THREE-DIMENSIONAL COMPUTER MODELING OF FRACTURE SURFACES

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In fracture mechanics, the analysis of fracture surfaces is based on the digital photogrammetric processing of images obtained with the help of a scanning electron microscope [1, 2].

In three-dimensional fractography, it is customary to compare the profilometric data of regular surfaces (cubic, conic, or spherical). However, the accuracy of this procedure is quite low due to the fact that the geometric approximations are not identical. These arguments enable us to make important generalizations.

1. Let $h = Q(x)$ be an *a priori* unknown function reflecting the dependence of the relative height of the investigated surface as a function of the abscissa in the stereoscopic image obtained with the help of a scanning electron microscope. As soon as the heights h_s at the points x_s are determined, it is necessary to estimate the function Q for a known collection of pairs $\{(x_s, h_s)\colon 0 \le S \le S-1\}$. This problem is stated as the problem of extrapolation of a function of two variables known for a finite set of points. To solve it, we represent the micropattern regarded as a random field in the form of a sum of cylindrical components. Indeed, let

$$Q(x) = \sum_{j=0}^{\tau-1} Q_j(x), \qquad Q_j(x) = C_j(x_1 \cos\alpha_j + x_2 \sin\alpha_j), \tag{1}$$

where x_1 and x_2 are the coordinates of the point x and $C_j(t)$ are *a priori* unknown functions of single variable

$$\alpha_j = \pi j \tau^{-1} \quad (0 \le \tau \le \tau - 1).$$

Also let

$$t_{js} = (x_1^{(s)} \cos\alpha_j + x_2^{(s)} \sin\alpha_j),$$

where $x_1^{(s)}$ and $x_2^{(s)}$ are the coordinates of x_s $(0 \le s \le s-1)$.

Suppose that the functions $C_j(t)$ are piecewise linear in the segments from $T(j,k)$ to $T(j,k+1)$ $(0 \le s \le s-2)$. We denote the slopes of these segments by $u_{j,k+1}$. Then

$$C_j(T(j,k)) = u_{j,0} + \sum_{m=0}^{k-1} [T(j,m+1) - T(j,m)]\, u_{j,m+1}, \tag{3}$$

where $u_{j,0}$ is the initial value of $C_j(t)$ and $q_s = h_s$ $(0 \le s \le s-1)$. By definition, we can write

$$q_s = \sum_{j=0}^{\Delta\tau-1} \left\{ u_{j,0} + \sum^{\mathrm{ord}:(s)^{-1}} [T(j,m+1) - T(j,m)]\, u_{j,m+1} \right\}. \tag{4}$$

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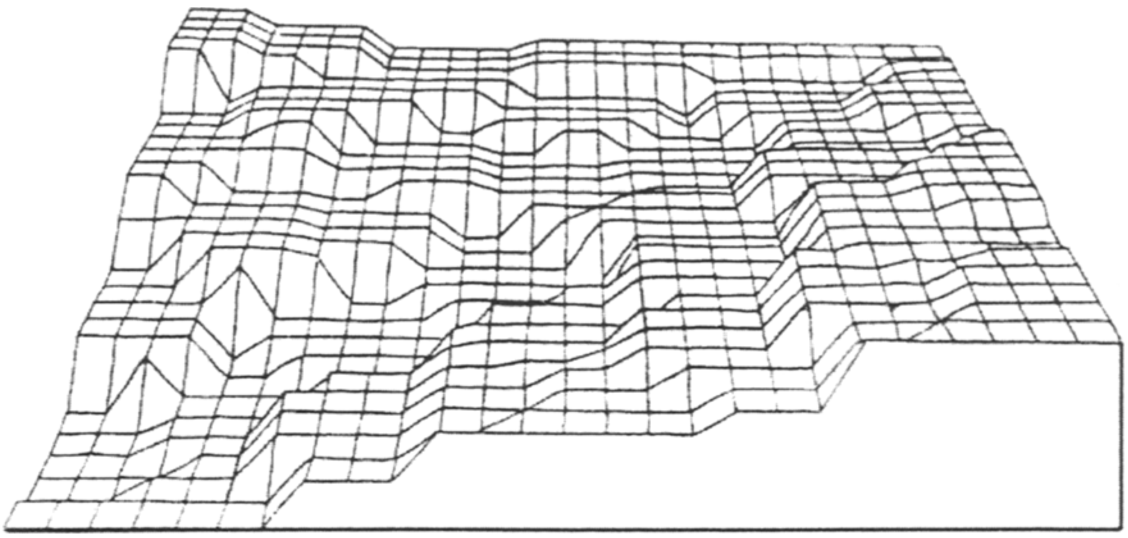

Fig. 1. Digital model of a micropattern of the fracture surface plotted by the method of extrapolation of the data of stereoscopic measurements in scanning electron microscopy.

