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The influence of microstructure on material properties

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THE paper concerns the discussion of the influence of microstructure of a material on its mechanical properties. Two types of phenomena connected with microstructure of a material are considered. In the first type the microstructure influences the values of macroscopic parameters and it appears directly only during some comparatively fine experiments. The microstructure effects on the second type are those which are observable in macroexperiments. Ideal models which can describe both phenomena are discussed. The stochastic character of some problems connected with structural defects in real bodies are pointed out. Some examples are considered.

Praca dotyczy wpływu mikrostruktury materiału na jego własności mechaniczne. Rozpatrzono dwa typy zjawisk związanych z mikrostrukturą. W pierwszym przypadku mikrostruktura wywiera wpływ na wartości parametrów makroskopowych nie ujawniając się bezpośrednio w makroeksperymentach. W drugim przypadku zmiany mikrostruktury są obserwowalne bezpośrednio w eksperymentach makroskopowych. Omówiono idealne modele ośrodków pozwalające opisywać oba typy zjawisk. Zwrócono szczególną uwagę na stochastyczny charakter problemów związanych z defektami strukturalnymi w ciałach rzeczywistych. Rozpatrzono kilka przykładów.

Работа касается влияния микроструктуры материала на его механические свойства. Рассмотрены два типа явлений связанных с микроструктурой. В первом случае микроструктура оказывает влияние на значения макроскопических параметров не проявляясь непосредственно в макроэкспериментах. Во втором случае изменения микроструктуры наблюдаются непосредственно в макроскопических экспериментах. Обсуждены идеальные модели сред, позволяющие описывать оба типа явлений. Обращено особенное внимание на стохастический характер проблем связанных со структурными дефектами в реальных телах. Рассмотрено несколько примеров.

1. General considerations

1.1. Introduction

LET us differentiate two types of microstructure effects. The first is one which vanishes in macroexperiments (for macroscopic volumes as well as for sufficiently long waves, etc.). Here, the microstructure contributes to the effective (averaged) properties of the material and this appears directly only when some comparatively exact experiments are carried out. The appropriate properties of materials called structurally-insensitive are observed both in thermodynamically-reversible processes (such as elasticity) and non-reversible ones (thermoconductivity, diffusion).

The microstructure effects of the second type are those which are retained in macroexperiments. Some structurally-sensitive materials usually observed in thermodynamically non-reversible processes (of plasticity, fracture, are related with these effects). As a rule, such processes are connected with a change of microstructure and hence with a variation of entropy configuration.

In both cases the characteristic feature of the microstructure is the presence of scale parameters. This is why microstructure effects are often interpreted as scale effects. The latter ones are observed in particular when structurally-sensitive properties are measured. On the one hand, they occur as the direct dependence on the microstructure parameters (for exact experiments) or, on the other hand, as the dependence on size and shape of a sample (for macroexperiments).

Now, we shall consider examples of microstructure effects of both types.

1.2. Microstructure effects in elastic media [1]

The scale parameters in the elastic medium having a microstructure can be of different origin. For example, these may be the parameters of the characteristic medium cell: the interatomic distance in a crystal, the size of the crystallite in a polycrystal or that of the cell of a composite, polymer net, etc. As for the medium with occasional characteristics, the correlation distance plays the role of scale parameters. The scale parameter in approximate equations of rods and shells of finite thickness has a geometrical character.

We shall briefly review below some effects which are closely related to the available scale parameters.

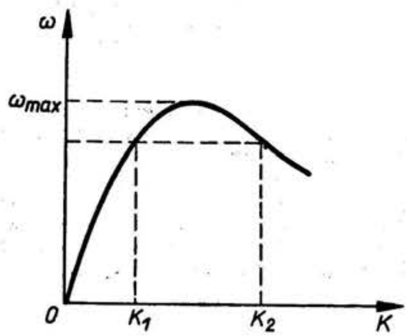

FIG. 1.

In a macroscopic homogeneous elastic medium without dissipation the undamped plane waves $\exp i(\mathbf{k}\cdot\mathbf{x}-\omega t)$ can propagate the frequency ω and wave vector $\mathbf{k}$ being connected with the dispersion equation $\omega = \omega(\mathbf{k})$. If the group velocity $\partial\omega/\partial\mathbf{k}$ depends upon $|\mathbf{k}|$ or, which is the same, $\omega(\mathbf{k})$ is a non-linear function of k (Fig. 1), then we can say that space dispersion takes place. The phenomenon is typical of all media having scale parameters. The dispersion of wave packets in the course of time is the direct consequence of velocity dispersion.

