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Petrographic structures and Hardy – Weinberg equilibrium

Yury L. VOYTEKHOVSKY, Alena A. ZAKHAROVA
Saint Petersburg Mining University, Saint Petersburg, Russia

The article is devoted to the most narrative side of modern petrography – the definition, classification and nomenclature of petrographic structures. We suggest a mathematical formalism using the theory of quadratic forms (with a promising extension to algebraic forms of the third and fourth orders) and statistics of binary (ternary and quaternary, respectively) intergranular contacts in a polymineralic rock. It allows constructing a complete classification of petrographic structures with boundaries corresponding to Hardy – Weinberg equilibria.

The algebraic expression of the petrographic structure is the canonical diagonal form of the symmetric probability matrix of binary intergranular contacts in the rock. Each petrographic structure is uniquely associated with a structural indicatrix – the central quadratic surface in *n*-dimensional space, where *n* is the number of minerals composing the rock. Structural indicatrix is an analogue of the conoscopic figure used for optical recognition of minerals. We show that the continuity of changes in the organization of rocks (i.e., the probabilities of various intergranular contacts) does not contradict a dramatic change in the structure of the rocks, neighboring within the classification. This solved the problem, which seemed insoluble to A.Harker and E.S.Fedorov.

The technique was used to describe the granite structures of the Salminsky pluton (Karelia) and the Akzhailau massif (Kazakhstan) and is potentially applicable for the monotonous strata differentiation, section correlation, or wherever an unambiguous, reproducible determination of petrographic structures is needed. An important promising task of the method is to extract rocks' genetic information from the obtained data.

***Key words*:** rock; petrographic structure; quadratic form; structural indicatrix; classification; nomenclature

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Introduction. Determining the structure of rocks is important for their correct diagnosis and reconstruction of the formation conditions. But today, the term of the petrographic structure is not well defined in comparison with, for example, the crystalline structure. In special dictionaries [12, 15] there are many terms that characterize the structure of rocks. Usually, morphological and genetic aspects are mixed in these definitions. This does not allow constructing a mathematical theory, full classification and relevant nomenclature of petrographic structures. Petrography lags behind crystallography by more than a hundred years in the creation of a mathematical theory of its object – rock. Moreover, there is a persistent bias against the very possibility of such a theory.

E.S.Fedorov noted: “If we take into account that various types of structure depend on the external constantly changing conditions that occurred during the rock's formation, it will become clear how difficult it is to distinguish rock types by their structure when rocks are originating from the same or similar magmas. The fundamental difference between the rocks is, of course, the initial chemical composition; but this composition is also very variable, and in this respect there are various transitional levels between different rocks that do not allow one to sharply distinguish one type of rock from another. ... It is easy to understand that with a wide variety in the composition it is impossible to establish a natural classification that could give each rock its rightful place” [18, p. 164].

The Cambridge petrologist A.Harker wrote about the same thing: “Petrology has not yet developed any philosophical classification of rocks. It could not be created a certain and accurate classification as it was successfully done in some other scientific areas. The mathematically precise laws of chemistry and physics, which give individuality to mineral species, do not help us in working with complex mineral aggregates, and some fundamental principle still needs to be found in petrology. There are continuous transitions between rocks of various types, that’s why no artificial classification with sharp dividing boundaries can truly represent the facts of nature. Today, therefore, the best taxonomy is one that combines, as far as possible for the convenience of description, rocks with common properties, primarily bearing in mind those properties that most directly depend on important formation conditions. The grouping used below should be considered more

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as one of the agreements than as a principle" [20, p.20]. By the way, a completely modern classification of rocks is "used below".

The attitude towards the situation is gradually changing: "No matter how diverse the associations of rocks mapped in different regions may seem, there is a confidence that, with a systematic approach, they, like chemical elements in the Periodic table, can be naturally classified, paving the way for the unification of legends to the geological maps of the new generation" [16, p.5]. The question is what is meant by a systematic approach and which mathematical apparatus to use.

Methodology. If a systematic approach to the description of petrographic structures means the use of as many parameters as possible, then this already takes place and is rather a weakness than a strength. The reason is clear – very different morphological (euhedral, xenomorphic, etc.), large-scale (even- and uneven-grained; fine-, medium-, coarse-grained, etc.) and genetic (blastasy, etc.) characteristics of minerals (elements) that compose the rock (rock system), cannot be linked within a coherent theory [14, p.110-121, 283-294]. By the principles of systems theory, it was previously proposed to shift the focus from the morphometric characteristics of minerals to the statistics of their contact relationships in the description of the rocks organization [3, 5, 7].

