Mathematical modeling of textural and structural features of magnetite-pyroxene shales of Pishchansk iron ore structure

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SUMMARY

The paper presents the results of modeling the influence of textural and structural features on the acoustic and elastic properties of rocks of the group of magnetite-pyroxene shales of the Pishchansk iron ore structure. The influence of the format, orientation of grains and microcracks, their concentration on the values of effective elastic constants, coefficients of linearity and shaleness, symmetry types, coefficients of integral acoustic and differential elastic anisotropy are established. The corresponding stereoprojections of the index surfaces of the calculated parameters are analyzed.

Introduction

Mathematical modeling of elastic and acoustic parameters of rocks can serve as a reliable basis for assessing the impact on their physical properties of the mineralogical composition of the rock, the orientation and shape of mineral grains, types and orientation of cavities. When considering rocks of the Pishchans`ka structure, which due to their structure are characterized by anisotropy, mathematical modeling of their effective elastic and acoustic properties is possible only with the use of perfect models that would adequately reflect their properties and structure, as well as deformation processes occurring in these rocks.

Method and Theory

Elastic and acoustic properties of rocks *(Aleksandrov and Prodayvoda, 2000)* are determined not only by their mineral composition, but also by the microstructure and texture of the rock. The microstructure means the shape and size of mineral grains, microcracks, their concentration and mutual orientation.

The method of mathematical modeling is based on a multicomponent matrix model, which is as close as possible to the structure of real rocks. The model matrix (mineral base) is divided into microcracks and minerals with different shape, size and orientation with different crystallographic orientation of grains of a certain shape with different concentrations of their inclusions.

To solve this problem, the method of conditional moment functions using the Mori-Tanaka calculation scheme is used. The inverse problem in modeling is reduced to the determination of elastic constants and is carried out by the known method of least squares using nonlinear optimization methods *(Bezrodnyi, 2008; Prodayvoda et al., 2010, 2011)*.

In practice, the substantiation of mathematical models is usually based on a priori results, in particular, the petrographic description of the samples of rocks under study. The models are based on elastic constants and mineral densities that make up the rock model.

Based on the developed models, in accordance with the mineral composition of rock-forming minerals and the structure of the void space of the model are calculated:

a) based on the parameters of the acoustic tensor, the analysis of the parameters of the acoustic ellipsoid - acoustic shale (S_μ) and linearity (L_μ) was performed;
b) the integral coefficient of acoustic anisotropy $A\mu$;
c) matrices of elastic constant models;
d) on the basis of calculated elastic constants and density - stereoprojection of isolines of indicative values of velocities of quasi-longitudinal and quasi-transverse waves and parameters of elastic anisotropy.

The next step is to analyze the data:

- according to the symmetry of the acoustic tensor, the textures of rock models are separated: spherical, transverse isotropic and rhombic symmetry;
- according to the ratios of the maximum, average and minimum values of the acoustic tensor, the classification of textures into planar (flattened) and axial (elongated) type of symmetry is performed;
- on the basis of the received information analyze influence of the set geological characteristics on change of speeds of elastic waves, and also acoustic and elastic parameters of anisotropy, form opinion concerning influence of geological processes on stages of formation of the modeled breeds.

Examples

The authors performed mathematical modeling of the influence of geological characteristics on the parameters of elastic and acoustic anisotropy of rocks of the Pishchans`ka iron ore structure.

Substantiation and creation of mathematical models was based on a comprehensive analysis of petrographic and petrophysical studies of 35 samples taken from the core of pyroxene-magnetite ores from well №3 Sand structure in the range of depths 144-273 m *(Entin, 2012).*

According to previous complex petrographic and petrophysical studies [references] among the rocks under consideration, three groups have been identified:

- magnetite-pyroxene crystalline shales;
- quartz-magnetite-pyroxene crystalline shales;
- biotite-amphibole plagiocrystals.