A maximum frequency of propagating waves (ω_{max} in Fig. 1) exists for discrete media and some other cases. Complex wave vectors correspond to the waves with $\omega > \omega_{max}$, i.e., such waves must damp exponentially. In this case the medium is obviously the filter for low frequencies.

As it can be seen in Fig. 1, a number of waves of different lengths may correspond to the fixed frequency $\omega < \omega_{max}$. Such new types of waves have no analogues in the classical theory of elasticity.

A specific effect of gyrotropy, the rotation of wave plane polarization, occurs in media deprived of central symmetry. It is essential that the gyrotropy is shown even at the weak dispersion, i.e., for comparatively long waves. Now, the boundary between two media is the layer of the order of the scale parameter. Hence, the boundary conditions are to be given not on the surface but rather in the thin boundary layer. A part from Rayleigh waves new types of surface waves damping deep into the medium may propagate.

Unlike the classical elastic medium the interaction force of defects is of a non-monotonous character and this may serve as a mechanism forming steady couples of point defects of dislocations.

The inner degrees of freedom (microrotations, microdeformations, etc.) which are in line with additional optical branches of vibrations may be important for sufficiently high frequencies (Fig. 2). These inner degrees of freedom are usually closely connected with scale parameters.

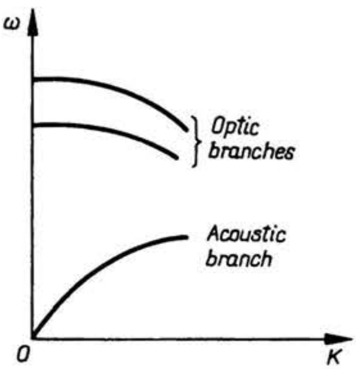

FIG. 2.

Finally, we should notice that a number of interesting effects appears when non-linear waves of finite amplitude propagate in media with scale parameters. Particularly, the wave packets tend to break asymptotically to the distinctive type of steady solitary waves, to the so-called solitons.

1.3. Microstructure effects in quasi-brittle fracture [2]

Scale parameters, at fracture and in the elastic media described above, follow from the peculiarities of the structure of solid bodies at microlevel. But, owing to the specificity of the fracture the effects of microstructure are found even in macroexperiments.

It is observed by many experimental data, that the failure stress σ^b depends on the site and shape of the samples at the fracture experiments.

The scale effect takes place not only when strength properties are studied but also when various structurally sensitive properties are investigated. The latter are typical by their dependence on the microstructure parameters. For instance, the failure stress σ^b depends essentially on the size d of the crystallite in polycristals. This dependence is approximated by linear relations between σ^b and $d^{1/2}$. The data on these dependences at various sorts of loadings are of special interest.

Microstructure reveals itself in a complicated manner at fracture in the presence of surface-active substances. The paradox is that in this case only the negligible part of the material interacts directly with the surfactant. The endurance and development of the fracture processes in time are also closely connected with the complicated microstructure change, microdefects progress, etc.

Many micromechanisms of such processes are still not clearly understood. Consequently, the most perspective approach to the investigation of these phenomena is the thermodynamical (phenomenologicical) one.

The clearly defined stochastic character of fracture is particularly interesting. Statistical regularities are rather different at fracture. They can be listed as follows: brittle strength dispersion, still further dispersion of long-time strength, the variety and stochastic character of fracture surfaces at identical exterior conditions, etc.

It should be noted that the statistical regularities found while studying these characteristics are rather informative. So, far example, when an experienced metallophysicst looks at the relief of the fracture surface he can give in detail the biography of the specimen and the causes of fracture. A problem which still remains unsolved is how to formalize the information included in the relief of the fracture surface.

2. Some mathematical models of media having microstructure

2.1

The very notion of a medium with microstructure indicates that proper mathematical models must contain some scale parameters, i.e., they must be nonlocal in essence. This is shown in the change of differential operators by integro-differential ones (strong non-locality) or in their appearance in equations of high-derivatives with small scale parameters (weak non-locality or long wave approximation). For example, the tensor of elastic constants $C^{\alpha\beta\lambda\mu}$ of the common theory of elasticity is changed for the integral operator $\hat{C}^{\alpha\beta\lambda\mu}$ with the kernel located in the region of the order of the scale parameter l. In the longitudinal approximation

$$\hat{C}^{\alpha\beta\lambda\mu} = C_0^{\alpha\beta\lambda\mu} + l^2 C_2^{\alpha\beta\lambda\mu\nu\varrho}\partial_\nu\partial_\varrho .$$

2.2

In regular structures (lattices) l coincides with the lattice parameter. When describing these structures it is convenient to include the concept of quasi-continuum (KRUMHANSL, ROGULA, KUNIN].