The organization of n-mineral rock is proposed to be expressed through the algebraic relation:

$$\sum_{i,j=1}^{n} p_{ij} m_i m_j = [m_1 \ m_2 \ \dots \ m_n] \begin{bmatrix} p_{11} & p_{12} & \dots & p_{1n} \\ p_{21} & p_{22} & \dots & p_{2n} \\ \dots & \dots & \dots & \dots \\ p_{n1} & p_{n2} & \dots & p_{nn} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ \dots \\ m_n \end{bmatrix} = 1,$$

revealing the fundamental role of the symmetric matrix $[P_{ij}]$ of probabilities (frequencies) p_{ij} of different intergranular contacts $m_i m_j$ of the minerals m_i and m_j. At the same time, it defines in space $(m_1, ..., m_n)$ non-degenerate central quadratic surfaces (n-dimensional ellipsoids and hyperboloids) – structural indicatrixes of rocks.

The mathematical expression of the petrographic structure is the canonical diagonal form $[D_{ii}]$ of the matrix $[P_{ij}]$, which determines the type of structure with the signs of the coefficients d_{ii}. The real symmetric matrix is always reducible to the diagonal form by the non-degenerate transformation $[D_{ii}] = [Q_{ij}]\ [P_{ij}]\ [Q_{ij}]^{-1}$, corresponding to the space rotation of the structural indicatrix $(m_1, ..., m_n)$ and reduction to the principal axes [9, 19]. The nomenclature of the petrographic structure S_n^m means that among the coefficients d_{ii} there are exactly m positive ones.

So, a continuous change in the probabilities p_{ij} of various intergranular contacts (rock organization) does not contradict a sharp change in the type of structural indicatrix (petrographic structure). A complete classification of petrographic structures, with which their nomenclature is strictly connected, is based on indicatrixes. It seems that the proposed methodology follows a systematic approach and at least partially resolves the doubts of E.S.Fedorov and A.Harker. The theory was used to differentiate the gabbronorites monotonic section of the Fedorovo-Panskii intrusion on the Kola Peninsula [4, 6, 8]. We present new applications of the theory with necessary additions.

Granites of the Salma pluton, Karelia. An important geological problem is the development of methods for granitoid intrusions mapping [16]. Let us consider the granites of the Salma pluton in terms of description and comparison of petrographic structures [2]. They consist of five mineral phases (Fig.1): quartz (yellow), plagioclase (blue), K-Na feldspar (red), biotite (dirty green), and accessory minerals (purple). Do petrographic structures differ in two thin sections?

In both cases, the matrices $[P_{ij}]$ are reduced to a diagonal form corresponding to the structure S_5^2. Structural indicatrix is a space three-cavity hyperboloid $(m_1, ..., m_5)$. Indexes correspond to rows and columns of matrices and mean: 1 – quartz, 2 – plagioclase, 3 – K-Na feldspar, 4 – biotite, 5 – accessory minerals. Thus, both samples belong to the same structural type, although their organization, fixed by the whole set of intergranular contacts probabilities p_{ij}, is different (typification of the structure does not require conversion of the numbers of intergranular contacts to probabilities):

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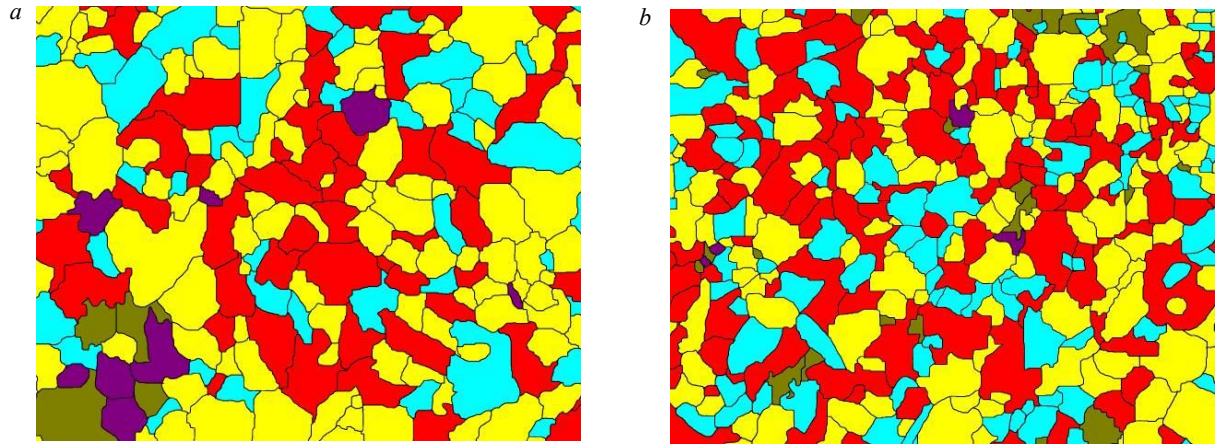