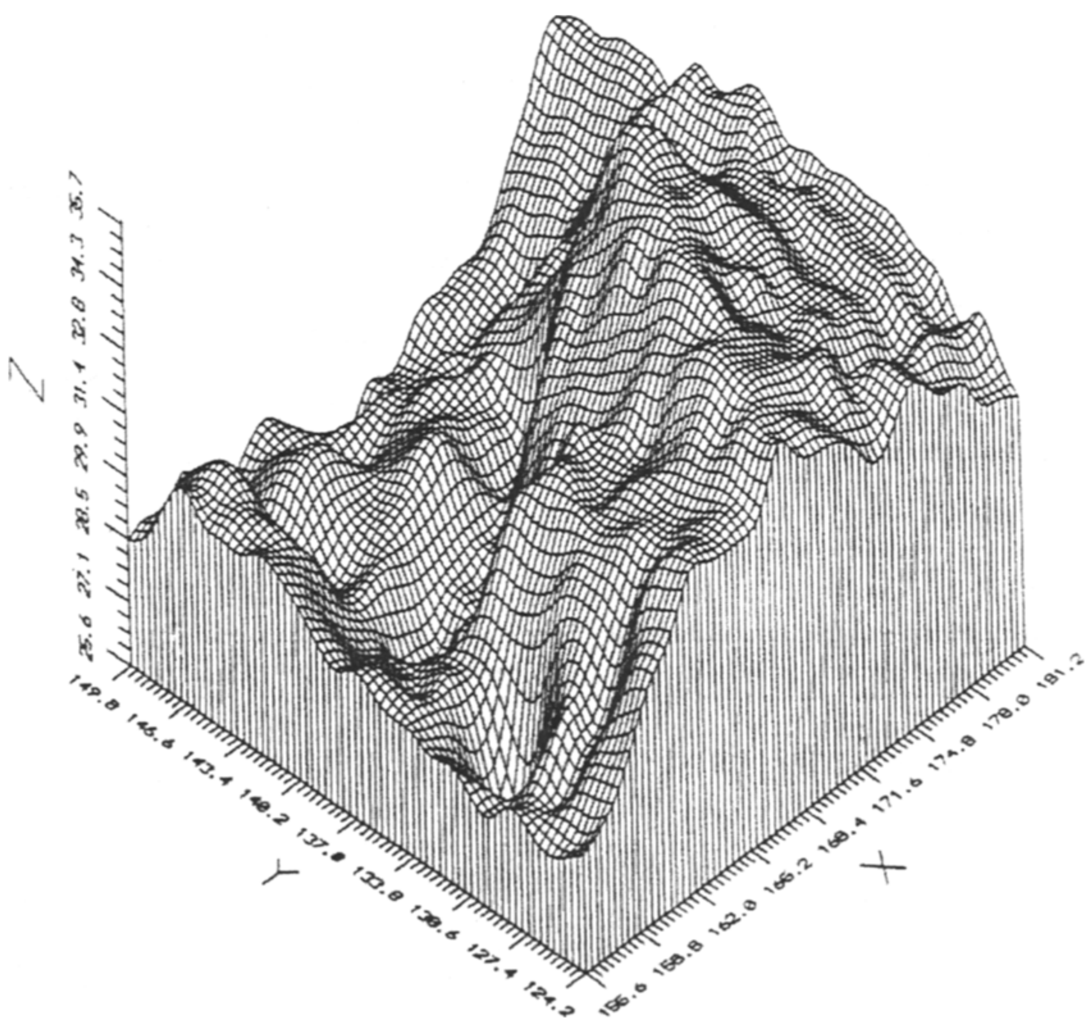

Fig. 2. Perspective projection of a stepwise brittle-fracture surface.