The authors created and analyzed seven mathematical models of "magnetite-pyroxene crystalline shales".

The skeleton of the rock model is mineralogically represented by pyroxene.

Among the non-matrix minerals for mathematical modeling, pyroxene, magnetite and quartz were chosen. Summarizing the macro- and micro-studies of the samples, a number of structural and textural parameters were selected, which are given in Table 1.

Table 1 *Types of models*

Model name	Rock-forming minerals				Cracks		
	Contents	Format	Orientation	Concentration	Format	Concentration	Orientation
Magnetite-pyroxene crystalline shales							
1a, 1b. "Magnetite-pyroxene crystalline shale layered coarse-grained"	magnetite - 12 quartz – 1	α=0,3	in the plane X1X2	in X3 – 2% in X1 and X2 – equally	α=0,005	1a ζ=0,005 1b ζ=0,009 in X3 – 2%	in the plane X1X2
2. "Magnetite-pyroxene crystalline shale fine-grained layered"	magnetite - 12 quartz – 1	α=0,5	in the plane X1X2	in X3 – 2% in X1 and X2 – equally	α=0,005	ζ=0,005 in X3 – 2%	in the plane X1X2
3. "Magnetite-pyroxene crystalline shale fine-grained layered"	magnetite - 12 quartz – 1	α=0,5	in the plane X1X2	in X3 – 2% in X1 and X2 – equally	α=0,005	ζ=0,009 in X3 – 2%	in the plane X1X2
4-5. "Magnetite-pyroxene crystalline shale is multigrained"	magnetite - 4	model 4 - α=0,3 model 5 - α=0,5	chaotic	in X3, X1 and X2 – equally	α=0,005	ζ=0,005	chaotic
6a, 6b. "Magnetite-pyroxene crystalline shale of various grains with high magnetite content"	magnetite – 38	model 6 –α=0,5	chaotic	in X3, X1 and X2 – equally	α=0,005	6a - ζ=0,005 6b - ζ=0,01	chaotic

The matrix of the model is divided into different in shape, size and orientation microcracks and minerals with different crystallographic orientation of grains of a certain shape with different concentrations of their inclusions. Substantiation of the mathematical model developed in the work is based on the results of complex geological-petrographic-geochemical studies of the team of authors of the Institute of Geology *(Bezrodnyi et al., 2019).*

Based on the obtained results, the authors analyzed the influence of mineral composition, format of mineral grains, their orientation, type and magnitude of microcracking on effective elastic and acoustic parameters of models of magnetite-pyroxene crystalline shales of the Pishchans`ka structure. (Table 2).

Table 2 *Summary results of parameter modeling*

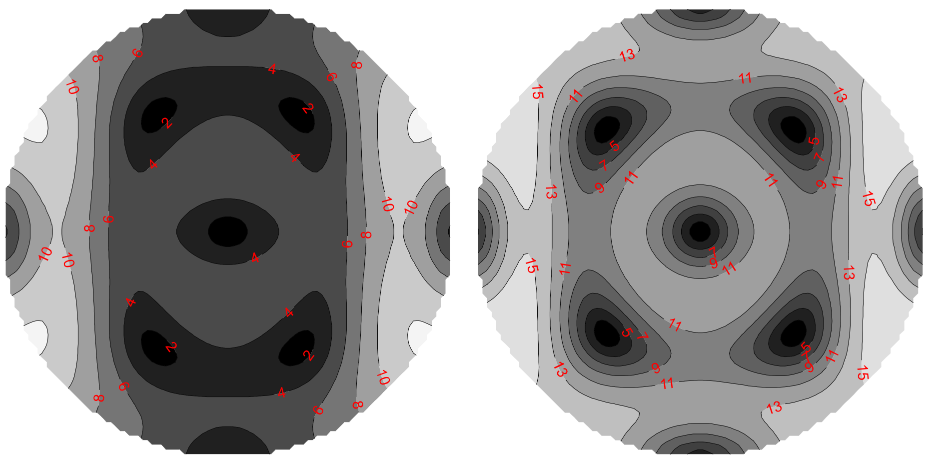
Parameters models	Magnetite-pyroxene crystalline shales								
	Model 1a	Model 1b	Model 2	Model 3	Model 4	Model 5	Model 6a	Model 6b	Model 7
A_μ	20,97	28,13	21,05	28,04	5,73	6,37	4,33	2,87	5,12
L_μ	1,45	1,72	1,46	1,71	1,03	1,01	1,01	1,04	1,01
S_μ	1,10	1,07	1,11	1,08	1,11	1,13	1,09	1,04	1,11
ρ	3,5	3,48	3,50	3,48	3,35	3,36	3,99	3,97	4,00

