PARAMETRIZATION OF STRUCTURE MATERIALS WITH OF APPLICATION THE FORMALISM OF MULTIFRACTALS

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SUMMARY: It has been worked out the procedure of multifractal parametrization of structure materials and production program that permits the determination of fractal dimension characteristic connected with mechanical properties. It has been shown that multifractal analysis reveals high information capacity in the studies of structure materials of various nature.

KEYWORDS: structure, multifractal, parametrization, steels, polymers.

INTRODUCTION

Much attention is given recently to the fractal analysis of structures in materials that undergo self-organization under various conditions [1-3]. However, in real physical systems self-similarity of structures occurs only over a limited scale, thus calling for the application of a multifractal approach. In this case the fractal measure is represented by interconnected fractal subsets which change following power functions with different exponents [3], meaning that the set we study is structurally uniform and comprises subsets differing in their fractal dimensions. Accordingly, sets of such kind became known as multifractals. The limitations of fractal analysis in the investigation of physical objects (such as metal fracture surfaces) demonstrated earlier [4] suggested the introduction of the characteristics of fracture structure related to the mechanical properties [4-8].

1.PROCEDURE FOR PARAMETRIZATION OF A MULTIFRACTAL SET OF LINES

The fundamentals of computerized analysis of multifractal structures have already been discussed [1-3].The analysis of multifractal characteristics of a two-dimensional structure involves representing it as a population of zeros and unities since each structure element can assume but two possible values corresponding to one bit of information. In order to convert 256-colour image into a monochrome version, the file in question (graphics BMP-format, 512x512 pixels) was loaded into the videomemory of PC. Further, the current range of shades was adjusted so as to fix the required threshold level of grey. Then all shades having an intensity of grey equal to or les than this level were taken is black, all shades exceeding this level Ö as white. The

monochrome image copied then to the on-line storage represented a two-dimensional array of 512x512 bytes that characterized the given structure.
It is apparent from the following expression [3]

$$\tau(q) = - \lim_{\delta \to 0} \; [\ \ln N(q,d) \,/\, (\ln \delta\ ) \qquad (1)$$

that the mass index ((q) is the derivative of the functional relationship: logarithm of the weighted number of cells N(q,d) versus logarithm of cell dimension δ. As applied to the given procedure, the values of $\tau(q)$ were found in the following way. The structure studied was superposed with sets (2, 4, 8, 16, 32, 64, 128,256) of square cells with side δ_k (k=1,... 8). The characteristic function N(q,d) was calculated for each set as the normalized number of points occupied by the given set in a given cell, then summed up over all cells for given k. The normalizing basis was the total number of cells of the same colour constituting the given set. These calculations were made for all k=1,..., 8 and the dependence $\ln\{N(q,d)\}$ versus $\ln(\delta_k)$ was plotted. Then the least squares procedure yielded the slope which actually was the index of mass τ for the given q. Similar calculations for all q in the range from -40 to 40 in steps of 1 were conducted and the dependence $\tau(q)$ plotted. Finally, the following formulas

$$\alpha(q) = - [\ d \,/\, (dq)\ ]\ \tau\ (q), \qquad (2)$$

$$f(\alpha(q)) = q\alpha(q) + \alpha(q) \qquad (3)$$

were used to calculated f, (and D for each q. The dependence $\tau(q)$ became the basis for determining the spectrum of Reniy dimensions. The measure offered in the algorithm considered here is the area covered by points of one of the two possible colours (black and white), so the initial 256-colour format image had to be converted into a monochrome image. This operation caused a loss of information since a three-dimensional relief was substituted by a planar image.

2. METHODICS FOR MULTIFRACTAL PARAMETRIZATION OF COMPACT AGGREGATED STRUCTURES

This procedure involves the analysis of not a monochrome image, as in the previous case, but rather of the initial 256-colour image of the structure, the intensity of the shade of grey in each image pixel being interpreted as the ‘depth’ or the distance to the obsever’s eye. The dareker regions with lesser intensity of grey correspond to more distant surface points of the structure studied, whereas the brighter regions correspond to points that are closer to the observer. Thus, the surface of the structure of the structure studied appears to be ‘immersed’ in a layer with a ‘depth’ of 256 arbitrary units each of width correlates with one shade of grey. With the measure reference tending to zero, this surface reveals fractal (multifractal) properties.