In this statement, the problem of extrapolation is reduced to the choice of variables $u_{j,k}$ $(0 \le j \le \tau - 1,\ 0 \le k \le s-1)$ satisfying the linear equations (3). Since this choice is ambiguous and we want to guarantee the maximum possible smoothness of the surface of approximation, it is reasonable to perform the choice of the variables $u_{j,k}$ by the method of least squares minimizing the quadratic functional of "action"

$$W = \sum_{j=0}^{\tau-1} \sum_{k=0}^{s-2} u_{j,k+1}[T(j, k+1) - T(j, k)] \tag{5}$$

under given linear restrictions imposed on the choice of variables.

Moreover, to take into account the errors accumulated in measuring heights h_s, it is reasonable to minimize the quadratic functional

$$\tilde{W} = W + \gamma \sum_{k=0}^{s-2} u_{j,k+1}^2, \tag{6}$$

where $\gamma > 0$ is a parameter taking into account the accuracy of measuring h_s and $u_{j,k}$ are the measurement errors of h_s. The origin of coordinates where the relative height is known and equal to zero corresponds to $s = 0$ in the list $\{x_s : 0 \le s \le s-1\}$.

2. As an important specific feature of the proposed method (two examples of its practical realization are presented in Figs. 1 and 2), one can mention the possibility of its application to the quantitative evaluation of three-dimensional roughness and angular distribution of the fracture faces. If, as a result of extrapolation, the space coordinates of points of the surface are sufficiently close to each other, then we can construct a triangular net in which every triangle corresponding to a fracture face is specified by two neighboring points of the surface determined by the coordinates of the same $x-z$ profile (y is constant) and the proximate point of the next profile. Thus, for a profile measured in the direction y, two pairs $y-z$ of the y-profile are combined with a single point of the next profile. For this choice of points, the computer software enables us to find the area of the fracture surface and the slopes of the facets (faces) relative to the direction of stresses (e.g., the $z(\alpha_z)$-axis), to the direction of crack propagation (the $x(\alpha_x)$-axis), or to the direction normal to these two axes (the $y(\alpha_y)$-axis). The entire area of the fracture surface S is estimated by adding the areas of all triangles $\alpha_{i,j}$, i.e.,

$$\bar{S} = \sum_{i,j} \alpha_{i,j}. \tag{7}$$

We can also find the area of a three-dimensional irregular fracture surface according to the density of vectors. The estimate of the actual fracture surface obtained by this method is denoted by S' and we can write [3–5]

$$S' = \frac{365}{A_z'}\Big\{P_L[001] + P_L[010] + P_L[100] + P_L[011] + P_L[101] + P_L[110] + P_L[\bar{1}10] + P_L[1\bar{1}0]$$

$$+ P_L[\bar{1}01] + \sqrt{\frac{3}{4}}(P_L[111] + P_L[\bar{1}11] + P_L[1\bar{1}1] + P_L[\bar{1}\bar{1}1])\Big\}, \tag{8}$$

where A_z' is the area of the surface projected in the direction z onto the plane corresponding to the actual area of the domain covered with $x-y$ data points in a noninclined micrograph made with a scanning electron microscope and $P_L[001]$ is the density of vectors normal to the fracture surface (in the direction z). For all other P_L, the interpretation is similar.

The values of S' obtained as indicated above are somewhat lower than the values computed by using triangular faces. This is a result of smoothing of the roughness of the fracture surface in both directions in the procedure used to obtain S'. At the same time, in the case of $\bar{S}$, only one direction is smoothed. It is thus obvious that the actual area of the surface S is greater. By performing simple corrections of smoothing at the equidistant points of the initial data, we can estimate the deviation of $\bar{S}$ (one smoothing) from S (no smoothing) according to the difference between S' and $\bar{S}$. Thus, we obtain the corrected empirical estimate S^C of the actual area of the surface S in the form

$$S^C = \bar{S}\left(\frac{\bar{S}}{S'}\right).$$

One can avoid the procedure of smoothing based on the use of equidistant profiles and proper collections of points. To do this, it is necessary to measure the coordinates of angles of the actual fracture faces or to use profiles distributed with sufficiently high densities.

