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NUMERICAL DESCRIPTION OF MICROSTRUCTURES OF SYNTHETIC MINERAL BODIES

Abstract. Quantitative and qualitative development of synthetic mineral bodies produced by industry, the precise characteristic of which should be often compared using computer technique, requires the unification of microscopic description of structures and their presentation by means of mathematical language. The present paper deals with a proposal of numerical description of structure based on the set of questions and answers deduced from the graph theory.

The dynamically growing demand for materials characterized by specific technical properties requires a precise comparison of their microstructures, taking into account their qualitative selection according to a particular application. In contrast to the approach of classical mineralogy and petrography, it requires progressive elimination of verbal descriptions for the benefit of computer language.

The views on classification of synthetic materials were gradually coming to the above conclusion. Beginning with the division of sintered materials proposed by Milligan (1950), via researches and analyses of Bielankin *et al.* (1957), Baumann (1958), Smith (1964), Smith (1968), Allen (1968), Lach (1971), Glibowski and Święcki (1975) applied graph theory to the digital expression of microstructure of ceramic bodies in green state and after firing. In their considerations they assumed after Lach that pores in the analysis of microstructure should be regarded as a zero-phase of the material.

The graph method is based on a list of questions (D^1 — list), allowing one to define the properties of the material, then to make a graph of possible answers to these questions (D-graph), and to classify the analysed material in the form D-description. The basic assumption is to answer only "yes" or "no" and to strictly obey the given sequence of questions.

Unlike the authors who classified the structures of ceramic materials with the help of 12 questions, we propose to describe microstructures by 24 questions concerning structural properties. The questions are divided into 8 groups, and each group contains 3 similar questions. The additional ninth group of 3 questions is open for specific properties that may be significant for a given material. The questions of the D^1-list (Table 1) allow one to make the D-description of microstructure (Table 3). Since the answers to the D^1—list questions may only be "yes" or "no",

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Table 1

D^1—list: Questions for description of x-body microstructure

No	Kind of question
1	Is the body fully crystalline?
2	Is the body partly crystalline (below 25% of the glassy phase)?[1]
3	Does the body contain much glassy phase (above 25%)?[1]
4	Does the body contain pores?
5	Do pores occur on grain boundaries?
6	Do pores occur inside the grains?
7	Does the body contain crystalline grains of different sizes?
8	Is the body composed of large oriented areas of different composition?
9	Is the body composition visibly crystalline (under optical microscope)?
10	If body mean grain size is coarse-grained (> 1.0 mm)?
11	If body mean grain size is medium-grained (0.1—1.0 mm)?
12	If body mean grain size is fine-grained (< 0.1 mm)?
13	Is the body composed of microcrystalline components?
14	Is the grain structure polycrystalline or twinned?
15	Does the body contain more than one crystalline phase?
16	If crystals composed body has only isometric shape?
17	Is the crystal habit regularly bordered — idiomorphic?
18	Is the crystal habit partly regularly bordered — hypidiomorphic?
19	Is parallel orientation of needle-like or plate-like grains observed?
20	Is wetting of crystalline grains by glassy phase good?[1]
21	Are mechanical stresses observed in the structure?
22	Does the microstructure show post-technological effects?
23	Are phase-changes observed as a result of No 22?
24	Is texture observed as a result of No 22?
25 26 27	Questions for special features not listed before

[1] In cermets intergranular metallic phase is similar to glass phase in ceramics.

in D-description they are marked as "1" or "0". The number of digits of all the answers to 27 questions is 27. When some questions are omitted, the answer has fewer digits, but the sum of digits in the position binary system equals the number of questions. On this basis, the author divised the D-graph showing the mechanism of microstructure classification (Fig. 1).

The graph peaks constitute the numbers of sub-sequent questions from 1 to 27 and they also constitute numbers which are equal to a sum digits of position

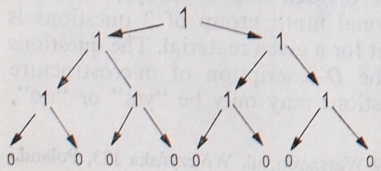


Fig. 1. Graph D_3 of D_n-graph group

Table 2

Schematic freehand drawings of more typical microstructures compared in Table 3

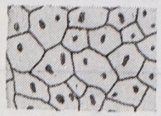
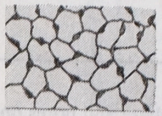
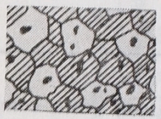
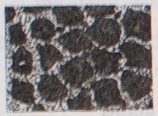
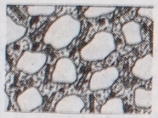
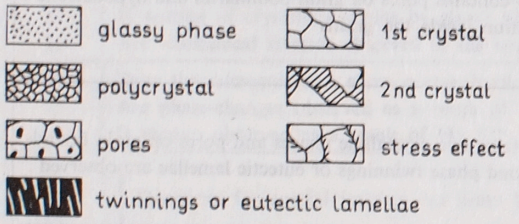
1		Body contains one crystalline phase, without glassy phase or pores. Visible stress effect
2		Body as *1* contains pores inside the grains
3		Body as *1* contains pores on grains boundaries
4		Body contains two crystalline phases and pores inside the grains
5		Body as *4* contains pores on grain boundaries and hypoeutectic crystallization inside the grains
6		Body contains two crystalline phases and pores on grain boundaries. Second phase twinnings or eutectic lamellae are observed
7		Body as *6* but with the third crystalline phase. It contains pores inside the grains
8		Body as *2* but composed of polycrystalline grains
9		Body contains one crystalline phase of two sizes composed of glassy-crystalline matrix. Two types of pores

