a step of 50 km. Despite all the conventionality and approximation of such estimates, they fully meet the task of studying the evolution of symmetry of mineral matter with depth.

To assess the average symmetry of the mineral aggregate, the Dolivo-Dobrovol'sky index σ (characterizing the average order of the holohedry group of the corresponding mineral system) and the mean atomic complexity parameter introduced for the first time in this work $\overline{I_G}$ (reflecting the average amount of structural information per atom in bits) were used.

Dolivo-Dobrovolsky Index σ was calculated using the formula:

$$\sigma = \sum_{i=1}^{n} x_i s_i \qquad (1)$$

where $x_i$ is the normalized atomic amount of phase $i$ in the aggregate; $s_i$ numerical characteristic of the mineral phase crystal system, equal to the order of the holohedry group in the given crystal system (= maximum order of the point group in the crystal system); $n$ is the number of phases in the aggregate. Note that

$$\sum_{i=1}^{n} x_i = 1 \qquad (2)$$

and the parameter $s_i$ equals 2, 4, 8, 12, 16, 24, and 48 for triclinic, monoclinic, orthorhombic, trigonal, tetragonal, hexagonal, and cubic crystal systems, respectively. V.V. Dolivo-Dobrovol'sky [6] used the fraction of the total mass of the aggregate attributed to phase i as the $x_i$ parameter, which does not seem entirely correct due to differences in molecular masses of various mineral components of the Earth shells.

To calculate the informational parameters of symmetry and complexity of crystalline matter, the methodology previously developed in [13, 14] was used. According to this approach, the complexity of a crystal structure is evaluated as the amount of information per atom in the reduced unit cell, using the following formula:

$$I_G = -\sum_{i=1}^{k} p_i \log_2 p_i \ \text{(bit/atom)} \qquad (3)$$

where $k$ is the number of crystallographic orbits (Wyckoff positions or number of sites) and $p_i$ is the

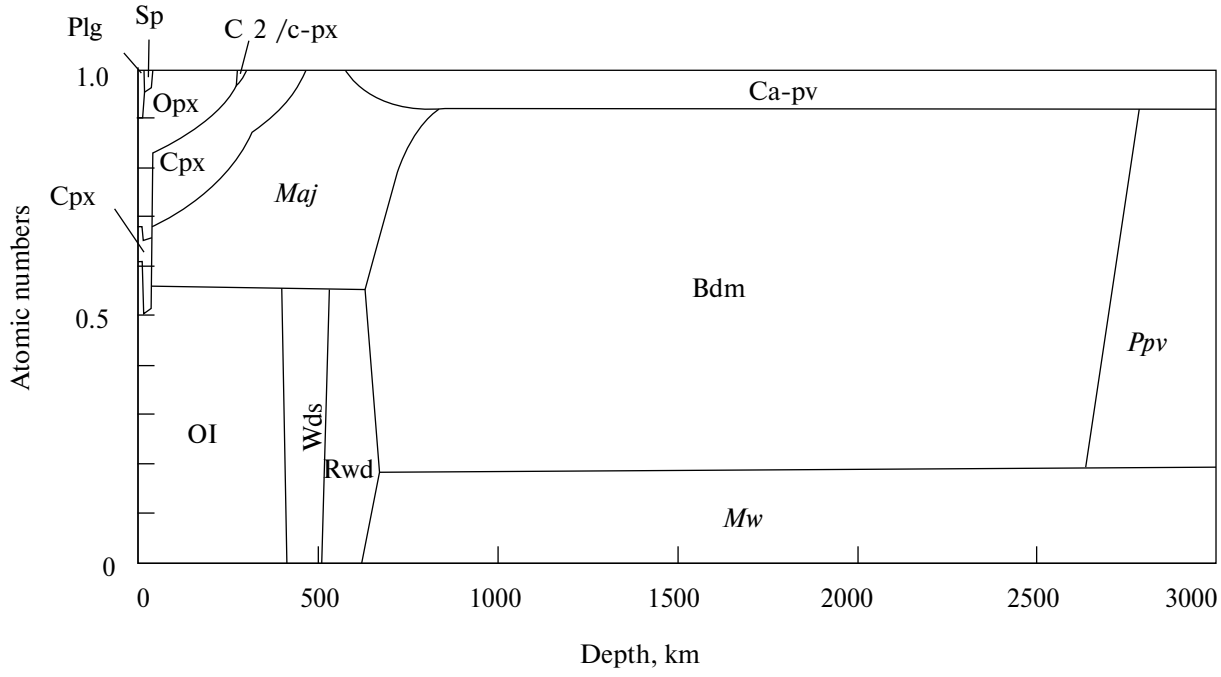


**Fig. 1.** Diagram of the structure of the Earth's deep geospheres to the "mantle-core" boundary (according to [11, 12]). The interpretation of mineral phase symbols is given in Table 1.

probability of randomly selecting an atom from the $i$-th Wyckoff position, i.e.:

$$p_i = m_i / v \,, \qquad (4)$$

where $m_i$ is the multiplicity of the orbit in the reduced cell, and $v$ the number of atoms in the reduced unit cell.