Fig.1. Medium-grained piterlite (*a*) and porphyry microcline-albite granite (*b*), no porphyry phenocrysts in the groundmass. The vertical size is 1 cm

$$\begin{bmatrix} 164 & 87.5 & 106.5 & 7 & 10.5 \\ 87.5 & 35 & 49.5 & 2.5 & 3.5 \\ 106{,}5 & 49.5 & 46 & 1.5 & 3.5 \\ 7 & 2.5 & 1.5 & 1 & 3.5 \\ 10.5 & 3.5 & 3.5 & 3.5 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} + & & & & \\ & + & & & \\ & & - & & \\ & & & - & \\ & & & & - \end{bmatrix} \rightarrow S_5^2;$$

$$\begin{bmatrix} 148 & 98 & 182 & 21.5 & 4.5 \\ 98 & 53 & 102.5 & 15 & 2 \\ 182 & 102.5 & 105 & 17.5 & 2.5 \\ 21.5 & 15 & 17.5 & 5 & 2.5 \\ 4.5 & 2 & 2.5 & 2.5 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} + & & & & \\ & + & & & \\ & & - & & \\ & & & - & \\ & & & & - \end{bmatrix} \rightarrow S_5^2.$$

Analysis of thin sections can be continued since accessory minerals and biotite make up a very small share in granite. We apply the method of accessory minerals subtraction [7], removing them from consideration one by one, that is, removing the corresponding rows and columns from the matrices $[P_{ij}]$. In both cases, we obtain the type of structure S_4^2, the indicatrix is a space two-cavity hyperboloid (m_1, ..., m_4):

$$\begin{bmatrix} 164 & 87.5 & 106.5 & 7 \\ 87.5 & 35 & 49.5 & 2.5 \\ 106.5 & 49.5 & 46 & 1.5 \\ 7 & 2.5 & 1.5 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} + & & & \\ & + & & \\ & & - & \\ & & & - \end{bmatrix} \rightarrow S_4^2;$$

$$\begin{bmatrix} 148 & 98 & 182 & 21.5 \\ 98 & 53 & 102.5 & 15 \\ 182 & 102.5 & 105 & 17.5 \\ 21.5 & 15 & 17.5 & 5 \end{bmatrix} \rightarrow \begin{bmatrix} + & & & \\ & + & & \\ & & - & \\ & & & - \end{bmatrix} \rightarrow S_4^2.$$

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But without biotite we get structures S_4^1 and S_4^2. Indicatrixes are space three-cavity and two-cavity hyperboloids (m_1, ..., m_4):

$$\begin{bmatrix} 164 & 87.5 & 106.5 & 10.5 \\ 87.5 & 35 & 49.5 & 3.5 \\ 106.5 & 49.5 & 46 & 3.5 \\ 10.5 & 3.5 & 3.5 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} + & & & \\ & + & & \\ & & - & \\ & & & - \end{bmatrix} \rightarrow S_4^2;$$

$$\begin{bmatrix} 148 & 98 & 182 & 4.5 \\ 98 & 53 & 102.5 & 2 \\ 182 & 102.5 & 105 & 2.5 \\ 4.5 & 2 & 2.5 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} + & & & \\ & - & & \\ & & - & \\ & & & - \end{bmatrix} \rightarrow S_4^1.$$

