INFORMATION-THEORETIC INTERPRETATION OF MULTIFRACTAL FORMALISM AND ANALYSIS OF METALLIC FRACTURE SURFACES

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We introduce and investigate new quantitative characteristics of uniformity and order of the natural structures on the base of our information - theoretic interpretation of multifractal formalism (MF). An practical algorithm for calculation of multifractal characteristics of metallic fracture surface is presented. Even relatively rough estimates of MF characteristics alongside with their qualitative implications stemming from the information-theoretic interpretation allows us to find out additional evidence on the fracture processes in real materials.

INTRODUCTION

It is well known that the self-similarity of natural and numerous model structures cannot be adequately described only in terms of single fractal dimension. More detailed description of disordered structures requires to calculate the spectrum of various dimensions, i.e., the multifractal formalism is needed (Feeder (1), Halsey at al(2), Vstovsky at al (3), Vstovsky and Bunin (4)).

In this paper we suggest a new information-theoretic interpretation of MF. This approach allow us to introduce and to examine the quantitative parameters characterizing homogeneity and ordering of the fractal structures related to fracture surface of metals. Such technique supplements the conventional ones.

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MULTIFRACTAL INTERPRETATION BASED ON INFORMATION THEORY

Consider some strange (porous, friable, etc.) object embedded into Euclidean space and divide it into cells of characteristic size l. Making this, we may ascribe to each cell its own measure (weight) corresponding to the nature of this object (portions of mass, area, energy, etc). Let P_i be the measure of i-th cell with the size $l_i \leq l$, where l is a characteristic cell size and $\sum_{i=1}^{N} P_i = 1$. Let us consider transformation of the $\{P_i\}$ measure included into the one-parameter set $[V_q]$

$$P_{1i}(q) = V[\{P_i\},q] = (P_i)^q / \chi(q); \quad \text{.....(1)}$$

$$\chi(q) = \sum_{i=1}^{N} (P_i)^q,$$

where $\chi(q)$ is the generalized correlation function of the $\{P_i\}$ measure, q is the real parameter continuously varying within the $-\infty \leq q \leq +\infty$ range. Transformation (1) presents a one-parameter group operating in the space of normalized measures (Vstovsky at al (5)). An appropriate measure of distinction between the $\{P_i\}$ and $\{P_{1i}(q)\}$ is the Kullback information (4,5)

$$I_{mfr}(q) = \sum_{i=1}^{N} P_i \ln[P_i/P_{1i}(q)], \quad \text{.....(2)}$$

where subscript "mfr" indicates that this quantity should describe the multifractal properties. The Legendre transformation of the function $\tau_I(q) = \lim_{l \to 0} I_{mfr}(q)/\ln l$ gives

$$\alpha_I(q) = d\tau_I/dq = \alpha(q) - D_1, \quad \text{.....(3)}$$

$$f_I(q) = q\alpha_I(q) - \tau_I(q) = f(q) - D_1, \quad \text{.....(4)}$$

where

$$\alpha(q) = d\tau/dq = \lim_{l \to 0} \sum_{i=1}^{N} P_{1i}(q) \ln(P_i)/\ln(l), \quad \text{.....(5)}$$

$$f(q) = q\alpha - \tau = \lim_{l \to 0} \sum_{i=1}^{N} P_{1i}(q) \ln(P_{1i}(q))/\ln(l). \quad \text{.....(6)}$$

The expression for α_q and f_q coincide with the definitions ref.(2) where they were introduced as formulas meeting the

Legendre transformation. These definitions were used at transition from the description in terms of generalized Renyi dimensionalities

$$D_q = \tau(q)/(q-1), \qquad \tau(q) = \lim_{\ell \to 0} \chi(q)/\ln \ell$$

to that in terms of so called $f(\alpha)$ spectrum: $\alpha = d\tau/dq$, $f = q\alpha - \tau$. Thus, equation (5) and (6) may be considered as explicit formulas for $f(\alpha)$ spectrum parametrized by group parameter q. The $f_I(\alpha_I)$ spectrum is simply a shifted $f(\alpha)$ spectrum. Simple transformations lead to the relation

$$\tau_I(q) = (q-1)(D_q - D_I). \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

The above discussion demonstrates that the multifractal description can be deduced by considering some degree of ordering (I_{mfr}) in system characterized by distribution $\{P_i\}$. A quantity $I_{mfr}(q)$ can be referred as a measure of order in the system (5). Its zero value corresponds to the complete disorder when all P_i are equal each other. A slightest non-uniformity of the $\{P_i\}$ distribution should affect appreciably f_q, α_q, and D_q at sufficiently large q-values. This provides an opportunity to take f_Q and $\Delta_Q = D_I - D_Q$ at certain fixed q=Q as effective measures of the uniformity and order. The larger is Q, the more sensitive become the above quantities to the features of $\{P_i\}$ distribution characterizing the system under study.

STUDY OF FRACTURE SURFACES

The multifractal characteristics of actual fracture surface structures were studied in the course of investigating

(i) the effect of rhenium coating on fracture surface after uniaxial tensile tension of molybdenum wires 1 mm diameter;

(ii) the effect of initial microstructure and impact loading conditions on mechanical properties and fracture surface structures of the Charpy specimens made of the ЭП-678 Maraging steel.

We used two different special algorithms for two above cases, respectively.