3. It is known [6, 7] that the roughness of the surface ~~R_S can be defined as~~ the ratio of the actual area of the fracture surface S to the area $A_{\sim}'$ of its projection onto the fracture plane, namely,

$$R_S = \frac{S}{A_{\sim}'}. \tag{9}$$

It is clear that $R_{\bar{S}}$ and $R_{S'}$ obtained by using $\bar{S}$ and S' are different. This difference is also caused by the procedure of smoothing. However, in this case, we can also find the actual values of these quantities by using the same correction as for the actual surface, i.e.,

$$R_S^C = \frac{S^C}{A_{\sim}'} = R_{\bar{S}}\,\frac{R_{\bar{S}}}{R_{S'}}. \tag{10}$$

This means that, according to the data of estimates of the actual area of the surface, we can determine the corrected roughness of the surface free of measurement errors and smoothing. Below, we present some results of the practical evaluation of the surface roughness according to the data of stereoscopic measurements.

$R_{\bar{S}}$	1.50; 1.45	1.90; 1.87
$R_{S'}$	1.20; 1.18	1.48; 1.42
Δ	0.30; 0.27	0.32; 0.45

4. We now clarify the agreement between the results of construction of a digital model of micropattern of the stepwise surfaces and the data of measurements carried our for arbitrary fracture surfaces. To this end, we use the theorem well-known in the profilometry of fracture surfaces according to which "the fracture surfaces with the same degrees of roughness (K_A) have almost equal profile indices of roughness (K_P)" [1, 6]. For the "ideal" stepwise fracture surface, we obtain the following general relationship between the mean characteristics of the roughness profile $\bar{K}_P$ and the corresponding indices of roughness of individual segments [6]:

$$\frac{1}{\bar{K}_P} = \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n(2-K_A)^n}{(2n+1)K_A^{n+1}}. \tag{11}$$

If we now rewrite relations (11) in the form of a finite series, then, after simple transformations, we obtain

$$\frac{1}{\bar{K}_P} = \frac{4}{\pi}\left[\frac{1}{K_A} - \frac{2-K_A}{3K_A^2} + \frac{(2-K_A)^2}{5K_A^3} - \frac{(2-K_A)^3}{7K_A^4}\right]. \tag{12}$$

The analysis of this relation shows that if $K_A = 2$, which corresponds to the surface of a random field of heights with arbitrary distribution of steepness and Gaussian curvature, then the distribution of orientations of elements of the surface and local curvature of some parts of the fracture surface do not affect the unambiguity of correlation between $\bar{K}_A$ and $\bar{K}_P$. This result can be interpreted as follows: If we assume that the first term in relation (12) takes into account the irregularity of the surface curvature, then the higher-order terms can be regarded as corrections for the deviations of the analyzed surface from the arbitrary fracture surface. Note that if $K_A = 1$, which corresponds to a "perfectly plane fracture surface," then $\bar{K}_P = 1$. The results of numerical calculations demonstrate that, for the values of K_A important for the purposes of fractography, these deviations do not exceed 2–3%, which is, in fact, inessential.

Thus, the application of three-dimensional computer modeling enables one to obtain the reliable three-dimensional quantitative characteristics of specific features of the fracture surfaces and the spatial distribution of facets in these surfaces as well as correct estimates of their roughness.

REFERENCES

1. V. M. Mel'nik, V. N. Sokolov, et al., "A procedure of three-dimensional reconstruction of the micropattern of the surface of solid bodies according to their stereoscopic images obtained with the help of a scanning electron microscope," *Izv. Ros. Akad. Nauk, Ser. Fiz.*, **E59**, No. 2, 28–34 (1995).
2. A. Boyde and H. F. Ross, "Photogrammetry and the scanning electron microscope," *Photogrammetrie Record.*, **8**, No. 46, 408–457 (1975).
3. S. A. Saltykov, *Stereometric Metallography* [in Russian], Metallurgiya, Moscow (1970).
4. K. S. Chernyavskii, *Stereology in the Science of Metals* [in Russian], Metallurgiya, Moscow (1977).
5. H. Exner and M. Fripan, "Quantitative assessment of three-dimensional roughness, anisotropy, and angular distribution of fracture surfaces by stereometry," *J. Microscopy,* **138**, 161–178 (1985).
6. A. P. Khusu, Yu. R. Vitenberg, and V. A. Pal'mov, *Surface Roughness. Probabilistic Approach* [in Russian], Nauka, Moscow (1975).
7. S. M. El-Soudani, "Profilometrie analysis of fractures," *Metalloghaphy,* **11**, 247–336 (1978).