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## Mathematical modeling of the connection between different types of cracks and elastic parameters of quartz-magnetite-pyroxene crystalline shales

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### SUMMARY

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The work is devoted to modeling the influence of different types of cracks on the acoustic and elastic parameters "quartz-magnetite-pyroxene" crystalline shales group of samples from the Pishchans'ka iron ore structure. Models include ordered, chaotic and combined cracks, as well as the influence of the format and concentration of cracks. The authors calculated the complete set of components of the matrix of elastic constants, determined the differential coefficient of elastic anisotropy.

The results showed high anisotropy of the models and a significant effect of ordered cracks on the value of the differential coefficient of elastic anisotropy and other elastic parameters. According to the results, stereoprojections of the index surfaces of the obtained parameters were constructed and analyzed. A comparison of the basic sample and models is also given.

## Introduction

Studies of the anisotropy of the physical properties of rocks, as well as the nature of its origin, are inextricably linked with the study of the influence of all components of a multicomponent geological object on the distribution of these properties (Aleksandrov and Prodaivoda, 2000). In particular, mathematical modeling of physical parameters is used to comprehensively characterize the lithological and petrographic features of rock samples and to reproduce the conditions of their formation. In this paper, such mathematical modeling allows us to track and evaluate the impact of such structural and textural elements as mineralogical composition of rocks, orientation and shape of mineral grains, types and orientation of cavities, on the distribution of acoustic and elastic properties.

## Method and/or Theory

In solving this problem, the method of conditional moment functions using the Mori-Tanaka calculation scheme was used. The inverse problem in the simulation was reduced to the determination of elastic constants and calculations by the least squares method (LSM) using nonlinear optimization methods (Bezrodnyi, 2008; Prodayvoda et al., 2010; Prodayvoda et al., 2011).

The development and selection of the models is based on a priori results, in particular, a petrographic description of the rock samples under study. The developed models are based on the elastic constants and densities of minerals that make up the rock model, as well as crack characteristics.

In general, the algorithm of the mathematical modeling can be represented as follows:

- Selection of basic samples, petrographic characteristics of which will be used in creating models.
- Development of mathematical models of rocks taking into account their mineralogical composition, orientation and shape of mineral grains, types and orientation of voids.
- Calculation of acoustic and elastic parameters, such as matrices of elastic constants, parameters of acoustic tensor, coefficients of linearity and slackness, coefficients of differential acoustic anisotropy ( $A_d$ ).
- Calculation of azimuthal anisotropy parameters of elastic waves represented by stereoprojections of index surfaces isolines.
- Analysis of the obtained data and comparison with the results of processing of petrophysical researches.

A set of original programs developed by the staff of the Institute of Geology was used to model and analyze the obtained parameters.

## Examples

According to previous complex petrographic and petrophysical studies (Bezrodnyi et al., 2019) three groups have been identified among the rocks under consideration:

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

Based on the results of research (Bezrodna et al., 2020), a group of quartz-magnetite-pyroxene samples of crystalline shales of the Pishchanka iron ore structure (Entin, 2012) was chosen as the basis. Ten models were developed based on petrographic and micropetrographic description of a typical sample (PS-9), which among this petrographic group has the lowest magnetite content - 10% and the average content of quartz - 11% (Figure 1).

Since the paper (Bezrodna et al., 2020) proved the minimal influence of the size and shape of mineral grains on the parameters of elastic anisotropy, the set of models is based on the variation of the shape, concentration, size and orientation of cracks. The skeleton of the rock model is mineralogically represented by pyroxene. Among the non-matrix minerals for mathematical modeling, magnetite and quartz were chosen. The grain format ( $\alpha$ ) is accepted on average according to the results of micropetrographic studies as 0,69.