Knowing the values of parameters $I_G^i$ for each mineral phase in the aggregate, the average atomic complexity parameter $\overline{I_G}$ can be calculated as

$$\overline{I_G} = \sum_{i=1}^{n} x_i I_G^i \,. \qquad (5)$$

Table 1 shows the values of parameters $s_i$ and $I_G^i$ for all mineral phases appearing in the diagram in Fig. 1. As already mentioned, the values of parameter were estimated directly from the diagram with a depth increment of 50 km.

## RESULTS

Fig. 2a shows a graph of the change in the Dolivo-Dobrovol'sky index σ with depth. It is clearly visible that, contrary to the conclusions of work [6], repeated in work [7], the average symmetry of mineral matter does not increase with depth, but behaves nonlinearly. Up to a depth of approximately 600 km, the index σ increases sharply (the substance on average becomes more symmetrical, with the maximum index value of 48 being reached, at which all matter has cubic symmetry), whereas after 600 km there is a sharp decline, and from ~880 km to the "mantle-core" boundary, the index σ has a constant value of 18.40.

The behavior of parameter $\overline{I_G}$ (Fig. 2b) with depth turned out to be even more uneven. Up to a depth of 600 km, its value generally decreases (which corresponds to an increase in symmetry and a decrease in structural complexity), after which there is an increase, a plateau (2.786 bits/atom; from approximately 850 to 2650 km), and a decrease to a value of 1.712, which is maintained to the "mantle-core" boundary are observed. Thus, the behavior of parameter $\overline{I_G}$, which describes structural complexity (or the symmetry of the crystal structure taking into account the space group and the size of the unit cell), is more

**Table 1.** Symmetry characteristics of the main minerals of the Earth's crust and mantle within the pyrolite model

| Mineral | Symbol* | Crystal system | Space gr.** | $s_i$ | $I_G^i$ [bit/atom] |
|---|---|---|---|---|---|
| "Plagioclase"*** | Plg | triclinic | $P\bar{1}$ | 2 | 4.700**** |
| "Spinel" | Sp | cubic | $Fd\bar{3}m$ | 48 | 1.379 |
| "Orthopyroxene" | Opx | orthorhombic | $Pbca$ | 8 | 3.322 |
| "Clinopyroxene" | Cpx | monoclinic | $P\,2_1/c$ | 4 | 3.322 |
| "High-temperature clinopyroxene"***** | $C\,2/c$-px | monoclinic | $C\,2/c$ | 4 | 2.522 |
| "Olivine" | Ol | orthorhombic | $Pnma$ | 8 | 2.522 |
| Majorite | Maj | cubic | $Ia\bar{3}d$ | 48 | 1.595 |
| Wadsleyite | Wds | orthorhombic | $Imma$ | 8 | 2.807 |
| Ringwoodite | Rwd | cubic | $Fd\bar{3}m$ | 48 | 1.379 |
| Bridgmanite | Bdm | orthorhombic | $Pnma$ | 8 | 3.374 |
| "Magnesiowüstite" | Mw | cubic | $Fm\bar{3}m$ | 48 | 1.000 |
| "Calcium perovskite" | Ca-pv | cubic | $Pm\bar{3}m$ | 48 | 1.371 |
| "Post-perovskite" | Ppv | orthorhombic | $Cmcm$ | 8 | 1.922 |

Note. * Mineral symbols in Table 1 correspond to those in Fig. 1.
** Sp. gr. = space group
*** Terms in quotes correspond to mineral names not approved by the International Mineralogical Association but widely used in geological literature
**** The parameter value $I_G^i$ for "plagioclase" is chosen as the average of the values for albite (3.700 bits/atom) and anorthite (5.700 bits/atom)
***** High-temperature modification of pyroxene with space group $C2/c$