Along with the previous result, this means that in one thin section (Fig.1, *a*) accessory minerals and biotite form statistically equivalent intergrowths, in another (Fig.1, *b*) they are different. Without accessory minerals and biotite, the main (carcass-forming) part of the studied granites has a structure S_3^1, indicatrix is a space two-cavity hyperboloid (m_1, m_2, m_3):

$$\begin{bmatrix} 164 & 87.5 & 106.5 \\ 87.5 & 35 & 49.5 \\ 106.5 & 49.5 & 46 \end{bmatrix} \rightarrow \begin{bmatrix} + & & \\ & - & \\ & & - \end{bmatrix} \rightarrow S_3^1;$$

$$\begin{bmatrix} 148 & 98 & 182 \\ 98 & 53 & 102.5 \\ 182 & 102.5 & 105 \end{bmatrix} \rightarrow \begin{bmatrix} + & & \\ & - & \\ & & - \end{bmatrix} \rightarrow S_3^1.$$

Thus, the suggested methodology for petrographic structures standardization according to the statistics of intergranular contacts makes it possible to identify even subtle features of rock organization. This allows it to be used for granitoid intrusions mapping. Routine algebraic operations with arbitrarily large matrices are computerized.

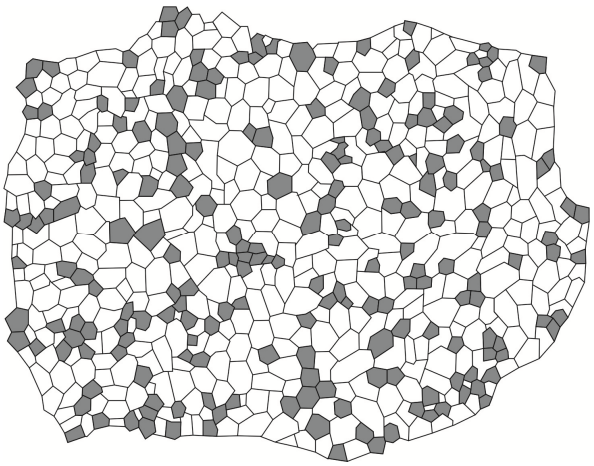

Fig.2. The typified physiography of granite of the Akzhailau massif [1]. Gray – quartz, white – feldspars, mica and amphiboles are not shown. Polished chip sample, 15 × 10 cm

Granites of the Akzhailau massif, Kazakhstan. Massive textures are very common in rocks of predominantly magmatic origin. They mean the random spatial distribution of rock-forming minerals, in contrast to layered, banded, or spotted textures. But is the random spatial distribution always consistent with the perfect mixing of minerals? To test the hypothesis, granite from the Akzhailau massif was taken (Fig.2).

Hardy – Weinberg equilibrium is accepted as a mathematical model corresponding to the ideal mixing of minerals [10; 11, p. 126-128]. In relation to our task, this means the following. If p and q are the frequencies (probabilities) of minerals A and B (conditionally $pA + qB = 1$), then the equilibrium frequencies of their contacts AA, AB (the same as BA) and BB in the rock can be calculated

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by the formula

$$(pA + qB)^2 = p^2\,AA + 2pq\,AB + q^2\,BB = 1.$$

Estimating deviations from equilibrium frequencies is a statistical routine. The Hardy-Weinberg formula is obviously generalized by the number of terms on polymineralic rocks

$$(p_1A_1 + \ldots + p_nA_n)^2 = \sum p_{ij}\,A_iA_j = 1, \quad \text{where} \quad i, j = 1, \ldots, n.$$

It is theoretically and practically important that it is generalized in degrees to:

• ternary

$$(p_1A_1 + \ldots + p_nA_n)^3 = \sum p_{ijk}\,A_iA_jA_k = 1, \text{ where } i, j, k = 1, \ldots, n;$$

• quarternary intergranular contacts

$$(p_1A_1 + \ldots + p_nA_n)^4 = \sum p_{ijkl}\,A_iA_jA_kA_l = 1, \text{ where } i, j, k, l = 1, \ldots, n.$$

The study of petrographic structures and textures should be done in 3D. Analysis in 2D (in thin section or polished samples) is justified only by the fact that their classification and nomenclature were formed from observations in 2D. Today it is technically impossible to obtain statistics of quaternary contacts of mineral grains in rock. The joints of four grains do not fall into the petrographic section. But the statistics of their ternary (triple) contacts in n-mineral rocks can be found in thin sections.

Ternary contacts. The use of quaternary and even ternary intergranular contacts in practice is interesting because the resulting classification of petrographic structures is much more extensive than in the case of binary contacts. It should be expected that in this case, through the statistics of intergranular contacts, more and more subtle details of the rocks organization are revealed and typed.