In developing this procedure we applied the main principles of the formalism described above. The necessary condition was that the structure studied (surface in the three-dimensional Euclidean space) is covered with a set of elementary parallelepipeds, their bases represented by squares with sides (k = 2, 4, 8, 16, 32, 64, 128, 256 shades of grey corresponding to each δ_k. The characteristic function N(q,d) was calculated by summing up over all the cells filling out the 512x512x256 parallelepiped, normalizing was conducted in relation to the total number of image points (512x512), and values of f, α and D were found for each q in the range from -40 to 40. Then we determined the relationship $D_q = f(q)$ and the surface area S of the structure studied expressed in arbitrary units: 'size of image pixel per unit shade of grey'.

3. COMPUTERIZED PARAMETRIZATION OF GRANULAR AND AGGREGATED STRUCTURES

A block diagram of the procedure is shown in Fig.1. A photomicrograph of the structure of a material is scanned and converted into a graphical BMP-format file. Much attention is paid to the selection of resolution because the resulting image must include an element sized 512x512 pixels covering the largest possible area. The dependence D(q) produced by computerized analysis of the structure permits the determination of the spectrum of Reniy dimensions: D_o - characterizing a uniform fractal; D_1 - the informative dimension; D_{40} and D_{-40} characterizing the degree of surface looseness (maximum for D_{40} and minimum for D_{-40}). The difference $\delta_s = D_1 - D_{40}$ (or else ($\Pi_c = D_o - D_{40}$) describes the latent ordering of the structure (see Fig.1).

We conducted multifractal parametrization of the granular structure of nonmagnetic austenitic Mn-Ni-Cu-V-C steels varying in Cu/Ni ratio from 0.05 to 0.9 [9]. The dependence of the parameter δ_s on the Cu/Ni ratio was determined (Fig.2), as well as the correlation between the cold brittleness temperature t_{k1} and parameter δ_s. It is obvious that the equality $\delta_{s1}^{max} = \delta_s^*$, as found in the analysis, is the critacal parameter controlling the type of the correlation dependence tk1=f(δ_s): when (s > (s*, tK1 decreases with the increase of the degree of latent ordering, but increases when $\delta s < \delta_s^*$ (Fig.3). The apparent inference is that multifractal parametrization of the initial grain structure can be useful for the optimization of the composition of steel (as well as for other modes of affecting alloy structure).

Another subject of inquiry was the the structure of specimens of polymethylmetacrylate (acrylic plastic) and of NiCu catalyst (Fig.4) [10]. The problem was to reveal the structure differences from the viewpoint of their multifractality in relation to parameters (c and S. The results of this study were as follows:

Material	D_0	D_{40}	($\Pi c = D_0 - D_{40}$	$S*10^{-6}$
Polymethylmetacrylate	2.703	1.911	0.792	2.702
NiCu catalyst	2.660	2.064	0.596	5.419

It is apparent that the values of D_0 for both specimens are close, but their multifractal structure differs: considering the fractal set with the greatest looseness (parameter D_{40}) planar clusters ($D_{40} < 2$) are predominant in the plastic, whereas three-dimensional clusters ($D_{40} < 2$) prevail in the catalyst. The transition to a volume-aggregate structure decreases the latent ordering of the structure (values of Πc for the catalyst are lower than those for the plastic). The higher value of S for the catalyst points to the higher sinuosity of its surface compared to that of the plastic.

CONCLUSION

Elaborated methodics and production program has been shown that multifractal parametrization, as a new method of structural studies, holds much promise for improving the structure and properties of materials.