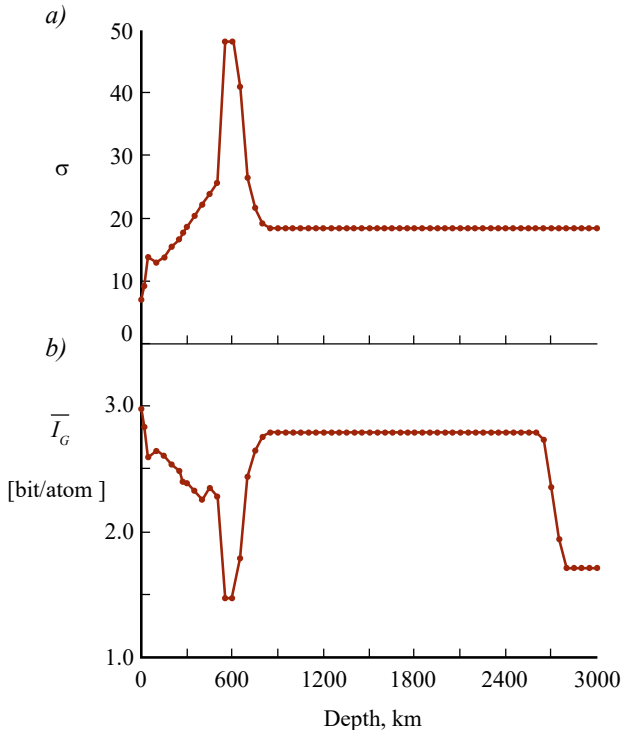


**Fig. 2.** Dependence of the Dolivo-Dobrovolsky index σ (a) and information parameter $I_G^i$ (b) on depth.

nuanced, i.e., this parameter appears to be more sensitive to changes in symmetry than the Dolivo-Dobrovol'sky index.

There is no doubt that the discrepancy between our results and the conclusion made in works [6, 7] is associated with the emergence of new data on the structure of the Earth's mantle and the symmetry of its constituent minerals. Thus, the symmetry of bridgmanite – perovskite-like $MgSiO_3$ – presumably the main mineral by mass of the Earth as a planet [15, 16] is not cubic, as V.V. Dolivo-Dobrovol'sky assumed, but orthorhombic (space group *Pnma*), and the orthorhombic symmetry is preserved throughout the entire range of temperatures and pressures of the lower mantle [17]. It should be noted that in his work, V.V. Dolivo-Dobrovol'sky noted that "for pure $MgSiO_3$, the perovskite-type phase has a distorted structure with orthorhombic symmetry" [6], however, he did not use this information in his further conclusions.

## DISCUSSION

The nonlinear change in parameters σ and $\overline{I_G}$ requires an explanation, which, in our opinion, should be sought in the relationship between the influence of temperature and pressure on the symmetry and structural complexity of matter. It is known that there is a statistically significant tendency for increasing symmetry [18] and decreasing structural complexity [14] of crystalline matter with increasing temperature. Despite the fact that increased pressure ambiguously affects structural complexity, the influence of pressure and temperature on matter has the opposite direction. There are known cases when, with increasing pressure, crystalline matter undergoes phase transitions in the same order that is observed when the temperature decreases. While increasing temperature leads to disordering of the crystal structure, increasing pressure is usually accompanied by processes of atomic ordering.

It is well known that the deep temperature and pressure gradients in the Earth's geospheres have different characteristics [19]. While pressure increases almost linearly with depth (up to the boundary of the mantle and core) with an intensity of about 30–35 MPa/km [20], deep geotherms have a more complex nature. Fig. 3 shows averaged geotherms for whole mantle convection (a) and layered mantle convection (b) models (for hybrid convection models, geotherms are between these extreme variants) [19]. The diagram shows that the dependence of temperature on depth has two (a) or three (b) inflection points (or rather, intervals) where the intensity of temperature increase changes. The temperature rises quite sharply to a depth of about 200 km (for both oceanic and continental geotherms), after which the temperature increase slows down. At the same time, the symmetry of matter increases, and structural complexity decreases (Fig. 2). According to generally accepted concepts [8], at a depth of about 410 km, olivine $Mg_2SiO_4$ transitions to wadsleyite (orthorhombic spinel-like structure), and this reaction is exothermic and accompanied by heat release in the amount of 90 kJ/kg [19]. This leads to additional heating of the substance and a sharp increase in the index σ and a decrease in the value of $\overline{I_G}$ to a depth of approximately 600–650 km. At a depth of 660 km, ringwoodite ($Mg_2SiO_4$ with cubic spinel structure) decomposes into cubic "magnesiowüstite" (isomorphic mixture of periclase MgO and wüstite FeO) and orthorhombic bridgmanite $MgSiO_3$. This reaction is endothermic with heat absorption in the amount of 70 kJ/kg, which causes a temperature decrease of 70 K [19]. This cooling of the substance against the background of constant pressure increase leads to a decrease in average symmetry and an increase in structural complexity. Further to a depth of approximately 2650 km (to the so-called *D*''-layer) the temperature increases monotonically

