

Developing application for thermobarometric calculation in geology

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Abstract. This article focuses on development of software for calculating the temperatures and pressures of rock formation. The assessment of the physico-chemical conditions of natural mineral formation is based on solving the inverse problem of convex programming - modeling mineral equilibria by minimizing the Gibbs free energy of a mineral system. The proposed algorithm includes the parametric minimization of the criterion function of deviation of the observed and calculated mineral paragenesis over the entire set of specified identifying parameters. The method was verified using the example of thermobarometric conditions for the formation of metamorphic rocks of the Okhotsk complex (North-East of Russia). In the conclusion, the main directions of using the obtained estimates in geological applications are outlined.

Keywords: Geothermobarometry, Inverse Problems, Convex Programming, Parametric Minimization.

1 Introduction

Determination of temperatures and pressures of formation of rocks in the thickness of the earth's crust is associated with laborious experimental or calculated geochemical studies. We propose a different approach to assessing the physicochemical conditions of natural mineral formation, as solving the inverse problem of convex programming - modeling mineral equilibria by minimizing the Gibbs free energy of a mineral system using all available petrological information, including the chemical composition of the rock and the composition of minerals in a given mineral paragenesis. A correct assessment of the parameters helps to understanding the natural laws in the history of the mechanism of formation and transformation of minerals in different geological eras.

2 Mathematical model

The main criterion for finding the optimal values of temperature and pressure for the formation of a reference rock sample is to find the maximum approximation of the observed and calculated mineral paragenesis over the entire set of specified identifying parameters.

In the mathematical description, the problem can be attributed to a special class of problems in the theory of pattern recognition - the method of comparison with the prototype [1-4], where a real rock sample, represented by a vector of basic parameters and chemical composition (Fig. 1), is selected as a standard. Experimental (model) rock samples obtained as a result of solutions for various temperature (T), pressure (P) and fluid compositions represent a set of recognizable classes. The measure of proximity between objects of classification and a given standard is established depending on the selected metric distance between them, which largely determines by the results of classification.

Okhotak complex

Minimization | Chemical Composition | Mode | Control | Precision | Output | Reservoirs | Thermobarometer | Uncertainty | Comments | Transformer

Additional parameters

	amphibole	clin amphib	ortho amphib	biotite	garnet	olivine	orthopyroxene	clinopyroxene	chlorite	corundum	staurolite	talc	chloritoid	white mica	spinel
Fe	0	0	0	35.4	65	0	0	0	0	0	0	0	0	0	0
Al	0	0	0	24.5	0	0	0	0	0	0	0	0	0	0	0
Ca	2.7	25.9	0												
Na					0	0	0								
Ti											4.5				
Fe+3															0

Sample Units: mole g weight % vol %

Fluid quantity: 1

Gas	5
Bi	11.5
CPyr1	0
Calc1	0
Camph	0
Chl	0
Chld	0
Crd	0
Ep	0
Garnet	19
Ilmdis	1
Kfs	37
Kfslow	0
Ky	0
Micas	0
OPyr	0
Oamph	0
Ol	0
Pl2	14
Qtz	8
Sil	4
Sph	0
Spil	0
St	0
Ta	0

Fig. 1. Software

The identification of thermobaric conditions is carried out by solving the problem of finding the minimum of the function f , which determines the proximity of the mod-

eled rock composition to the reference at different T and P from a given T_{\min} - T_{\max} and P_{\min} - P_{\max} intervals:

$$f = \min\left(\sqrt{\sum_i w_i (A_i - B_i)^2} + \sum_j (A_j - B_j)^2\right), \quad i \in M, j \in C$$

where A is a standard (real rock), B is a model calculation,

M is a set of parameters of the mineral composition,

C is a set of data on the quantitative chemical composition of a rock.

The weighting factors w_j allow to assign a certain weight for the parameter in proportion to the degree of importance of the feature in the classification problem ($w_j > 0$). If such additional information is absent, all w_j are taken equal to one. The search for the minimum of the criterion function is carried out by the golden ratio method. This method provides high reliability, reliability and efficiency in solving deterministic problems.

It is considered to use a combined measure of distance: weighted Euclidean distance (for parameters of mineral composition) and squared Euclidean distance (for rock composition). Typically, the second measure of distance is used when you want to give more value to objects that are more distant from each other. But in this case, since the parameters are determined in relative units in the interval (0, 1), the second measure represents a smaller contribution to the overall functional. Thus, the composition of minerals (parameters) make a more significant contribution to finding a solution than the value of the amount of minerals in the rock. This ratio is accepted due to the fact that determining the composition of minerals is the most reliable and verified information available to almost any petrologist. In the case of the chemical composition of the rock, a certain gap is in the calculations due to accuracy of silicate analysis, determination of the degree of oxidation, not always complete and objective assessment of the role of volatile components in the formation of the rock, and other factors that increase the degree of error in the initial data.