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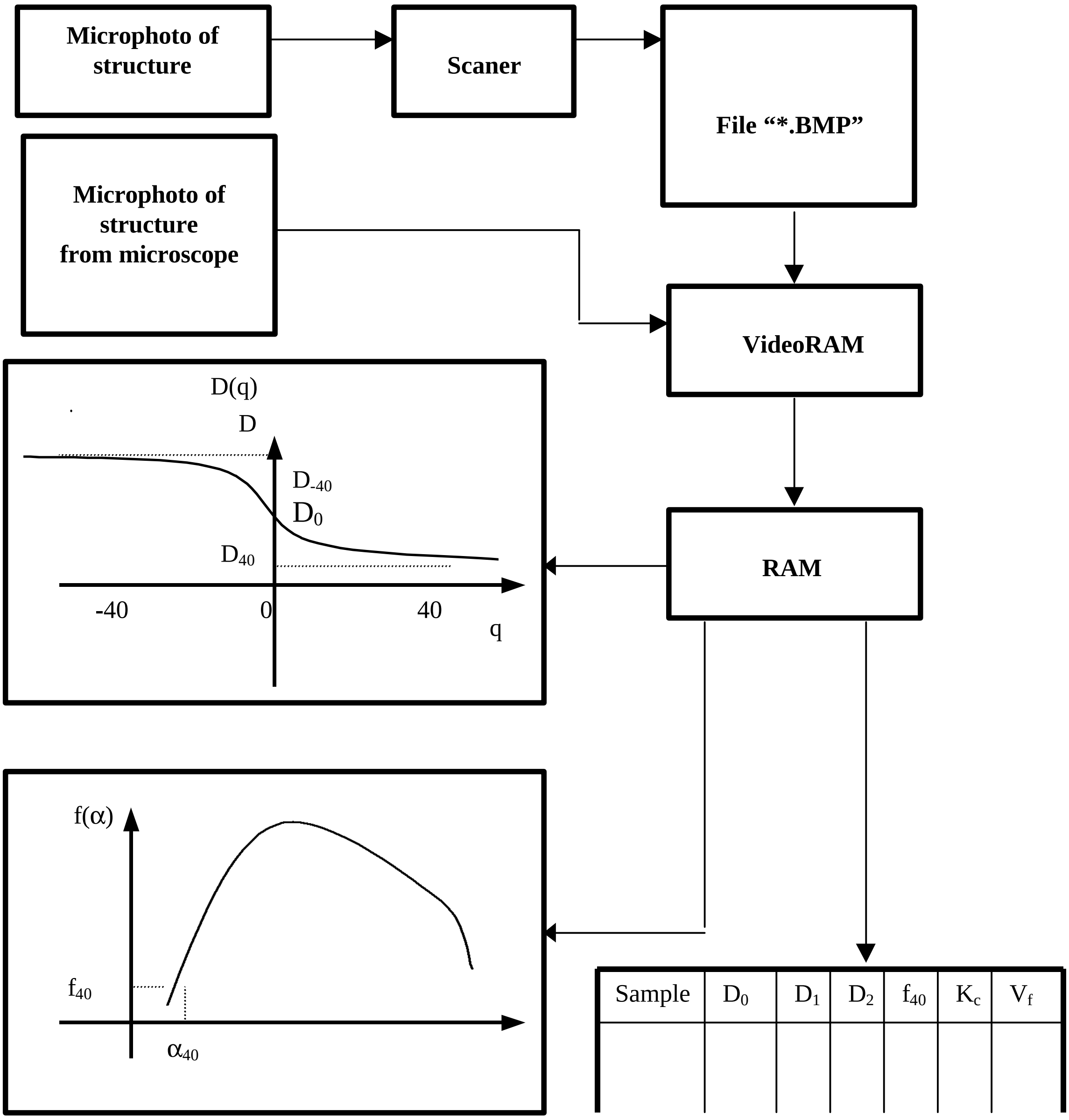
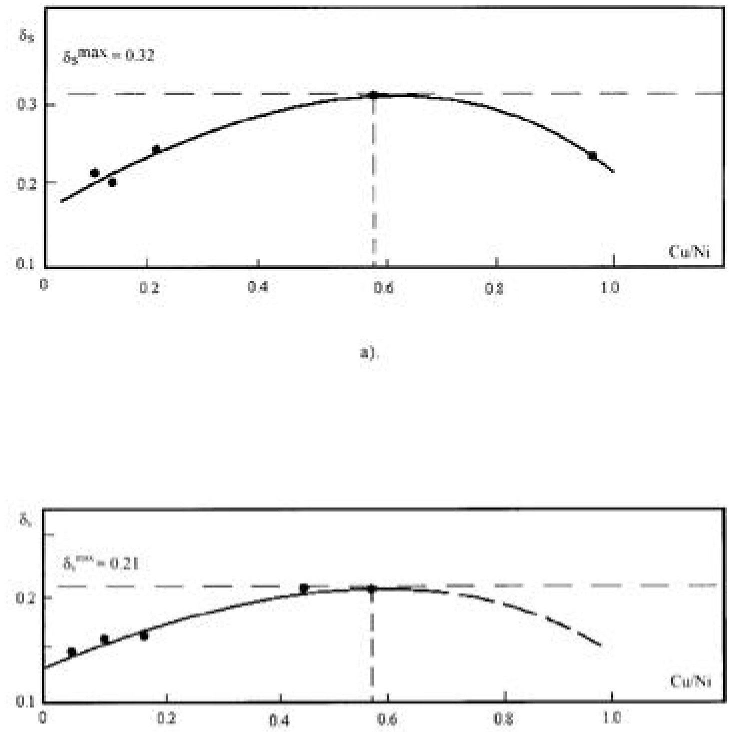