It is possible to establish a one-to-one correspondence between the functions $u(\mathbf{n})$ on lattice and analytical functions $u(\mathbf{r})$ of a special type. It also permits one to translate all discrete operations into continuum language.

This allows for translating all discrete operations to continuum language, so as to include correctly such operators as grad, div, rot, def, etc., together with the stress and deformation tensors and to write the motion equations in a form analogous to the classical theory of elasticity (simple structure medium)

$$\varrho\ddot{u} - \operatorname{div}\sigma = q, \quad \sigma = \hat{C}\varepsilon, \quad \varepsilon = \operatorname{def} u.$$

It should be noticed that the function space on a quasi-continuum is isomorphic to that on the lattice. That is why quasi-continuum is to be treated not as a new mathematical model but only as another description of a lattice.

When the inner degrees of freedom are considered, we can effectively describe in terms of quasi-continuum some continuous periodical structures, that is, we have the model of the medium of complex structure.

In cases when anisotropy of the lattice is not essential, it can be described approximately by means of an isotropic model or Debye's quasi-continuum. Fourier-images $u(\mathbf{k})$ are here considered to be located not in the cell of the reciprocal lattice but in the sphere with the radius of the order of l^{-1} where l is the lattice parameter. This model retains the main property of the lattice: the presence of the elementary length unit.

Debye's model together with the dispersion law provides an effective method of describing isotropic linear media. However, when trying to extend this model onto the non-linear media, one can encounter some principal difficulties resulting from the fact that it is impossible to define correctly non-linear operations with the field variables (as distinct from the quasicontinuum model). Indeed, the function product in the x-space is followed by integral convolution in the k-space which expends the convolution support beyond Debye's sphere. Some modifications of Debye's model will be discussed further on.

2.3

In the most practically interesting cases — such as crystal defects, polycrystals, composites, etc., the microstructure is of a stochastic character. The correlation distance usually appears in these structures as the scale parameter.

It is rather difficult to give an exact description of the stochastic structures in terms of probability measures on the stochastic fields. Such a description usually carries excessive information. Therefore, it is only natural that approximate mathematical models should appear (one of them is a stochastic geometry, SCHWEITZER, MARKOV, BLOKHITSER). It is based on the suggestion that the distance between any points is the stochastic variable. This complies with the idea about the stochastic arithmetization of the space which requires a transition from the traditional analysis to the stochastic one. For example, if $u(x, t)$ is the field variable in this space, then, instead of the common derivative $\frac{\partial u}{\partial t}$, the stochastic one should be used:

$$\frac{Du}{Dt} = \frac{\partial u}{\partial t} + a^{\alpha\beta}\partial_\alpha \partial_\beta u, \quad a^{\alpha\beta} = \lim \frac{1}{\Delta t} < \Delta x^\alpha, \Delta x^\beta \rangle .$$

From this equation it can be seen in particular, that the scale parameter appears in the differential operator. One can point out a number of physical situations where stochastical geometry is used:

a) the device measuring the distance has an unavoidable error $\Delta x \sim l$,

b) the medium where the signal for distance measurement propagates is microheterogeneous which causes signal velocity fluctuations;

c) "particles" that help to fix the space points have final sizes $\sim l$.

Let us consider some other possibilities of an approximate description of stochastic structures.

When stochastic space is statistically homogeneous and isotropic, it is characterized geometrically by the scale parameter — the correlation distance. The simplest method to control this fact is the transition to Debye's model of quasi-continuum. But as we have already mentioned above, it is impossible to define correctly the non-linear operations with the field variables within this model.

There are two ways of overcoming this difficulty.

In quantum theory there have been many attempts to include the fundamental length beyond which all the common presentations on the space-time continuum lose their validity. To perform the space-time quantization, SNYDER proposed to substitute the space of constant curvature for the common momentum space. Here, the coordinate operators correspond to the space-time points, the commutators of the operators being of the order of fundamental length. The momentum space is closed relative to convolution and this allows to define accurately the product in space-time and, subsequently, the non-linear operations.