№ of models	Type of cracking	Rock-forming minerals			Cracks		
		Composition	Orientation	Concentration	Format	Concentration	Orientation
1-2	weakly fractured (1) and strongly fractured (2)	quartz-11, pyroxene - 79, magnetite - 10	in the plane X1X2	in X3 – 2% in X1 and X2 – equally	$\alpha=0,007$	1 $\zeta=0,002$ 2 $\zeta=0,009$ in X3 – 2% in X1 and X2 – equally	in the plane X1X2
3-4.	weakly fractured (3) and strongly fractured (4)	quartz-11, pyroxene - 79, magnetite - 10	in the plane X1X2	in X3 – 2% in X1 and X2 – equally	$\alpha=0,003$	3 $\zeta=0,002$ 4 $\zeta=0,009$ in X3 – 2% in X1 and X2 – equally	in the plane X1X2
5-6.	Weakly cracked	quartz-11, pyroxene - 79, magnetite - 10	Chaotic	in X3, X1 and X2 – equally	model 5 - $\alpha=0,003$ model 6 - $\alpha=0,007$	$\zeta=0,002$ in X3, X1 and X2 – equally	Chaotic
7-8.	Strongly cracked	quartz-11, pyroxene - 79, magnetite - 10	Chaotic	in X3, X1 and X2 – equally	model 7 $\alpha=0,003$ model 8 - $\alpha=0,007$	$\zeta=0,009$ in X3, X1 and X2 – equally	Chaotic
9.	Combined fracture	quartz-11, pyroxene - 79, magnetite - 10	Chaotic	in X3, X1 and X2 – equally	$\alpha=0,005$	$\zeta=0,007$ in X3, X1 and X2 – equally $\zeta=0,001$ in X3 – 2% in X1 and X2 – equally	Chaotic, in the plane X1X2
10.	Combined fracture	quartz-11, pyroxene - 79, magnetite - 10	Chaotic	in X3, X1 and X2 – equally	$\alpha=0,005$	$\zeta=0,002$ in X3, X1 and X2 – equally $\zeta=0,001$ in X3 – 2% in X1 and X2 – equally	Chaotic, in the plane X1X2

**Figure 1** Types of models of the "quartz-magnetite-pyroxene" group of crystalline shales

Based on the obtained results, the authors analyzed the influence of the type and magnitude of fracture on the effective elastic and acoustic parameters of the models of "quartz-magnetite-pyroxene" crystalline shales of the Pishchans`ka structure (Figure 2).

The results showed that for models with ordered crack orientation (model 1-4), the change in the format and concentration of voids is a defining characteristic. Thus, an increase in the grain format at low concentrations of microcracks leads to an increase in the differential anisotropy coefficient from 17 to 23%, and at high concentrations the coefficient increased from 28 to 38%

For samples with a chaotic arrangement of structural elements, this effect is significantly smaller. In particular, with the increase of the grain format of low-fractured models of rocks (model 5 and 7) the value of anisotropy remained unchanged (11%). However, the density decreased by 20 kg/m<sup>3</sup>. For models with larger fractures (model 6, 8) the increase in the format led to a slight change in the value of A<sub>d</sub> (from 10.5 decreased to 10%). At the same time, the density decreased by 10 kg/m<sup>3</sup>. In general, all models can be attributed to highly anisotropic, as the coefficient A<sub>d</sub> for all models ranges from 10-38%.

This is confirmed by a significant difference in the values of the effective elastic constants  $C_{11}^*$ ,  $C_{22}^*$ ,  $C_{33}^*$ . According to the analysis of the ratios of the main components of the matrix, it was found that most models have a rhombic type of elastic symmetry. However, models 4 and 7 can be conditionally attributed to the transverse isotropic type, because:

$$(C_{11}^* \approx C_{22}^* < C_{33}^*; C_{44}^* = C_{55}^* > C_{66}^*).$$

These models are characterized by high cracking with the format  $\alpha=0,003$

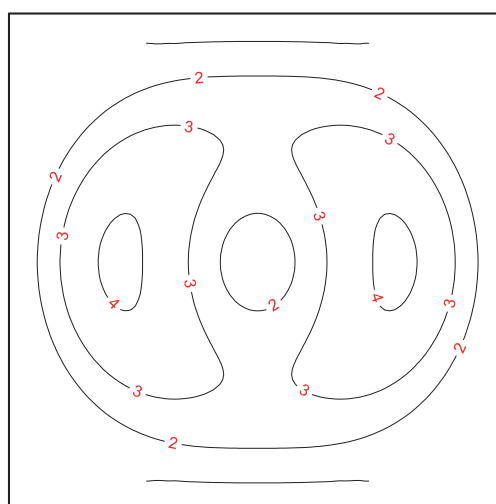
№ Model	Elastic constants, density and differential anisotropy coefficient for models 1- 10, MPa									
	1	2	3	4	5	6	7	8	9	10
C <sub>11</sub>	125,26	64,60	91,33	39,00	102,97	86,59	48,35	76,43	73,38	108,46
C <sub>22</sub>	98,56	57,20	76,17	37,04	82,98	72,03	44,25	65,02	62,84	86,39
C <sub>33</sub>	160,72	144,39	152,76	133,68	109,13	93,95	53,46	83,91	92,75	154,79
C <sub>44</sub>	56,95	44,04	51,58	32,21	47,86	42,97	26,94	39,41	40,26	53,59
C <sub>55</sub>	56,28	43,66	51,05	32,03	47,37	42,58	26,81	39,08	39,92	52,96
C <sub>66</sub>	44,93	30,52	38,41	19,99	40,80	37,02	24,05	34,22	33,20	41,11
C <sub>12</sub>	31,73	-0,32	11,81	-6,89	18,76	10,01	-4,74	5,11	3,84	22,68
C <sub>13</sub>	36,67	14,89	24,81	6,56	17,45	10,59	9,21	6,92	8,28	31,84
C <sub>23</sub>	30,68	11,74	19,66	5,14	13,23	7,71	-0,75	4,75	5,94	25,08
A <sub>d</sub> , %	17,0	28,0	23,0	38,0	11,0	10,5	11,0	10,0	13,5	20,0
ρ, kg/m <sup>3</sup>	3410	3390	3410	3390	3350	3340	3330	3330	3330	3350