Microphoto of structure
Scaner
File “*.BMP”
Microphoto of structure from microscope
VideoRAM
RAM
D(q)
D
D-40
D0
D40
-40
0
40
q
f(α)
f40
α40
Sample
D0
D1
D2
f40
Kc
Vf

Fig.1


δs
δs max = 0.32
0.3
0.2
0.1
0
0.2
0.4
0.6
0.8
1.0
Cu/Ni
a).
0.2
0.1
0
0.2
0.4
0.6
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1.0
Cu/Ni

b).

Fig.2.

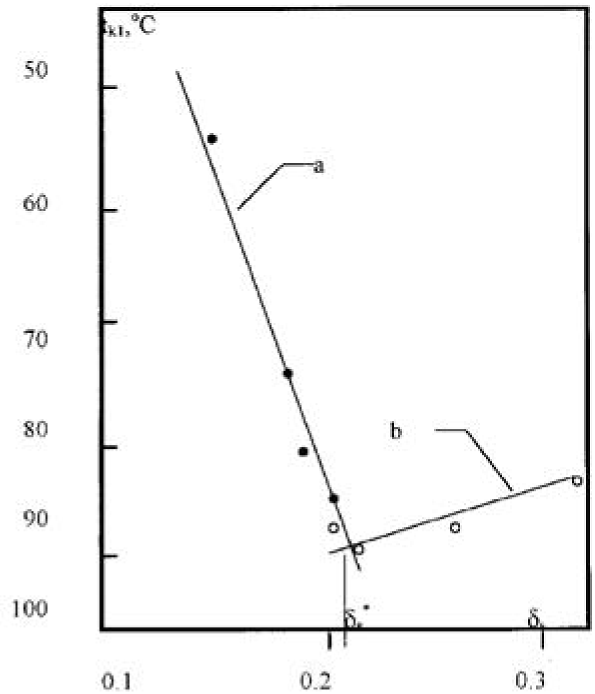
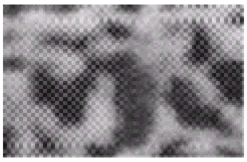
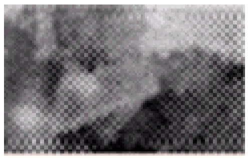

°C
50
60
70
80
90
100
a
b
0.1
0.2
0.3

Fig.3



a)



b)

Fig.4

SIGNATURE TO F I G U R ES

Fig.1. Block diagram of the computerized parametrization of structures.

Fig.2. δ_s versus Cu/Ni ratio for the nonmagnetic austenite 1_% Mn-7%Ni-(0.5-4%)V-Cu steels after hardening (1150 ^oC) and ageing (650 , 10h); a is for steels for which
Petch law are satisfing; b is for steels for which Petch law are not satisfing.

Fig.3. t_K versus δ_s for steels for which Petch law are satisfing (a) and not satisfing (b).

Fig.4. Microstructure of polymer (a) and catalyst (b).