Table 2

10		Body with one crystalline phase and pores inside the grains, composed of glassy matrix
11		Body with one crystalline phase composed of glassy matrix. Pores inside the matrix
12		Body as *11* but with second lathlike crystalline phase with idiomorphic grain habitus
13		Body as *12* but with need like second phase and pores on the grain — glass phase boundaries
14		Body contains two crystalline phases and pores, composed of glassy phase (more than 50 vol. %)



binary system answers to questions. The peak "1" is only one, peaks "2" are two, peaks "3" are four, peaks "27" are $2^{26} = 67109056$ and the answers to the last questions will then amount to 134218112.

As it is difficult to present the D_{27}-graph, we may use directly the D-description as an ungraphic answer to the D^1-list questions. This ungraphic answer in the binary system is a D_2 structure indicator (Table 3). It may be shortened to an indicator of the octal system by grouping similar questions in threes. Then every three digits of the binary system will be equalled by one digit in the octal system according to the principle:

Binary system	Octal system
000	0
001	1
010	2
011	3

Table 3

D-description of typical microstructures compared in the pictures (Table 2)

Microstructure according to No in Table 2	D_2-indicator: answers on D^1-list questions ("0" for "no", "1" for "yes") — Number of question																										D_8-structure indicator
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	
1	1	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0	0	401204140
2	1	0	0	1	0	1	0	0	1	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	451204000
3	1	0	0	1	1	0	0	0	1	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	461204000
4	1	0	0	1	0	1	0	0	1	0	1	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	451214000
5	1	0	0	1	1	0	1	0	1	1	0	0	0	0	1	0	0	0	0	0	0	1	1	0	0	0	0	465410060
6	1	0	0	1	1	0	1	1	1	0	1	0	0	0	1	0	0	1	1	0	0	1	1	0	0	0	0	467211460
7	1	0	0	1	1	1	1	0	1	0	0	1	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	475112400
8	1	0	0	1	1	1	0	0	1	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	471424000
9	0	1	0	1	1	1	1	1	1	1	0	0	1	0	0	0	0	0	1	1	0	0	0	0	0	0	0	277440600
10	0	1	0	1	0	1	0	0	1	0	1	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	251205200
11	0	1	0	1	0	0	0	1	1	0	1	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	241204200
12	0	0	1	1	0	0	1	0	1	0	1	1	0	0	1	0	0	1	0	1	0	0	0	0	0	0	0	145311200
13	0	0	1	1	1	0	1	0	1	0	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	163314000
14	0	0	1	1	1	0	1	0	1	1	1	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	165615000

100	4
101	5
110	6
111	7

The microstructure indicator given in the octal system (D_8-indicator, Table 3) allows one to describe every material by nine digits (27 : 3) which constitute a numerical parameter of the material. This enables one to use mathematical methods for the evaluation of technological processes.

Table 2 compiles schematic drawings of 14 typical cases of microstructure, which are compared in Table 3, basing on the answers for the D^1-list questions presented in Table 1. The given D_8-indicators also describe a particular microstructure in the range of D^1—list questions, emphasizing the similarities and differences. Higher digits in the indicators generally point to materials that are structurally more complex.

In this manner of microstructure description, numeral indicator must be supplemented with type of material and investigation method.

The application of the presented principle allows one to avoid optional description of microstructure, generally used in petrography, and to eliminate significant differences in descriptions presented by different scientists and laboratories.

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OPIS CYFROWY MIKROSTRUKTUR SYNTETYCZNYCH TWORZYW MINERALNYCH

Streszczenie

Rozwój ilościowy i jakościowy wytwarzanych przez przemysł tworzyw mineralnych, których precyzyjna charakterystyka coraz częściej musi być oceniana porównawczo z zastosowaniem technik komputerowych, wymaga ujednolicenia mikroskopowego opisu struktury i przedstawienia go za pomocą języka matematycznego. W artykule przedstawiono metodę cyfrowego opisu struktury w oparciu o zestaw pytań i odpowiedzi wyprowadzony z teorii grafów.

Анджей ШИМАНЬСКИ

ЦИФРОВОЕ ОПИСАНИЕ МИКРОСТРУКТУР СИНТЕТИЧЕСКИХ МИНЕРАЛЬНЫХ ПЛАСТМАСС

Резюме

Количественное и качественное развитие производимых промышленностью минеральных пластмасс, которых точную характеристику всё чаще надо сравнительно оценивать с применением техник основанных на вычислительных машинах, требует унификации микроскопического описания структуры и её представления при помощи математического языка. В статье представлен метод цифрового описания структуры на основании состава вопросов и ответов, выведенного из теории графов.