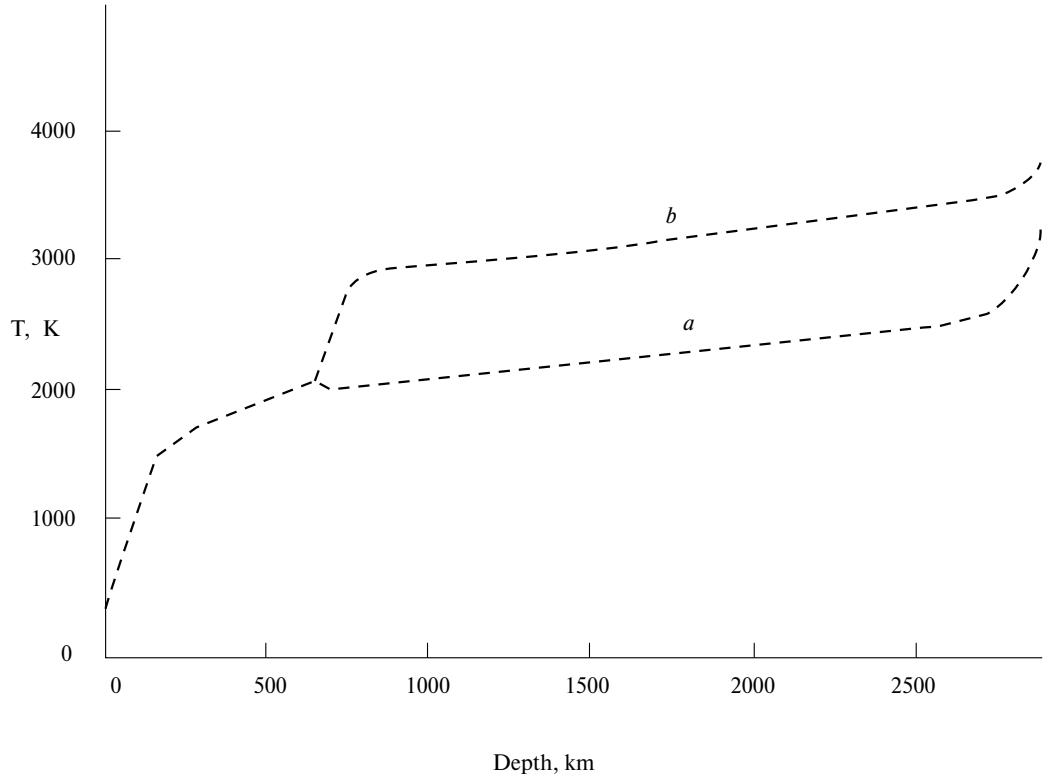


**Fig. 3.** Averaged geotherms of the Earth for models of whole-mantle (a) and layered (b) mantle convection (based on data from [19] with modifications).

and (according to currently accepted models) the phase composition of the mantle does not change. As it approaches the Earth's core, the temperature increases and bridgmanite transitions to "post-perovskite" with a $CaIrO_3$ structure, which also has orthorhombic symmetry [9]. This does not affect the value of the Dolivo-Dobrovol'sky index, but directly influences the information parameter of structural complexity $I_G$, which in "post-perovskite" is lower (1.922 bits/atom) than in bridgmanite (3.374 bits/atom), which corresponds to the general principle of decreasing structural complexity with increasing temperature [14].

Thus, the nonlinear behavior of the index σ and parameter $\overline{I_G}$ with increasing depth can be explained by the uneven influence of temperature and pressure on the crystalline matter of the Earth's mantle. While pressure monotonically increases with depth, the intensity of temperature change varies, which leads to a change in the predominant role of one or another thermodynamic parameter in determining the symmetry and structural complexity of matter.

## CONCLUSIONS

Based on the pyrolite model of the Earth's mantle, using quantitative parameters (the Dolivo-Dobrovol'sky index and information parameters of complexity), it is shown that the symmetry and structural complexity of mineral matter behave nonlinearly with increasing depth, which contradicts the previously made conclusions about the monotonic increase in the symmetry of minerals in the deep geospheres of the Earth [6, 7]. Such behavior may be associated with the uneven and opposite effects of temperature and pressure on the symmetry and complexity of crystalline matter, which is caused by the nonlinear nature of the averaged geotherm of the Earth's crust and mantle. It is also important that the information parameters of structural complexity are a more sensitive indicator of symmetry than the Dolivo-Dobrovol'sky index, which is due to the former's consideration of fine details of the structural organization of specific minerals. While the Dolivo-Dobrovol'sky index only takes into account the crystal system of a mineral, the information parameters characterize its space group and the distribution of atoms among crystallographic orbits.

When evaluating the conclusions of this work, one should take into account the conditionality of the pyrolite model of the Earth's mantle and the existence of other models, which will be considered in subsequent works.

The author dedicates this article to the memory of Professor V.V. Dolivo-Dobrovol'sky from St. Petersburg Mining University, an outstanding scientist and remarkable person.

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