**Figure 2** Summary results of parameter modeling

For models with combined fracture (model 9 and 10), rocks with the same grain format were modeled. Model 9 used a combination of a high concentration of chaotically located cracks and a small part of the cracks oriented in the X1X2 plane, in model 10 - a small concentration of chaotic and ordered cracks. The results showed that even a small content of unidirectional microcracks significantly affects the overall anisotropy of rocks, even in conditions of combined fracture (the value of A<sub>d</sub> for model 9 was 13.5%, and for model 10 - 20%).

For each of the models, the stereoprojections of the pointing surfaces isolines were also constructed: the phase velocity of the quasi-longitudinal wave, the difference between “fast” and “slow” quasi-transverse waves, the angle of deviation of the elastic displacement vector from the wave normal direction, and the differential coefficient.

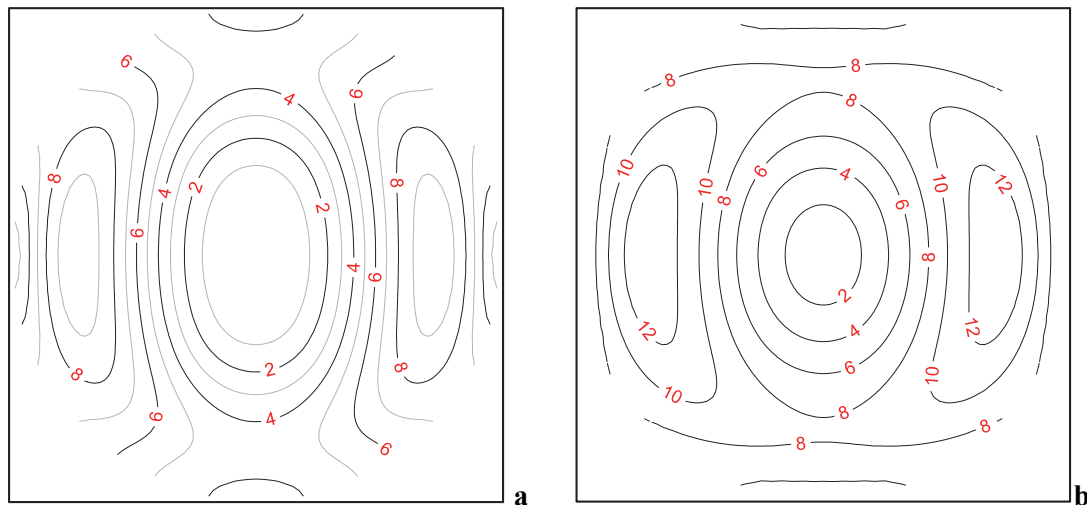
Comparison of the obtained constructed stereo projections with the reference mineralogical composition sample PS-9 showed that the nature of the distribution of isolines in the models is close to real. However, it should be noted that as a result of modeling, the coefficient of differential elastic anisotropy A<sub>d</sub> varies from 10 to 38%, while this value is significantly smaller in the sample (for PS-9 A<sub>d</sub> = 4.2%) (Figure 3).



**Figure 3** Stereoprojection of the index surface of the differential coefficient of elastic anisotropy for the sample PS-9

It should be noted that the closest in value to the real sample were model 8 and model 9 (Figure 4).

Comparing the stereoprojections of other samples with the stereoprojections obtained during the simulation, the authors found that in most samples there is a double system of cracking.



**Figure 4** Stereoprojections of the index surfaces of the differential coefficient of elastic anisotropy for Model 8 (a) and Model 9 (b)

Figure 3 and Figure 4 (a), (b) show that the nature of the distribution of isolines is similar for the standard and models. In particular, there is a zone with minimal values in the center, and two zones of increased values in the peripheral areas. This indicates the correct choice of models and high reliability of the calculations.

## Conclusions

According to the results of mathematical modeling, the influence of different types of cracks on the acoustic and elastic properties of quartz-magnetite-pyroxene crystalline shales was established. The influence of changes in the format, concentration and orientation of microcracks on the elastic parameters of the models is shown. When comparing the stereoprojection of real samples with the stereoprojections obtained during modeling, the authors found that in most samples there is a double system of cracking: chaotic and directed in the area of shale.

In addition, it is shown that this technique allows you to create and operate models close to the real geological environment.

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