The problem of determining the equilibrium rock composition at fixed T, P and fluid composition is solved by minimizing the Gibbs energy of the system for the model calculation of the rock sample. The reduced potential of the Gibbs energy of the mineral system has the form [11]:

$$G(x) = \sum_{j \in S} \left(\frac{g_j}{RT} + \ln a_j^{id} + \ln \gamma_j \right) x_j$$

where g_j is the standard isobaric-isothermal potential of the j -th component;

a_j^{id} - the activity of the minal j in a mineral with ideal mixing, which allows to take into account the contributions of configuration factors to the ideal activity;

γ_j is the activity coefficient;

x_j is the molar amount of the j -th minal;

S - a set of indices j , denoting the components of the mineral system.

In the case of solid solutions in which the mixing of components occurs at one position of the crystal structure, the activity is equal to the molar fraction of the minal in

the mineral phase $a_j^{id} = x_j / X_\alpha$, where X_α is the molar amount of the α phase of the solid solution.

From a practical point of view, it is necessary to take into account that the error in calculating the values of T and P can be associated with small variations in the criterion function in the case of systems with a sufficiently wide PT-range of stability of a certain paragenesis. Therefore, increased requirements are applied to the accuracy of the initial data on the composition of minerals. It can also be recommended to consider several mineral systems at once in one area of the metamorphic strata, represented by rocks with different compositions of coexisting minerals.

3 Verification of the model

All calculations were carried out on the basis of rock samples from the Okhotsk metamorphic complex of the southwestern part of the Verkhoyansk-Chukotka fold region (North-East of Russia) [12]. The weight ratio fluid / rock (W / R) in the models was 0.005-0.0005.

Table 1 shows a comparison of modeling data with estimates derived from the basis of known experimental and empirical classical thermobarometers [5-7, 9-10] and P-T estimates under the PET program [8].

Table 1. Comparison of estimates P (kbar) and T(°C)

Sample	A-433		441-g		251-A		A-218		138		A-234-1		A-208	
	T	P	T	P	T	P	T	P	T	P	T	P	T	P
Grt-Bt thermometer [5]	634	-	660	-	640	-	-	-	583	-	635	-	660	-
Grt-Opx thermometer [6]	-	-	-	-	-	-	700	-	700	-	750	-	-	-
Grt-Opx-Pl-Q barometer [7]	-	-	-	-	-	-	-	6.2	-	5.5	-	4.5	-	-
PET [8]	680	6.7	-	-	690	6.5	890	8.3	690	6.7	700	5.7	710	6.1
Grt-Bt thermometer [9]	680	-	720	-	690	-	-	-	690	-	700	-	676	-
Grt-Bt-Pl barometer [10]	-	6.1	-	-	-	7.0	-	-	-	7.0	-	4.8	-	5.1
This study	690	6.0	770	6.1	620	5.6	630	7.0	652	5.2	700	5.6	650	5.6

There is a good convergence in pressure in samples (A-218, 138, A-234-1) for which there are well-developed experimental thermobarometers, since the differences in pressure estimates are on average no more than 1 kbar. Differences in temperature

estimates reach 50-700 °C. Good convergence is observed between the Grt-Bt-Pl of the Wu barometer readings [10] and our data. Only in one sample (sample 138) the divergence in the pressure estimates exceed the error in determining the pressure using the Wu geobarometer [10]. But sample 138 is distinguished by an increased content of magnetite and increased oxidation of garnet and biotite, which, apparently, introduces an error in the pressure estimate according to Wu [10]. Quite good convergence (except for sample 218) is noted between our calculation and the PET program.

The P-T estimates obtained in this work for the Okhotsk granulite complex are 5.2–7 kbar in pressure and 620–770 °C in temperature (Table 1). On the whole, they are quite close to earlier estimates [13]. The probable error in finding the P-T estimates was (except for sample 441-g) 1-1.5 kbar in pressure and 200-500 °C in temperature.