(i) The photos of fracture surface regions LxL in size (L=32 [μm]) near the surface of the specimens were divided into nxn (n=64) "elementary" cells. Then, the cells were marked by unities if they coincided with the transcrystalline fracture domains and by zeroes in the case of intercrystalline fracture domains. The measure was calculated for each photo by using eight rougher partitions into cells: l_kxl_k unit cells, k=1,...,8. Here, l_k were taken from the {4,6,8,10,12,16,21,32} set. We performed a simple summation of unities in each cell and divided this sum by the total sum of unities in the cells. Then, we calculated functions $\chi_k(q)$ at each $q \in [-30,40]$ for all eight rough partitions. After that, we plotted log-log diagram describing the $\chi_k(q)$ dependence on l_k and calculated the $\tau(q)$ slope using the least-square method. The Renyi dimensions and $f(\alpha)$ spectra were calculated according to the canonical procedure:

$$D_q = \tau(q)/(q-1), \quad \alpha = d\tau/dq, \quad f = q\alpha - \tau(q).$$

(ii) The second algorithm involved the similar steps with the following parameters: L=170 [μm], n=128, and l_k (k=1,...,15) were taken from the {4,5,6,7,8,9,11,12,14,16,18,21,32,42,64} set. The $f(\alpha)$ spectra were calculated straightforwardly by approximating log-log dependencies of the sums in equations (5) and (6) on l_k using the least-square method. The quantities $\tau(q)$ and D(q) were calculated according to the relations $\tau(q) = q\alpha - f$, $D_q = \tau(q)/(q-1)$, respectively.

In both studies, the values of Δ_{40} and f_{40} may be considered as good estimated of Δ_∞ and f_∞. These values were used as effective quantitative measures of the order and homogeneity for the structure of fracture surfaces. The results of calculations are illustrated in Fig.1. These results are in good qualitative agreement with modern concepts concerning the fracture processes in the materials under study. Moreover, the use of MF characteristics provides an opportunity to draw qualitative conclusions about the evolution of defect structure and characteristic times, to name but a few. For example, it was shown in (3) that the self-organization processes of fractal structures in subsurface layers of molybdenum wires occur faster than in the bulk of the material. The changes in wire surface geometry can be caused by decreasing the size of surface microdefects (in the course of polishing). These changes affect the dynamics of metal

structure evolution in subsurface layers during the static tension. As a result, the structure becomes more homogeneous (f_{40} grows) and its localization near the defects is smoothed off (Δ_{40} decreases). The rhenium coatings slow down the self-organization rate of fractal structures in the subsurface layers and stimulate the growth of their homogeneity. With the growth of coating thickness, the dynamics of self-organization processes in the subsurface layers becomes closer to that in the bulk.

The behavior of MF characteristics of Maraging steel fracture surface can be interpreted in the following way. The nearly absence of diffusion processes, intense heat transfer from local prefracture zones at the test temperature -196 ^{o}C, and more homogeneous distribution of the hardening phase particles make the fracture surface of aged steel more homogeneous in comparison to those characteristic of quenched steel. At the test temperature 20^{o}C, the activation of microdamage diffusion process at the tip of macrocrack makes the structure of fracture surface of the quenched steel more homogeneous than at -196 ^{o}C. However, the more intense diffusion of microdefects in aged steel at 20 ^{o}C gives rise to more intensive localization of them at the hardening phase particles. Thus, the fracture surface becomes more structurally inhomogeneous than at -196 ^{o}C. Therefore, it may be inferred, in general, that the aged steel is in a highly nonequilibrium state, and the fracture processes give rise to self-organization of more ordered structures owing to the diffusion processes.

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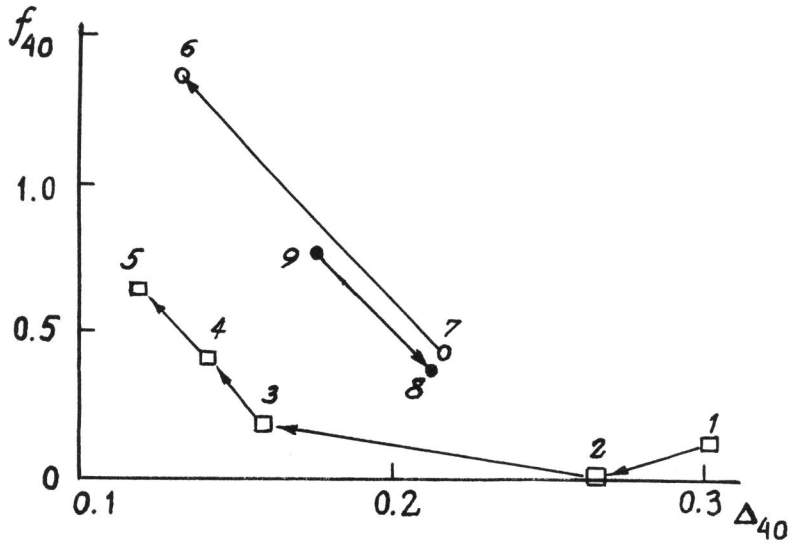

Figure 1 Variation of parameters characterizing "homogeneity" f_{40} and "ordering" Δ_{40} of fracture surface structures for molybdenum wire samples coated by rheniun (points 1-5):
(1) specimen without coating, (2) similar specimen with electropolished surface, (3 and 4) specimens with coating 0.4 and 3.2 μm thick, respectively, and (5) bulk of the metal.
The same for fractures of macrospecimens with the Charpy V-notch made of the ЭП-678 Maraging steel (points 6-9): (6 and 7) quenched steel and (8 and 9) aged steel; the corresponding values of impact toughness are $(30.8, 8.4, 16.5, \text{ and } 0.86)\times10^{-2}$, $MJ*m^{-2}$; the test temperature equals to 20 °C (6 and 8) and -196 °C (7 and 9).