The results of mathematical modeling show that the acoustic anisotropy coefficient of the models varies from 2.87% for model 6b and reaches 28.13% for model 1b. A sharp difference in the values of the effective elastic constants $C^*_{11}, C^*_{22}, C^*_{33}$ indicates an increase in the anisotropy of the model, which is associated with an increase in the concentration of microcracks.
But the authors obtained against the background of generalized results and some exceptions.

Models 4 and 5 have the same mineral composition (pyroxene-60%, magnetite - 38%), orientation and concentration of microcracks, but different grain format. As established (Table 2), the values of the main acoustic and elastic parameters are very close, in particular, the value of the integral coefficient of acoustic anisotropy, these models are the average anisotropic value A_μ respectively. However, a completely different picture is observed when analyzing the values of the differential coefficient of elastic anisotropy A_d. In particular, for Model 4 A_d = 19%, and for Model 5 - 18%. These results show an increase in the elastic anisotropy in the modeling of elongated grains, whereas for the anisotropy of acoustic properties the situation is opposite. As for the nature of the distribution of isolines of the pointing surfaces, the difference is insignificant, the number of extremum points and their relative position remains constant.

Model 6a is characterized by average values of the integral coefficient of acoustic anisotropy A_μ = 4.33% and high values of the differential coefficient of elastic anisotropy A_d = 12%. Regarding Model 6b, the increase in the concentration of microcracks caused a decrease in A_μ to 2.87%, and a significant increase in A_d values to 17%. As can be seen in Figure 3, the number of extremums is the same for both models, the nature of the distribution of isolines is very similar, with a clearer separation of the minimum in the center, and the zone of high values (11%) around the center.
Four models are considered, according to the type of acoustic symmetry of textures are planar rhombic.

Modeling the effect of microcrack concentration showed significant differences in acoustic and elastic parameters of models with the same mineral composition, grain shape and orientation, as well as microcrack orientation. For example, the following (Table 1) stereoprojections of the index surfaces of the differential coefficient of elastic anisotropy Ad (%) of Model 6a and Model 6b.
These models are characterized by the same mineral content (pyroxene 94% - magnetite 4%), the same format, grain orientation and different concentration of chaotically oriented microcracks, 0.5 and 1%, respectively.
According to the simulation results, it is established that the considered models have significant differences in the values of acoustic and elastic parameters.



a **b**

Figure 1 *Stereoprojections of isolines of the pointing surfaces of the differential coefficient of elastic anisotropy A_d (%) of Model 6a (a) and Model 6b (b)*

Conclusions

Analysis of the simulation results showed that:

- most of the presented models of magnetite-pyroxene crystalline shales are highly anisotropic ($A_{\mu}>10\%$);
- an increase in the concentration of microcracks in all cases leads to a sharp difference in the values of the elastic constants and indicates an increase in the anisotropy of the model;
- change in grain format has much less effect on the value of acoustic and elastic properties than the concentration of microcracks; The obtained results require additional modeling taking into account the identified mineralogical and petrographic features.

The obtained results require additional modeling taking into account the identified mineralogical and petrographic features.

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