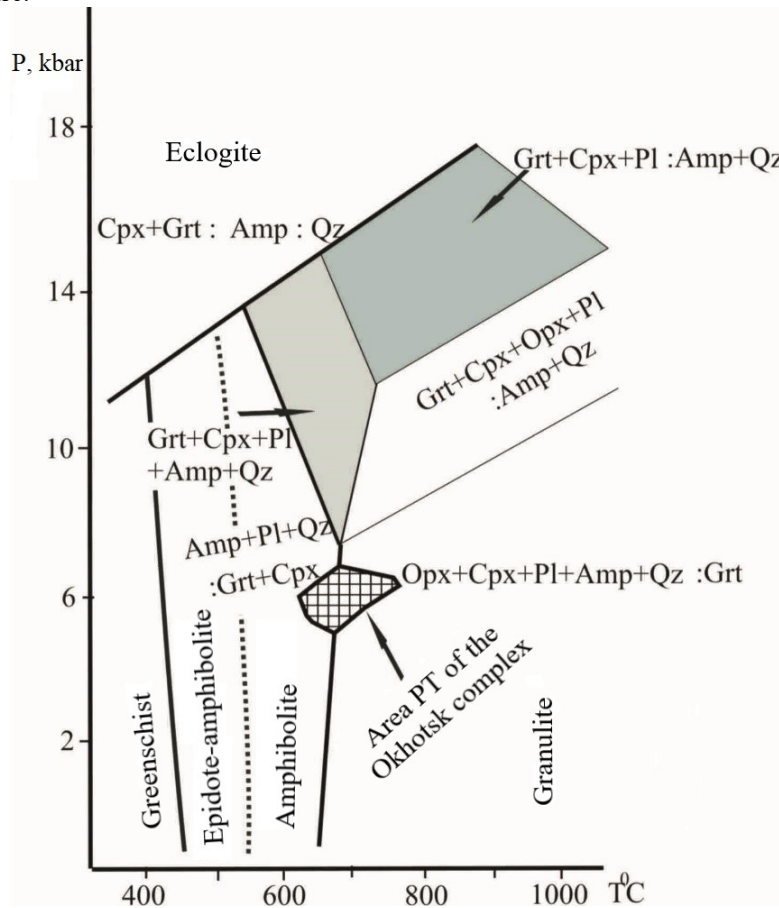


Fig. 2. P–T field of the conditions of formation of metamorphic rocks of the Okhotsk complex on the Pattison diagram [14]. A colon in front of mineral indices indicates that these minerals may be missing. Minerals: Grt - garnet, Cpx - clinopyroxene, Opx - orthopyroxene, Pl - plagioclase, Amp - amphibole, Qz - quartz.

The P-T parameters of the Okhotsk complex metamorphism are shown on the P-T diagram [14], where they form a small field (Fig. 2) corresponding to the boundary conditions of the amphibolite and granulite facies, which corresponds to all available data on the Okhotsk complex metamorphism regime.

4 Conclusions

The developed software is a rapid temperatures and pressures of rock formation assessment tool. It allows to significantly enhance the capabilities of classical geothermobarometry tools, which are rely on experimental studies or calculation methods based on the equations of a geothermobarometer or a fugometer, representing a set of chemical reactions of the formation of natural mineral associations. The obtained values can be used in the construction of models of the evolution of the geological environment, including ore deposit formation process.

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References

1. Tu, J., Gonzalez, R.: Principles of pattern recognition: Moscow: Mir, 410 p. (1978)
2. Duda, R., Hart, P.: Pattern recognition and scene analysis. Moscow: Mir, 510 p. (1978)
3. Simankov, V.S., Lutsenko, E.V.: Adaptive control of complex systems based on the theory of pattern recognition. Krasnodar: Tech. un-t Kuban. state technol. University, 318 p. (1999)
4. Fomin, Ya. A.: Pattern recognition: theory and applications. 2nd ed. Moscow: FAZIS, 429 p. (2012)
5. Perchuk, L.L.: Magmatism, metamorphism and geodynamics. Moscow: Nauka, 190 p. (1993)
6. Lavrentyeva, I.V., Perchuk, L.L.: Experimental study of the phase correspondence in the garnet-orthopyroxene-amphibole system at 700 and 800 °C. Essays on physical and chemical petrology, Vol. XVI. Moscow: Nauka, pp. 139-164 (1991)
7. Grafchikov, A.A., Fonarev, V.I.: Garnet-orthopyroxene-plagioclase-quartz barometer (experimental calibration). Essays on physical and chemical petrology. Moscow: Nauka, Issue 16, pp. 199–225 (1991)
8. Dachs, E.: PET: Petrological elementary tools for mathematica. Computers & Geosciences. V. 24, no.3, pp. 219-235. (1998)
9. Holdaway, M.J.: Application of new experimental and garnet Margules data to the garnet-biotite geothermometer. American Mineralogist. V. 85. pp. 881-889 (2000)
10. Wu, C.M., Zhang, J., Ren, L.D.: Empirical garnet-biotite-plagioclase-quartz (GBPQ) geobarometry in medium - to high-grade metapelites. Journal of Petrology. V.45, pp. 1907-1921 (2004)

11. Chudnenko, K.V.: Thermodynamic modeling in geochemistry: theory, algorithms, software, applications. Novosibirsk: Academic publishing house "Geo", 287 p. (2010)
12. Avchenko, O.V., Chudnenko, K.V., Vakh, A.S.: Analysis of mineral paragenesis by the Gibbs energy minimization method. Moscow: GEOS, 252 p. (2018)
13. Avchenko, O.V.: Mineral equilibria in metamorphic rocks and problems of geobarothermometry. Moscow: Nauka, 184 p. (1990)
14. Pattison, D.R.M.: Petrogenetic significance of orthopyroxene-freegarnet + clinopyroxene+plagioclase \pm quartz-bearing metabasites with respect to the amphibolite and granulite facies. *Journ. Metamorph. Geol.*, V. 21, pp. 21-34. (2003)