As applied to our problem, it would be the same as to transform Debye's sphere in three-dimensional space of wave-vectors into the space of constant curvature, i.e., three-dimensional sphere in a four-dimensional space.

It is likely that the change of Debye's sphere by the proper compact group — e.g., SO(3) or SO(2) — would have been more consistent. The harmonic analysis of the group allows to introduce the conjugate coordinate space with the elementary length unit. Such an approach widens algebraic and analytical possibilities as compared to Snyder's scheme.

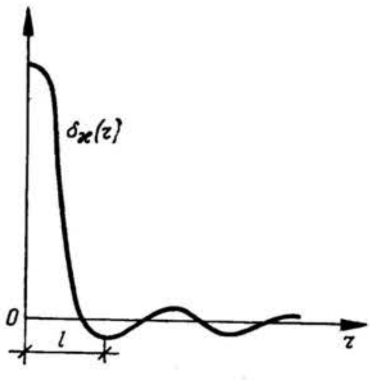

FIG. 3.

All the schemes described can be considered as different definitions of isotropic quasi-continuum with the elementary unit of length. Here, the field variables (in part, the coordinates) become operators which do not admit localizations in the region with sizes less than an elementary unit of length. For instance, instead of the common singular δ-function localized in a point, there appears $\delta_\varkappa(\mathbf{r})$ where $\varkappa \sim l^{-1}$ is Debye's sphere radius or the curvature of the appropriate homogeneous space (Fig. 3).

It should be noted that isotropic quasi-continuum, in contrast to the lattice one, has no distinguished points.

The transition to the continuum is performed for distances much larger than l or, which is the same, at $l \to 0$ $(\varkappa \to \infty)$.

2.4

Because quasi-continuum, it is allowable to give sense to the generalized stochastic processes. Indeed, if the trial functions are given on the quasi-continuum, the generalized stochastic processes (or fields) can be considered as the roughness of the actual processes (or fields) at the distances of the order of the typical scale parameter. When there is no detailed information on the stochastic field and only the correlation scale is known, then, it is natural to approximate it by the white noise with the correlation function $\delta_\varkappa(\mathbf{r})$ where $\varkappa \sim l^{-1}$.

In general cases a special construction of the trial function space is possible and it must be in agreement with the desirable degree of detal.

It is known that to generalize the processes of the white-noise-type, the stochastic differential equations substitute the classic ones. The stochastic equations not only describe these processes adequately but are also perspective in the construction of new effective solutions. It is essential that the introduction of quasi-continuum allows to use the formalism of stochastic differential equations in the mechanics of media with microstructure.

3. Some illustrations

Let us give number of exemples showing the specificity of media with microstructures.

3.1. Green's function for Debye' quasi-continuum with dispersion (Kunin 1967)

Green's tensor $G_{\alpha\beta}(\mathbf{r}, t)$ in the unbounded homogeneous isotropic medium can be expanded into longitudinal and transverse components by the proper projection operators. In $(\mathbf{k}, \omega)$ representation

$$G_{\alpha\beta}(\mathbf{k}, \omega) = G^l_{\alpha\beta}(\mathbf{k}, \omega) + G^t_{\alpha\beta}(\mathbf{k}, \omega) = \pi_{\alpha\beta}(\mathbf{k}) G^l(k, \omega) + o_{\alpha\beta}(\mathbf{k}) G^t(k, \omega),$$

$$\pi_{\alpha\beta}(\mathbf{k}) = \frac{k_\alpha k_\beta}{k^2}, \quad o_{\alpha\beta}(\mathbf{k}) = \delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2},$$

and the scalar functions $G^l(k, \omega)$ and $G^t(k, \omega)$ are defined by the dispersion laws $\omega(k)$

$$G^j(k, \omega) = \frac{1}{\varrho[\omega_j^2(k) - \omega^2]}, \quad j = l, t.$$

This gives the presentation

$$G^j(r, \omega) = \frac{1}{4\pi r} \sum_{m=0}^{\infty} A_m(\omega) e^{ik^j_m(\omega) r},$$

where $k_m^j(\omega)$ are the roots of the dispersion equation

$$\omega_j^2(k) = \omega^2.$$

In the case of statics in the first zeroes approximation (fairly long waves)

$$G_{\alpha\beta}^l(\mathbf{r}) = \frac{1}{8\pi(\lambda_0+2\mu_0)}\partial_\alpha\partial_\beta\left\{r+\mathrm{Re}\left[c(\varkappa)\frac{1-e^{i\varkappa r}}{r}\right]\right\},$$
$$\varkappa = \varkappa'+i\varkappa'', \quad |\varkappa| \sim l^{-1}$$

and similarly for $G_{\alpha\beta}^t(\mathbf{r})$.