For Akzhailau granite, the probabilities of quartz and feldspar grains in thin sections (208 and 428, respectively) are $p_1 = 0.327$ and $p_2 = 0.673$. The calculated probabilities of ternary contacts corresponding to the Hardy-Weinberg equilibrium are $p_{111} = 0.035$, $p_{112} = 0.216$, $p_{122} = 0.444$, $p_{222} = 0.305$. Of the total number of 1116 ternary contacts, this is: 39, 241, 496, and 340. The actual number of contacts is calculated in the section: 17, 211, 490, and 398. The value of the nonparametric chi-square criterion of 26.02 significantly exceeds the threshold value of 11.3 for a confidence probability of $p = 0.99$ and the number of degrees of freedom $df = 3$. Thus, the hypothesis of the correspondence of the studied granite massive texture to the Hardy – Weinberg equilibrium is rejected. The reason is clearly lower frequencies p_{111}, p_{112} and overestimated p_{222}.

The peculiarity of the situation is that even if the calculated probabilities correspond to theoretical ones (i.e., the real texture to the Hardy – Weinberg equilibrium), the conclusion about the correspondence is made with a certain probability. The calculated probabilities always differ from the equilibrium ones. Hardy – Weinberg equilibria determine classification boundaries in a variety of statistically nonequilibrium situations (in our case, rock structures). To typify them as structural indicatrices, by analogy with [3, 5, 7], we use the Newtonian classification of plane cubic curves [17, p. 44-53]. Unfortunately, for $n > 2$, the mathematical theory for petrography is not adapted [13]. The equation of the desired curve

$$\sum p_{ijk}\,A_iA_jA_k = 1, \text{ where } i, j, k = 1, \ldots, n$$

for the case $n = 2$ (bimineral rock) is as follows (the coefficients of the equation are the probabilities of ternary contacts calculated in the thin section)

$$0{,}015\,m_1^3 + 0{,}189\,m_1^2\,m_2 + 0{,}439\,m_1\,m_2^2 + 0{,}357\,m_2^3 = 1$$

and defines a curve of two hyperbolic and one rectilinear branches (Fig.3). This is one of two dozen possible structural indicatrices [17], whereas in the description based on binary intergranular contacts at $n = 2$, only two structures are possible. The study of structural indicatrices of the third order at least for $n = 3$ (trimineral rocks) by computer simulation methods is a promising development of the theory.

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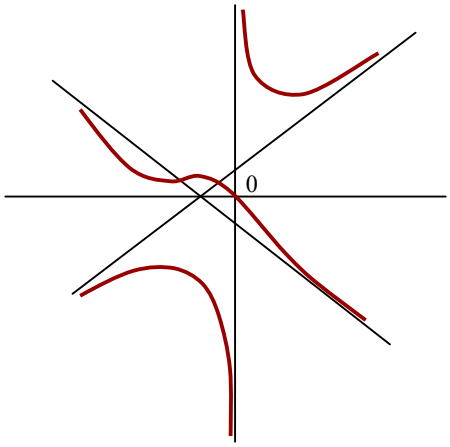

Fig.3. The third order structural indicatrix of granite of Akzhailau massif

Conclusions. Thus, the proposed methodology allows us to construct a complete classification and nomenclature of petrographic structures according to the statistics of binary (for polymineral) and ternary (for bimineral rocks) intergranular contacts.

A continuous change in the organization (probabilities of intergranular contacts) of a rock does not contradict a dramatic change in the structure of the rocks, located at the classification boundaries corresponding to Hardy – Weinberg equilibria.

Correspondence of petrographic structures to one or another state (for example, Hardy – Weinberg equilibria) is checked by statistical criteria and reflects their probabilistic nature. Rock is the realization of a spatially distributed random function of the initial field of concentrations, conditions and mechanisms of crystallization.

The study of petrographic structures and textures should be performed in 3D. Analysis in 2D is justified only by the fact that their classification and nomenclature were also formed from observations in two-dimensional space. But this situation reveals the problem of stereo reconstruction of any parameters.

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***Authors*: Yury L. Voytekhovsky,** *Doctor of Geological and Mineralogical Sciences, Professor, Voytekhovskiy_YuL@pers.spmi.ru* (*Saint Petersburg Mining University, Saint Petersburg, Russia*), **Alena A. Zakharova,** *Postgraduate Student, zakharova.alena27614@gmail.com* (*Saint Petersburg Mining University, Saint Petersburg, Russia*).

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