It follows from here that together with classical amplitude $\sim r^{-1}$ there are the terms $\sim r^{-3}$ and those damping exponentially.

At $r \to 0$ Green's function, as it must be, has no singularities for quasi-continuum:

$$G_{\alpha\beta}(0) \sim \frac{\varkappa}{\varrho}\left(\frac{1}{C_l^2}+\frac{1}{C_t^2}\right),$$

where C_l, C_t are velocities of longitudinal and transverse waves.

It should be noted that for the theory of defects in quasi-continuum the following quantity is also of interest.

$$g_{\alpha\beta\lambda\mu} = -\partial_\lambda\partial_\mu G_{\alpha\beta}(0) \sim \varkappa^2 G_{\alpha\beta}(0).$$

3.2. Point defects, dislocations and cracks in a medium with microstructure

It is convenient to present Green's function for a medium with defects as follows:

$$G = G_0 - GRG_0,$$

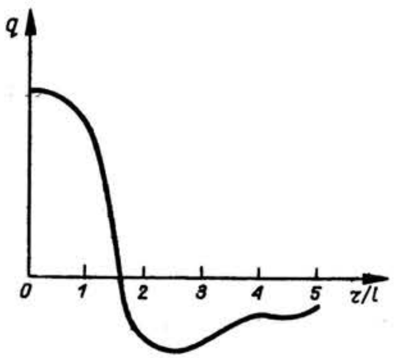

FIG. 4.

where G_0 is Green's function of the homogeneous medium, R is the subsidiary operator. The latter one is convenient to include because it is connected with the defect features more directly than G and is located, in part, in the same region with defects. It is essential that for many important cases (point system), rectilinear dislocations, etc.) the kernel $R(x, x', t-t')$ of the operator R can be constructed in the explicit form.

There is a close connection between the operator R and the scattering matrix S. One can show that $S(\mathbf{k})$ is expressed in terms of the kernel $R(\mathbf{k}, \mathbf{k}', \omega(\mathbf{k}))$ on the "diagonal"

$$S(\mathbf{k}) \sim I - R(\mathbf{k}, \mathbf{k}', \omega(\mathbf{k})),$$

where I is the unit operator. This, in particular, allows for analyzing the direct and reverse problem of scattering on the defect system (KUNIN, KOSILOVA, 1973).

Green's function helps to solve effectively a number of statistic and dynamic problems of theory of defects in media with microstructure.

Therefore, Fig. 4 shows the character of dependence of the interaction force between dislocations on the distance between them. This result is obtained for Debye's quasi--continuum with dislocation (KUNIN, 1967).

It is seen that at the distance of the order of several interatomic distances the force can change its sign and this gives the possible interpreting of the existence of steady dislocation dipoles.

An obvious distinctive feature of the theory of defects in the media with the elementary scale parameter is the lack of singularity on small distances which is typical for continious media. Particularly, the stress at the top of the crack turns to be finite. This is of importance for the study of fracture mechanisms and the construction of kinetic equations of the moving crack. It should be noted that the study of conditions in the crack top within the scope of common elastic media is not sufficient.

3.3. Fracture of composites

Now, we shall consider the composite given in Fig. 5. It is suggested that inclusions are more robust than the matrix and the fracture takes place on the trajectories which realize the minimum of a functional J — this is the difference between surface and elastic energy.

FIG. 5.

As a result of the fluctuation of surface energy and the stress field, the fracture trajectories are of a stochastic character and J is a stochastic quantity. Accordingly, instead of a common limiting strength curve there occurs a set of curves of similar fracture probability (Fig. 6). (CHUDNOVSKII, SHREIBER, 1975). Figure 7 shows an example of dependence of fracture probability $p(A)$ at $\sigma = \text{const}$ on the inclusion concentration c. Now, the validity of the problem on optimization of microstructure of composites becomes evident.

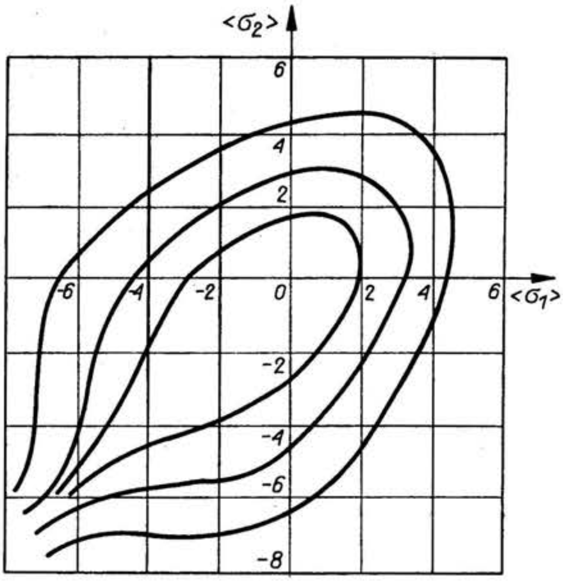

FIG. 6.

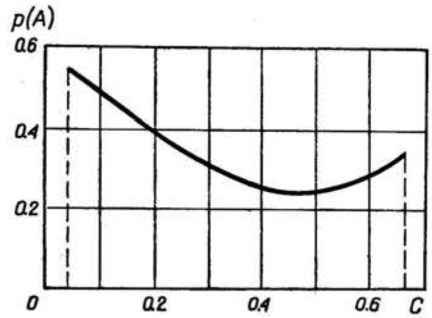

FIG. 7.

3.4. The equation of stochastic crack

As it can be seen from the above example, a study of the microstructure leads naturally to the stochastic formulation of fracture condition. It is essential to note that the fracture orientation in each point and hence a trajectory of the crack motion have a the stochastic character.

According to the considerations given above this may be simulated by the introduction of crack trajectory perturbation in the form of white noise. In particular, for the crack extending towards the x-axis perpendicular to the stretching stress σ, the equation of stochastic crack relief $y(x)$ takes a very simple form (CHUDNOVSKII, 1972).

$$y''_x + k(\sigma, \dot{x}) y'_x = a(\sigma, \dot{x}) \omega'_x,$$

where $\dot{x}$ is the crack velocity (related to the sound velocity), $\omega(x)$ is the Wienner process with a zero expectation value and unit dispersion.

The solution of this stochastic equation is the Gauss process. Its expectation value $\langle y(x)\rangle$ and correlation function $r(x, x')$ can be defined by means of a simple algorithm. In the case considered at the additional conditions

$$\langle y(x)\rangle|_{x=0} = 0, \quad \langle y(x)\rangle'|_{x=0} = 0, \quad a = \text{const}$$

we have $\langle y(x)\rangle = 0$ and

$$r(x, x') = a_1(x, a, k)\left[\min(x, x') + f\left(\dot{x}, \frac{x-x'}{l}\right)\right],$$

where

$$a_1 \sim a, \quad f \sim l\dot{x}\exp\left(-\frac{x-x'}{l\dot{x}}\right).$$

The first term is the correlation function of the Wienner process, the second one takes into account the additional correlation conditioned by the "inertia" of the crack.

The expression given for $r(x, x')$ relates the statistical characteristics of relief to those of micro-heterogeneity a and l which allows to find the latter ones experimentally.

3.5. Scale effect in fracture

The dependence of strength of a sample on its geometrical dimensions and shape is a problem closely connected with what has been discussed above. The greater the measure of set of possible fracture surfaces the greater the probability of the fracture samples, all other things being equal. This measure depends on the statistical properties of crack relief. In the class of Gauss stochastic surfaces the measure is defined uniquely by the solution of the stochastic relief equation as given above.

A comparison of the measure of the set of possible fracture surfaces in geometrically similar samples of different dimensions allows to distinguish the criterion of the similarity of fracture processes.

So, at the axial stretching of cylindrical samples of length H and radius R the parameter $H/\sqrt{lR}$ appears naturally and coincides with the measure of the set of the Wienner fracture surface. This parameter is the geometrical similarity criterion. The form of the similarity criterion points to the fracture sensibility to the microstructure and is in good agreement with the experimental data.

4. Conclusion

Now, we shall indicate some principal problems connected with the development of the microstructure medium theory.

1. Further development of the geometry considering the existence of the elementary length unit.

2. A broadening of the class of continuous medium problems solved effectively by the methods of stochastic differential and integral equations.

3. Definition of the notion "material" relative to the properties in which the scale effects reveal thermselves.

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